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à Brigue les 5 et 6 octobre 1978
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Rapport de la Session d'automne de la Société Suisse de Physique à Brigue les 5 et 6 Octobre 1978

Président: Prof. PH. CHOQUARD, EPF Lausanne
Vice-Président: Madame Prof. IRIS ZSCHOKKE-GRÄNACHER, Université
de Bâle
Secrétaire: Prof. PAUL ERDÖS, Université de Lausanne
Membres du bureau: Prof. PETER F. MEIER, Université de Zürich
Prof. ALEXANDRE HEYM, EPF Lausanne

Partie administrative

I. Membres

Les membres ordinaires suivants ont été reçus au sein de notre Société:
PETER BOCHSLER (Berne), EMMANUEL BUFFET (Lausanne), JEAN-MARC DE
SIEBENTHAL (Genève), THOMAS FINK (Fribourg), MARC ILEGEMS (Lausanne),
ABDUL-HAMID KAYAL (Neuchâtel), JÜRIG K. LANG (Zürich), JAMES LEWIS
(Lausanne), EBERHARD LÖFFLER (Bâle), ERIC LÜDIN (Bâle), FRANCIS W. MÜLLER
(Bâle), THONG NGO (Lausanne), PETER PSCHIED (Constance), RESHEF TENNE
(Genève), TARIK YALCIN (Lausanne), PETER ZÜRCHER (Zürich).

La Société comprend actuellement 1186 membres individuels, 6 membres
collectifs et 13 bibliothèques.

II. Séance Administrative

Ouverture de la séance, vendredi 6 octobre 1978 à 14 h 00, dans les locaux
du Collège de Brigue. Présents: 36 membres.

1. *Procès-verbal de la réunion précédente* (30 mars 1978, Neuchâtel): pas de
commentaire
2. *Communications du bureau*

Cette année, sur l'initiative du Prof. E. Kaldis, la Société accueille le groupe
'Croissance des Cristaux' de la Section Suisse de Cristallographie. Il faut souhaiter
que cette expérience se renouvelle, vu l'intérêt évident qu'elle suscite.

3. *Lieux et dates des réunions de printemps 1979 et d'automne 1979.*

La réunion de printemps se tiendra à Bâle les 5 et 6 avril 1979 et marquera
le début du prochain bureau.

La réunion d'automne sera commune avec les Sociétés Allemande et Au-
trichienne de Physique à Ulm, à l'occasion de trois anniversaires (dont celui



d'Einstein). Messieurs P. Trüol et P. Brüesch ainsi que Madame I. Zschokke formeront une délégation chargée de mettre au point le programme avec les allemands.

4. *Communications des représentants des groupements spécialisés*

– Accueil de MM. P. Trüol (Physique Nucléaire et Corpusculaire), P. Brüesch (Matière Condensée) et Ch. Gruber (Théorie) dans le Comité en tant que délégués de leur propre groupement de spécialité. A noter que l'Assemblée Générale n'a pas à se prononcer sur leurs nominations. Le Comité est convenu de nommer les membres du bureau pour 2 ans renouvelables année par année trois fois au plus (5 ans en tout).

– D'une manière générale on pose le problème de la pluralité des communications présentées par une seule et même personne lors d'une session. Il est proposé que, dans ce cas, une seule communication soit présentée oralement et les autres par posters. La proposition est acceptée.

5. *Communications des présidents des commissions et du service de placement*

– Pour l'Orientation Professionnelle, Monsieur J.-P. Amiet, absent, est excusé et n'a rien à transmettre.

– Monsieur S. Steinemann démissionne de la présidence de la Commission de Politique de la Science.

– Dans cette même commission on enregistre également les démissions de Messieurs Roland Hofmann et Christian Risch.

– Monsieur F. Kneubühl du Service de Placement fait le point sur la situation actuelle: il ressort qu'il n'y a pas assez de physiciens et particulièrement d'expérimentateurs et par contre trop de théoriciens (*voir tableau en fin de rapport*).

– Monsieur Peter Meier, délégué du Comité des H.P.A. est absent et s'est fait excuser. Monsieur G. Wanders, le rédacteur des H.P.A., pose un problème concernant le comité de rédaction: après chaque session, l'essentiel des communications est publié dans H.P.A. et une partie des communications de Physique Appliquée dans Z.A.M.P. La situation est telle que ce sont les abonnés des H.P.A. qui paient pour ces dernières. Faut-il donc maintenir ce système? ou bien tout publier dans H.P.A.? A noter que pour cette session les publications dans Z.A.M.P. sont peu nombreuses. La question est posée pour réflexion et décision lors de la prochaine assemblée. Le Comité pour sa part a déjà envisagé ceci: sauf désir exprès de l'auteur, tout serait publié dans H.P.A. (les exceptions devraient être dûment motivées). L'Assemblée Générale est d'avis de recommander cette solution.

6. *Propositions du Comité pour les membres du prochain bureau*

En ce qui concerne la succession de Monsieur Steinemann au poste de Président de la Commission de Politique de la Science, les statuts demandent que cette nomination soit approuvée par l'Assemblée Générale. Monsieur H.-P. Baltes de Landis et Gyr, Privat-docent à l'E.P.F.-L, est proposé et sa nomination approuvée par applaudissements.

Composition du prochain Comité: au vu de la composition des comités depuis 1945, on s'aperçoit que l'Université de Neuchâtel en a été exclue depuis

1959. Il serait donc souhaitable que Neuchâtel fournisse prochainement un vice-président. Après enquête le nom du Prof. Paul Dinichert, directeur du L.S.R.H. a été retenu. Le bureau propose donc les noms suivants pour le prochain comité 1979-1981:

- Présidente: Madame Iris Zschokke-Gränacher
- Vice-Président: M. Paul Dinichert
- Secrétaire: M. Ingo Sick

ce qui est approuvé par applaudissements.

Le Comité 1981-83 devrait être fourni par Fribourg.

7. *Propositions du Comité pour l'utilisation des bénéfices de la Société*

Ceci pour répondre à une question posée par un membre, à savoir la réduction éventuelle des cotisations. Cependant le Comité propose d'autres utilisations:

- Subsidés pour frais de publication: il est possible d'envisager des subsides pour les H.P.A. de façon à soutenir les abonnements qui deviennent trop chers. Mais la situation n' a rien de critique. Monsieur Wanders rappelle que pour l'instant les H.P.A. disposent d'un fonds de Fr. 80.000.-- et il souhaite seulement pour l'avenir garder un fonds de sécurité de Fr. 50.000.--. Le problème n'est donc pas urgent. D'autre part, ces dernières années les frais de publication des bulletins des réunions ont été nuls car fournis gratuitement par l'E.P.F.-L, d'où la réserve accumulée. Or ceci n'existera plus dès le déplacement du prochain comité à Bâle.
- Subsidés pour frais de délégation: Jusqu'ici plusieurs membres du comité se sont vus offerts leurs déplacements par leurs instituts. Ceci devient également improbable pour l'avenir. Le Comité propose que dorénavant, les voyages effectués par les membres en tant que délégués de la S.S.P. soient dans une large mesure pris en charge par la Société.
- Subsidés pour réunions et conférences: diverses réunions et symposia sont organisés en Suisse tous les ans. La Société pourrait favoriser de telles réunions par une contribution matérielle aux frais d'organisation.

En conclusion, l'Assemblée approuve le maintien des cotisations à Fr. 35.-- par 25 voix de majorité et 5 abstentions.

8. *Action éventuelle de la S.S.P. en faveur du Prof. Orlov*

La Société a reçu de plusieurs institutions et également du Prof. W. Känzig des demandes de prise de position en faveur du Prof. Orlov. Le Comité a débattu de cette question et souhaite avant tout ne pas rendre cette intervention émotionnelle car elle pourrait aussi bien aller dans le sens de l'allègement que de l'aggravation de la pression exercée sur la personne. Le Comité ne souhaite pas déposer un manifeste, mais propose une action ponctuelle et modérée. Il est donc demandé à l'Assemblée de se prononcer pour l'une ou l'autre de deux possibilités:

- envoi d'une lettre avec en-tête de la Société, signée par le Président, au nom de la Société;

– envoi d'une lettre sur papier d'un institut avec signature des instituts et personnes qui le souhaitent.

L'Assemblée se déclare en faveur de la première solution avec la répartition suivante: pour, 32; abstentions, 3; contre, 1.

La lettre ne sera pas communiquée à la presse, par contre cette action sera communiquée aux sociétés soeurs par lettre.

9. Divers et propositions

Pas d'intervention.

Fin de la séance à 15 h 15.

Statistik Stellenvermittlung 1978

Zirk. Nr.	Datum	Anzahl Kandid.	Anzahl Zirkulare	Anzahl Angeb.	Anzahl Firmen	Anzahl verm. Stellen	Dipl. phys.	Dr. sc. nat.	Div.
1	30.3	14	384	57	25	2	4	10	—
2	24.5	11	357	65	22	4	3	6	2
3	9.8	13	357 $\geq$	(36)	(15) $\geq$	1	3	7	3

19.10.1978

Physique de la matière condensée

Métaux

Relaxations α et γ dans le niobium de haute pureté

F. DE LIMA et W. BENOIT

(Laboratoire de Génie Atomique, EPF-Lausanne)

Les pics de frottement intérieur α et γ dans les métaux à structure cubique centrée sont associés à la formation thermiquement activée des doubles décrochements sur les dislocations coins (α) et sur les dislocations vis (γ). Dans un certain nombre de métaux, dont le niobium, l'observation de la relaxation γ est difficile car elle apparaît dans un domaine de température où l'oxygène a diffusé vers les dislocations et les a bloquées. Dans cette étude on détermine l'influence de l'oxygène sur l'évolution du réseau de dislocations dans Nb fortement dégazé et les conditions optimales pour observer la relaxation γ .

Mesures des constantes élastiques près de la transformation martensitique sur un alliage AuCuZn_2 monocristallin

J. J. MEISTER et S. KOSHIMIZU

(Laboratoire de Génie Atomique, EPF-Lausanne)

La transformation martensitique de l'alliage AuCuZn_2 fait passer la maille de cet alliage de la structure cubique centrée ordonnée à une structure orthorhombique. Cette transition est suivie par la mesure des constantes élastiques par ultrasons en fonction de la température. Ces mesures montrent pour la valeur de ces constantes des anomalies qu'on peut associer soit à l'apparition du mode mou phononique, soit au mouvement des dislocations d'interfaces avancées comme origine de la transformation martensitique.

Enfin, on constate que la variation de la constante de cisaillement $C' = \frac{1}{2}(C_{11} - C_{12})$ calculée d'après les mesures de C_{11} et C_{12} diffère de celle trouvée par mesure directe de C' .

Spectre de frottement intérieur lié à la précipitation dans les alliages Al-Ag

R. SCHALLER et W. BENOIT

(Laboratoire de Génie Atomique, EPF-Lausanne)

Les alliages Al-Ag ($C_{\text{Ag}} = 10, 20, 30\%$ poids) présentent deux pics de frottement intérieur lors d'une première montée en température après trempe. Après recuit d'une dizaine de minutes à 520 K, le spectre ne se compose plus que d'un pic lié à la présence des précipités γ' ($\text{Ag}_2\text{Al-hc}$). Le premier pic observé à l'état trempé semble être le pic de Zener dû à la réorientation sous la contrainte appliquée des paires d'atomes d'Ag en solution solide. Le deuxième pic peut être lié à la réversion des zones GP ou à la nucléation des γ' . Le troisième pic peut naître de dissipations d'énergie aux interfaces (γ' -matrice).

Frottement intérieur dû à une interaction dislocation-boucle de dislocation dans l'aluminium¹⁾

F. BAUDRAZ et B. VITTOZ

(Laboratoire de Génie Atomique de l'Ecole Polytechnique Fédérale de Lausanne)

Nous avons étudié l'évolution, en fonction des recuits, du spectre de frottement intérieur d'échantillons d'Al 99.999% déformés de 1000 cycles de 1.5×10^{-3} à 80 K. L'installation de mesure est un pendule de torsion oscillant à environ 2.4 Hz.

Le spectre de frottement intérieur en fonction de la température contient essentiellement deux pics entre 80 et 330 K. L'un vers 80 K est le pic de Bordoni (B_2): sa hauteur est proportionnelle à la densité de dislocations et au carré de la longueur des segments de dislocations. Il apparaît aussi bien après écrouissage qu'après déformation cyclique.

Un autre pic vers 250 K n'apparaît bien qu'après déformation cyclique [1]. Nous l'appelons pic de fatigue (P_F). Il y a coïncidence entre les températures de recuit après lesquelles ce pic croît et celles après lesquelles on observe, au microscope électronique, une mise en mouvement des boucles créées par déformation cyclique [2]. Pour ces mêmes températures de recuit on remarque, par une diminution du pic de Bordoni, un épinglage des dislocations. Ces

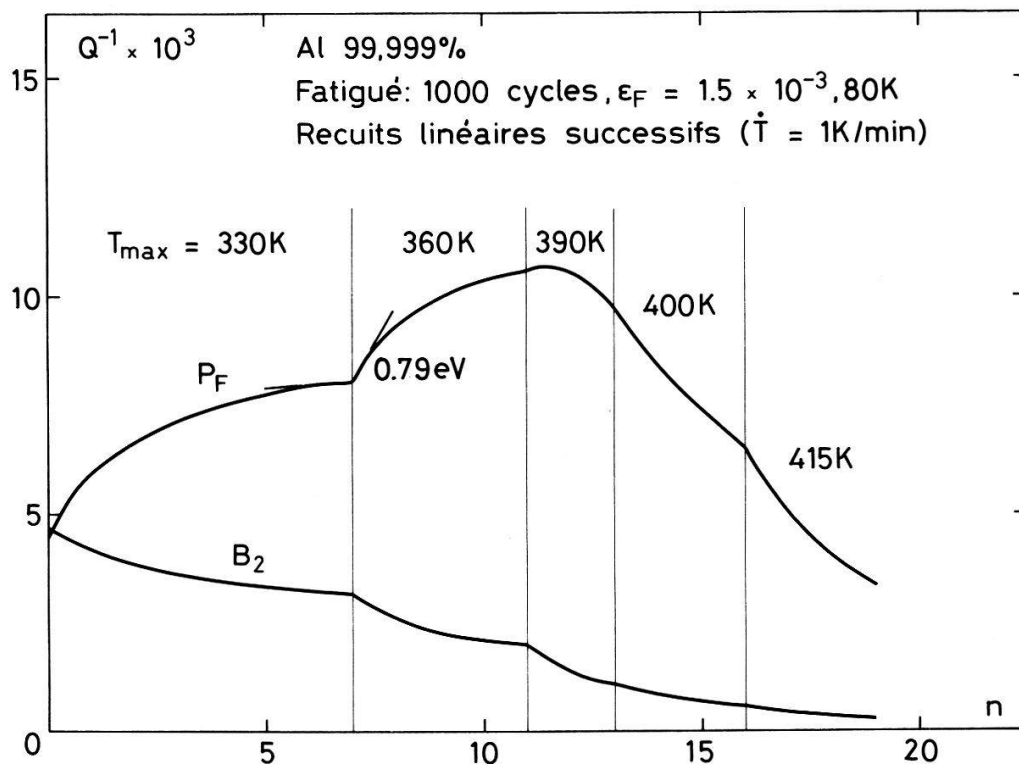


Figure 1

¹⁾ Recherche partiellement subventionnée par le Fonds National Suisse de la Recherche Scientifique, subside no. 2.932-0.77.

constatations suggèrent que le pic vers 250 K est dû à une interaction dislocations – boucles de dislocations [1].

Le frottement intérieur est alors causé par le freinage des dislocations par les boucles qui les épinglent et qui deviennent mobiles vers 250 K. Dans ce cas, l'énergie de relaxation de ce pic (qui vaut 0.43 eV) doit correspondre à l'énergie de migration des boucles (modèle de 'dragging').

Nous avons déterminé l'énergie de restauration attachée à la croissance du pic par la méthode des changements de pente [3]: une suite de montées linéaires jusqu'à 330 K est suivie d'une autre jusqu'à 360 K, puis jusqu'à 390 K, etc. Le spectre de frottement intérieur est mesuré pendant les montées de température.

Les hauteurs des pics B_2 et P_F tracées en fonction du numéro de la montée montrent un changement de pente lorsque la température maximale des montées change. Le calcul de l'énergie de restauration par la méthode du changement de pente entre 330 et 360 K (croissance de P_F) donne 0.79 eV.

Cette énergie est nettement supérieure à l'énergie de relaxation du pic (0.43 eV). Il convient donc de distinguer le mécanisme de relaxation responsable du pic de celui de la croissance de sa hauteur. On peut toutefois supposer que le modèle d'interaction dislocation – boucle est correct mais qu'il est nécessaire de désépingler les boucles des impuretés avant qu'elles puissent migrer vers les dislocations, ce qui expliquerait la valeur élevée de l'énergie de restauration.

RÉFÉRENCES

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- [2] R. GOTTHARDT, Proc. 6th European Congress on Electron Microscopy, Jerusalem (1976), vol. I, 512.
- [3] P.-A. GRANDCHAMP, B. BAYS et W. BENOIT, Mém. Sc. Rev. Mét., 68, 617 (1971).

Effets anélastiques dûs aux phénomènes de précipitation et recristallisation dans les alliages aluman 100¹⁾

C. DIALLO et M. MONDINO

(Laboratoire de Génie Atomique, EPF-Lausanne)

L'étude de l'évolution du spectre de frottement intérieur lors des traitements thermiques effectués sur des échantillons écrouis d'ALUMAN 100 a permis de confirmer l'extrême sensibilité de la technique aux changements structureux ayant lieu lors de la recristallisation et de la précipitation.

Nos résultats montrent que la croissance du fond de frottement intérieur est liée à la recristallisation et que la chute de ce fond accompagnée de l'apparition d'un pic de relaxation apparaît lors de la précipitation.

Ces observations ont permis d'optimiser les traitements thermomécaniques afin d'obtenir une structure recristallisée à grain fin.

¹⁾ Recherche subventionnée par la Commission pour l'encouragement des recherches scientifiques, projet no. 916.

Elastische und anelastische Eigenschaften amorpher Metalle

H. U. KÜNZI, K. AGYEMAN und H.-J. GÜNTHERODT

(Institut für Physik der Universität Basel, Basel)

Der Elastizitäts- und Schubmodul sowie die innere Reibung einiger amorpher Metalle (wie $\text{Mg}_{70}\text{Zn}_{30}$, $\text{Cu}_{50}\text{Zr}_{50}$, $\text{Gd}_{67}\text{Co}_{33}$ u.a.m.) wurden in Abhängigkeit der Temperatur untersucht. Elastizitäts- und Schubmodul wurden aus den Eigenfrequenzen von Biege- resp. Drillungsschwingungen berechnet und die innere Reibung mit der freien Abklingmethode bestimmt. Als Funktion der Frequenz zeigt die innere Reibung ein Maximum, das seine Ursache im thermoelastischen Effekt hat. Aus Höhe und Breite dieses Debye-Peaks werden der lineare thermische Ausdehnungskoeffizient und die Wärmeleitfähigkeit bestimmt.

Photoemissionsuntersuchung der fest-fest und fest-flüssig Phasenumwandlung des Thalliums

F. GREUTER und H. P. VATERLAUS

(Laboratorium für Festkörperphysik ETHZ)

U. GUBLER

(Institut für Physik der Universität Basel, Basel)

Die allotropen α - und β -Modifikationen sowie die flüssige Phase des Thalliums wurden mittels Photoemission bis zu Photonenenergien von 6.6 eV untersucht. Die Energieverteilungskurven des flüssigen Thalliums weisen, wenigstens im oberen Teil des Leitungsbandes, auf ein Sommerfeld-Verhalten der Elektronen hin. Der Uebergang von der kubischen Hochtemperaturphase in die hexagonale Raumtemperaturphase findet auch an der Oberfläche bei 230°C statt und äussert sich ausgeprägt sowohl in der Energieverteilung der Photoelektronen wie im Photostrom. Die in beiden festen Phasen für ein Metall ungewöhnlich kleine Zahl der Photoelektronen im Bereich der Fermikante muss dem k -erhaltenden Charakter des optischen Uebergangs zugeschrieben werden.

Anisotropy of the atomic displacements near an impurity in dilute metallic alloys*

G. SOLT

(IPT, Université de Lausanne, 1015 Lausanne),

and

A. P. ZHERNOV

(Kurchatov Institute of Atomic Energy, Moscow)

In strongly anisotropic metals the static displacement of a host atom far from the solute impurity depends strongly on the orientation of its relative position

*) With partial support of the Swiss National Science Foundation, grant No. 2.748-0.77.

within the crystal, as elasticity theory predicts it. The microscopic local displacements corresponding to the static equilibrium of the alloy lattice are calculated both near and far from the solute atom by the method of pseudopotentials. In the particular case of an alkali host the *limits* of the asymptotic region, where the deformation is already that of an anisotropic elastic continuum, are found and it is shown that the *amplitude* of the lattice distortion is substantially smaller near the foreign atom than is the elastic prediction, while the degree of *anisotropy* is more or less the same all over the lattice.

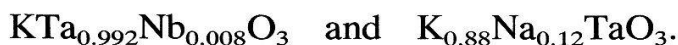
Ferroélectricité, systèmes amorphes, centres

Dielectric susceptibility in the ferroelectric quantum limit

D. RYTZ¹⁾ and U. T. HÖCHLI

(IBM Zurich Research Laboratory, 8803 Rüschlikon, Switzerland)

Deviations from the Curie-Weiss law $\varepsilon^{-1} \sim (T - T_c)^\gamma$ with $\gamma = 1$ have been found in incipient ferroelectrics. They are characterized by $\gamma \sim 1.4$ and have been attributed to coupling between acoustic and ferroelectric soft modes. We establish here, for the first time, a third regime characterized by the dominance of zero point fluctuations of the polarization. We find that below ~ 30 K, $\gamma = 2$ and that this can be observed only under quantum-limit conditions such as are met in



The discovery of a region with $\gamma = 2$ validates the scaling argument put forward for the condition of vanishing T_c .

¹⁾ Present address: Laboratoire de Physique Expérimentale, EPF-Lausanne, Switzerland.

Dielectric susceptibility and local freeze-out of Li in KTaO_3

U. T. HÖCHLI and H. E. WEIBEL

(IBM Zurich Research Laboratory, 8803 Rüschlikon, Switzerland)

L. A. BOATNER

(Solid-State Division, Oak Ridge National Laboratory,¹⁾ Oak Ridge, Tennessee 37830, USA)

Traces of Li added to KTaO_3 render the crystal dispersive. The dispersion is attributed to hopping of Li between equivalent off-center positions at the K site. Its activation energy is determined as 0.125 eV and its one-well frequency as 10^{12} Hz. Below 30 K Li freezes-out and exhibits a static (but not spontaneous) polarization indicative of collective displacement of the Li plus ligand ions. The lack of hysteresis and of any acoustic anomaly above 0 K for samples with Li concentrations up to 20% shows that static polarization, as obtained by cooling

¹⁾ Operated by Union Carbide Corporation under contract W-7405-eng-26 with the U.S. Department of Energy.

the biased sample through the freeze-out temperature, is not due to bulk ferroelectricity.

Neutronenstreuung am weichen optischen Phonon in $\text{Ca}_x\text{Sr}_{1-x}\text{TiO}_3$

W. BÜHRER

(Institut für Reaktortechnik, Eidg. Technische Hochschule Zürich, 5303 Würenlingen)

J. G. BEDNORZ

(Laboratorium für Festkörperphysik, Eidg. Technische Hochschule, 8093 Zürich)

K. A. MÜLLER

(IBM Forschungslaboratorium, 8803 Rüschlikon)

Eine ausführliche Publikation ist in Vorbereitung.

Electronic properties of amorphous phosphorus prepared by chemical transport in a glow discharge¹⁾

W. E. SPEAR and P. G. LE COMBER

(Carnegie Lab. of Physics, Univ. of Dundee)

S. VEPŘEK and R. WILD

(Inst. of Inorganic Chemistry, University of Zurich)

Amorphous films of remarkable chemical stability have been prepared by chemical transport in a low pressure plasma. The conductivity was measured as a function of temperature between 290 and 450 K. Following values were found: r.t. conductivity between 10^{-12} and $10^{-15} \text{ (cm)}^{-1}$, act. energy 0.9–1.1 eV and pre-exponential factor σ_0 200 to 1000 (cm)^{-1} . Photoconductivity measurements show a sharp onset at 1.1 eV and an estimated optical gap between 2.5 and 3 eV.

¹⁾ Phil. Mag. B38, 349 (1978).

Erzwungene Rayleigh Streuung in Glas

DIETER POHL

(IBM Forschungslaboratorium Zürich, Säumerstr. 4, 8803 Rüschlikon, Schweiz)

Aufgrund der besonderen Natur des amorphen Zustandes werden Anomalien in der Rayleigh-Streuung bei tiefen Temperaturen erwartet [1]. Erzwungene thermische Rayleighstreuung [2] besitzt eine grosse Nachweisempfindlichkeit und kann mit Vorteil in einem solchen Fall angewandt werden. Die Streulichtintensität ist u.a. ein Mass für die Kopplungskonstante (dn/dT), die ihrerseits Information über den thermischen Ausdehnungskoeffizien-

ten, Konfigurationseffekte und dynamische Eigenschaften enthält. Für die beiden Schott Gläser BG20 und FG18 beobachten wir ungewöhnlich starke Streuung (im Vergleich zu entsprechenden Kristallen) für Temperaturen unter 30K in Einklang mit theoretischen Erwartungen [2].

LITERATUR

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Magneto-optical effects on the emission of self-trapped and localized excitons in alkali halide crystals [1]

Y. MORI, J.-P. VON DER WEID and M. A. AEGERTER

(Institut de Physique, Université de Neuchâtel, 2000 Neuchâtel)

The optical recombination of trapped hole (V_k center) and electron far or near monovalent cation impurities has been studied by optical detection of ESR (DC and transient behaviour) as well as magnetic circular and linear dichroism of the intrinsic (self trapped exciton) and perturbed excitonic emissions (localized-exciton) in several alkali halide crystals. Information on decay time kinetics, spin-lattice relaxation (one phonon process) and tunneling probabilities between pair of nearby defects (V_k -impurity) has been obtained and they will be explained quantitatively with a simple theoretical model.

REFERENCE

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Systèmes magnétiques, méthodes de résonance

Critical Heisenberg spin dynamic structure factor

J. S. HELMAN

(CIEA-IPN, México)

S. ALEXANDER

(RIP-HUJ, Israel)

Using general thermodynamic identities and inequalities, the critical behavior of integrals involving the critical spin dynamic structure factor $\Gamma(t, q, \omega)$ are discussed. Here, t is the reduced temperature, q is the wave vector and ω is the energy transfer. For a large class of integrands, including most cases of physical interest, it is shown that the most singular terms are of two types:

- (a) The instantaneous approximation result obtained by considering scattering from the thermodynamic correlation functions

- (b) A term which for intrinsic spin dynamics, e.g. for a Heisenberg model, has leading energy like singularities. This term can exhibit more complicated behaviour when the time dependence has external sources.

It is shown that this holds for the Fourier transform of $\exp(\beta\omega/2)\Gamma(t, q, \omega)$ itself, where $\beta = 1/kT$.

Magnetic excitations in ferromagnetic CeSb

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Circular polarization of the spectral thermal emission from polycrystalline iron

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Abstract. The spectral thermal emission from iron exhibits a partial circular polarization. Identical spectral dependence of the polarization was observed for a single crystal and for a polycrystal.

The spectral thermal emission from a single crystal of ferromagnetic iron was found to be partially circular polarized [1]. Identical results have now been obtained for polycrystalline iron.

The electropolished sample of polycrystalline iron (purity 99.99%) was heated in an uhv-chamber and magnetized. The radiation was analysed with a Soleil-Babinet compensator, a photoelastic modulator and polarizers. The arrangement of these optical components had to be adapted to the properties of the different detectors used for the various spectral regions.

The degree of polarization P was determined in the wavelength range $0.6 \mu\text{m} \leq \lambda \leq 5.5 \mu\text{m}$ and in the temperature range 900–1150 K. P is defined by the intensity ratio

$$P = \frac{I_{\text{LCP}}(B) - I_{\text{RCP}}(B)}{I_{\text{LCP}}(B) + I_{\text{RCP}}(B)}$$

The results for polycrystalline iron are given in Figs. 1 and 2.

In Fig. 1 the degree for polarization P at the constant wavelength $\lambda = 5.4 \mu\text{m}$ is plotted versus the temperature. The curve follows the magnetization of iron and diminishes above the Curie-temperature $T_c = 1043 \text{ K}$. The frequency dependence

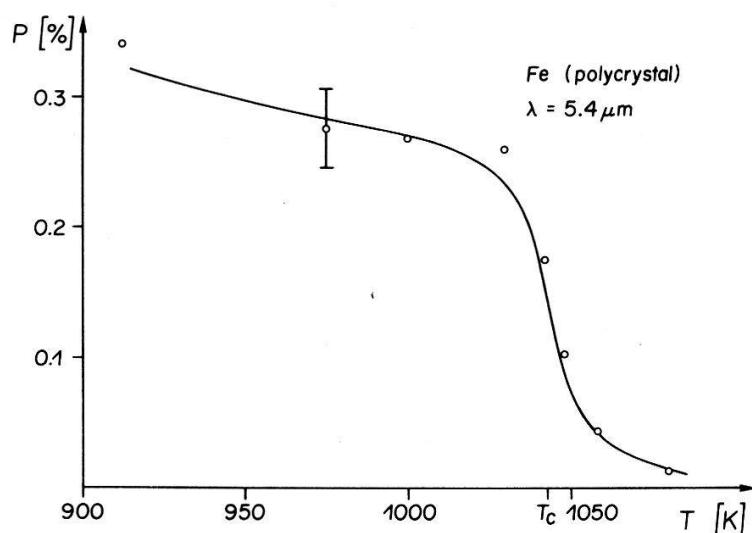


Figure 1

Degree of circular polarization P as a function of temperature at a constant wavelength.

of P is shown in Fig. 2. The result is the same as in the case of a single crystal [1]. The degree of polarization reaches a peak at 0.3 eV and changes sign at about 1.3 eV. The errors in Fig. 2 vary because of different methods of measuring and due to the variation of the intensity of the spectral thermal emission. The curve exhibits a fine structure in the region $1.5 \text{ eV} \leq h\nu \leq 2 \text{ eV}$. On expanded scale we found small oscillations of P with a period of about 90 meV which corresponds to $k \cdot T_{\text{Curie}}$.

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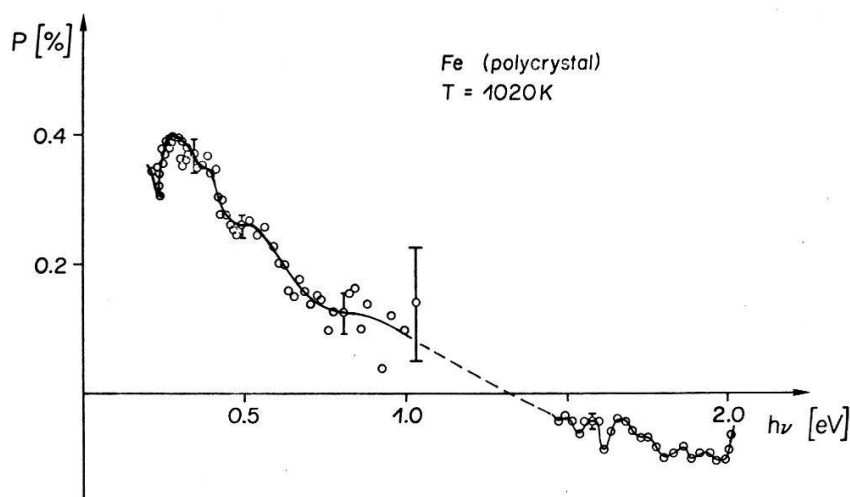


Figure 2

Degree of circular polarization P as a function of photon energy at constant temperature.

Electron spin resonance of Mn^{2+} -single ions, clusters and layers in the compounds $[\text{NH}_3-(\text{CH}_2)_2-\text{NH}_3]\text{Cd}_{1-x}\text{Mn}_x\text{Cl}_4$

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Abstract. The layer compounds $[\text{NH}_3-(\text{CH}_2)_2-\text{NH}_3]\text{Cd}_{1-x}\text{Mn}_x\text{Cl}_4$ with manganese concentrations $x \leq 0.005$, $x \approx 0.01$, and $x = 1$ have been investigated by electron spin resonance.

For $x < 0.005$, the single ion Mn^{2+} -spectra have been analysed. The crystal field splitting reflects the distortion, rotation and tipping of the Cl-octahedra. For $x \approx 0.01$, an exchange narrowed line has been found which broadens with $\Delta H \propto T^{-1}$ and weakens below about 50 K. Probably, small Mn^{2+} -clusters are present. In the manganese compound ($x = 1$) no paramagnetic line is seen below 51 K. The critical line broadening $\Delta H \propto (T/T_N - 1)^{-p}$ yields $T_N = 51 \pm 1$ K and $p = 1.2 \pm 0.1$.

Single crystals of the layer compounds $[\text{NH}_3-(\text{CH}_2)_2-\text{NH}_3]\text{Cd}_{1-x}\text{Mn}_x\text{Cl}_4$ have been grown by evaporation [1]. An electron spin resonance (ESR) spectrum recorded at room temperature and 9.5 GHz is shown in Fig. 1 for a sample of about $x \approx 0.005$. Clearly, a single ion spectrum of Mn^{2+} is seen with the characteristic hyperfine and crystal field splittings [2]. In addition, a narrow line is present at $g \approx 2$. This exchange narrowed line is attributed to small Mn^{2+} -clusters. At concentrations $x \approx 0.01$ only the narrow line is present. For low concentrations $x < 0.005$ only the single ion spectrum is measured. The values x have been estimated by comparing the intensities of the ESR signals with the exchange narrowed line in the manganese compound ($x = 1$).

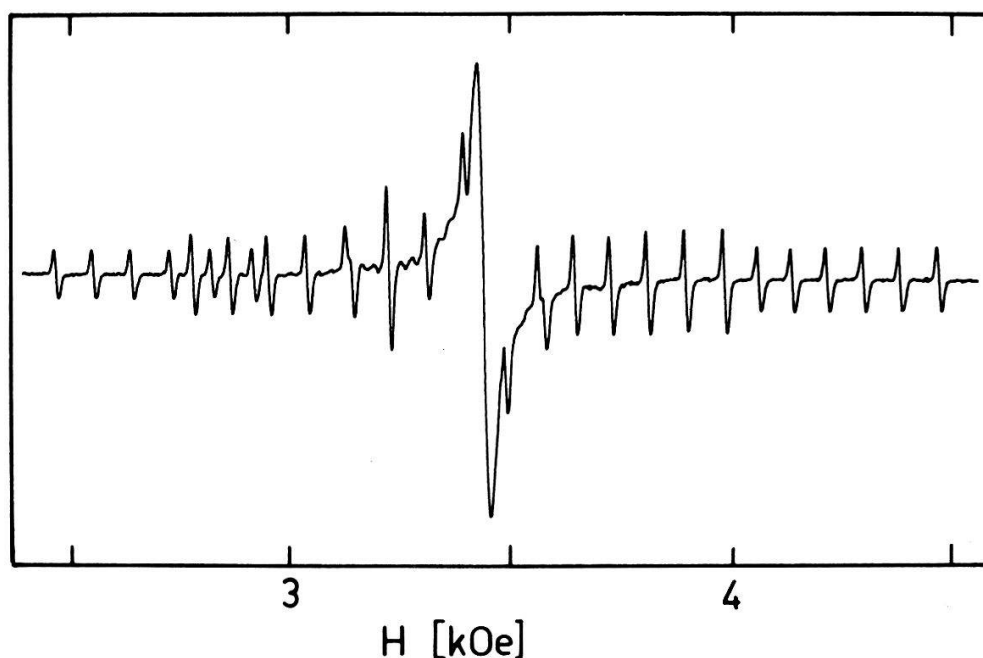


Figure 1

ESR-single ion and cluster spectrum of Mn^{2+} in $[\text{NH}_3-(\text{CH}_2)_2-\text{NH}_3]\text{Cd}_{1-x}\text{Mn}_x\text{Cl}_4$ with $x \approx 0.005$, measured at 9.5 GHz and room temperature, $H \perp c$ -axis.

First, the single ion results will be presented. Then, preliminary investigations of the cluster line will be described and compared with the critical line broadening in the manganese compound.

The single ion spectra of Mn^{2+} have been measured at room temperature in compounds with $x < 0.005$. The spectra reflect the mirror plane symmetry of the space group $P2_1/b$ ($Z = 2$) as determined by diffraction studies [3, 4]. Two sets of Mn^{2+} -lines are present when the applied field H is not parallel to the mirror plane. In order to find the symmetry axes xyz of the crystal field interaction tensor, the sample and the magnet have been rotated along perpendicular axes. The strongly anisotropic z -axis is tipped by $1.67 \pm 0.08^\circ$ from the mirror plane (which is normal to the c -axis) and has an angle of $7.3 \pm 0.2^\circ$ to the direction $\vec{b} \times \vec{c}$ normal to the layer plane bc . The weaker anisotropy in the plane normal to z has its symmetry axis x at an angle of $32 \pm 1^\circ$ to the axis b . These directions agree with the directions of the rotated and tipped Cl-octahedra as determined by diffraction methods [3, 4]. Hence, the Mn^{2+} -ions occupy regular Cd^{2+} -positions. Preliminary values of the usual parameters of the spin Hamiltonian [2] have been evaluated by second order perturbations:

$$\begin{aligned} g &= 2.004 \pm 0.001. \\ |D| &= (361.4 \pm 0.8) \times 10^{-4} \text{ cm}^{-1}. \\ |E| &= (20.4 \pm 0.6) \times 10^{-4} \text{ cm}^{-1}. \\ |a - F| &< 5 \times 10^{-4} \text{ cm}^{-1}. \\ |A| &= (80.3 \pm 0.9) \times 10^{-4} \text{ cm}^{-1}. \\ |B| &= (78.1 \pm 0.9) \times 10^{-4} \text{ cm}^{-1}. \end{aligned}$$

The compounds with concentrations x around 0.01 exhibit only the exchange narrowed line of nearly Lorentzian shape. The angular and temperature dependencies differ for samples of different growings. For two samples, the temperature dependencies of the line width ΔH_{pp} (peak-to-peak separation of absorption derivative) are plotted in Figs. 2a and 3a for H normal and parallel to the layers. Below about 50 K the line width is proportional to T^{-1} , see solid line in Fig. 2a. However, the intensity drops drastically around 50 K. As a crude estimate, the value $(\Delta H_{pp})^2 \cdot y_{pp}$ with the peak-to-peak amplitude y_{pp} is shown in Figs. 2b and 3b. The observed behavior might be interpreted by the presence of small Mn^{2+} -clusters. The smaller clusters remain superparamagnetic, while the larger clusters order antiferromagnetically around the Néel temperature of the manganese compound. It is not clear why the magnitude of the angular dependence is different in these samples.

The manganese compound ($x = 1$) has been investigated similar to the compound $[\text{NH}_3-(\text{CH}_2)_4-\text{NH}_3]\text{MnCl}_4$ [5]. In contrast to that compound, the critical broadening of the line width seems to follow a power law

$$\Delta H \propto (T/T_N - 1)^{-p}.$$

A fit to both T_N and p yielded $T_N = 51 \pm 1$ K and $p = 1.2 \pm 0.1$. No paramagnetic line is seen below 51 K.

The authors would like to thank H. Reimann and J. Mettler for valuable help and the Swiss National Science Foundation for partial financial support.

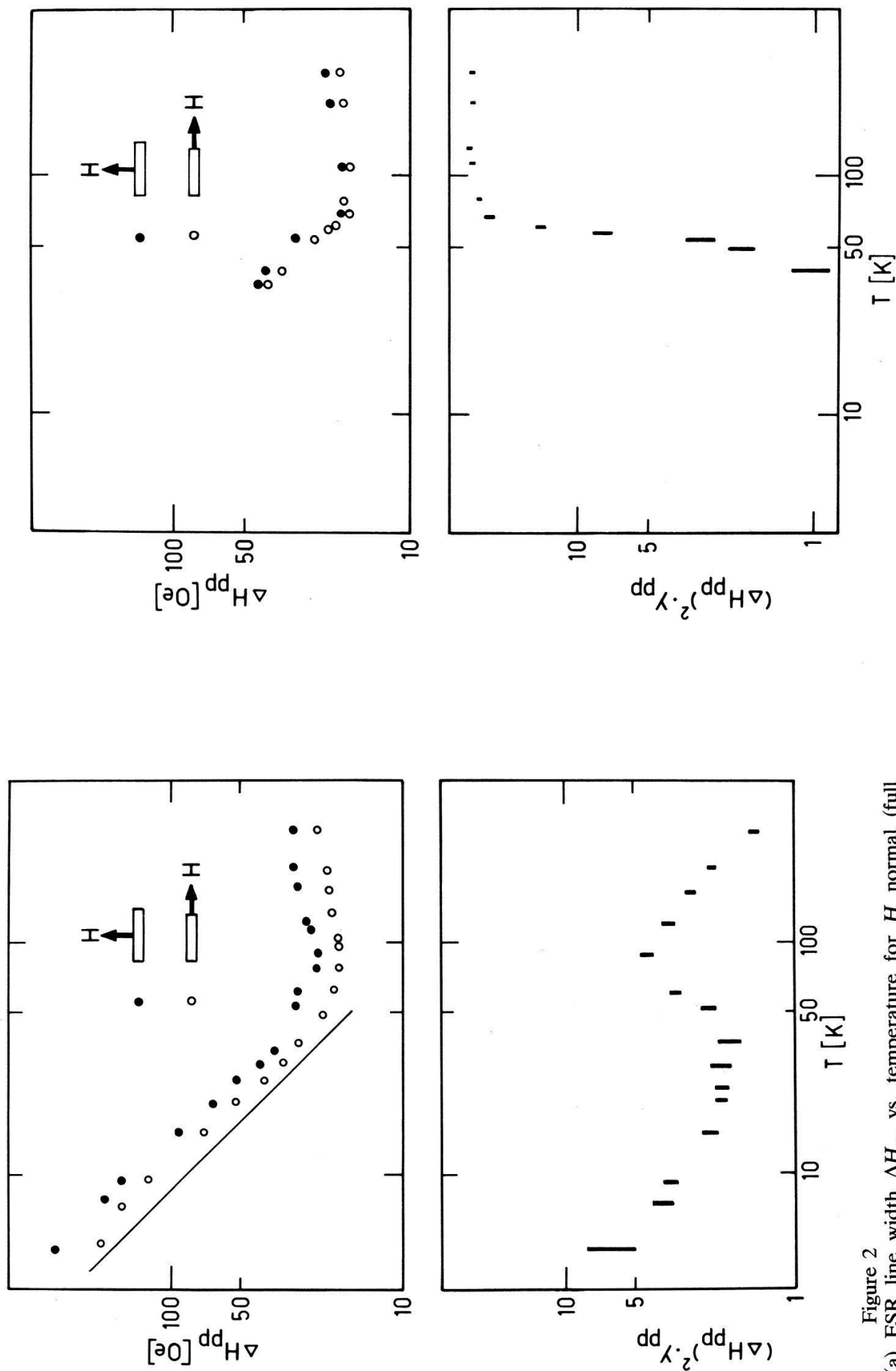


Figure 3

Same as Fig. 2, but for sample of different growing.

Figure 2

(a) ESR line width ΔH_{pp} vs. temperature for H normal (full circles) and parallel (open circles) to the layers in $[\text{NH}_3-(\text{CH}_2)_2-\text{NH}_3]\text{Cd}_{1-x}\text{Mn}_x\text{Cl}_4$ with $x \approx 0.01$. Solid line $\propto T^{-1}$. (b) The value $(\Delta H_{pp})^2 \cdot \gamma_{pp}$ is a crude estimate of the intensity of the ESR lines.

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Lithium-Diffusion im Superionenleiter Li_3N

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Die NMR-Quadrupol-Kopplungskonstanten und die Spin-Gitter-Relaxation der ^7Li -Kerne in den beiden nicht-gleichwertigen Lithium-Lagen in Li_3N wurden zwischen 230 und 600 K gemessen. Insbesondere die Abhängigkeit der Relaxation von Larmorfrequenz und Kristallorientierung wurde bestimmt. Daraus ergibt sich, dass unterhalb 370 K die Li-Diffusion vornehmlich innerhalb der beiden Schichten der Li-Lagen stattfindet, wobei auf eine Verteilung von Potentialbarrieren für diese Diffusion geschlossen werden muss. Bei höheren Temperaturen setzt via Zwischengitterplätze ein chemischer Austausch zwischen diesen Schichten ein, der schliesslich oberhalb 500 K zu einem flüssigkeitsähnlichen Verhalten führt und die Anisotropie der Leitfähigkeit stark reduziert. Die Anisotropie der Relaxation, Anomalien der 'Versuchsfrequenzen' sowie Aktivierungsenergien werden diskutiert.

Eichung der Isomerieverschiebung der Mössbauerisotope ^{127}I und ^{129}I

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Die in der Mössbauerspektroskopie gemessene Isomerieverschiebung δ ist proportional zum Produkt aus der Kernradiusänderung ΔR beim γ -Uebergang und der durch chemische Bindungsunterschiede bedingten Änderung der Elektronendichte $\Delta\rho(0)$ am Kernort:

$$\delta = \frac{4\pi}{5} Ze^2 R \Delta R \Delta\rho(0).$$

Aus Isomerieverschiebungsmessungen ist das Verhältnis $\Delta R_{127}/\Delta R_{129} = -0.78$ für die beiden Jodisotope $^{127,129}\text{I}$ bekannt. Die für $\Delta\rho(0)$ Bestimmungen notwendigen Absolutwerte ΔR lassen sich jedoch nur durch unabhängige Messungen von $\Delta\rho(0)$ an den entsprechenden Jodverbindungen erhalten. Wir haben für eine

solche Bestimmung die chemische Beeinflussung der Uebergangswahrscheinlichkeiten λ beim Elektroneneinfang von ^{125}I verwendet: $\Delta\lambda/\lambda = E_0^2 \Delta\rho(0)/\sum (\rho_i(0)(E_0 - E_{Bi})^2)$. E_0 ist die Uebergangsenergie ($E_0 = 143 \text{ keV}$) und E_{Bi} die Bindungsenergie der $K, L, M \dots$ -Schale. Die Lebensdauerunterschiede wurden mit einer differentiellen Ionisationskammer für 5 Jodverbindungen gemessen. Die Lebensdauer von ^{125}I wurde zu $\tau = \lambda^{-1} = 86.080 \pm 0.022 d$ bestimmt. Z.B. beträgt der Lebensdauerunterschied der Quells Kombination $\text{Na}_3\text{H}_2\text{IO}_6\text{-CsICl}_4: (\lambda(\text{Cs}) - \lambda(\text{Na}))/\lambda = (1.5 \pm 0.2) \times 10^{-4}$, woraus vorläufig $(\Delta R/R)_{129} = 6 \times 10^{-4}$ resultiert.

Mössbauer effect study of some binuclear ferricyanides

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Abstract. In the tetraphenylphosphonium salt of pentacyanoferrate(III)- μ -cyanotetracyanomonoammineferrate(III), $[(\text{C}_6\text{H}_5)_4\text{P}]_4[(\text{NC})_5\text{FeNCFe}(\text{CN})_4\text{NH}_3] \cdot 6\text{H}_2\text{O}$, the two inequivalent iron atoms are linked by a cyanide bridge. Mössbauer measurements on polycrystalline samples show two quadrupole doublets (at 300 K: $\Delta_1 = 1.11 \text{ mm/s}$ and $\Delta_2 = 1.92 \text{ mm/s}$), that can be assigned to two distinct crystallographic sites. As a function of temperature the Mössbauer parameters show anomalous behaviour. A 0.133-molar solution of the complex in methanol indicates that the complex is strongly altered upon dissolving. Furthermore a Mössbauer spectrum of the tetraphenylphosphonium salt of pentacyanoferrate(III)-pyrazine-pentacyanoferrate(III), $[(\text{C}_6\text{H}_5)_4\text{P}]_4[(\text{NC})_5\text{FepyrFe}(\text{CN})_5] \cdot 4\text{H}_2\text{O}$, was recorded.

I. Introduction

Cyano complexes of iron and their derivatives have raised interest for a long time, and many of them have been investigated by Mössbauer spectroscopy because of their interesting magnetic properties [1]. Dimeric iron cyano complexes are relatively unknown both from a chemical point of view as well as with respect to their magnetic properties. In the binuclear tetraphenylphosphonium salt of pentacyanoferrate(III)- μ -cyano-tetracyanomonoammineferrate(III), $[(\text{C}_6\text{H}_5)_4\text{P}]_4[(\text{NC})_5\text{FeNCFe}(\text{CN})_4\text{NH}_3] \cdot 6\text{H}_2\text{O}$, the two iron atoms are linked by a cyanide bridge, thus yielding two inequivalent iron sites (cf. Fig. 1). Whereas the full crystallographic structure will shortly be published elsewhere [2], we will here describe Mössbauer studies on this complex. Since the subject of cyanide bridging is of current chemical interest [3, 4], we investigated also a frozen solution of this complex in methanol solvent. Furthermore we extended the measurements to the tetraphenylphosphonium salt of pentacyanoferrate(III)-pyrazine-pentacyanoferrate(III), $[(\text{C}_6\text{H}_5)_4\text{P}]_4[(\text{NC})_5\text{FepyrFe}(\text{CN})_5] \cdot 4\text{H}_2\text{O}$, in which each of the iron atoms is coordinated by five cyanide groups and by one nitrogen atom of the

pyrazine molecule, which provides the bridge (pyr is pyrazine, ).

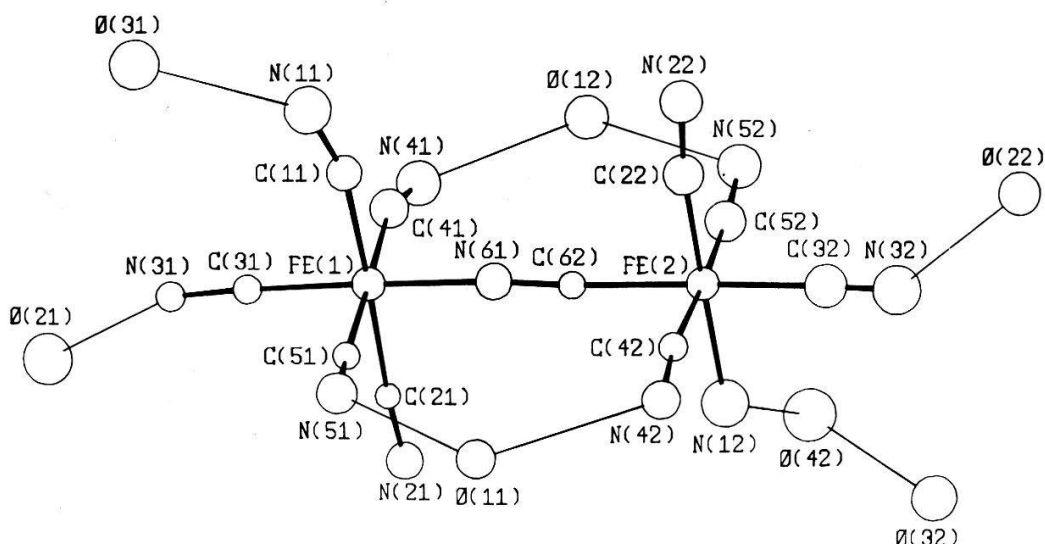


Figure 1

X-ray structure of pentacyanoferrate(III)- μ -cyano-tetracyanomonoammineferrate(III), $[(\text{NC})_5\text{FeNCFe}(\text{CN})_4\text{NH}_3]^{4-}$.

II. Experimental results

Mössbauer spectra of the $[(\text{NC})_5\text{FeNCFe}(\text{CN})_4\text{NH}_3]^{4-}$ complex were recorded as a function of temperature between 6 K and 300 K. Two representative spectra are shown in Fig. 2. The spectra were interpreted in terms of two quadrupole doublets. The quadrupole splittings and the isomer shifts were evaluated by fitting the data with four lines of Lorentzian shape. The results of

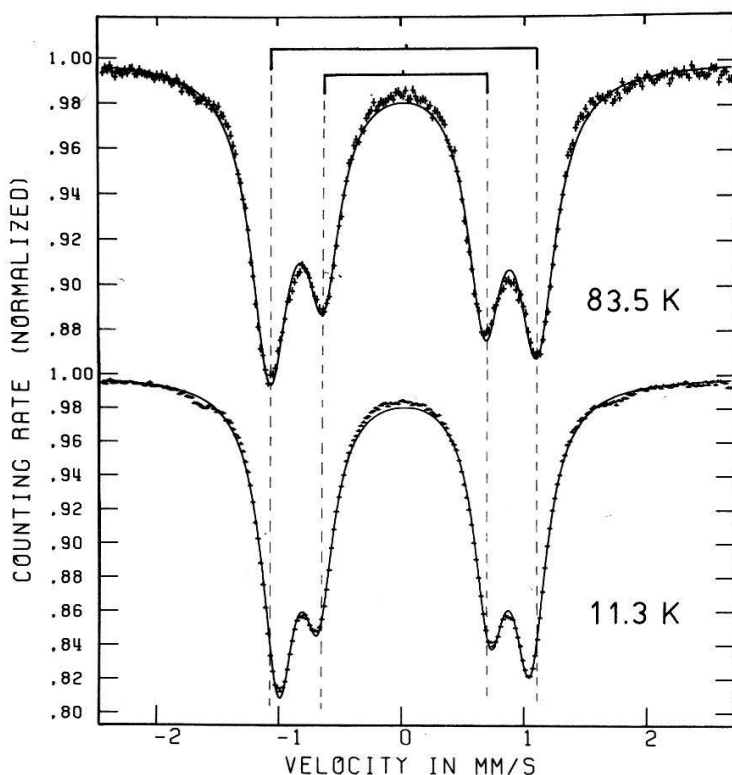


Figure 2

Mössbauer spectra of the tetraphenylphosphonium salt of pentacyanoferrate(III)- μ -cyano-tetracyanomonoammineferrate(III), $[(\text{C}_6\text{H}_5)_4\text{P}]_4[(\text{NC})_5\text{FeNCFe}(\text{CN})_4\text{NH}_3] \cdot 6\text{H}_2\text{O}$.

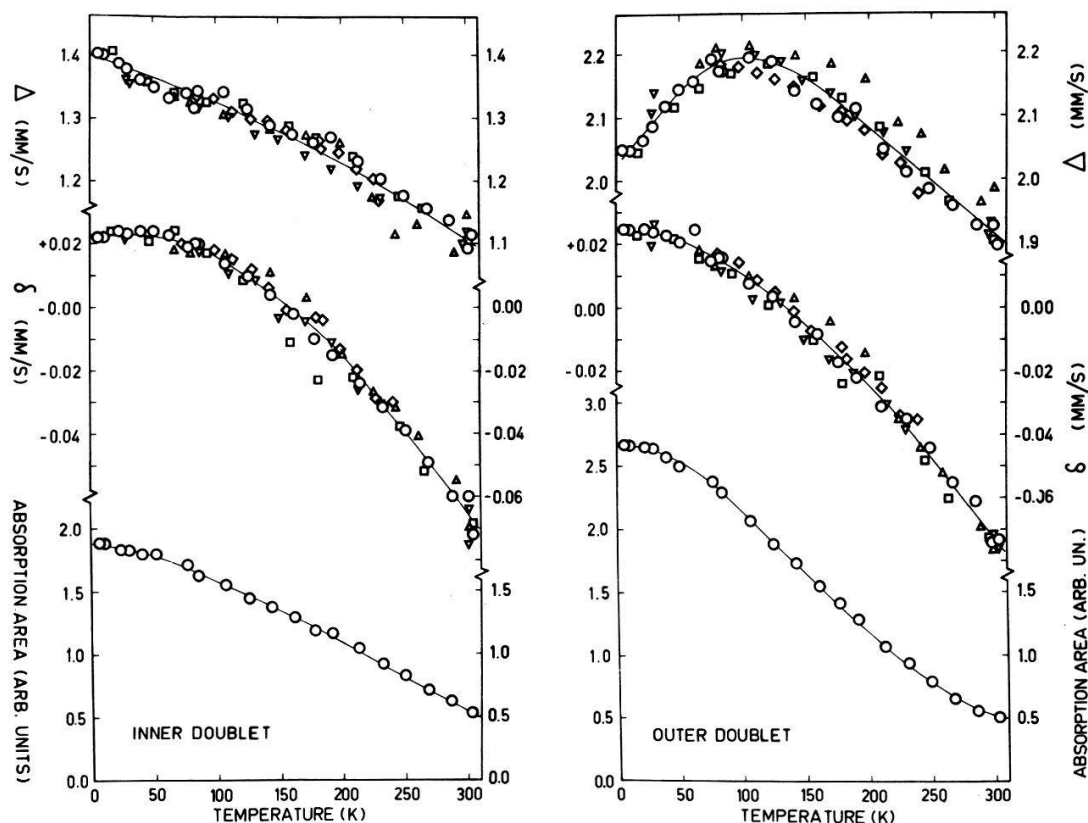


Figure 3

Temperature dependence of the quadrupole splittings (Δ), the isomer shifts (δ) and the absorption areas in $[(C_6H_5)_4P]_4[(NC)_5FeNCFc(CN)_4NH_3] \cdot 6H_2O$. Symbols of different shapes indicate the different measurement series.

several series of measurements on polycrystalline samples of different batches are shown in Fig. 3. For one particular set of measurements no adjustments to the counting circuit were made (Fig. 3). At room temperature the average values of the quadrupole splittings (Δ) and isomer shifts (δ), relative to natural metallic iron, are: $\Delta = 1.92 \pm 0.03$ mm/s and $\delta = -0.073 \pm 0.003$ mm/s for the outer doublet and $\Delta = 1.11 \pm 0.03$ mm/s and $\delta = -0.067 \pm 0.003$ mm/s for the inner doublet.

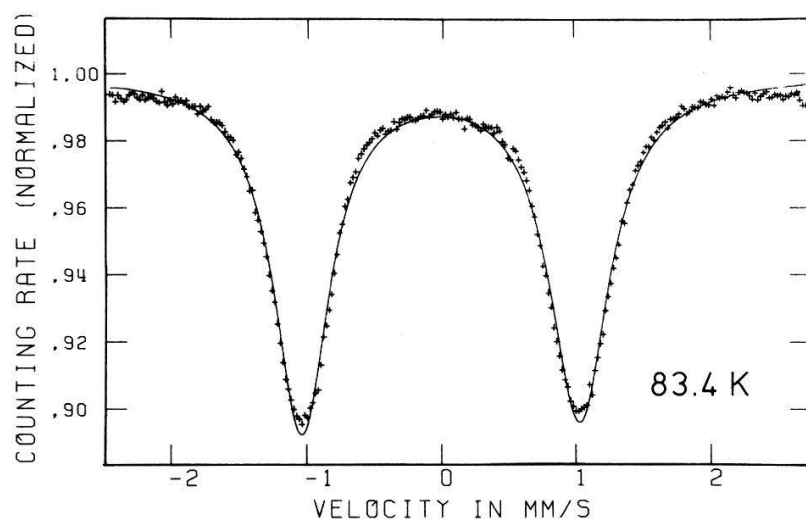


Figure 4

Mössbauer spectrum of a frozen 0.133 molar solution of $[(C_6H_5)_4P]_4[(NC)_5FeNCFc(CN)_4NH_3] \cdot 6H_2O$ in methanol.

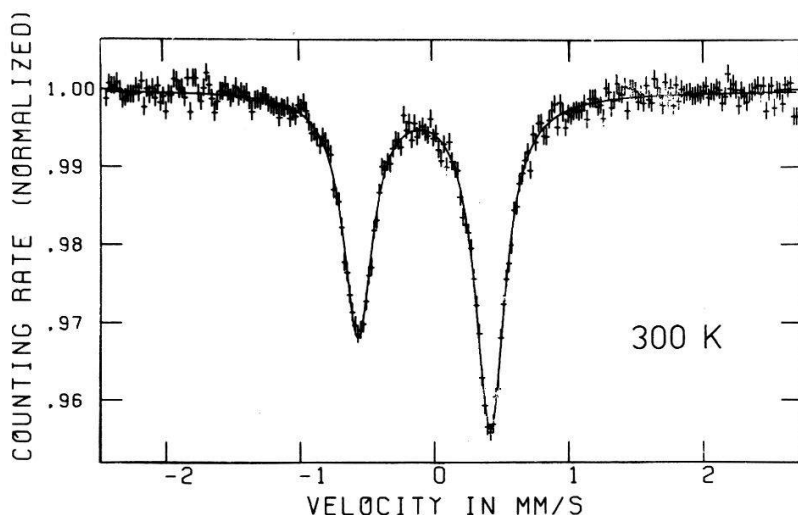


Figure 5

Mössbauer spectrum of the tetraphosphonium salt of pentacyanoferrate(III)-pyrazine-pentacyanoferrate(III), $[(C_5H_6)_4P]_4 \cdot [(NC)_5FepyrFe(CN)_5] \cdot 4H_2O$.

The dark green crystals are soluble in methanol, yielding a violet solution. On evaporation of the solvent the green product is obtained again giving an X-ray powder pattern identical to that of the starting material. The Mössbauer spectrum of the frozen solution is shown in Fig. 4 and could be described with only one quadrupole doublet. At 83.8 K the spectral parameters of this doublet are: $\Delta = 2.06 \pm 0.02$ mm/s and $\delta = 0.00 \pm 0.02$ mm/s. The lines are somewhat broadened; linewidth $\Gamma = 0.52 \pm 0.02$ mm/s.

The Mössbauer spectrum of the symmetrically bridged $[(NC)_5FepyrFe(CN)_5]^{4-}$ -complex is shown in Fig. 5 and could be described as expected in terms of one quadrupole doublet. The spectral data at room temperature are: $\Delta = 0.985 \pm 0.005$ mm/s and $\delta = -0.077 \pm 0.005$ mm/s.

III. Discussion

The values obtained of the quadrupole splittings and isomer shifts establish that the iron atoms at both crystallographic sites in the $[(NC)_5FeNCFe(CN)_4NH_3]^{4-}$ complex, as well as in the $[(NC)_5FepyrFe(CN)_5]^{4-}$ complex are in the low spin $S = \frac{1}{2}$ state.

In order to assign the quadrupole doublets to the two different crystallographic sites in the $[(NC)_5FeNCFe(CN)_4NH_3]^{4-}$ complex one may compare the results with those of other monosubstituted ferricyanides (cf. Table 1). For a comparison with the Fe(1)-site, which is coordinated by five cyanide carbons and by one nitrogen of the cyanide bridge (cf. Fig. 1), one may consider the $[(NC)_5FepyrFe(CN)_5]^{4-}$ complex. The quadrupole splitting of the latter ($\Delta = 0.985$ mm/s) suggests that the inner doublet ($\Delta = 1.11$ mm/s) should be ascribed to the Fe(1)-site.

The Fe(2)-site, located at the carbon end of the cyanide bridge, is coordinated by 5 cyanide carbons and by the NH_3 group. As a comparison serves the compound $Na_2Fe(CN)_5NH_3 \cdot H_2O$ [5], which has a quadrupole splitting ($\Delta = 1.78$ mm/s) quite similar to that of the outer doublet ($\Delta = 1.92$ mm/s). This

Table 1
Mössbauer data of some substituted ferricyanides

Compound	T(K)	Δ (mm/s)	δ (mm/s) (rel. to Fe)	Reference
[(C ₅ H ₆) ₄ P] ₄ [(NC) ₅ FeNCFc(CN) ₄ NH ₃]-6H ₂ O, crystalline	300	1.92 ± 0.03	-0.073 ± 0.003	this work
		1.11 ± 0.03	-0.067 ± 0.003	
	77	2.18 ± 0.03	+0.015 ± 0.003	
		1.34 ± 0.03	+0.020 ± 0.003	
	6	2.04 ± 0.03	+0.024 ± 0.003	
[(C ₅ H ₆) ₄ P] ₄ [(NC) ₅ FeNCFc(CN) ₄ NH ₃]-6H ₂ O, 0.133 molar solution in methanol		1.40 ± 0.03	+0.023 ± 0.003	this work
	83.4	2.06 ± 0.02	0.00 ± 0.02	
[(C ₅ H ₆) ₄ P] ₄ [(NC) ₅ FepyrFe(CN) ₅]-4H ₂ O	300	0.985 ± 0.005	-0.077 ± 0.005	this work
Na ₂ [Fe(CN) ₅ NH ₃]-H ₂ O	300	1.78 ± 0.05	-0.09 ± 0.05	[5]

confirms the site assignment proposed above, the outer doublet thus corresponding to the Fe(2)-site.

The relative absorption intensity of the doublets is somewhat puzzling. Whereas at low temperature the outer doublet is about 40% more intense than the inner doublet (cf. Fig. 3), both doublets have approximately equal intensity at room temperature. It may be reminded that in a simple approach to the recoilless fraction, as is e.g. offered by the Debye model, one would expect an increase of the intensity ratio towards higher temperatures, rather than the behaviour observed here.

The isomer shifts show a gradual decrease with increasing temperature. This is due to the second order Doppler shift.

The temperature dependence of the quadrupole splitting of low spin trivalent iron has been studied by Gibb [6], and shows for a wide range of crystal field splittings hardly any temperature dependence below 100 K. As can be seen in Fig. 2, the present measurements feature a maximum at approximately 100 K for the outer doublet, whereas a continuous increase towards lower temperature is observed for the inner doublet. A possible influence of the crystal field states of the iron atom at the Fe(1)-site due to the vicinity of the non-equivalent iron atom at the Fe(2)-site and vice versa was investigated by diagonalizing the full crystal field Hamiltonian of the dimer, including spin-orbit coupling and magnetic exchange. However it was not possible to obtain a satisfactory description of the experimental data, thus indicating that the observed behaviour is not due to this mechanism.

This unusual behaviour of the Mössbauer parameters as a function of temperature is at present not understood. A possible explanation may be that they are partly a consequence of structural changes at low temperatures. Also from the susceptibility measurements [2] indications in that direction could be inferred.

The frozen solution spectrum of the [(NC)₅FeNCFc(CN)₄NH₃]⁴⁻ complex clearly shows that the site inequivalency which is obvious in the crystals, does not persist in methanol solution. This result can only be explained by assuming considerable alterations of the complex on going into solution. Also the striking change from dark green to violet colour points in that direction. The possibility should be considered that the original complex is split into two equal pentacyano

complexes. In this respect one can perhaps think of the violet pentacyano-monoaquo complex $[\text{Fe}(\text{CN})_5\text{H}_2\text{O}]^{2-}$ described by Hofmann [7]. Alternatively the formation of a binuclear species, $[\text{Fe}_2(\text{CN})_{10}]^{4-}$, with a symmetric double cyanide bridge cannot be excluded [3, 4]. Whatever may be the case, the present measurement indicates that the NH_3 group no longer coordinates directly to the iron in methanol solution.

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Structures cristallines, divers

Elektronendichtebestimmung und elektrostatische Grössen

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Die genaue Kenntnis der räumlichen Elektronendichte in einem Kristall erlaubt die Berechnung elektrostatischer Grössen. Die Präzision röntgenographisch bestimmter Elektronendichten ist jedoch zumeist ungenügend, wobei die Fehler in der Nähe der Atomzentren maximal sind. Wir suchen deshalb nach derjenigen (quasi-vibrationsfreien) Elektronendichte, die gleichzeitig die Diffraktionsdaten und mit NQR-Methoden bestimmte Feldgradienten möglichst gut reproduziert. Dies führt zu erhöhter Präzision, sofern nur das zur Parametrisierung der Ladungsdichte verwendete Pseudoatom-Modell (Multipolfunktionen mit variablen Besetzungszahlen [1]) genügend flexibel ist, gleichzeitig die Quadrupolverzerrungen im Atominneren und die Bindungsdichten zu simulieren. Das Verfahren wurde auf die Quarzstruktur von AlPO_4 erfolgreich angewendet. Diplomomente könnten in Strukturen starrer Molekeln ähnlich verwendet werden.

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Local ordering of the Na^+ -ions in Na_xTiS_2

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To understand the physical properties of alkali ion intercalates of transition metal chalcogenides in connection with their use as electrodes in electrochemical devices, the local arrangement of the Na^+ -ions in electrochemically intercalated single crystals of TiS_2 was studied by means of diffuse X-ray scattering. For $x < \frac{1}{2}$ a series of stoichiometric compounds appears to exist. Superlattices in the hexagonal c -direction correspond to structures, in which one out of two, three or more van der Waals layers are filled with sodium ions. Within the intercalate layers the ions are organized into three different types of superlattices. The almost flat Na^+ -activity in this stoichiometry range is consistent with these observations. Above $x = \frac{1}{2}$, where all planes are intercalated the structure becomes disordered.

Electron-optical analysis of Gd_2SiO_5 in the 3 Å resolution range

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An electron-optical analysis of the structure of Gd_2SiO_5 (monoclinic) has been made based on a large amount of through-focus series of n -beam images for the [100]- and [001]-projections using a JEM-100 C electron microscope with a high resolution objective lens pole piece, with $C_s = 0.7$ mm. Image contrast calculations using the multislice (Cowley-Moodie) approximation were performed in collaboration with Dr. L. Kihlberg, Arrhenius Laboratory, Stockholm. The comparison of calculated and observed contrast serves to investigate the possibility of recognizing the heavy atom positions (Gd) in this silicate structure and to analyse fine structure in both the observed and the calculated contrast of the [100]-projection. In the observed images, for approx. -200 and -300 Å under-focus, a bee-hive shaped arrangement of white dots approximately 1.7 Å apart is resolved and related to the projected potential.

Flussquantisierung (FQ) der (kovalenten) chemischen Einzelbindung

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Das Studium der Festkörper (FK) valenz-abhängigen – schon im 2-atomigen Fall extrem komplexen – Molekülionenformation im FK-Stereoplasma aus dem nichtmolekularen kovalenten und/oder ionogenen (realen) FK führt zu neuartigen Einblicken in den Mikroprozess der Bindung. Es gelingt der Nachweis, dass die Bildung eines Valenzelektronenpaares der FQ unterliegt, und, pro Einzelektron, quantitativ mit dem Befund am Atom übereinstimmt [1]. Minimale

Flussänderung: $\phi_0 = h/2e$. Anstelle des Ionisierungsgrads tritt die Valenzstufe als Niveau eines Quantenrotators.

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Un spectromètre de haute masse

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Dans le but d'étudier des amas d'atomes identiques à très haute masse un spectromètre classique, à relativement basse résolution, à simple secteur magnétique de 60° , à champ uniforme focalisant dans les directions horizontale et verticale a été construit. Sa limite supérieure en masse est de 26000 u.m.a. pour une tension d'accélération de 2000 V. Les caractéristiques principales de l'électro-aimant sont, un rayon de courbure de 80 cm, un entrefer de 5 cm et un champ max. de 13 KG. La ionisation est du type à bombardement électronique et la détection se fait à l'aide d'un multiplicateur d'électrons secondaires suivit soit d'un électromètre, soit d'une chaîne de comptage avec ratemeter.

Le double-emploi de la vitesse en hydrodynamique

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Les phénomènes électromagnétiques, n'agissant que très indirectement sur nos sens, sont restés longtemps enveloppés d'une sorte de mystère. Mais il a suffi d'un siècle à peine, de Franklin à Maxwell, pour faire de l'électromagnétisme le paradigme des théories de la physique mathématique classique; l'abstraction même des faits a forcé les Gauss, les Ampère, les Faraday, à concevoir l'objet de leurs découvertes directement dans le cadre de l'analyse mathématique.

Ce qui donne aux équations de Maxwell leur caractère *fondamental*, c'est leur signification topologique; et cette signification topologique est établie par la possibilité d'exprimer les équations de Maxwell au moyen du calcul différentiel extérieur [1, 2]. Dans l'espace-temps, une première forme Φ , d'espèce paire, groupe les composantes du *champ électrique* E et de l'*induction magnétique* B ; une seconde forme Ψ , d'espèce impaire, contient les composantes de l'*induction électrique* D et du *champ magnétique* H . Les équations de Maxwell consistent simplement à écrire

$$\begin{aligned} d\Phi &= -P, \\ b\Psi &= Q, \end{aligned} \tag{1}$$

où P contient les densités de *pôle magnétique* m et de *force électromotrice* e , tandis que Q contient les densités de *charge* ρ et de *courant* j . Dans l'espace, ces deux

équations se décomposent en quatre équations

$$\begin{aligned} dE + \dot{B} &= e, \\ bH - \dot{D} &= j, \end{aligned} \quad (2)$$

$$\begin{aligned} dB &= m, \\ bD &= -\rho. \end{aligned} \quad (2')$$

Les *inductions* sont les deux formes qui apparaissent par leur *dérivée temporelle* dans le système (2), tandis que les deux *champs* sont celles qui y figurent respectivement par leur différentielle et leur bord. Le système (2') est, moyennant une condition initiale, conséquence du système (2) et des relations de *conservation*

$$de = \dot{m}, \quad bj = \dot{\rho}. \quad (3)$$

Tout ce formalisme est presque entièrement *a priori*; l'exactitude *axiomatique* des relations (1) est possible grâce à la distinction des champs et des inductions, d'où résulte une indétermination qui permet l'ajustement nécessaire. Les *relations phénoménologiques* entre les champs et les inductions sont *a posteriori*, et traduisent les observations de l'expérience.

Il est facile de trouver pour la thermodynamique un système d'équations fondamentales répondant au modèle Maxwellien [3]. La chose n'est pas si aisée pour l'hydrodynamique; peut-être cela vient-il de la familiarité des faits: les préjugés de l'expérience entravent l'abstraction de la pensée.

Il y a cependant une première équation de l'hydrodynamique qui s'offre immédiatement sous une forme fondamentale: c'est l'équation de continuité $\text{div } w + \dot{\rho} = \kappa$, où w est le *flux de matière*, ρ la *densité de matière*, et κ la *densité de création de matière*; nous poserons en conséquence, dans l'espace-temps

$$\tilde{\rho} = \rho[0] + w^1[1] + w^2[2] + w^3[3], \quad (4)$$

$$\tilde{\kappa} = \kappa[_x], \quad (5)$$

et nous écrirons

$$b\tilde{\rho} = -\tilde{\kappa}; \quad (6)$$

dans l'espace, nous aurons

$$-bw + \dot{\rho} = \kappa. \quad (7)$$

Selon l'analogie des équations de Maxwell, w apparaît donc comme un *champ*, et ρ comme une *induction*. A la forme spatio-temporelle (4), d'espèce impaire de dimension 1, doit correspondre une forme d'espèce paire de degré 1, dont pour le reste nous ignorons tout pour l'instant, mais que nous nommerons $\tilde{\eta}$, et développerons ainsi:

$$\tilde{\eta} = -\eta[0] + v_1[1] + v_2[2] + v_3[3]; \quad (8)$$

nous écrirons encore

$$\begin{aligned} \tilde{g} &= -g_1[01] - g_2[02] - g_3[03] \\ &\quad + \omega^1[23] + \omega^2[31] + \omega^3[12], \end{aligned} \quad (9)$$

et poserons

$$d\tilde{\eta} = \tilde{g}. \quad (10)$$

Dans l'espace, (10) donnera

$$d\eta + \dot{v} = -g, \quad (11)$$

$$dv = \omega, \quad (11')$$

ce qui, vectoriellement, se traduit respectivement par $\text{grad } \eta + \dot{v} = -g$ et $\text{rot } v = \omega$; η est un *champ* et v une *induction*. De (11) et (11') on tire l'équation de conservation

$$dg + \dot{\omega} = 0, \quad (12)$$

ou $\text{rot } g + \dot{\omega} = 0$.

Ecrivant l'une sous l'autre l'équation (11) et l'équation (7), multipliant la première par w , la seconde par η :

$$\begin{array}{r|l} d\eta + \dot{v} = -g & w \\ -bw + \dot{\rho} = \kappa & \eta \end{array} \quad (13)$$

$$\eta \wedge \dot{\rho} + \dot{v} \wedge w - b(\eta \wedge w) = -g \wedge w + \eta \wedge \kappa,$$

nous obtenons le *bilan de l'énergie*; cela nous fait apercevoir quelles doivent être les significations respectives des formes η et v : si $\dot{v} \wedge w$ est la dérivée temporelle de la densité d'énergie cinétique, v est alors la *vitesse*; quant à η , c'est le facteur de $\dot{\rho}$ dans l'expression de la dérivée temporelle de la densité d'énergie non-cinétique: c'est donc le *potentiel chimique*.¹⁾

Suivant cette conjecture, nous rapprocherons l'équation (11) de l'équation d'Euler

$$\frac{1}{\rho} \text{grad } p + D_t v = -\bar{g}, \quad (14)$$

où p est la *pression*, $-\bar{g}$ le *champ d'accélération*, et D_t le symbole de la *dérivée convective*

$$D_t = \partial_t + v^1 \partial_1 + v^2 \partial_2 + v^3 \partial_3. \quad (15)$$

Ce qui est embarrassant dans la comparaison des équations (11) et (14), c'est que dans cette dernière v est soumis au symbole D_t , tandis que dans la première le point qui surmonte v représente la dérivation ∂_t .

Voici comment on se tire d'affaire. Comme on le sait, l'équation d'Euler peut se mettre sous la forme suivante

$$\frac{1}{\rho} \text{grad } p + \text{grad } \frac{v^2}{2} + \partial_t v = -\bar{g} + v \times \text{rot } v \quad (16)$$

¹⁾ La nature *chimique* de cette forme d'énergie n'est pas évidente du fait que nous ne considérons ici qu'une seule sorte de matière; mais si nous avons à distinguer deux *espèces chimiques* (1) et (2), nous devrions écrire $\eta \wedge \dot{\rho} = \eta^{(1)} \wedge \dot{\rho}_{(1)} + \eta^{(2)} \wedge \dot{\rho}_{(2)}$, et l'expression des $\eta^{(i)}$ en fonction des $\rho_{(i)}$ dépendrait bien de la chimie. D'ailleurs, le mot *chimie* ne vient-il pas de la racine égyptienne *kem*, signifiant *noir*, et dont dérivait *Kemet*, qui était le nom même de l'Égypte [4]? Parce que *kem* était la couleur du célèbre limon, présent du Nil, qui était aussi le symbole de la *matière* sous sa forme la plus générale.

Il ne reste plus alors qu'à poser

$$\eta = \int \frac{\delta p}{\rho} + \frac{v^2}{2} \quad (17)$$

$$g = \bar{g} - v \times \text{rot } v, \quad (18)$$

pour identifier les équations (11) et (16).

Mais il faut remarquer maintenant que la vitesse v apparaît dans $\tilde{\eta}$ par ses composantes *covariantes* v_i , tandis que dans D_t figurent les composantes *contravariantes* v^i ; pour faire rentrer ces dernières dans le cadre du calcul différentiel extérieur, nous poserons

$$\hat{v} = v^1[{}_1] + v^2[{}_2] + v^3[{}_3], \quad (19)$$

et nous distinguerons la *vitesse convective* $\hat{v}$, d'espèce impaire, de la *vitesse inductive* v , d'espèce paire.

Ainsi, la vitesse nous apparaît sous deux aspects, liés, il faut le dire, par une propriété très profonde de l'univers physique, à savoir sa métrique; mais fondamentalement, la métrique est un phénomène expérimental, qui ne doit pas s'exprimer dans des équations fondamentales. Aussi est-ce l'induction v qui est *a priori*, et que l'on soumet à l'équation (11) avant toute détermination expérimentale; la convection $\hat{v}$ est *a posteriori* et ses coefficients sont, comme nous allons le voir, des coefficients phénoménologiques.

D'après le bilan (13), si la densité d'énergie U est une fonction d'état, on aura pour sa variation

$$\delta U = \eta \delta \rho + w \cdot \delta v; \quad (20)$$

les *relations matérielles* consisteront dans l'expression des variations des champs $(\delta \eta, \delta w)$ en fonction de celles des inductions $(\delta \rho, \delta v)$. Supposons que $U(\rho, v)$ soit de la forme

$$U = \phi(\rho) + \frac{\rho v^2}{2}; \quad (21)$$

nous aurons alors

$$\delta U = \left(\phi'(\rho) + \frac{v^2}{2} \right) \delta \rho + \rho v \delta v, \quad (22)$$

d'où

$$\eta = \phi'(\rho) + \frac{v^2}{2}, \quad (23)$$

$$w = \rho v,$$

et enfin

$$\begin{pmatrix} \delta \eta \\ \delta w \end{pmatrix} = \begin{pmatrix} \phi'' & \hat{v} \\ \hat{v} & \hat{\rho} \end{pmatrix} \begin{pmatrix} \delta \rho \\ \delta v \end{pmatrix}. \quad (24)$$

C'est à dessein que nous avons écrit $\hat{v}$ dans la matrice, car la demi-variation du carré du module de la vitesse est bien $v^i \delta v_i$; nous avons aussi écrit $\hat{\rho}$ à la place de ρ dans la matrice; car il est clair que si $w = \rho \hat{v}$, on n'aura pas, en toute rigueur, le droit d'écrire $w = \rho v$; cependant, tant que le tenseur métrique s'exprime par la matrice unité, on a numériquement $v^i = v_i$, et donc $\hat{\rho} = \rho$.

Quant à ϕ'' , il est tel, d'après l'équation (17), que l'on ait

$$\phi'' \delta \rho = \frac{\delta p}{\rho}, \quad (25)$$

c'est-à-dire

$$\hat{\rho} \phi'' = \frac{dp}{d\rho} = c^2 \quad (c = \text{célérité des ondes acoustiques}). \quad (26)$$

On pourrait trouver que le *double-emploi* de la vitesse, comme induction et comme convection, n'est fondé que sur une subtilité d'orthographe tensorielle, et ne devrait prendre de consistance physique qu'en théorie de la relativité. Il y a cependant une circonstance très pratique où cette distinction se révèle indispensable: c'est l'application de la méthode du *complexe topologique* [5, 6] à la discrétisation d'un problème d'hydrodynamique.

Dans ce cas, on posera [7]

$$\begin{aligned} \eta &= \eta_i P^i, & v &= v_i L^i, \\ \rho &= \rho^i P_i, & w &= w^i L_i, \end{aligned} \quad (27)$$

où les P sont attachés à des *points*, et les L à des *lignes* du complexe *primaire*; les coefficients v_i , étant les intégrales $\int_{L_i} v$, auront pour dimension physique $[m^2 \cdot s^{-1}]$, tandis que les coefficients ρ^i se mesureront en $[kg]$. En revanche, la vitesse convective aura pour support des lignes Λ du complexe *secondaire*

$$\hat{v} = \hat{v}^{ij} \Lambda_{ij}, \quad (28)$$

et les coefficients $\hat{v}^{ij}$ auront pour dimension physique $[s^{-1}]$. Quant à la matrice $\hat{\rho}$, discrétisation de la densité considérée comme coefficient matériel, ses éléments $\hat{\rho}^{ij}$ auront pour dimension physique $[kg \cdot m^{-2}]$.

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Probenhalter für Tieftemperatur-in-situ-Verformungsversuche in einem 200 kV-Durchstrahlungs-Rasterelektronenmikroskop

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Es wird ein Probenhalter gezeigt, der es ermöglicht, Proben bei Temperaturen < 20 K im Mikroskop zu verformen. Solche Halter wurden bisher nur in Hochspannungselektronenmikroskopen verwendet. Die hohe Energie der abbildenden Elektronen erzeugt jedoch in der Mehrzahl aller Metalle atomare Gitterfehler oder deren Agglomerate. In einem 200 kV-Mikroskop ist die Energie genügend klein, trotzdem können noch relativ dicke Folien durchstrahlt werden. Ausserdem können in einem Rasterelektronenmikroskop Veränderungen der Anordnung von Gitterfehlern ohne Kamera auf Magnetband aufgezeichnet werden. Mit dem Probenhalter wurde zum ersten Mal beobachtet, wie sich Versetzungssegmente bei 20 K bewegen, wenn sie unter dem Einfluss von inneren Spannungen und einer variierenden angelegten Spannung stehen (vgl. Messung der inneren Reibung bei niedrigen Frequenzen). Zusätzlich wurde beobachtet wie sich die Lage einzelner Segmente bei konstanter Spannung bei verschiedenen Beobachtungstemperaturen reversibel ändert.

Production of A-15 compounds by condenser discharge

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Multiwire samples (consisting of two or more twisted wires of two different pure metals) are heated and melted by condenser discharges in a protective He atmosphere, in a similar way as this has been described earlier for single pure metals [1]. The product is a large number of small spheres which represent almost the whole phase diagram (e.g. Nb-Al) each sphere having typically a different composition, but being individually mostly homogeneous (consisting of a single phase or containing a second one in microsegregation). A-15 or 'sigma' phase spheres can be selected optically and by hardness analysis. Lattice parameter analysis of individual spheres shows that not only stable compositions occur, but also such corresponding to metastable phase extensions.

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Matériaux

Méthode de préparation et quelques propriétés physiques des amas d'atomes

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Pour fixer les idées, nous considérons ici des amas comportant un nombre d'atomes compris entre 100 environ et quelques milliers. Les méthodes de production de ces amas sont exposées (sources à ajutage, évaporation en phase gazeuse, évaporation sur un support, préparation en matrices solides, etc).

Quelques propriétés physiques d'amas métalliques sont discutées. La température de fusion, le facteur Debye-Waller, la susceptibilité magnétique, certaines propriétés optiques, ainsi que la structure.

Festkörperchemie von Verbindungen mit Valenzfluktuation: TmSe und Legierungen

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TmSe ist unter normalen Bedingungen eine Verbindung mit Valenzinstabilität ($4f^{13}$; $\text{Tm}^{2+} \leftrightarrow 4f^{12}5d^1$; Tm^{3+}), deren Präparate eine bis jetzt nicht verständliche starke Streuung der Gitterkonstante zeigen. Diese konnte kontrolliert werden durch Variation der Störchiometrie im Bereich $0.87 < x < 1.05$ ($x = \text{mol Tm/mol Se}$) die zur Veränderung der Valenz von Tm zwischen 3^+ und 2.71^+ führt. Grund dafür sind nicht nur die Spannungen des Gitters (innere Druck) aber auch die damit gekoppelten elektronische Effekte. Untersuchungen des Phasendiagramms Tm-Se bis 2200°C , der Reaktionsenthalpie mit 4NHCl (kalorimetrisch), der Dichten, der chemischen Zusammensetzung, der Struktur (Röntgen) und der Homogenität (elektronenmikr.), im ganzen nicht-stöchiometrischen Bereich zeigen dass, sowohl bei Zimmertemperatur als auch beim Schmelzpunkt Instabilitäten auftreten für $x \cong 0.98$, eine Zusammensetzung für die das Eintreten der Valenzfluktuation postuliert wird. Daraus kann man beschliessen dass, das Eintreten der Valenzfluktuation eine Instabilität des Gitters herbeiführt. Durch Zulegierung von TmSe mit TmTe oder EuSe ist es möglich die Valenz von Tm viel stärker zu variieren (Zwischen 3^+ und 2^+). Es zeigte sich dass die Beimischung von TmSe in TmTe eine hohe Konzentration von Schottky-leerstellen erzeugt, die bei $\text{TmSe}_{0.5}\text{Te}_{0.5}$ und $\text{TmSe}_{0.2}\text{Te}_{0.8}$ zu druckinduzierten Phasenübergänge ($\text{Tm}^{2.3} \rightarrow \text{Tm}^{2.5+}$, resp. $\text{Tm}^{2.5+} \rightarrow \text{Tm}^{2.9+}$) führt.

Physikalische Eigenschaften von Verbindungen mit Valenzfluktuationen (TmSe und Legierungen)

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In einigen Verbindungen der Seltenen Erden (SE) Ce, Sm, Eu, Tm und Yb sind zwei elektronische Konfigurationen, die zwei verschiedenen Valenzzuständen des SE Ions entsprechen, energetisch gleichwertig. Der daraus resultierende neue Grundzustand stellt eine Mischung der Valenz eines jeden Ions dar und ist bei tiefen Temperaturen allgemein durch einen temperaturunabhängigen Paramagnetismus gekennzeichnet. Lediglich TmSe ist als Metamagnet ($T_N \sim 3K$) die einzige bekannte Ausnahme. Der Grad der Valenzmischung kann in TmSe durch die Stöchiometrie variiert werden und hat auf alle physikalischen Eigenschaften grundlegenden Einfluss. Wird TmSe mit TmTe oder EuSe legiert, so bilden sich aus dem gemischtwertigen Metall zum Teil reinwertige Halbleiter. Externer Druck transformiert diese Halbleiter wegen ihrer kleinen Energielücke zu Metallen zurück.

Bedeutung halogenperovskitischer Schichtstrukturen mit organischen Aminen für die Festkörperwissenschaften

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Halogenperovskitische Schichtstrukturen der Formeln $(C_nH_{2n+1}NH_3)_2MX_4$ und $NH_3(CH_3)_nNH_3MX_4$ enthalten alifatische Kohlenwasserstoffketten, die von einer oder beiden Seiten über primäre Aminköpfe durch Wasserstoffbrücken mit den planaren, aus Oktaedern bestehenden MX_4 -Makroanionen gekoppelt sind. Die Variation von $n(1-18)$, $M(Cd, Cu, Fe, Mn, Pd)$ und $X(Cl, Br)$, sowie die einfache Deuterierung am Stickstoff zusammen mit der unterschiedlichen Befestigung der Kohlenstoffketten macht aus diesen Verbindungen ein interessantes Objekt zum Studium struktureller Phasenumwandlungen, magnetischer Phänomene und einer Reihe weiterer festkörperchemischer Probleme.

Einige neue Erkenntnisse auf dem Gebiete der Supraionenleitung

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Supraionenleiter sind Festkörper mit aussergewöhnlich hoher Ionenleitfähigkeit ($\sim 10^{-2} - 1(\Omega \text{ cm}^{-1})$). Die hohe Ionenbeweglichkeit bedingt sehr spezielle Voraussetzungen, nämlich die Existenz von zusammenhängenden, nur teilweise besetzten Leitungswegen. Anhand der Struktur einer erst kürzlich entdeckten Familie ionenleitender Metasilikate wird gezeigt, dass in der Natur diese Voraussetzungen auf viele, völlig verschiedene Arten erfüllt werden. Bedingt durch die ausserordentlich hohe Dichte beweglicher Ionen ($\sim 10^{22} \text{ cm}^{-3}$)

herrscht in diesen Materialien ein hoher Unordnungsgrad, der die Dynamik des beweglichen Gitters und dadurch indirekt auch die Sprungdynamik der beweglichen Ionen beeinflusst. Ferner spielt die direkte Wechselwirkung zwischen den beweglichen Ionen eine wichtige Rolle, sie beeinflusst wesentlich die Aktivierungsenergie der Leitfähigkeit. Ein verallgemeinertes Gittergasmodell gestattet erstmals die vollständige Erfassung aller die Dynamik eines Supraionenleiters bestimmenden Effekte. Die wesentlichen Züge dieses Modells werden anhand von konkreten Rechnungen für einen eindimensionalen Ionenleiter (Holandit) diskutiert.

Stockage d'hydrogène

Neutronenbeugungsuntersuchungen am Wasserstoffspeichersystem FeTi

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Die metallische Verbindung FeTi mit CsCl-Struktur ist ein technisch interessantes Speichersystem für Wasserstoff [1]. Zur Lokalisierung von Deuterium wurden Neutronenbeugungsmessungen an polykristallinem FeTiD_x ($x = 0 \div 1.74$, Phasen α , β , γ) entsprechend D₂-Drucken bis 84 bar durchgeführt. In FeTiD (β -Phase) [2] ist Deuterium auf zwei Typen von Oktaederplätzen verteilt. Als Folge der Deuteriumeinlagerung erniedrigt sich die Symmetrie der Metallstruktur (Raumgruppe P222₁ oder P2/c).

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Oberflächensegregation beim Wasserstoffspeicher FeTi¹⁾

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Zusammenfassung. Die Magnetisierung von FeTi nimmt als Funktion der Zahl der durchlaufenen Hydrierzyklen stark zu, ähnlich wie diejenige von LaNi₅. Die Zunahme weist auf lokale Unordnung im Gitter oder auf Oberflächensegregation hin. Durch Messung der magnetischen Suszeptibilität und Untersuchung der chemischen Zusammensetzung der Oberfläche mit Augerelektronenspektroskopie (AES) nach verschiedenen Probenbehandlungen haben wir festgestellt, dass in einer Oberflächenschicht Ti an die Oberfläche diffundiert und Fe-reiche Ausscheidungen entstehen.

¹⁾ Forschungsprojekt im Rahmen des Nationalen Forschungsprogramms 'Energie'.

FeTi gehört, wie LaNi_5 , vorläufig zu den besten Verbindungen zur Speicherung von Wasserstoff und wird z.B. schon zum Automobylantrieb eingesetzt [1].

Die Analogie zu LaNi_5 [2], bei dem durch Oberflächensegregation Ni Ausscheidungen entstehen, an welchen der molekulare Wasserstoff dissoziieren kann und Resultate aus verschiedenen Publikationen liessen uns vermuten, dass auch bei FeTi Oberflächensegregation vorliegt.

Unsere Vermutung stützte sich auf folgende Resultate:

- FeTi reagiert mit Wasserstoff erst nach einer Wärmebehandlung bei 400°C . Es ist nicht zu erwarten, dass bei dieser Wärmebehandlung die vorhandene Oxidschicht der Oberfläche verschwindet. Hingegen könnte die Segregation angeregt und somit die Dissoziation des Wasserstoffs ermöglicht werden.
- Sandrock [3] machte die ersten AES-Tiefenprofile an FeTi. Er fand folgendes: Die unaktivierte Probe hat dieselben Fe und Ti Konzentrationen an der Oberfläche wie im Bulk. Die Oberfläche einer 1500 mal hydrierten Probe besteht aus zwei Schichten, einer äusseren Ti reichen und Fe armen und einer inneren Fe reichen Schicht. Unterhalb dieser Schichten fand Sandrock die Bulkkonzentration.
- FeTi ist wie LaNi_5 ein Pauliparamagnet mit einer magnetischen Suszeptibilität von $(2-4) \cdot 10^{-6} \text{ emu/g}$. Hempelmann et al. [4] fanden einen irreversiblen Anstieg der magnetischen Suszeptibilität mit der Anzahl Hydrier- Dehydrierzyklen, analog zum Anstieg, den wir in LaNi_5 festgestellt haben [5].
- Wir bestimmten die magnetische Suszeptibilität von unaktivierten FeTi Bulk- und Pulverproben bei Zimmertemperatur und während einer Wärmebehandlung bei 400°C (Fig. 1). Die Suszeptibilität nimmt, während der Wärmebehandlung, bei beiden Proben zu, jedoch bei der Pulverprobe bedeutend stärker. Das zeigt, dass der Hauptteil der magnetischen Ausscheidungen an der Oberfläche gebildet wird.

Diese Ergebnisse liessen uns annehmen, dass in FeTi Oberflächensegregation vorliegt.

Wir untersuchten unaktivierte FeTi und FeTi nach verschiedenen Wärmebehandlungen bei unterschiedlichen Sauerstoffkonzentrationen, um einerseits unsere Modellvorstellungen zu testen und um andererseits den Aktivierungsprozess zu verstehen. Durch Messung der Konzentration von Fe, Ti, O und C in einer Oberflächenschicht von ca. $20 \text{ \AA}$ mit AES und gleichzeitigem Abtragen der Oberfläche durch Bombardieren mit Ar-Ionen haben wir Tiefenprofile bestimmt (Fig. 2).

- Die Oberfläche der an Luft ausgesetzten Probe war mit einer Kohlenstoffschicht bedeckt. Dies erklärt den Anstieg der Ti Konzentration zusammen mit der O Konzentration während des Abtragens.
- Nach verschiedenen Wärme- und Sauerstoffbehandlungen der Probe (Fall B, C) haben wir ähnliche Tiefenprofile gefunden wie Sandrock bei einer 1500 mal gezykelten Probe: Eine äussere Ti reiche und Fe arme und eine innere Fe reiche Schicht.
- Im Fall D besteht die Oberfläche sogar aus drei Schichten.

Wir reinigten die Oberfläche durch Abtragen mit Ar-Ionen und betrachteten die Oberflächenkonzentration von Fe, Ti und O in Funktion der Zeit. Die Fe

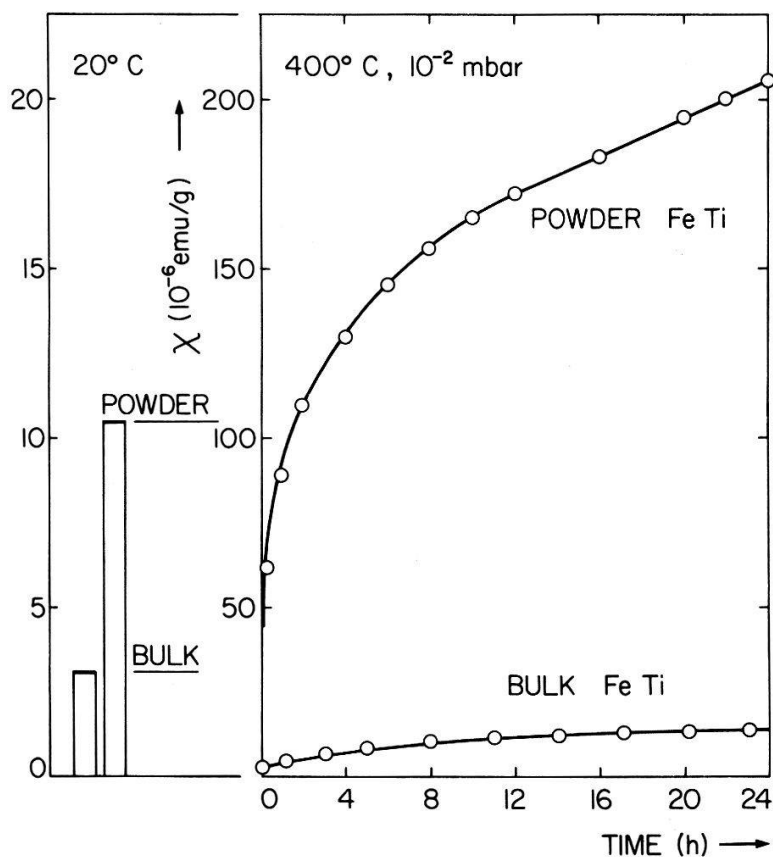


Figure 1

Anstieg der magnetischen Suszeptibilität von FeTi durch das Pulverisieren (20°C) und während einer Wärmebehandlung bei 400°C.

Konzentration blieb konstant während die Ti Konzentration leicht anstieg (<3%). Verglichen mit den entsprechenden Resultaten von LaNi_5 bei denselben Bedingungen (20°C, 10^{-8} Torr) sehen wir, dass bei LaNi_5 der Segregationsmechanismus bei Zimmertemperatur bedeutend effektiver ist als bei FeTi.

Interpretation:

- An der Oberfläche von FeTi ist wie bei LaNi_5 eine Segregation festzustellen. Ti diffundiert an die Oberfläche und erzeugt so eine Ti reiche äussere und eine Fe reiche innere Schicht.
- Die Fe-reichen Gebiete an der Oberfläche sind verantwortlich für die magnetischen Eigenschaften sowohl bei Wärmebehandlungen, wie auch beim Hydrieren.
- Die Zunahme der Suszeptibilität mit der Anzahl Hydrier-Dehydrierzyklen zeigt, dass mit jedem Hydrierzyklus neue Fe Ausscheidungen gebildet werden. Es besteht also ein Selbstregenerationsprozess.
- Der Selbstregenerationsprozess ist jedoch nicht so aktiv wie bei LaNi_5 . Dies könnte ein Grund sein für die schwierige Aktivierung von FeTi wie auch für die leichte Deaktivierung.

Danken möchten wir H. Scherrer und D. Spörri für die Probenpräparation und ihre Unterstützung bei Laborarbeiten.

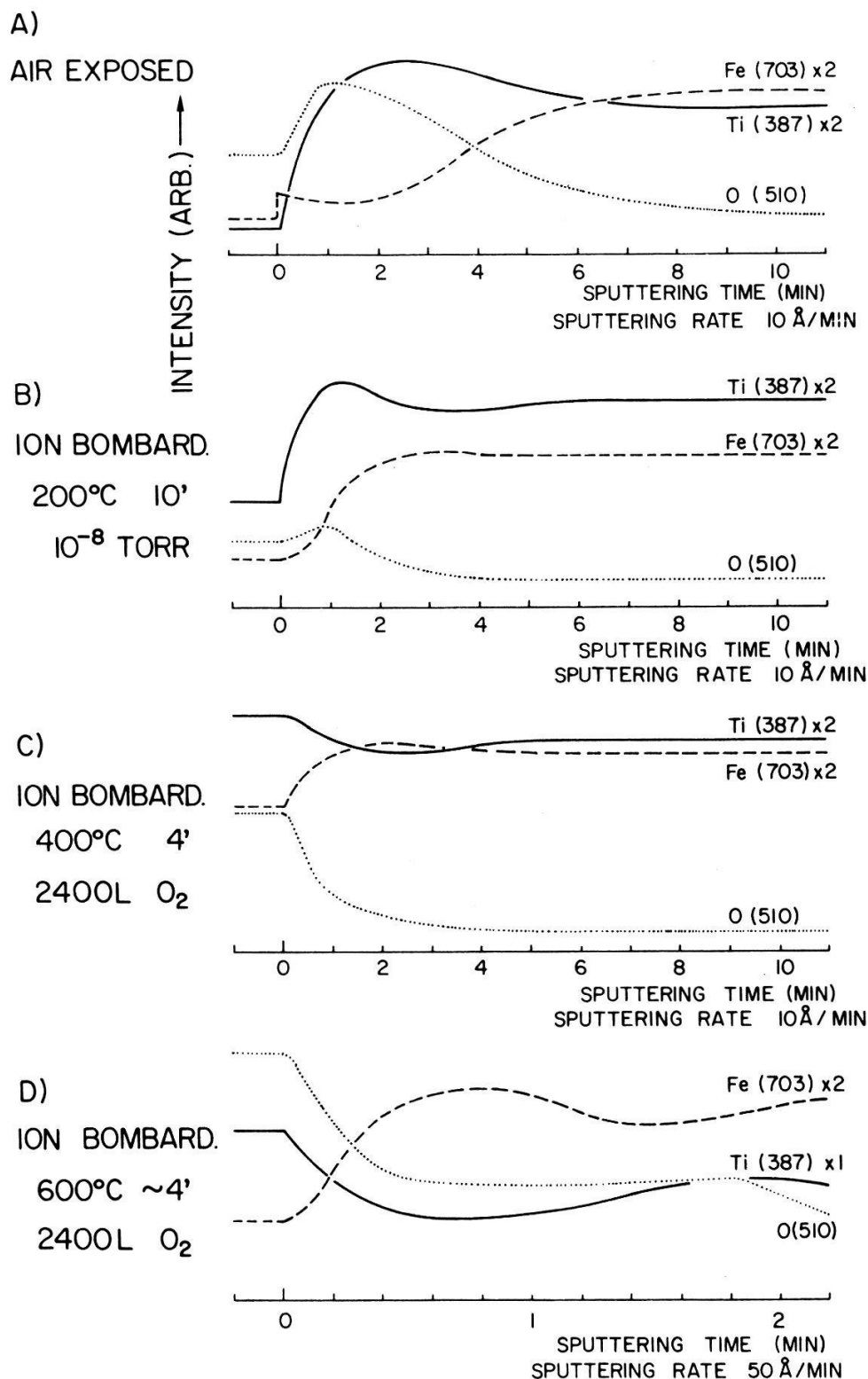


Figure 1
AES Tiefenprofile von FeTi.

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Katalytisch aktive Fe-Ausscheidungen an der Oberfläche von FeTi

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Metallisch reine Oberflächen von d-Metallen haben die Fähigkeit, H_2 zu dissoziieren. Mit Hilfe der Photoemissionsspektroskopie spin-polarisierter Elektronen haben wir festgestellt, dass bei der oben erwähnten Oberflächen-segregation *metallische* Fe-Ausscheidungen entstehen. An ihnen kann die Dissoziation des molekularen Wasserstoffs erfolgen.

Structure électronique, semiconducteurs

Fermi surface studies by the positron annihilation technique

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Abstract. We discuss the two-dimensional angular correlation of annihilation radiation measured in Cu and V_3Si single crystals.

Positron annihilation is an experimental method used in material properties research. On the one hand it contributes to studies of point defects and on the other hand to studies of electronic properties and more particularly to Fermi surface (FS) investigations in metals and alloys. This last application was our aim in developing [1] an experimental set-up for the two-dimensional detection of the angular correlation of annihilation radiation, by means of high density proportional chambers [2].

The principle of the measurement is the following: positrons emitted by a radioactive source (~ 30 mCi of ^{22}Na) strike a single crystal sample. They lose their kinetic energy (thermalization process) prior to annihilation with an electron. Focusing our interest on the two-photon annihilation, due to linear momentum conservation, the two 511 keV radiations are almost colinear. The small angle θ between them is related to the annihilated electron momentum p by:

$$\theta = p/mc$$

Therefore for each angle θ , the counting rate is proportional to the number of occupied electronic states with momentum p . Hence, the angular correlation

distribution $N(\theta)$ is proportional to the electronic momentum density $\rho(\vec{p})$. This function is continuous for the core electrons but has a discontinuity for the conduction electrons at the Fermi wavevector p_F .

The peculiarity of our system is the use of high resolution ($0.78 \text{ mrad} \times 0.68 \text{ mrad}$) two-dimensional detectors mentioned above. In such a way two components (p_x, p_y) of the electronic momentum are resolved simultaneously, for each annihilation, by measuring the angular components (θ_x, θ_y) of the photons emitted in the z direction perpendicular to the detectors. Therefore the following relation holds for the angular distribution:

$$N(\theta_x, \theta_y) \div \int_{-\infty}^{\infty} \rho(p_x, p_y, p_z) dp_z$$

For instance, consider the case of an hypothetical metal in which the conduction electrons are free, then $\rho(\vec{p})$ is spherical. Due to the positron-core Coulomb repulsion, let us assume, for simplicity, that there is no annihilation with core electrons. The reader may convince himself easily that within these approximations the angular distribution $N(\theta_x, \theta_y)$ is a semi-sphere whose radius is the Fermi wavevector p_F . In aluminum the above approximations are satisfied to some extent and in fact the measured $N(\theta_x, \theta_y)$ has, in general, the expected shape [3]. Moreover, information concerning deviations from sphericity such as zone boundary interaction, many body effects and core annihilation contributions are revealed.

We have also measured the angular correlation distribution in copper [4] and V_3Si [3]. In this communication we would like to present the detailed analysis of these measurements.

The copper single crystal was aligned with the $[\bar{2}11]$ and $[110]$ axes along θ_x and θ_y respectively. In this configuration the $[111]$ axis is parallel to the integration axis, therefore the outgrowth present at the top of the experimental distribution (see Fig. 4 in Ref. 3) is due to the neck in the FS. Figure 1 shows partial derivatives $|\partial N(\theta_x, \theta_y)/\partial \theta_x|$ of the measured distribution, at different θ_y spaced by 0.4 mrad . The small peak near the center is due to the necks, while the important peak is due to the FS cut-off at k_F . The position of those two structures in the derivative allows the determination of the neck radius and of the Fermi wavevector (for this specific partial derivative $k_F [110]$ is determined). Both values are in complete agreement with those obtained by dHvA effect [5]. By subtracting from the experimental distribution the contribution of the conduction electrons, calculated from the FS parametrized by Halse [5], we could extract the core electrons and many body effects contributions. Figure 2 shows the result and it reveals an anisotropy. Assuming that the integral over p_z of the core electron contribution is isotropic, this result suggests that the many body effects may depend on the character of the electronic wavefunction, i.e. the enhancement for a d -like wavefunction seems to be smaller than for a s -like one. Another possibility is that the many body effects are isotropic. Then the anisotropy may be attributed to a band structure effect. We do not have a criterium to tell which of these two possibilities is the correct one.

V_3Si is more complicated. The main feature of this A-15 intermetallic compound is its high superconductivity transition temperature ($T_c = 17 \text{ K}$). The single crystal was aligned with two $[100]$ axes along θ_x and θ_y respectively. In Fig. 3 are shown the partial derivatives $|\partial N(\theta_x, \theta_y)/\partial \theta_x|$ and $|\partial N(\theta_x, \theta_y)/\partial \theta_y|$ computed

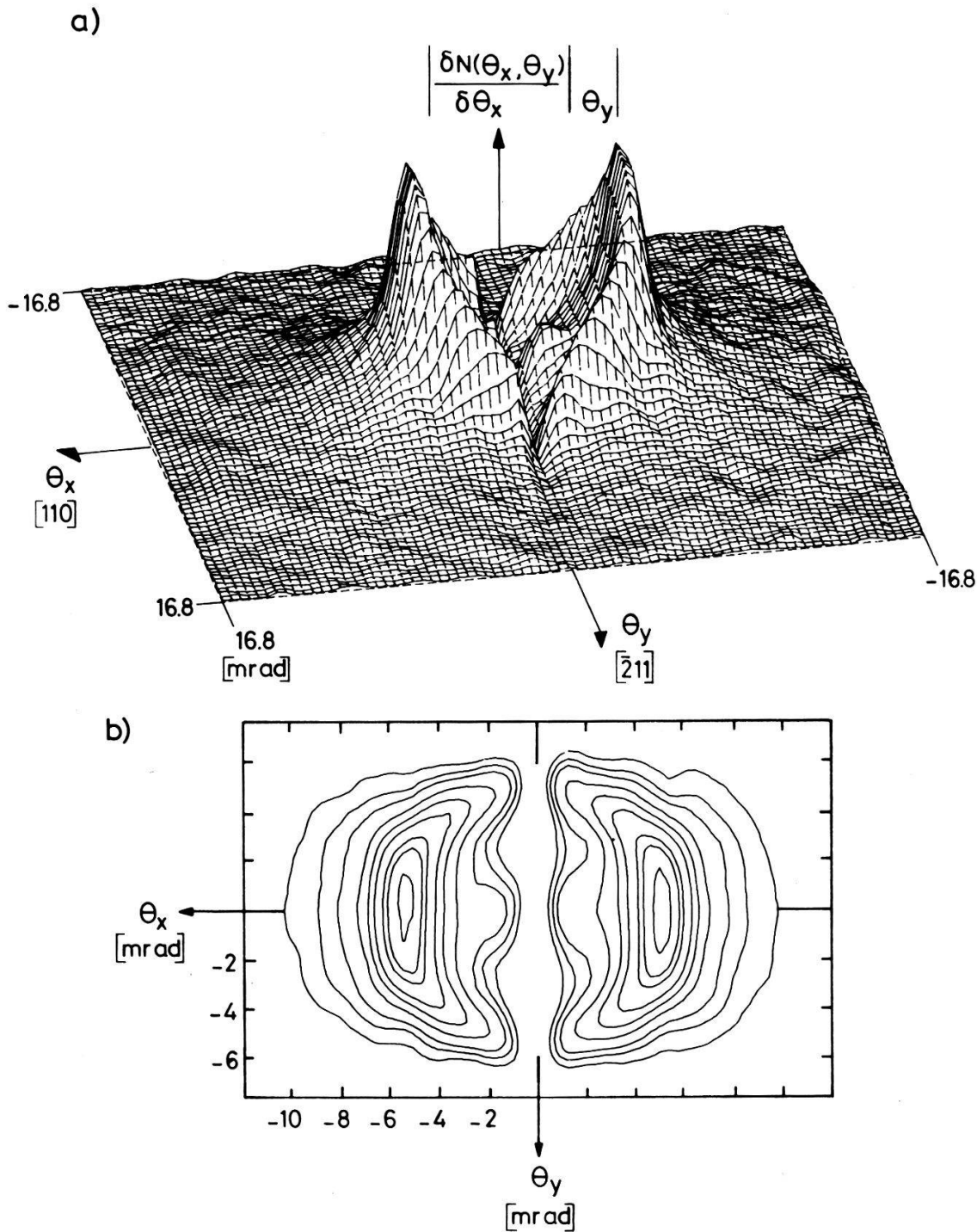


Figure 1

Partial derivative of the measured angular correlation distribution with the $[\bar{2}11]$ and $[110]$ axes along θ_x and θ_y , respectively. The spacing between two consecutive partial derivatives is 0.4 mrad. Contour lines are also shown.

as mentioned previously. Our results seem to be in good agreement with previous two-dimensional experiments [6]. The observed structure was analysed [1] in terms of an anisotropic FS. It is consistent with an APW band structure calculation published recently [7]. Its main features are a parallelepipedic electron surface centered at Γ and empty pockets centered at M in the Brillouin zone.

Finally let us mention an interesting possible medical application of our detection system: tomography [8, 9]. The aim is to localize the spatial distribution

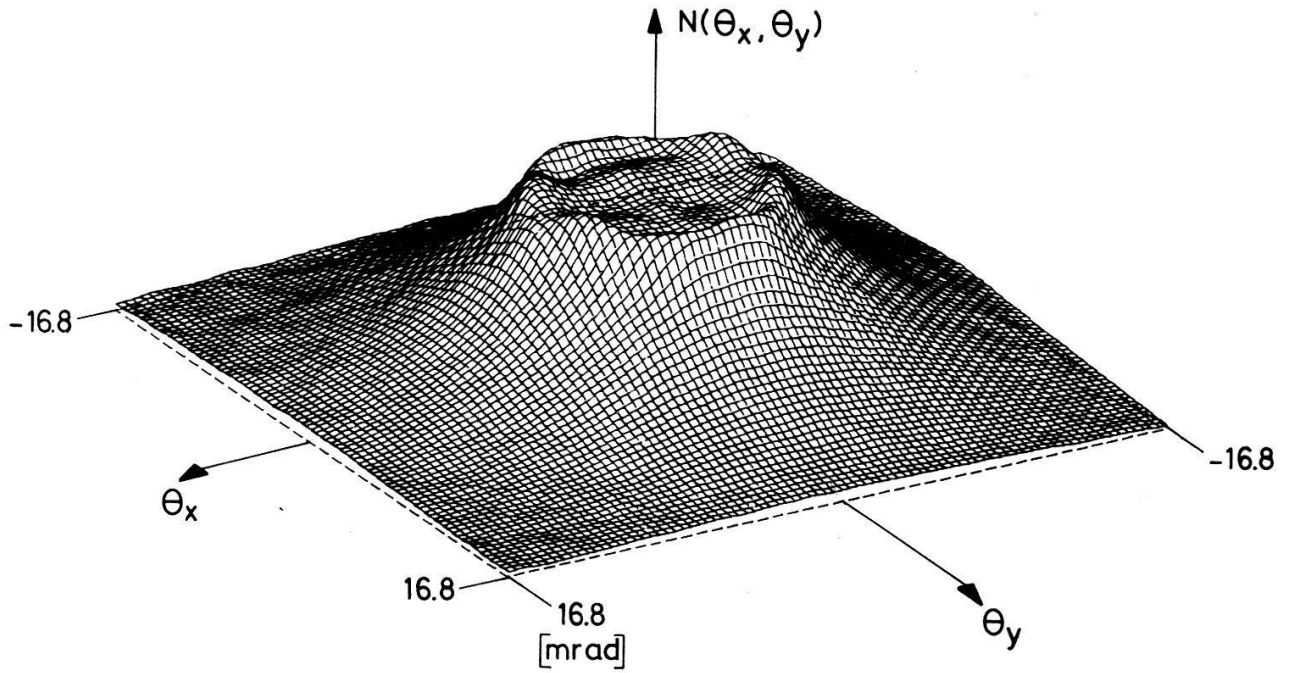


Figure 2

The core annihilation and many body effects contributions in copper, obtained by subtracting the parametrized Halse FS from the experimental angular correlation distribution.

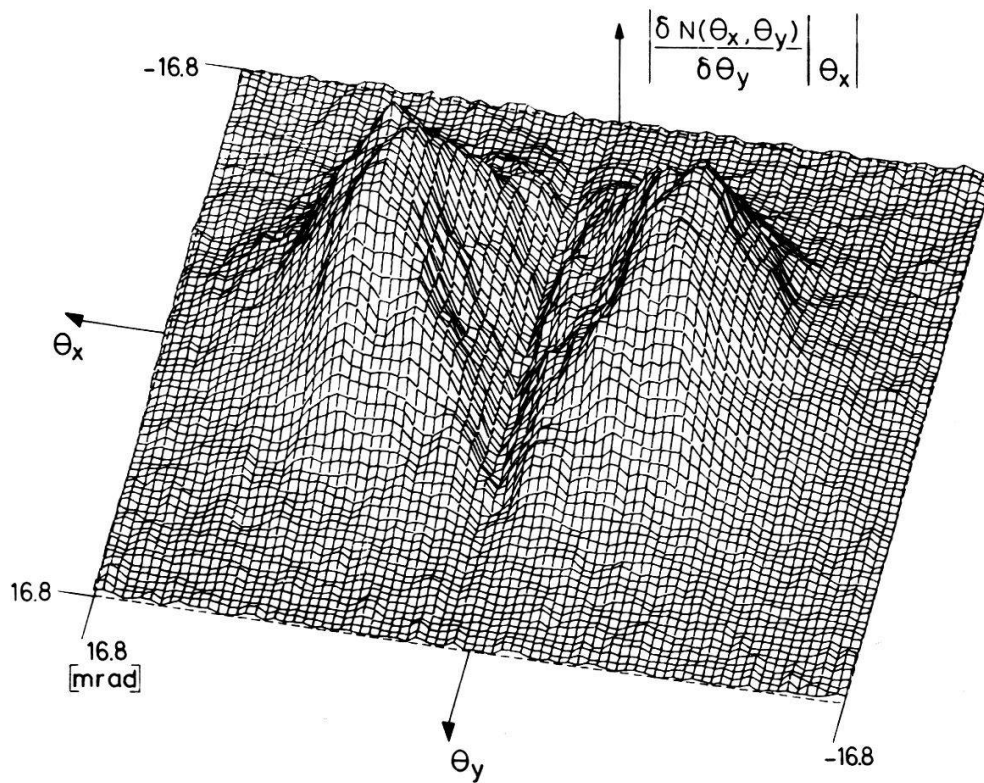


Figure 3

Partial derivatives of the measured angular correlation distribution in V_3Si with two $[100]$ axes along θ_x and θ_y respectively. The spacing between two consecutive partial derivatives is 0.4 mrad.

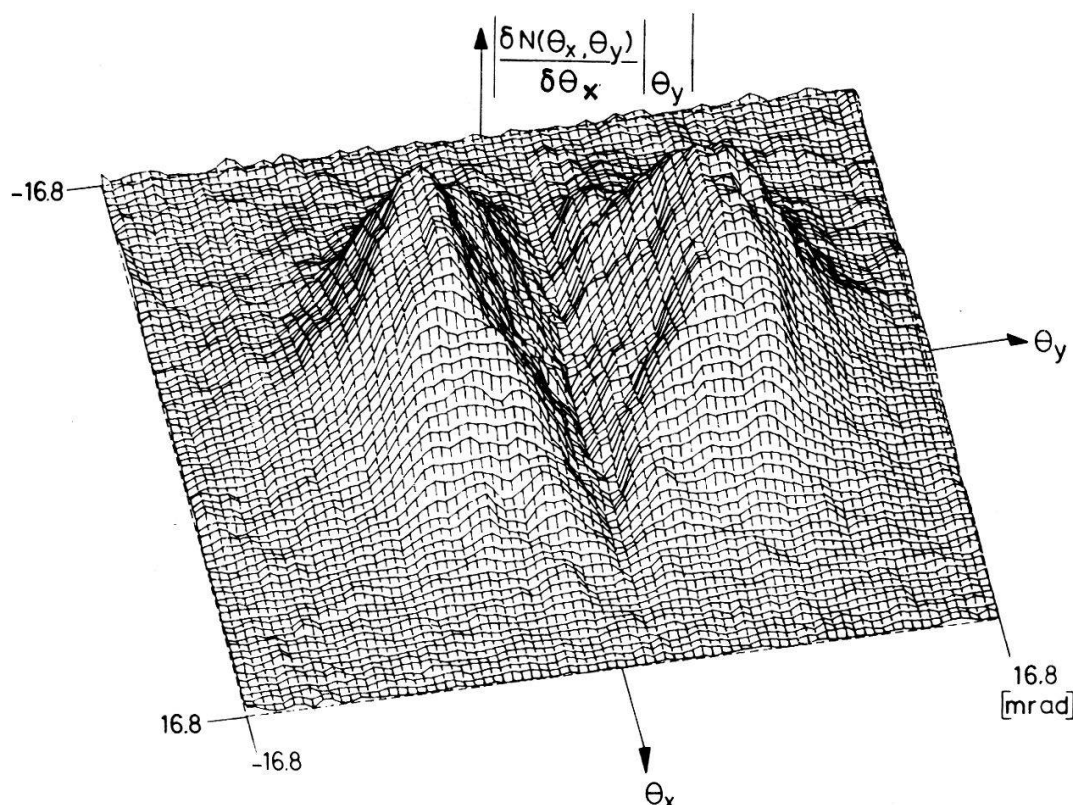


Figure 3 (Contd)

of β^+ emitters assuming that the annihilation radiation is colinear (neglecting thus the small, 0.5° , angular deviations). Measurements performed on a mouse injected with ^{18}F β^+ emitter [8] allow us to consider with some optimism the development of such a diagnostic tool on the basis of the proportional chambers used in this work.

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Méthode d'interpolation de Slater-Koster pour les actinides

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Nous présentons le formalisme de la méthode d'interpolation de Slater-Koster [1] pour des électrons s , p , d et f complètement relativistes. L'applicabilité de cette méthode aux actinides est discutée.

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The structure of brominated $(\text{SN})_x$

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Recently several authors [1, 2] have studied the appreciable changes in the physical properties of the superconducting polymer $(\text{SN})_x$ on bromination. In this paper a model of the molecular structure of the brominated polymer will be discussed based primarily on X-ray photoelectron and resonance Raman spectroscopic results. The data is shown to support a charge transfer-type structure in which the polymer chain acts as donor and Br_3 and Br_5 ions as acceptors.

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Elektronische Zustände und chemische Bindung in ionischen Halbleitern

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Wir zeigen, dass sich übliche Pseudopotential- und tightbinding Modelle bei der Beschreibung sowohl der Leitungsbandzustände als auch der chemischen Bindung in ionischen Halbleitern widersprechen. Pseudopotentialrechnungen weisen darauf hin, dass insbesondere die angeregten Anionenzustände, die im TB-Bild üblicherweise nicht berücksichtigt werden, eine wichtige Rolle spielen. Das Druck-Ionizitäts-Phasendiagramm für kubische Halbleiter unterstützt die Pseudopotentialbeschreibung.

Spin-polarisierte Photoemission an ternären Chalcopyrit-Halbleitern

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Die Chalcopyrit Struktur ist ein tetragonales Uebergitter der kubischen Zinkblende Struktur mit drei nicht-kubischen Aspekten: (1) Kompression des Kristallgitters entlang der z -Achse, (2) Verschiebung der Anionen weg von der normalen Position, (3) Verdopplung der Einheitszelle in z -Richtung. Die dadurch entstehenden elektrischen Feldgradienten sind u.a. für die Kristallfeldaufspaltung des Valenzbandes verantwortlich. Spin-Bahn-Wechselwirkung und Kristallfeld spalten nun das 6-fach entartete Valenzband in drei 2-fach entartete Niveaus auf. Durch Anregung mit zirkular polarisiertem Licht in das Γ_1 -Leitungsbandminimum werden hochpolarisierte Photoelektronen erwartet. An ZnSiAs_2 wurde das folgende Polarisationspektrum gemessen: $P=0\%$ an der Photoschwelle ($h\nu=1.7\text{ eV}$), $P_{\text{max}}=51\%$ bei einer Photonenenergie von 2.2 eV , ein Absinken der Polarisation auf Null bei $h\nu=3.0\text{ eV}$. Die Austrittsarbeit der Elektronen wurde durch Aufdampfen von Cäsium herabgesetzt. Sowohl die niedrige Photoschwelle als auch die kleinen Polarisationswerte in deren Nähe kann durch die Existenz von 'pseudodirekten' Bandlücken ($\Gamma_6^5 \rightarrow \Gamma_7^3$ resp. $\Gamma_6^5 \rightarrow \Gamma_6^2$) erklärt werden. Die Γ_7^3 - resp. Γ_6^2 -Leitungsbandminima liegen energetisch tiefer als das Γ_6^1 -Minima, das die direkte Bandlücke $\Gamma_6^5 \rightarrow \Gamma_6^1$ bildet.

Metal-non-metal transition in vanadium doped TiSe_2

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Single crystals of TiSe_2 doped with V have been prepared from the vapor phase. The electrical properties have been measured as a function of the temperature and drastically depend on the vanadium concentration. For $x \leq 0.008$ in $\text{Ti}_{1-x}\text{V}_x\text{Se}_2$, the electrical resistivity is similar to that of TiSe_2 with a maximum shifted to lower temperatures. For $0.008 \leq x \leq 0.05$ the crystals behave as semiconductors but without well defined activation energies. For $x > 0.05$, the temperature dependence of the resistivity has a metallic character. This behavior is discussed in relation to the Hall effect results and considering that the low temperature $2 \times 2 \times 2$ superstructure is present in crystals with $x < 0.05$.

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RMN sur du Li en matrice de CO_2

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Des atomes de Li, ainsi que des petites particules métalliques, dispersés dans une matrice de CO_2 solide ont été étudiés par RPE et RMN. Les petites

particules sont formées par diffusion des atomes de Li lors d'un 'recuit'. Ce passage est contrôlé par les mesures de RPE [1]. Par comparaison des mesures RMN avant et après traitement thermique, nous déduisons le spectre de résonance nucléaire du Li 'atomique' dispersé en matrice de CO₂.

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Structure and electronic configuration of Pd₈₀Si₂₀

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We analyse a structural model of amorphous alloys which reproduces the RDF of glassy Pd-Si.

Total energy and free energy are evaluated. The cellular multiple scattering cluster method is used for the electronic structure calculation.

Physique appliquée

Laserinduziertes anisotropes Schmelzen und epitaktisches Wachstum in Silizium

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Einkristallines Silizium wurde mit 100 μ s Pulsen eines Nd:YAG Lasers bestrahlt. Dabei zeigte sich, dass laserinduziertes Schmelzen bevorzugt entlang der Kristallachsen verläuft. Dies führte zu einem charakteristischen Oberflächenmuster im wiedererstarteten Silizium, falls nur eine dünne Oberflächenschicht geschmolzen wurde. Dieses Muster ist verschieden für (111) und (100) Silizium. Die kristallographische Untersuchung zeigte epitaktisches Wachstum der geschmolzenen Schicht.

Temperature dependence of optical absorption at $\lambda=1.06\ \mu\text{m}$ in amorphous and crystalline silicon

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Abstract. The absorption coefficient is a crucial parameter in laser assisted annealing and doping of semiconductors. Its temperature dependence is especially strong if the photon energy approximately equals the energy gap. This is the case if silicon is irradiated with Nd laser pulses. We report measurements made with different types of monocrystalline and amorphous silicon.

Recently there has been a lot of interest in laser annealing [1, 2, 3] and doping [4, 5] of silicon. The absorption coefficient is an important parameter in laser heating of silicon surfaces. This absorption coefficient, however, depends critically on the properties of the silicon sample and on temperature [6]. Especially if the photon energy of the laser approximately equals the energy of the silicon band gap. This is the case if Nd-Lasers are used. In this paper we report results on the temperature dependence of absorption in Nd:YAG laser irradiated monocrystalline and amorphous silicon.

Most of the experiments were performed at the wavelength of a Nd:YAG laser [$1.06\ \mu\text{m}$]. We measured the index of refraction of monocrystalline and amorphous silicon. Amorphous layers, with and without an H_2 content, were used. The samples of amorphous silicon were prepared by depositing silicon on glass substrates by sputtering. Sputtering was performed in either a pure Ar atmosphere or in an Ar atmosphere containing 32% of H_2 . The thickness of the deposited layer was determined by counting interference fringes [7, 8] and tally step measurements. Different samples, 130 to 730 nm thick, were used in the experiments. The uniformity of the layers was checked by microdensitometer measurements and found to be homogeneous within 1%.

In general, the index of refraction can be determined by reflectivity measurements. In the present case, however, this is difficult because of interference effects. In order to find the index of refraction of the thin layer, we measured the transmission as a function of wavelength with the aid of a spectrometer [7].

The refractive index, n , at $1.06\ \mu\text{m}$, for samples of different thickness is shown in Table 1. The values of n are smaller than those of monocrystalline silicon (about 3.65). This is probably due to the reduced density of the sputtered material. The differences of the measured values can be explained by the large number of parameters involved in the sputtering process that are not perfectly controlled [8, 9].

With the same samples the absorptivity was also measured at $1.06\ \mu\text{m}$. The measurement was performed in the setup shown in the Fig. 1. We used $5\ \mu\text{s}$ pulses of a free running Nd:YAG laser at an intensity of about $1\ \text{Watt per cm}^2$. The laser output was monitored with a first photodiode. With a second photodiode the power of transmitted light and with a third photodiode the power of reflected light near normal incidence were measured. The samples were temperature controlled.

The measured values of transmission and reflection were evaluated with formulae given in literature [8]. The results from room temperature measurements are shown in Table 1. The values of the absorption coefficient of samples

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Table 1
Thickness d , refractive index n and absorption coefficient α
(room temperature, $1.06\ \mu\text{m}$) of amorphous silicon layers.

Samples:	$d(\text{nm})$	n	$(10^4\ \text{cm}^{-1})$
sputtered	210	3.29	1.70
in Ar	240	3.39	1.60
sputtered	130	3.46	0.99
in Ar and	300	3.29	0.65
H_2	610	3.20	0.52
	730	3.46	0.44

containing hydrogen was markedly smaller than with the samples sputtered in pure Ar atmosphere [10]. The former show a decreasing absorption coefficient with increasing thickness of the layer. The same effect was observed by Schlötterer [11] measuring at 588 nm.

In the same setup the temperature dependence of the absorption of amorphous layers and of monocrystalline silicon wafers has been determined. It was not possible to measure the temperature dependence of absorptivity of the samples containing hydrogen because during the heating process the hydrogen content of the layers is reduced thus leading to irreproducible results. Figure 2 shows the temperature dependence of the absorption coefficient of an amorphous silicon layer prepared by sputtering in pure Ar atmosphere (sample with a thickness of 210 nm) and of a monocrystalline wafer of n -type, 4 Ohm cm silicon, $275\ \mu\text{m}$ thick.

The figure shows absorptivity as a function of temperature. The absorption coefficient of amorphous silicon remains rather constant. On the other hand, the

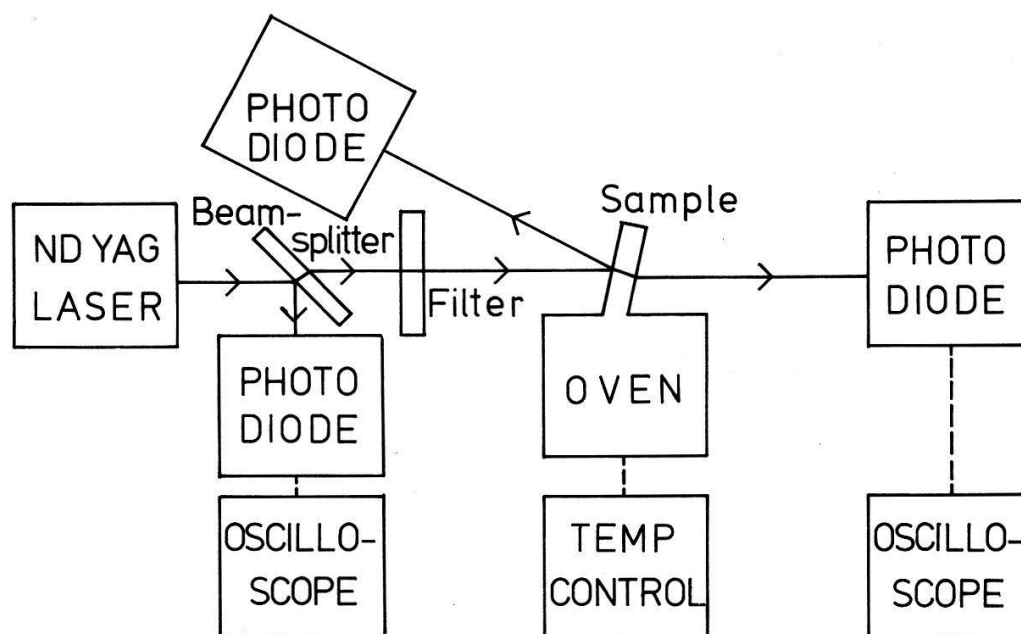


Figure 1
Experimental setup for the measurement of transmission and reflection at $1.06\ \mu\text{m}$ as a function of temperature.

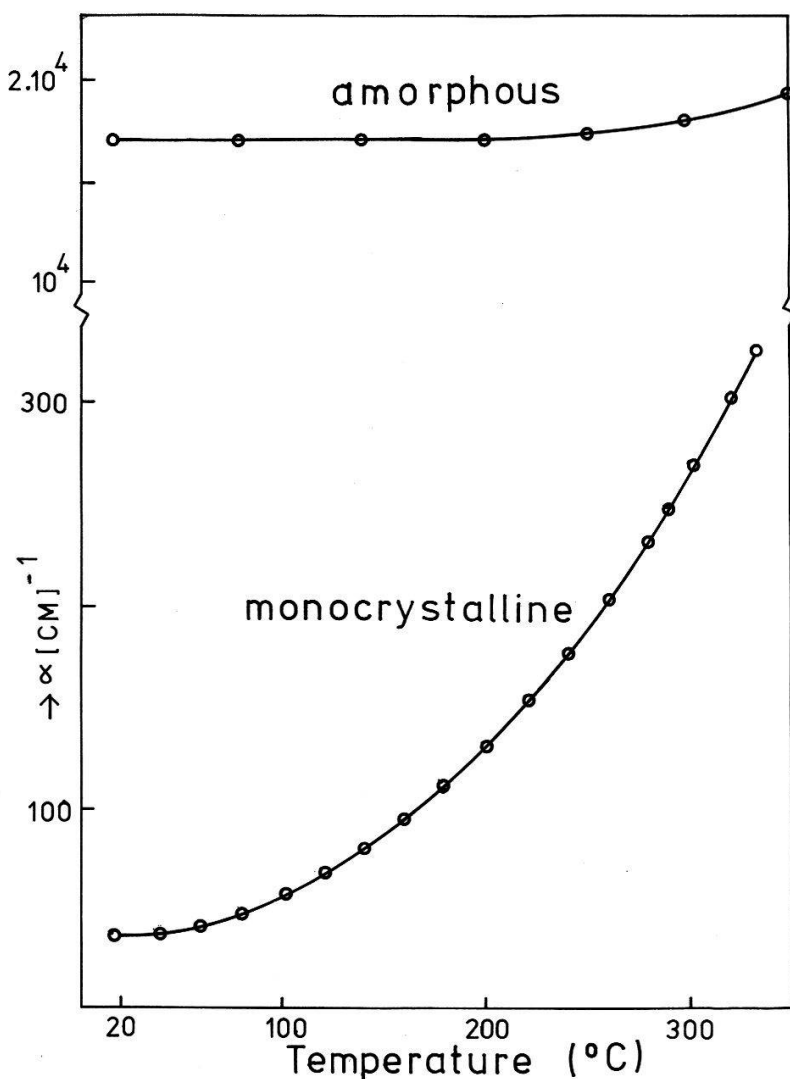


Figure 2

The absorption coefficient of monocrystalline (*n*-type, 4 Ohm cm, 275 μm thick) silicon and of an amorphous silicon layer (sputtered in pure Ar atmosphere, 210 nm thick, deposited on a glass substrate) as a function of temperature.

absorptivity of monocrystalline material increases by a factor of 10 from room temperature to about 350°C.

This behaviour is due [6] to the close proximity of the photon energy to the band gap of monocrystalline silicon.

In conclusion we have given values of absorption coefficient for amorphous silicon layers produced by a sputtering technique with different layer thicknesses and we have shown that the temperature dependence of the absorption coefficient only slightly changes with temperature in the range from 20 to 350°C. Further we have demonstrated the strong increase of absorption coefficient with temperature for monocrystalline material.

Acknowledgments

We would like to thank J. M. Mackowski, (IPN, Villeurbanne, France) for providing samples. Further we thank R. Rubin (PTT research laboratories) for the possibility to perform 'tally step' measurements. M. Fuhrer we thank for technical assistance and H. P. Weber for stimulating discussions.

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Kontaktieren von GaAs-Laserdioden mit Hilfe von Laserstrahlen

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Das Kontaktieren von GaAs-Laserdioden wird konventionell durch Aufdampfen von Metallschichten und anschliessender thermischer Behandlung in einem Legierungsofen durchgeführt. Wir haben den Legierungsschritt durch Bestrahlen mit Pulsen eines Nd:YAG Lasers ausgeführt. Die resultierenden Kontaktwiderstände entsprechen denjenigen guter konventionell hergestellter Kontakte. Das neue Verfahren bietet gegenüber dem bisherigen verschiedene Vorteile.

Bestimmung des effektiven Brechungsindex von monolithisch integrierten, mit einer Gitterstruktur versehenen, Wellenleitern

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Zur Untersuchung der optischen Eigenschaften von monolithisch integrierten Wellenleiterstrukturen aus Gallium-Aluminium-Arsenid wurde ein abstimmbarer Diodenlaser im Dauerstrichbetrieb verwendet. Die Intensität des mittels eines Gitters in den Wellenleiter eingekoppelten Lichtes wurde als Funktion des Einstrahlwinkels gemessen. Aus diesen Messungen konnte der effektive Brechungsindex des Wellenleiters und seine Temperaturabhängigkeit zwischen 10 und 50°C mit einer Genauigkeit von besser als ein Promille bestimmt werden. Anhand der Intensitätsverteilung des austretenden Lichtes, welches durch den Wellenleiter geführt wurde, kann der Wellenleiter noch detaillierter charakterisiert werden.

Tunable narrowband subnanosecond dye laser

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Abstract. Using the 50 kW subnanosecond output pulse of a N_2 laser, we transversally pump a miniature dye laser built up of a 2.5 cm long optical resonator containing a grating as reflector. Tunable laser oscillation was obtained with Rhodamine 6 G from 580 to 600 nm and Stilbene from 420 to 470 nm. With a coated 0.15 mm thick etalon within this resonator, the bandwidth could be reduced closely to the transform limited width given by the time duration.

The optical resonator of a typical narrow bandwidth dye laser is of the Hänsch configuration [1]. Unfortunately the beam expander leads to a relatively long cavity, so it can only be used for pumping pulses of several nanoseconds to fulfill the requirements for the build up of the laser oscillation. In the case of subnanosecond pulses (length e.g. 20 cm), one needs a cavity of about 2.5 cm, because a resonator requires at least some 4 roundtrips for the build up of the field.

For these reasons, we used for bandwidth narrowing a thin Fabry-Perot etalon (0.15 mm thickness, 60% reflectance) placed inside the cavity formed by a 80% reflectance mirror (for outcoupling), a dye cell of 1 cm length and a 1800 lines/mm grating. The pumping laser was a 0.6 nsec width, 30 kW output power N_2 laser.

Figure 1 shows the time behaviour of the dye pulse without and with etalon. No time deformation appears in contrast to an other work performed with a longer pumping pulse [2]. However, intensity fluctuations are responsible for the peaky appearance of the pulse if an etalon is used. The traces are taken with a 0.3 nsec risetime diode and a 0.1 nsec risetime sampling oscilloscope.

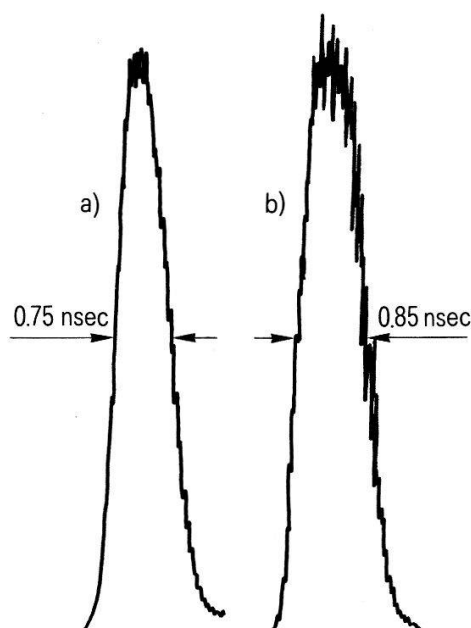


Figure 1

(a) mirror + grating.

(b) mirror + grating + etalon.

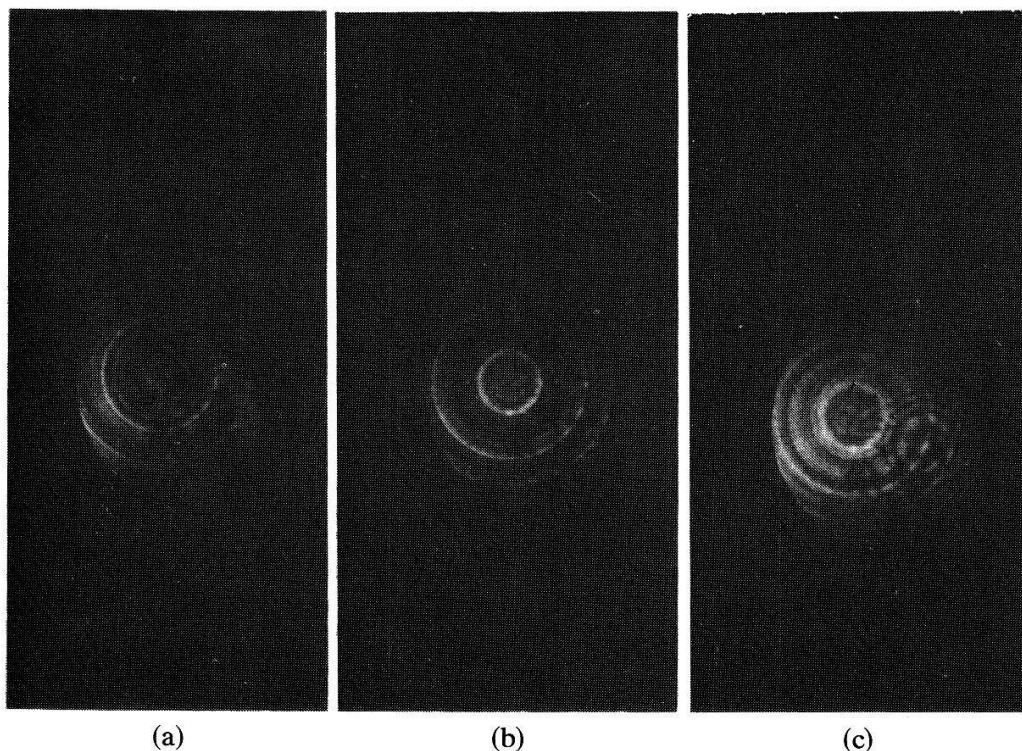


Figure 2

Figure 2 presents rings taken with a 2 mm thick Fabry-Perot of finesse 20.

Figures 2(a, b) are single shots recorded close to threshold showing lasing on a single etalon mode, but still several cavity modes. The width is 0.005 nm. This is about 8 times wider than that of a bandwidth limited 0.6 nsec monochromatic pulse. The position of the center of the line fluctuates within 0.02 nm from shot to shot.

This variation of position of the linecenter and the intensity fluctuations respectively, may be explained by the fact, that the index of refraction of the dye is not equal from shot to shot due to the thermally induced density fluctuations. This leads to different transmission angles through the etalon. Thus frequency selectivity may vary from shot to shot and intensity variations associate the frequency variations.

Conversion efficiency for these measurements for single line lasing was 1%.

Figure 2(c) shows rings with higher pumping power: multiline lasing appears, resulting from excitation of other etalon modes.

Acknowledgments

We thank Dr. C. Voumard for helpful discussions.

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Kurzer optischer Korrelator

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Die Baulänge optischer Korrelatoren kann durch Ersetzen der Fouriertransformationslinse durch ein kurzbrennweitiges Linsenraster um den Faktor 4–6 verkürzt werden. Damit wird der Korrelatoraufbau unempfindlicher gegen mechanische Erschütterungen. Zudem ist durch die Aufteilung des Bildfeldes eine Informationsunterteilung möglich, welche ein leichteres Interpretieren der Objektabweichungen ermöglicht. Die optischen Eigenschaften des Systems, insbesondere der Einfluss auf die Korrelationsantwort und das Uebersprechen zwischen den Einzellinsen werden diskutiert.

Taper-coupled Laser mit langen, passiven Wellenleitern für monolithische Integration

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In Taper Coupled (TC-) Laser wird das Licht in einem kurzen, aktiven Teil verstärkt und über eine keilförmig auslaufende Schicht in einen passiven Wellenleiterresonator gekoppelt. Der passive Wellenleiter ist so aufgebaut, dass weitere optische Elemente (Modulatoren, Wellenleiterschalter etc.) integriert werden können. Die Lumineszenzeigenschaften der Grundstrukturen im $\text{Al}_x\text{Ga}_{1-x}\text{As}$ -System werden beschrieben. Mit ersten TC-Lasern mit zweidimensionalen, passiven Wellenleitern und mit planaren Wellenleitern bis zu 1.7 mm Länge ist Dauerstrichbetrieb bei Zimmertemperatur erreicht worden. Die Schwellströme lagen im Bereich von 300 mA. Die aus verschiedenen Grundstrukturen hergestellten Elemente zeigen charakteristische Unterschiede in den Emissionsspektren und in den Licht-Strom-Kennlinien.

Kontinuierlicher Fiber-Raman-Laser

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Eine Single-Mode-Glasfiber wurde als lichtverstärkendes Element für einen kontinuierlichen Raman-Oszillator verwendet. Als Pumpquelle dienten verschiedene Linien eines Argon-Lasers. Für die 40 m lange Fiber mit einem Core-Durchmesser von $3.3 \mu\text{m}$ wurde bei 514.5 nm ein Transmissionsverlust von 20 dB/km gemessen. Die Pumpschwelle wurde für die Oszillation der 1. Stokes-Linie mit ~ 1 Watt, bzw. für die 2. Stokes-Linie mit ~ 3.5 Watt erreicht. Einfachheit im Aufbau, hohe Effizienz, sowie Abstimmbbarkeit machen Fiber-Raman-Laser zu interessanten, kohärenten Lichtquellen.

Absorptionseffekte beim Rekristallisieren amorpher Halbleiterschichten durch Nd-Laserstrahlung

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Bei der Bestrahlung von Si mit Nd Laserpulsen im ns Bereich führt die starke Zunahme der Absorption mit der Temperatur in der Regel zu inhomogener Aufheizung. Dies verhindert beim Bestrahlen amorpher Schichten, dass die erwärmte Zone gleichmässig kristallisiert. Das Problem kann umgangen werden durch Bestrahlung erwärmten Siliziums oder durch Verlängerung der Pulsdauer auf einige 10 μ s. Epitaktisches Wachstum in beiden Fällen wird demonstriert.

Abhängigkeit der Impulsenergie eines transversal angeregten HCN-Lasers vom Gasgemisch ($\text{CH}_3\text{CN-He}$, $(\text{CN})_2\text{-H}_2\text{-He}$, $\text{HCN-CH}_4\text{-He}$)

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Ein transversal angeregter HCN-Laser mit einer Hilfsentladung (UV-Vorionisierung) wurde mit den Gasgemischen $\text{CH}_3\text{CN-He}$, $(\text{CN})_2\text{-H}_2\text{-He}$ und $\text{HCN-CH}_4\text{-He}$ im durchfliessenden und abgeschlossenen System betrieben. Die besten Resultate wurden mit durchfliessendem $\text{HCN-CH}_4\text{-He}$ -Gemisch erhalten. Eine umfangreiche Beschreibung erscheint demnächst in "Infrared Physics."

Holographie mit geführten optischen Wellen

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Die untersuchten Wellenleiter-Hologramme [1, 2] sind durch die Verwendung des quergedämpften Anteils eines Wellenleitermode als Referenzwelle gekennzeichnet. Die Hologramme wurden aufgezeichnet durch Interferenz der quergedämpften Referenzwelle und des Objektwellenfeldes in einer Schicht aus Dichromatgelatine (DCG) auf einem planaren Wellenleiter aus Araldit. Dieser und die DCG-Schicht wurden mit einem Tauch-Zieh-Verfahren auf Glassubstraten hergestellt. Die Hologramme haben eine Fläche von mehreren Quadratzentimetern, was durch das Einkoppeln einer geführten Referenzwelle von 17 mm Breite mit einem speziellen Prismenkoppler ermöglicht wurde. Anhand rekonstruierter Testobjekte wird die Qualität der Hologramme diskutiert.

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Sättigungseffekte bei Laser-induzierten akustischen Wellen in Flüssigkeiten

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Bei Laserenergiedichten, wo der thermoelastische Prozess für die Druckerzeugung allein verantwortlich ist [1], wurde in CCl_4 eine Sättigung der Druckmaxima für steigende Laserintensität festgestellt. Dieses Phänomen steht im Gegensatz zu ähnlichen Beobachtungen bei der Laserwechselwirkung mit Festkörpern, wo die Plasmabildung dafür verantwortlich gemacht wird. In unserem Fall konnte die Drucksättigung mit einer reduzierten Absorption der Laserstrahlung in CCl_4 bei höheren Intensitäten erfolgreich erklärt werden.

LITERATUR

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Diese Arbeit wird in Appl. Phys. Lett. publiziert.

Influence of the transverse mode structure on laser-induced acoustic waves

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Abstract. It has been demonstrated that the amplitude of laser-generated stress waves in liquids drastically depends on the molecular transition of the involved hybrid CO_2 laser. This phenomenon can be explained by a correlation of the molecular transition with the transverse mode pattern of the laser beam. Experimental results are discussed and the importance of mode control and mode stability for interaction studies is emphasized.

In previous publications [1, 2, 3] we reported experimental results as well as a theoretical model on the generation of acoustic waves in liquids by laser impact. Both the amplitude and the temporal shape of the laser-induced stress waves in various liquids had been measured with the aid of self-developed stress transducers. Special attention was paid on the dependence of the acoustic signal characteristics on the physical properties of the liquid and on the laser pulse power. In this letter we wish to demonstrate the drastic influence of the transverse mode structure of the laser beam on the stress amplitude.

The present investigations were performed with water for a laser power range where the vaporization dominates the stress generation. The experimental setup used for this study was the same as described in Ref. 2. First our hybrid CO_2 laser

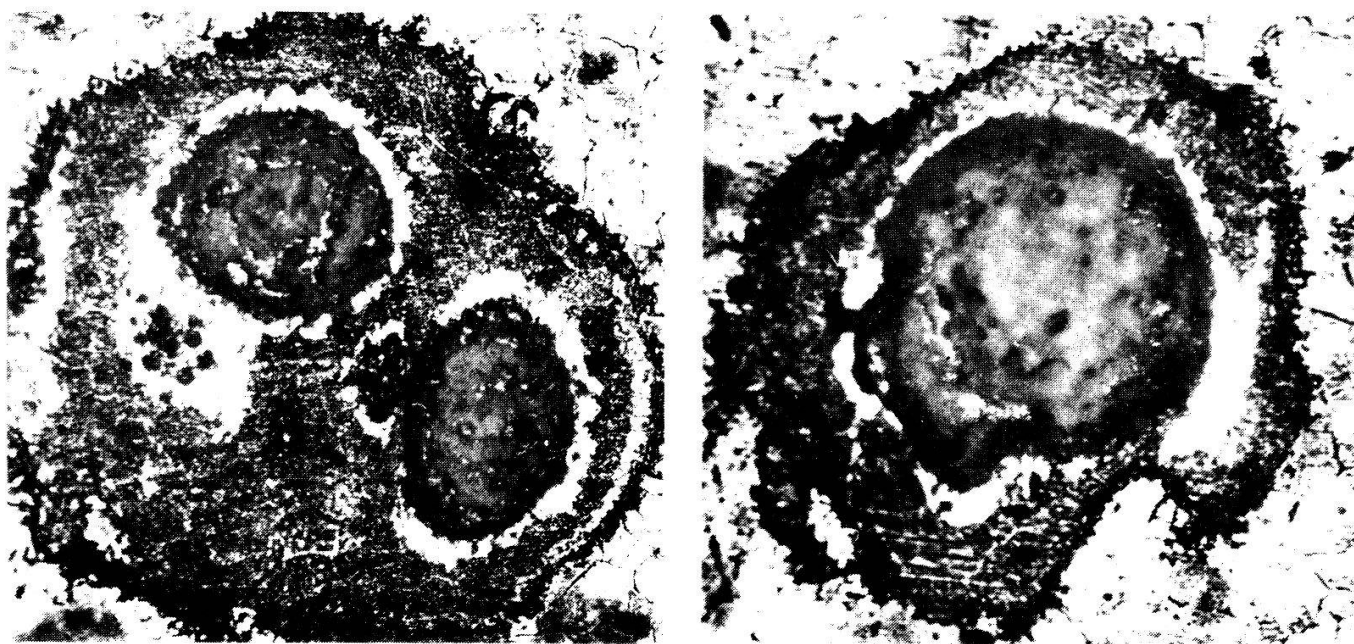


Figure 1

Two different transverse mode patterns, corresponding to adjacent P transitions, near the focus of the laser beam.

was run with one totally reflecting mirror and without a limiting aperture inside the cavity. With this version the average peak power of a pulse is 400 kW and its halfwidth is 350 ns. At the focus of a Ge lens with $f = 20$ cm a peak intensity of approximately $4 \cdot 10^8 \text{ Wcm}^{-2}$ is achieved.

The wavelengths of the pulsed emissions of this laser were checked with a spectrum analyzer (Optical Engineering, Inc., Model 16-A). We noticed that the laser output occasionally jumps from one pulse to another between various molecular transitions of a branch of the $10.4 \mu\text{m}$ band, e.g. between P (18) and P (20). Simultaneous observation of the transverse mode structure of the laser beam indicated that a change of the molecular transition is accompanied by a change of the mode pattern. An example is given in Fig. 1 showing the two different mode patterns of adjacent P transitions. These patterns were recorded on Polaroid film and represent the mode structure incident on the free surface of the liquid. The correlation mentioned above can be explained by the characteristics of the cw CO_2 laser, described in a review by Patel ([4], p. 117). It is due to the configuration of the hybrid laser which consists of a TEA-discharge tube in series with a cw-laser tube, both of which are contained within the same resonator. This combination gives rise to strong competition among the molecular transitions and implies the correlation of a line jump with a change in the transverse mode structure (Fig. 1). The mode pattern in the laser focus can thus be varied.

The influence of the mode structure of the laser beam on the induced peak stress is shown in Fig. 2. In this figure the peak stress recorded by the transducer, placed 20 mm below the free surface of the water, is plotted versus the incident laser peak power. The resulting straight curves correspond to two different molecular laser transitions. For an identical laser power, e.g. 400 kW, the stress amplitudes differ by more than a factor of two. This phenomenon cannot be explained by the negligible difference of the absorption coefficient α for the neighbouring frequencies of the two molecular transitions. The respective fre-

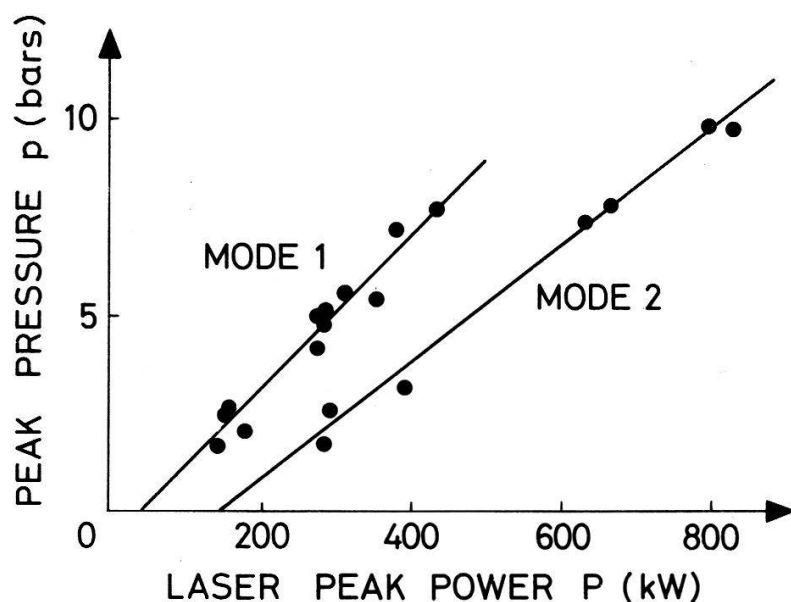


Figure 2

Peak pressures in water for two different transverse modes of the hybrid CO_2 laser as a function of the incident laser peak power at a constant distance from the impact.

quency separation of approximately 50 GHz is much less than the width of the absorption band of water. Consequently the change of the transverse mode pattern, which involves a change of the laser intensity in the focus, is alone responsible for the drastic difference of the peak stresses. Since the laser intensity in the case of mode 2 is considerably smaller than that of mode 1 (Fig. 1), the corresponding stress amplitudes are lower (Fig. 2). In addition the threshold power for stress generation is only 44 kW for mode 1 in comparison with 144 kW for mode 2. This can be explained by the vaporization threshold of water which has to be exceeded by the absorbed laser energy density. In the case of mode 1 this threshold is reached already at a lower laser power because of better focusing for this mode pattern.

In conclusion, our measurements of laser-induced stresses in liquids with piezoelectric transducers have demonstrated the drastic influence of the transverse mode pattern on the stress amplitude. This indicates the importance of the mode control and the mode stability of the laser beam for interaction studies. This may also be of importance for laser-induced chemistry.

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Lampe pulsée dans le domaine de la nanoseconde

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On présente une lampe à arc pulsé, utilisable pour des études de fluorescences. Le domaine d'émission s'étend de l'IR à l'UV, la durée d'une impulsion de lumière est ≥ 1 ns et la puissance émise est < 1 Watt par impulsion. Les opérations suivantes peuvent être effectuées sous tension: (a) changement de la fréquence de répétition des impulsions (5 à 35 KHz); (b) changement du gaz de remplissage et de sa pression (0 à 3 bar); (c) changement de la distance entre électrodes (0.2 à 8 mm); d) alignement de l'arc par rapport à l'optique de la lampe. Un réglage de la position de la lampe selon x , y et z est possible; en plus elle est facilement démontée pour le nettoyage, avec une précision de ~ 0.01 mm pour le remontage.

Acetylene formation by laser pyrolysis of methane

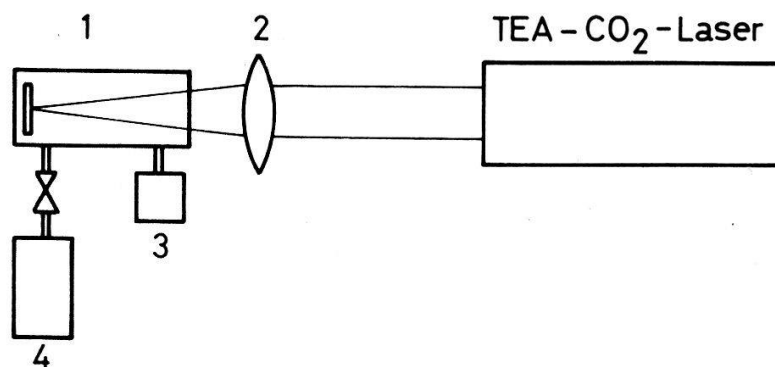
H. P. GRAF, M. W. SIGRIST and F. K. KNEUBÜHL
(Solid State Physics Laboratory ETH Hönggerberg, 8093 Zürich, Switzerland)

Abstract. The formation of acetylene from methane was studied by means of pulsed laser pyrolysis. Plasmas were generated on different metal targets in a methane atmosphere with the aid of a TEA-CO₂-laser. The influence of the laser intensity, the gas pressure, and the target materials on the acetylene formation was investigated. A strong dependence of the acetylene yield on these parameters was found.

The production of acetylene (C₂H₂) from methane (CH₄) by means of high temperature pyrolysis in an electric arc or in a plasma jet has been studied extensively, see e.g. [1]. With the pulsed laser pyrolysis technique temperatures above 10⁴ K and quenching times of the order of μ sec are obtained easily. These quenching times are orders of magnitude shorter than those obtained by conventional pyrolysis techniques. Over 90% of the pulse heated methane can be converted to acetylene plus hydrogen by the laser pyrolysis as demonstrated by Yogev and Lowenstein-Benmair [2].

In order to clarify the catalytic effect of metal vapors on the pyrolysis of methane we vaporized different metals in a methane atmosphere by TEA-CO₂-laser impact.

The experimental setup is shown in Fig. 1. The TEA-CO₂-laser has an output energy of 0.8 J per pulse. The pulse shows a half-width of 120 nsec followed by a tail of 1 μ sec. The plasma is produced by focusing the radiation by a Ge-lens of 10 cm focal length on a metal target placed in the reaction chamber. Lead, tungsten, nickel and brass plates have been used as targets. The reaction chamber has a diameter of 2 cm and a total volume of 95 cm³, which is filled with methane at pressures between 1 and 410 torr. The total quantity of reaction products in the chamber is determined with a capacitance pressure gauge. The gas composition is analyzed after the laser irradiation with a quadrupole mass spectrometer. For quantitative analysis the mass spectrometer has been calibrated with H₂, CH₄, C₂H₂, and C₂H₄, mixed in a gas mixing unit.



- 1 Reaction chamber with target
 2 Ge lens (focal length 10 cm)
 3 Pressure gauge (MKS Baratron 221A)
 4 Quadrupole mass spectrometer
 (Balzers QMG 101)

Figure 1
 Experimental setup.

The maximum conversion rate of methane is achieved with the highest laser intensity on the target. Decreasing the laser pulse energy from 0.6 J to 0.3 J by attenuation of the beam reduces the quantity of converted methane by a factor 4 to 5. Obviously, the higher plasma density obtained with higher laser intensity favours the energy transfer from the laser beam to the methane.

In Fig. 2 the gas composition is plotted as a function of the number of laser pulses when methane at a pressure of 67.5 torr is filled in the chamber. The main products are hydrogen and acetylene. 3 vol% of ethylene (C_2H_4) are found after

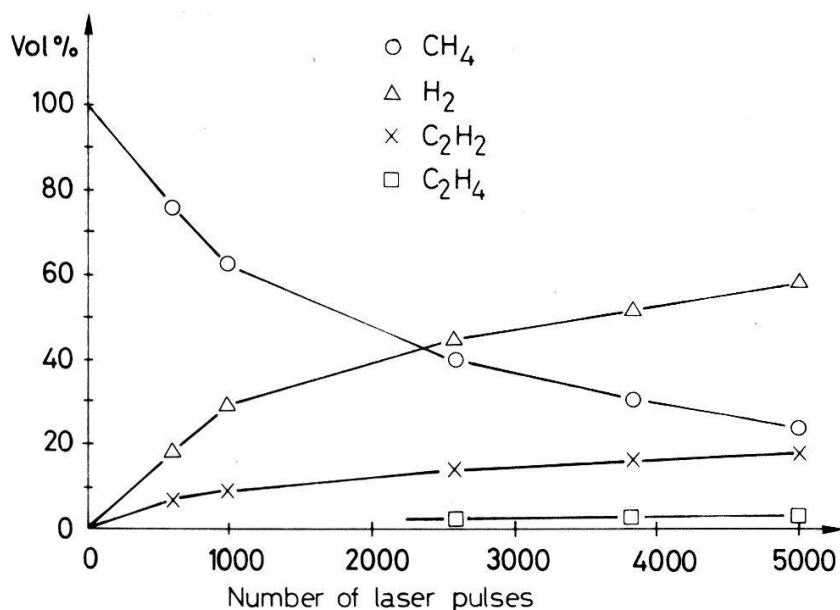


Figure 2
 Concentrations of H_2 , CH_4 , C_2H_2 , C_2H_4 as a function of pulse number. Target: nickel, laser energy per pulse: 0.6 J, pulse repetition frequency: 1 Hz, methane pressure: 67.5 torr.

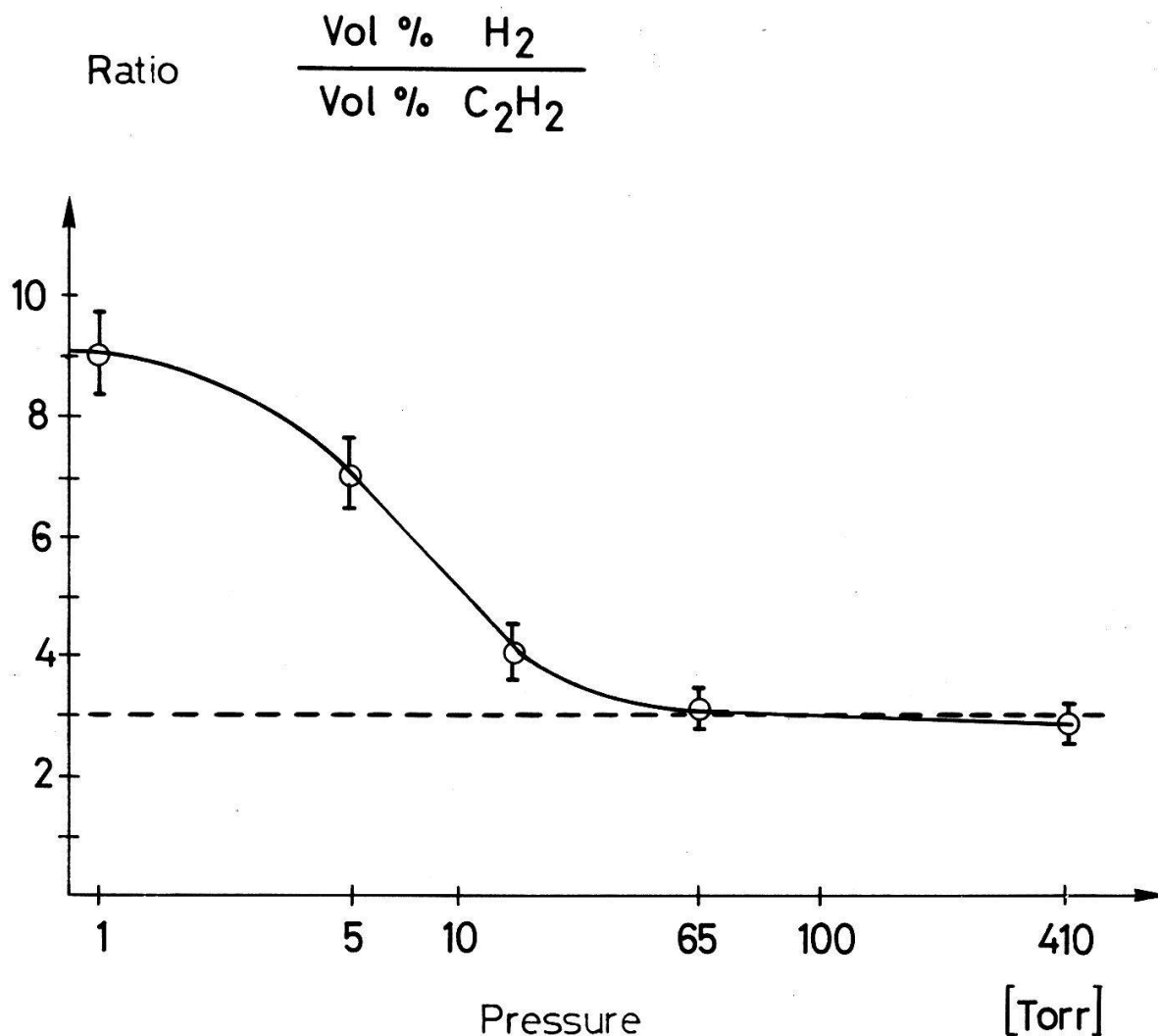


Figure 3

Concentration ratio of H₂ and C₂H₂ as a function of the methane pressure filled in the reaction chamber. Target: nickel.

5000 pulses. No other products with concentrations higher than 0.3 vol% were detected.

If methane at pressures below 65 torr is filled in the chamber, more hydrogen and less acetylene are produced. For 1 torr methane and a nickel target the concentrations of H₂, C₂H₂, and C₂H₄ increase up to 78 vol%, 8.6 vol%, and 3.1 vol% respectively after 80 laser pulses. For higher pulse numbers the concentrations of both, C₂H₂ and C₂H₄, decrease as well as that of CH₄. Consequently, after 500 pulses only H₂ is left, while all the carbon has condensed on the walls of the reaction chamber and on the target.

Figure 3 shows the influence of the methane pressure filled in the chamber on the concentration ratio of H₂ and C₂H₂. This ratio was determined at low pulse numbers where the methane concentration is higher than 80 vol%. Above 65 torr the ratio is approximately 3 as expected from the equation $2\text{CH}_4 \rightarrow \text{C}_2\text{H}_2 + 3\text{H}_2$ if C₂H₂ and H₂ are produced exclusively. The ratio increases up to 9.0 ± 0.8 at 1 torr methane. At this pressure 50%–60% of the hydrogen is produced by the reaction $\text{CH}_4 \rightarrow \text{C}_s + 2\text{H}_2$. The condensation of carbon on the chamber walls at lower ambient pressures was also observed by Hanson [3] and Taki et al. [4] in laser

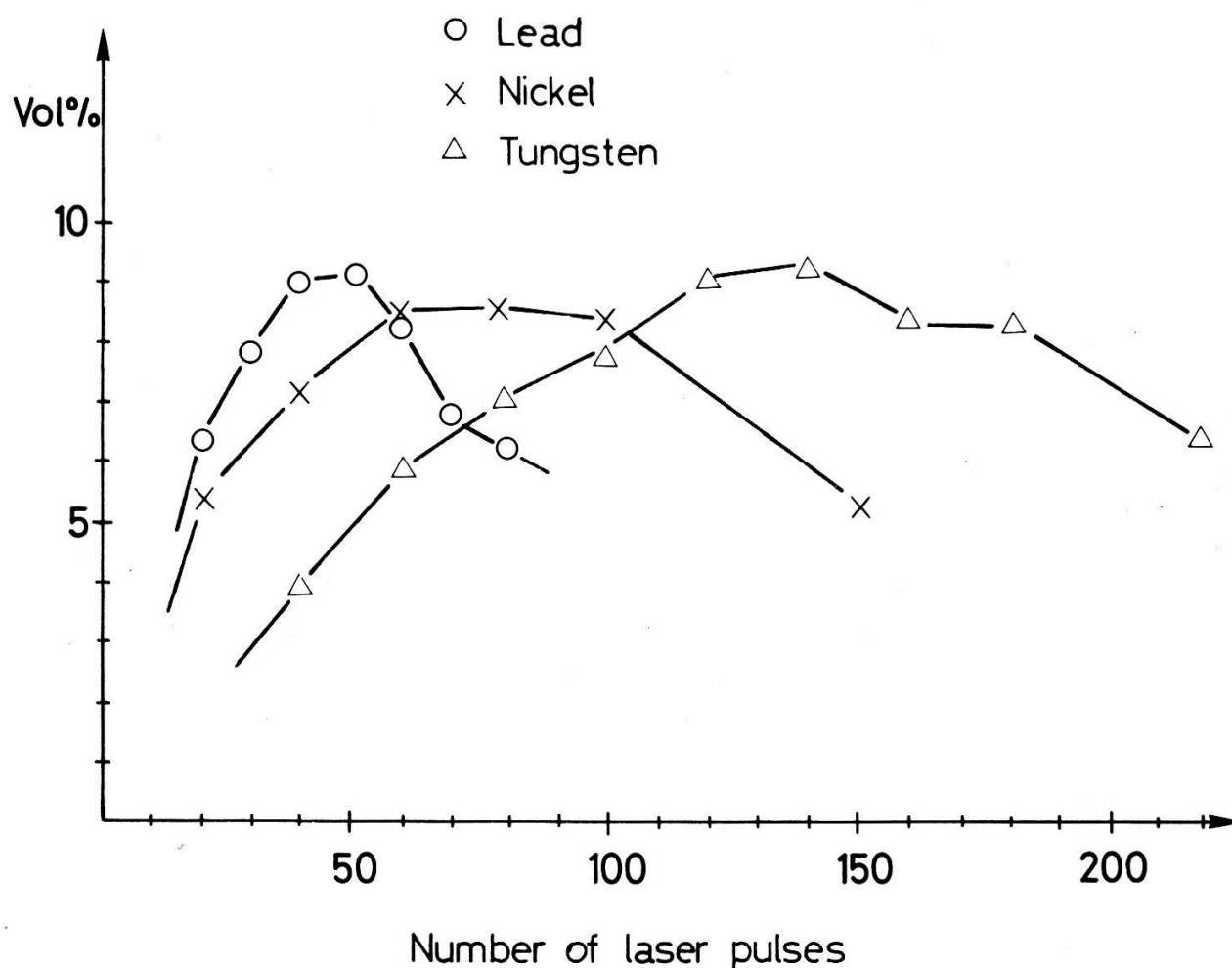


Figure 4

Concentration of acetylene as a function of the number of laser pulses focused on different targets. Laser energy per pulse: 0.6 J, pulse repetition frequency: 1 Hz, methane pressure: 1 torr.

pyrolysis experiments performed with coal and graphite in a hydrogen atmosphere.

The influence of the different target materials on the reaction is shown in Fig. 4. The same products are found with all metal targets used and the concentration ratios vary only slightly. The amount of converted methane varies drastically between $8.6 \cdot 10^{-8}$ mole/pulse for a lead target and $3.3 \cdot 10^{-8}$ mole/pulse for a tungsten target. This effect is probably due to the different amounts of vaporized metals, approximately $3 \cdot 10^{-8}$ mole/pulse for lead, $0.9 \cdot 10^{-8}$ mole/pulse for nickel, and $0.2 \cdot 10^{-8}$ mole/pulse for tungsten (ambient pressure 1 Torr, 0.6 J per pulse, 0.4 to 0.5 mm focus diameter). It is not yet clear whether the metal vapors have a catalytic effect on the methane conversion or whether the influence of the target materials on the expansion, temperature and density of the plasma is responsible. Further experiments are planned to clarify these questions.

We wish to thank Dr. C. von Planta (F. Hoffmann-La Roche & Co., Basel) for suggestions and Mr. H. R. Vogt for valuable assistance in the course of the experiments. This work was supported by the Kommission zur Förderung der wissenschaftlichen Forschung.

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Schockwellen in axial beblasenen Hochdruck Lichtbögen

R. GRAF, R. T. REINHARDT und H. J. SCHÖTZAU
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Es wird die experimentelle Anordnung beschrieben, bei der eine intensive axiale Strömung den Hochdruck-Lichtbogen stabilisiert.

Die in der Kaltgasströmung beobachteten Schockwellen können auch im Lichtbogen identifiziert werden. Ihr Einfluss auf den Lichtbogen wird diskutiert.

Collisional 2-D transport for finite beta tokamaks

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In Tokamaks with large parallel heat conductivity the two dimensional heating and transport problems can be reduced to a set of one dimensional parabolic equations with two dimensional effects appearing explicitly in the equilibrium equation. The method is outlined and the equations derived. We describe an application to the intense heating of a plasma in presence of classical thermal transport. Finally by means of major radius compression we show that a conventional Tokamak can approach a spheromak, with vanishing external toroidal field.

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Magnetoakustische Resonanz bei der Ionenzyklotronfrequenz¹⁾

H. P. ELMIGER, B. G. VAUCHER, B. A. HOEGGER und H. SCHNEIDER
(Physikinstitut der Universität Freiburg, Schweiz)

In einem magnetisierten Plasmazylinder ($B_0 = 8.3 \text{ kG}$, $10^{14} \text{ cm}^{-3} < n_e < 10^{16} \text{ cm}^{-3}$, $T_e = 1.5 \text{ eV}$) wurde die magnetoakustische Resonanz bei unterschiedlichen Dichten untersucht. Die Anregung erfolgte mittels einer kurzen Sendespule

¹⁾ Diese Arbeit wurde durch die Unterstützung des Schweizerischen Nationalfonds ermöglicht.

(2 cm) in der Umgebung der Ionenzyklotronfrequenz. Messungen des Wellenfeldes in Abhängigkeit der Frequenz, sowie der radialen und axialen Profile zeigen den typischen Verlauf für geometrische Resonanzen.

Distribution d'énergie des électrons dans les plasmas de gaz moléculaires

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Les électrons influencent considérablement les propriétés des plasmas de gaz moléculaires, en particulier la dissociation, par leur distribution d'énergie. Nous avons étudié cette distribution dans les décharges d'azote et d'oxygène au moyen de la méthode de la deuxième dérivée. Pour l'oxygène, nous avons trouvé une distribution différente dans la forme T et la forme H de la décharge. L'analyse des fonctions de distribution permet de tirer certaines conclusions sur les réactions homogènes dans les plasmas d'oxygène.

Einfluss von magnetischen und elektrischen Störfeldern auf die Energieanalyse niederenergetischer Elektronen

H. MARTIN und W. BAUMGARTNER

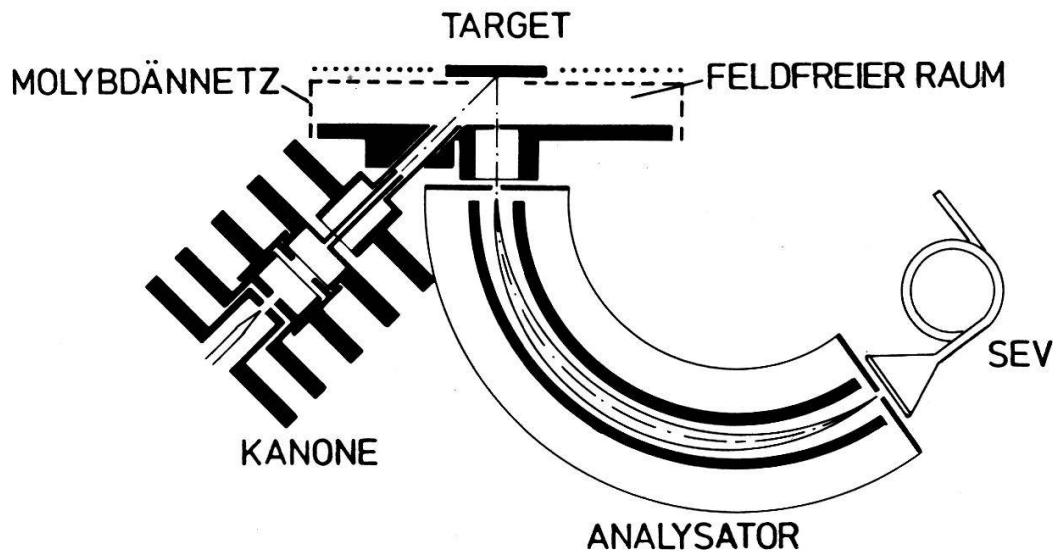
(Institut für Technische Physik, ETH Zürich)

Von Steiner [1] wurde die Energieverteilung von Sekundärelektronen an Gold, Wolfram und Bleiglas untersucht. Dabei traten die für Arbeiten mit langsamen Elektronen typischen Probleme auf:

1. Empfindlichkeit der Elektronenbahnen auf elektrische Störfelder von Aufladungen oder Kontaktpotentialen.
2. Empfindlichkeit der Elektronenbahnen auf magnetische Störfelder wie Erdfeld oder Streufelder elektrischer Geräte.
3. Sicherstellung eines definierten Zustandes der Targetfläche über längere Messzeiten.

In Fortführung der erwähnten Arbeit wurde unter verschärfter Berücksichtigung dieser drei Punkte die Messapparatur teilweise modifiziert. Mit dem neuen Rezipienten kann ein Arbeitsdruck im 10^{-11} Torr Bereich sicher gehalten werden. Zusätzlich kann mittels Sekundärionen-Massenspektroskop die Targetfläche gesputtert und in ihrer Zusammensetzung untersucht werden.

Analysiert werden jetzt die senkrecht zur Targetfläche emittierten Sekundärelektronen. Der feldfreie Raum (vgl. Fig. 1) ist nun einseitig durch ein Molybdännetz begrenzt und damit ist eine bessere Entgasung von Flächen in Nähe des Targets garantiert. Zusätzlich kann dieses Netz durch Elektronenbombardement geheizt werden, um Kontaminationen möglichst zu verhindern. An Stelle der doppelten – die Entgasung beeinträchtigenden – Permalloyabschirmung werden Helmholtz-Spulenpaare zur Kompensation von Magnetfeldern in den drei Raumrichtungen verwendet.



Figur 1
Messprinzip.

Der Analysator arbeitet nach der Beziehung $E = c \cdot V$, wobei E die detektierte Energie, c die sogenannte Analysatorkonstante und V die Ablenkspannung über den Analysatorplatten bedeuten. Die Energieabhängigkeit von c wurde, bei Anwesenheit von magnetischen und elektrischen Störfeldern, mit am Target elastisch reflektierten Primärelektronen untersucht.

Bei Anwesenheit eines zur Bahnebene senkrechten Magnetfeldes $H_{\perp}$ (A/m) sollte nach [2] für die Analysatorkonstante c_{em} gelten:

$$c_{em} = c_e \cdot \left(\frac{1}{1 - q \frac{H_{\perp}}{\sqrt{E}}} \right)$$

c_e = Konstante ohne Magnetfeld; E = detektierte Energie (eV); $q = 1.77 \cdot 10^{-2}$.

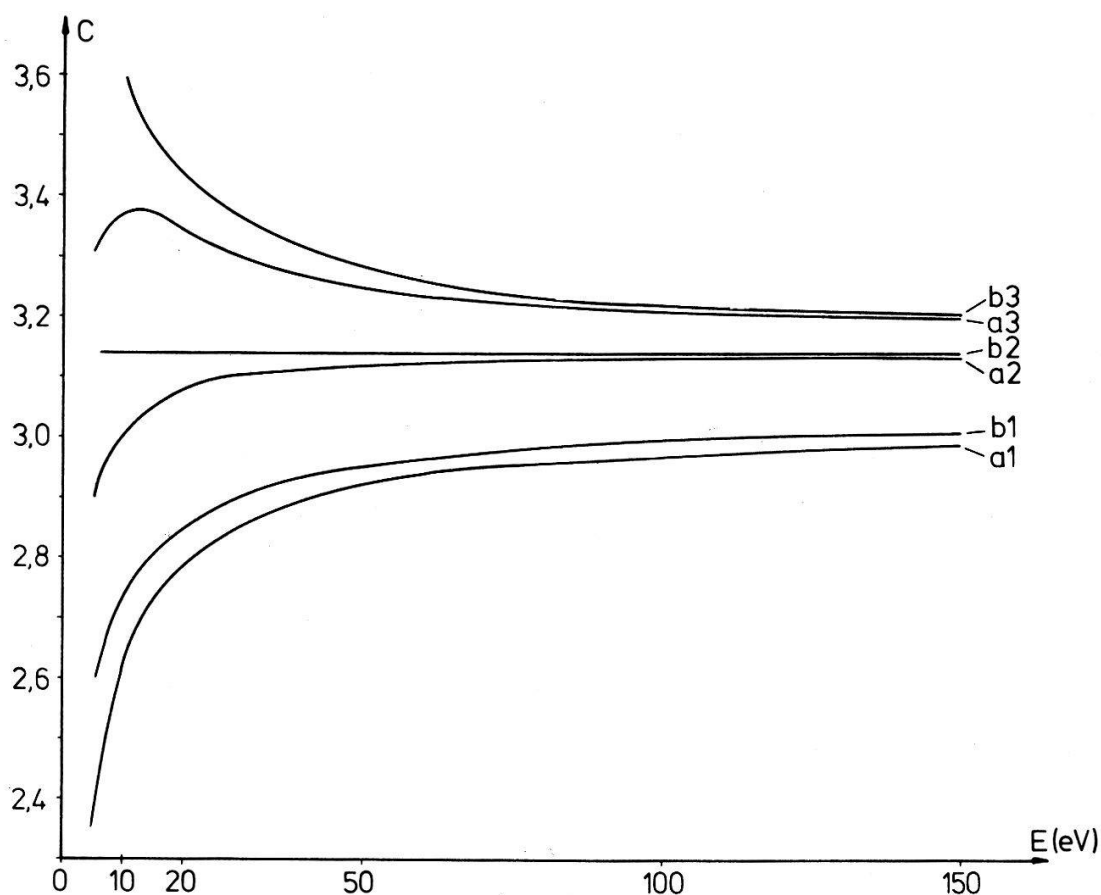
Figure 2 zeigt die gemessene Energieabhängigkeit von c für:

- a1: Magnetfeld nicht kompensiert
- a2: Magnetfeld kompensiert
- a3: Magnetfeld überkompensiert

Diese Kurven weichen bei tiefen Energien stark vom theoretischen Verlauf von c_{em} ab. Als verantwortlich für diese Abweichung erwies sich die Kontaktpotentialdifferenz zwischen Kathode und Analysator. Sie kann durch Zuschalten einer Spannungsquelle in den Primärelektronenkreis kompensiert werden. Nach Kompensation der Kontaktpotentialdifferenz ergeben sich folgende Kurven:

- b1: Magnetfeld nicht kompensiert
- b2: Magnetfeld kompensiert
- b3: Magnetfeld überkompensiert

b1 und b3 zeigen nun für c_{em} den Magnetfeldeinfluss gemäss obiger Formel, und b2 liefert tatsächlich eine energieunabhängige Analysatorkonstante über den Energiebereich 6–150 eV. Aus Intensitätsgründen ist eine Kontrolle der Konstanz unterhalb 6 eV zur Zeit nicht möglich.



Figur 2
Energieabhängigkeit der Analysatorkonstante.

Diese Arbeit wurde durch den Schweizerischen Nationalfonds unterstützt.

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Anpassungsglied für die Sekundärionen-Analyse mit Quadrupol-Massenfilter

P. BUCHMANN und W. BAUMGARTNER
(Institut für Technische Physik, ETH Zürich)

Wird die Sekundärionen-Massenspektrometrie (SIMS) mit einem Quadrupol-Massenanalysator betrieben, so stellt sich das Problem der Anpassung des Sekundärionenstrahls an die Einschussbedingungen des Quadrupol-Massenfilters (QMF) [1]. Der ins QMF eintretende Sekundärionenstrahl sollte folgende Bedingungen erfüllen:

- (1) Er enthält keine hochenergetischen Neutralteilchen und Sekundärelektronen mehr.

- (2) Die Sekundärionen-Bündelachse soll mit der Achse des Quadrupols zusammenfallen, dies bei möglichst kleiner Bündelöffnung. Nach einer von W. Paul [2] gegebenen Abschätzung für die maximal zulässige Radialgeschwindigkeit findet man für das von uns verwendete Massenfilter QMA140 der Balzers einen maximalen halben Öffnungswinkel:

$$\alpha_{\max} \approx 10.4^\circ (E_0 = 30 \text{ eV}) \quad (E_0 \text{ Ionenenergie})$$

$$\alpha_{\max} \approx 5.2^\circ (E_0 = 60 \text{ eV})$$

- (3) Die Ionenenergie darf den Wert

$$E_{\max} \approx 0.04 \cdot \Delta m \cdot l^2 \cdot \nu^2$$

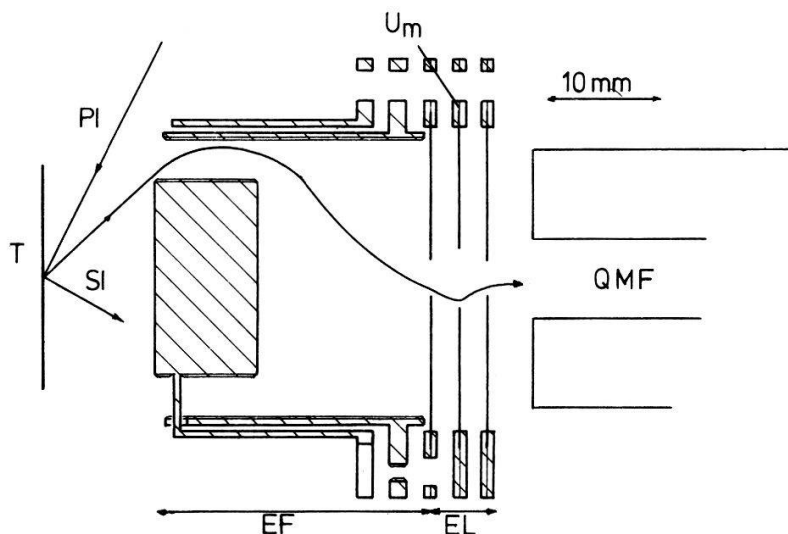
(Δm Halbwertsbreite des Massenfensters, l Quadrupolstablänge, ν Hochfrequenz) nicht überschreiten. Für den QMA140 ergibt sich ein Maximalwert von ca. 66 eV bei axialem Einschuss.

Um diese Bedingungen optimal zu erfüllen und zugleich die Ionenausbeute nicht allzu stark zu verringern, wurde das System nach Fig. 1 entworfen.

Es besteht aus einem Energiefilter – modifizierter zylindrischer Spiegel-feldanalysator – und einer Einzellinse. Die rotationssymmetrische Eintrittsöffnung ermöglicht eine gute Ausnützung der Sekundärionen. Um die Reflexion von Neutralteilchen und hochenergetischen Ionen in Richtung Quadrupol zu unterdrücken, wurden Innen- und Aussenzyylinder mit Rillen versehen. Die Einzellinse ermöglicht die Parallelisierung und Bündelung des Ionenstrahls. Beim Entwurf des Systems mussten auch die beschränkten Platzverhältnisse berücksichtigt werden.

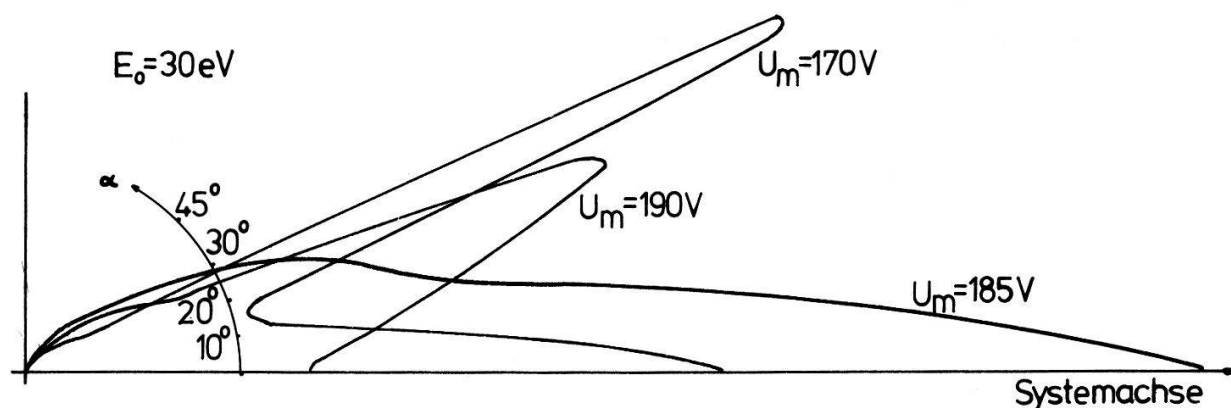
In einem ähnlichen System von T. Satake et al. [3] durchqueren die Ionen streifend zwei Gitter, was zur Entstehung von unerwünschten Sekundärpartikeln führen kann. In unserem System wurde deshalb auf den Einsatz von Gittern verzichtet.

Das Energiefilter sowie das Gesamtsystem aus Energiefilter und Einzellinse wurden mit Hilfe monochromatischer Natriumionen ausgemessen. Für das Energiefilter mit 3 mm-Blendenöffnung wurden folgende Daten bestimmt:



Figur 1

Masskizze des Anpassungsglieds mit Target T, Primärionen PI, Sekundärionen SI, Energiefilter EF, Einzellinse EL und Quadrupolmassenfilter QMF; U_m Potential der Mittelelektrode.



Figur 2

Strahlprofile für Ionenenergie $E_0 = 30$ eV und verschiedene Potentiale U_m . Für $U_m = 185$ V haben ca. 55% der Ionen einen halben Öffnungswinkel α kleiner als 10° .

Transmission (zwischen Eintrittsöffnung und erster Blende) ca. 15%, Energie – Auflösungsvermögen $\Delta E/E \approx 0.06$.

Bei kleiner Ionenenergie genügt die Auflösung, um eine Aufspaltung des Peaks infolge des Spannungsabfalls über das Filament der Ionenquelle (ca. 400 mV) sichtbar zu machen.

Die mit den optimalen Blendenspannungen – in Bezug auf Transmission und Winkelverteilung der Ionen – erreichbare Bündelung des Strahls ist aus dem Strahlprofil ersichtlich (Fig. 2).

Die Transmission des Gesamtsystems beträgt noch 1.7% und 0.5% innerhalb des optimalen Öffnungswinkels von 5° . Erste Messungen mit SIMS zeigen eine deutlich verbesserte Massenauflösung und völliges Fehlen eines Untergrundsignals, während die Empfindlichkeit des Systems zurückgegangen ist. Wie weit die Intensitätsverhältnisse noch verbessert werden können, muss die weitere Optimierung der Betriebsbedingungen zeigen. Die Ergebnisse der Messung der Energieverteilung von Aluminiumionen bei Beschuss einer Al-Probe mit 3 keV Argonionen stimmen gut überein mit entsprechenden Daten aus der Literatur [4].

Diese Arbeit wurde vom Schweizerischen Nationalfonds finanziell unterstützt.

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Installation pour l'étude par ultrasons des dislocations¹⁾

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Une nouvelle installation de mesure a été construite dans le but d'étudier la mobilité des dislocations et leurs interactions avec le réseau et les défauts

cristallins dans les métaux. Elle consiste à mesurer la vitesse et l'amortissement d'ondes ultrasonores longitudinales ou transversales (4 à 40 MHz) par la technique des échos.

La précision sur la vitesse absolue des ultrasons est de l'ordre de 100 ppm (mesure manuelle). Quant aux variations de vitesse et d'amortissement des ondes, elles sont faites automatiquement (jusqu'à 10 000 mesures/seconde) avec une précision voisine du ppm sur la vitesse et du ‰ sur l'amortissement.

Une contrainte mécanique (de compression), lentement variable, peut être appliquée sur l'échantillon selon un axe perpendiculaire à la direction de propagation des ultrasons. Une boucle de réglage automatique permet de donner à la contrainte une forme quelconque en fonction du temps, par la poursuite d'une référence analogique. Il est possible entre autres de générer une contrainte sinusoïdale (amplitude comprise entre 0.1 et 20 N/mm², jusqu'à 1 Hz) pour simuler les mesures de frottement intérieur basse fréquence faites en pendule ou pour comparer les résultats avec les observations faites sous contrainte et à basse température en microscopie électronique à transmission.

Les mesures sont effectuées dans un cryostat à He entre 10 K et l'ambiante. Il est en outre possible d'irradier l'échantillon sous un flux de γ , en cours de mesure, pour y créer des défauts ponctuels.

Les premières mesures ont confirmé la grande sensibilité des mesures d'ultrasons et la précision du système de contrainte mécanique.

¹⁾ Recherche partiellement subventionnée par le Fonds National Suisse de la Recherche Scientifique, subside no. 2.932-0.77.

A portable rapid spectral-scanning instrument for color studies

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A portable dual-channel instrument for rapid optical spectral reflectance measurements was constructed. Twenty discrete wavelengths spanning the range from 365 nm to 690 nm are scanned using an interference wedge filter. Seven more infrared wavelengths from 700 nm to 1000 nm are obtained with discrete interference filters. The 27 fully digitized values of the ratio measurements obtained in three seconds from this instrument are recorded on cassettes for further data processing.

The light source is a xenon flash lamp and fiber optics are used for the measuring heads (sample and reference). The single detector is a fast PIN diode operated in the photo conductive mode.

This instrument is being used in our laboratory for extensive measurements involving samples of ink printed onto paper. The computer evaluation is especially useful for evaluating subtle spectral variations while at the same time compensating for density variations. The instrument is also being used for the evaluation of food-stuffs in view of improved means for sorting according to ripeness.

A more detailed description is being submitted to *Journal of Physics E*.

Influence des vitrages et des murs dans le bilan thermique saisonnier d'une construction

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Resumé. Les deux tiers environ des déperditions thermiques d'un bâtiment sont dues aux pertes au travers des vitrages et des parties opaques de la construction.

Dans le cas des vitrages le résultat du bilan thermique hivernal dépend de la constitution de la fenêtre, de son orientation, ainsi que du climat. Sur la base d'un modèle mathématique, le bilan a été établi pour divers types de vitrages en utilisant des données climatiques hivernales réelles.

Le mur pour sa part, reçoit la lumière du soleil, il en capte et en stocke une partie, ce qui provoque une variation de sa résistance thermique apparente. Les mesures montrent que la résistance apparente du mur varie d'un facteur deux lorsque l'insolation journalière du mur passe de zéro à 3 [kWh/m² · jour].

Les déperditions thermiques d'un bâtiment standard normalement isolé se répartissent comme suit:

- pertes au travers des vitrages $\approx 35\%$
- pertes au travers des murs, du sol et du toit $\approx 30\%$
- pertes dues aux renouvellements d'air $\approx 35\%$

Du fait que les trois composants sont du même ordre de grandeur, il nous faudra, pour observer un effet notable, agir au moins sur deux d'entre eux. Dans le cadre de cet article, nous allons nous concentrer sur les vitrages et sur les murs.

1. Bilan thermique saisonnier d'un vitrage

Considérons le modèle simple représenté sur la Fig. 1, schématisant un élément d'une construction

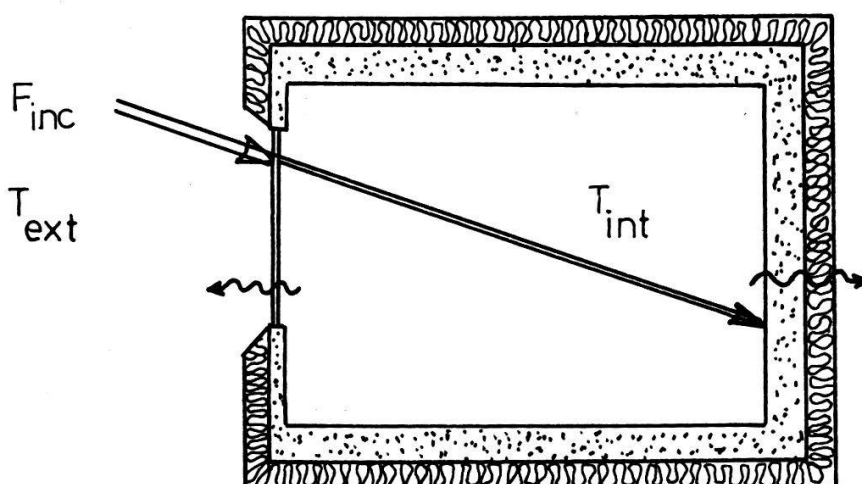


Figure 1

En présence de rayonnement solaire, le bilan thermique d'un tel local peut s'écrire comme suit:

$$Q = F_{inc} \cdot S \cdot \alpha \cdot \tau - (q_c + q_r)S - \bar{k} \cdot S_1 \cdot \Delta\theta$$

où

F_{inc} = flux solaire incident [W/m^2]

S = surface du vitrage

α = facteur d'absorption du local

τ = facteur de transmission du vitrage

$q_c = h_c \cdot \Delta\theta$ = pertes par conduction-convection au travers du vitrage

$q_r = 4\sigma\epsilon\bar{T}^3 \Delta\theta$ = pertes par rayonnement

k = facteur k moyen des murs en contact avec l'extérieur

S_1 = surface de murs en contact avec l'extérieur

$\Delta\theta = (T_{\text{int}} - T_{\text{ext}})$

Q est négatif lorsque les déperditions thermiques sont supérieures aux apports solaires, il est positif dans le cas contraire. L'équation d'équilibre ci-dessus est semblable à celle d'un capteur solaire.

Examinons les conditions qui devraient être remplies par notre 'capteur', afin de lui assurer un rendement optimal.

(a) $\alpha \approx 1$ (pour $0.3 < \lambda < 3 [\mu\text{m}]$)

le local doit présenter un facteur d'absorption maximal pour le rayonnement solaire incident.

(b) $\tau \approx 1$

le facteur de transmission du vitrage doit être aussi grand que possible.

(c) $\bar{k}$ petit

l'isolation des murs doit être aussi bonne que possible.

(d) $\epsilon \approx 0$

les pertes par rayonnement infra-rouge au travers du vitrage doivent être aussi faibles que possible.

(e) $16 < T_{\text{int}} < 25^\circ\text{C}$

C'est une condition additionnelle qui vient du fait que nous ne nous trouvons pas en présence d'un capteur habituel, puisque celui-ci doit être habitable. Cette condition pourra être satisfaite si l'on a soin de réaliser une construction *massive* présentant une isolation thermique à l'extérieur.

L'orientation du 'capteur' est très importante: une surface verticale Sud reçoit en hiver plus de rayonnement solaire que les autres surfaces verticales, elle en reçoit également moins en été qu'une surface Est ou Ouest. On choisira donc autant que possible, une orientation Sud ou proche du Sud.

1.1. Type de vitrage à choisir pour le 'capteur'

De par son coefficient de transmission de chaleur élevé, une vitre est, en l'absence de soleil, un élément de déperdition important dans une construction.

Pour remédier à ce défaut, plusieurs solutions peuvent être envisagées:

(a) *Augmenter le nombre des couches de verre*

Une idée simple, mais pas forcément économique, consiste à augmenter le nombre des couches de verre. Si le passage du simple au double vitrage procure une augmentation sensible de l'isolation: $\Delta k = 2.6 [\text{W/m}^2 \text{ K}]$ (voir Fig. 2), le passage du double au triple vitrage est déjà moins spectaculaire: $\Delta k = 1.1 [\text{W/m}^2 \text{ K}]$. Au-delà de trois verres, l'avantage thermique que l'on retire est mince et

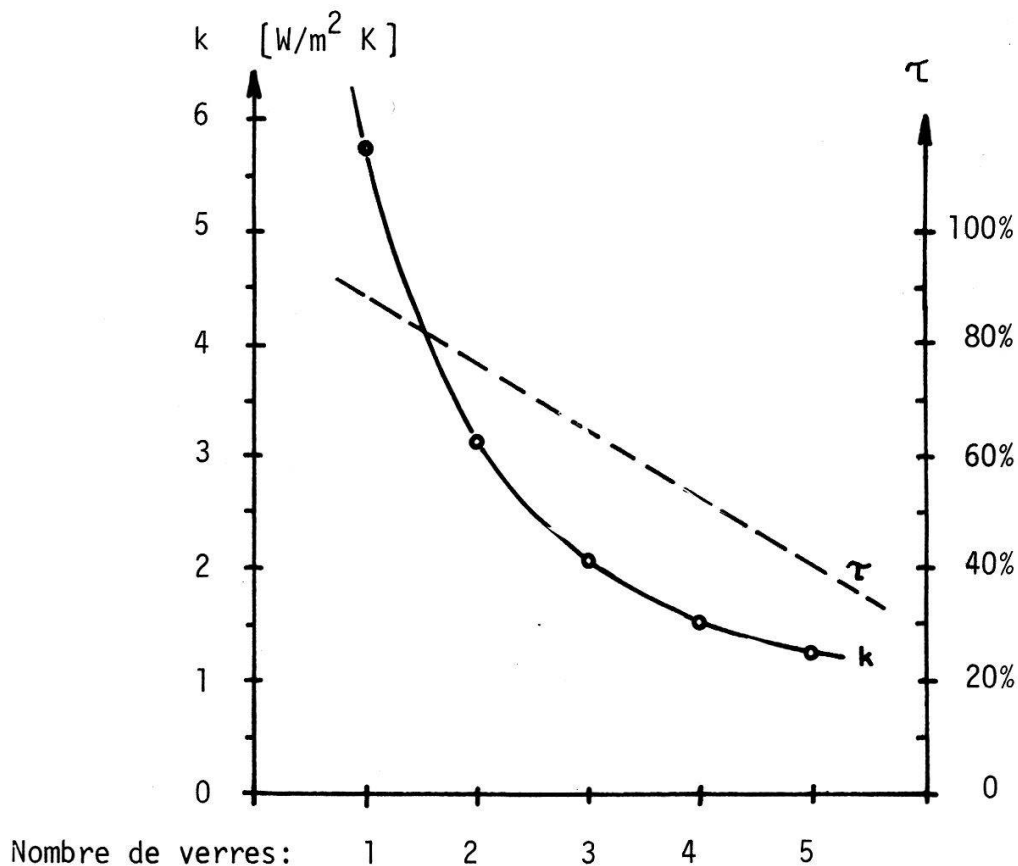


Figure 2

s'accompagne d'inconvénients sérieux: le système devient lourd, les pertes de lumières deviennent importantes ce qui diminue les apports solaires et augmente l'utilisation de l'éclairage artificiel.

1.2. Faire le vide entre les verres d'un double vitrage

Si une telle solution est loin d'être simple, elle a toutefois été réalisée expérimentalement par M. Freyholdt à Lausanne. Les problèmes techniques sont les suivants: d'une part le vitrage doit résister à la pression atmosphérique (10^5 N/m^2 !), d'autre part, le vide doit pouvoir être maintenu au cours du temps. Dans le cas de la fenêtre évacuée de M. Freyholdt, le premier problème est résolu par la pose d'entretoises métalliques qui évitent l'écrasement des verres, le second est résolu par l'utilisation d'un 'gatter' chimique qui permet de maintenir un vide élevé (10^{-4} mm Hg).

Cette solution permet de réduire considérablement les pertes par conduction-convection qui représentent 40% du total. Il reste à éliminer les pertes par rayonnement, ce que l'on fait à l'aide de couches réfléchissantes à l'infra-rouge.

1.3. Utiliser des couches sélectives réfléchissant l'infra-rouge

Du point de vue thermique, de telles couches peuvent présenter des avantages énormes. Elles doivent toutefois posséder les qualités suivantes si elles veulent avoir une chance de s'imposer:

- (a) La couche doit être transparente au visible ($\tau = 1$), tout en réfléchissant l'infra-rouge ($\epsilon_{\text{IR}} \approx 0$).

- (b) La couche doit avoir une durée de vie suffisante (≥ 20 ans).
- (c) Son prix doit être raisonnable.

Actuellement des vitrages munis de telles couches font leur apparition sur le marché.

1.4. Etude quantitative

Nous venons de comparer qualitativement l'effet des différentes améliorations qui peuvent être apportées à un vitrage, tentons de chiffrer ces effets:

1.4.1. *Modèle statique.* L'approche la plus simple consiste à utiliser un modèle statique: on se fixe les conditions extérieures et intérieures ainsi que le flux solaire incident, on peut alors calculer le bilan thermique instantané pour un type de vitrage donné. Le tableau ci-après permet de comparer le comportement statique d'un vitrage simple, d'un double et d'un triple vitrage. On notera que selon la température extérieure et le flux solaire incident, un type de vitrage peut être supérieur à un autre: pour une température extérieure de 5°C par exemple, le vitrage triple est supérieur aux deux autres lorsque le flux solaire est inférieur à $250 [\text{W/m}^2]$, le double est supérieur lorsque le flux est compris entre 250 et $600 [\text{W/m}^2]$, finalement le vitrage simple s'impose au-dessus de $600 [\text{W/m}^2]$.

Température extérieure [$^{\circ}\text{C}$]	Flux solaire incident [W/m^2]								
	NV	100	200	300	400	500	600	700	800
-10	1	-98	-28	43	113	183	253	324	394
	2	-12	52	115	178	241	304	368	431
	3	8	65	123	180	237	294	352	408
-5	1	-68	2	72	143	213	283	353	424
	2	0	63	127	190	253	316	379	442
	3	16	73	130	188	244	302	358	416
0	1	-39	32	102	172	242	312	382	452
	2	12	76	139	202	265	327	391	454
	3	24	80	138	195	252	309	367	424
5	1	-10	60	131	200	271	341	411	481
	2	24	88	151	214	277	340	402	465
	3	32	88	146	203	260	318	375	433
10	1	19	88	158	228	298	368	438	508
	2	37	100	163	226	289	352	415	477
	3	40	97	154	211	268	326	383	441
15	1	45	115	185	254	324	394	464	533
	2	50	113	176	239	302	364	428	491
	3	48	105	163	220	278	335	393	450

Bilan instantané en [W/m^2] pour un vitrage formé de un, deux ou trois verres (NV = 1, 2, 3) en fonction de la température extérieure et du flux solaire incident.

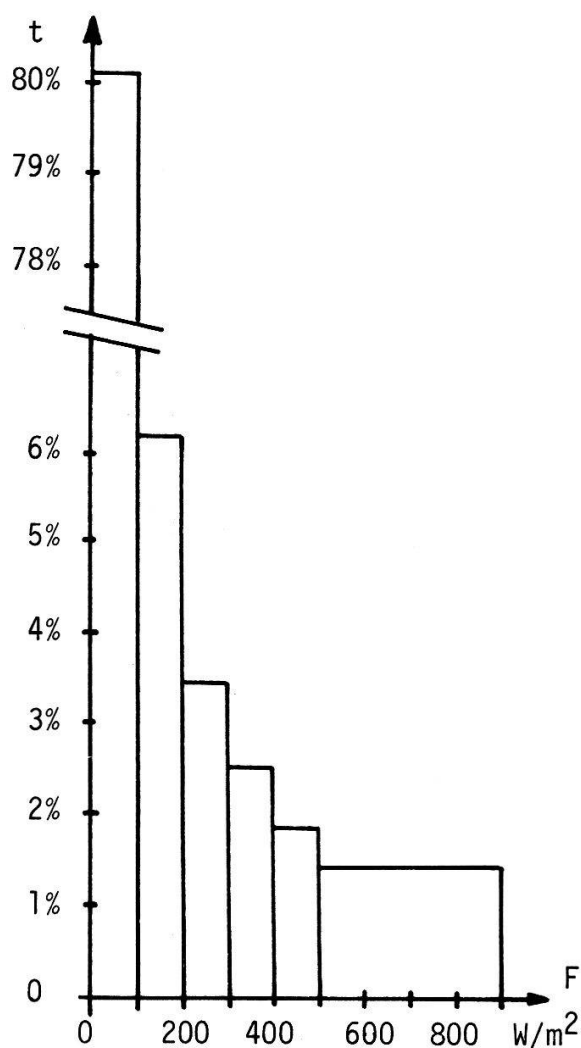


Figure 3
Rayonnement solaire sur une surface verticale sud (Ecublens 10.1-10.4.78).

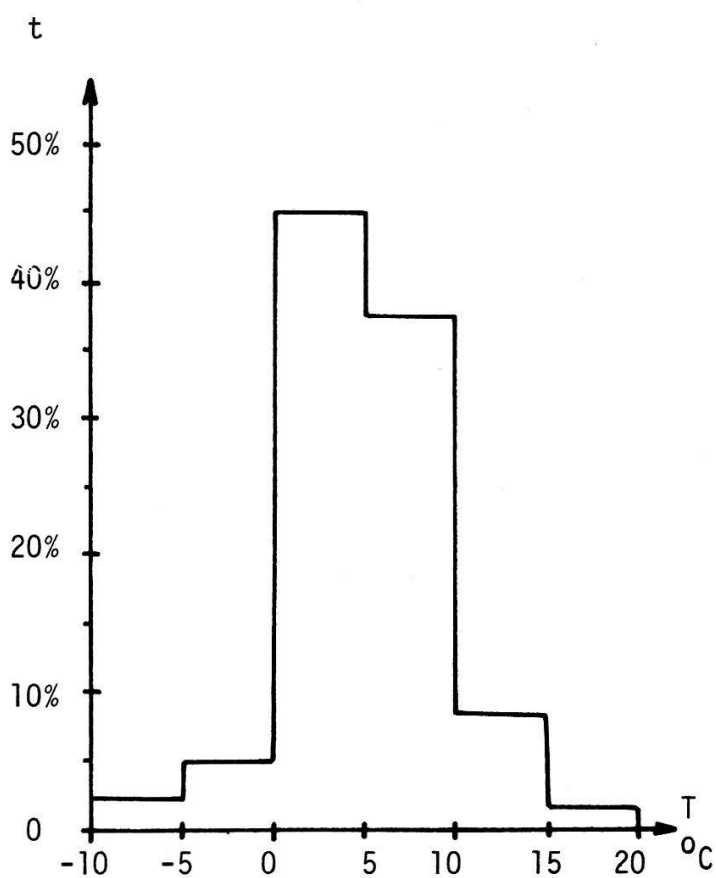


Figure 4
Températures extérieures.

1.4.2. *Modèle dynamique.* Le modèle statique nous permet de savoir ce qui se passe à un instant donné. Si l'on désire toutefois pouvoir effectuer des comparaisons pratiques, il faut considérer le bilan thermique du vitrage envisagé tout au long d'une saison de chauffage. Ceci nécessite la connaissance de données météorologiques précises sur l'ensemble du laps de temps considéré. Dans le cas particulier, nous avons utilisé des mesures météorologiques effectuées demi-heure par demi-heure durant la période du 10 janvier 1978 au 10 avril 1978 sur le site d'Ecublens.

A titre d'illustration, les Figs. 3 et 4 nous donnent, en pourcents, les distributions du flux solaire (mesuré sur une surface verticale Sud) et de la température extérieure pour la période considérée.

Sur la base de ces données météo, nous avons utilisé un modèle dynamique et avons effectué, pour la période de 3 mois, un bilan pour divers types de vitrages placés en façade Sud. La Fig. 5 illustre les résultats de la simulation pour un vitrage simple, un vitrage double, un vitrage double évacué et un vitrage triple.

Type de vitrage

Bilan sur 3 mois

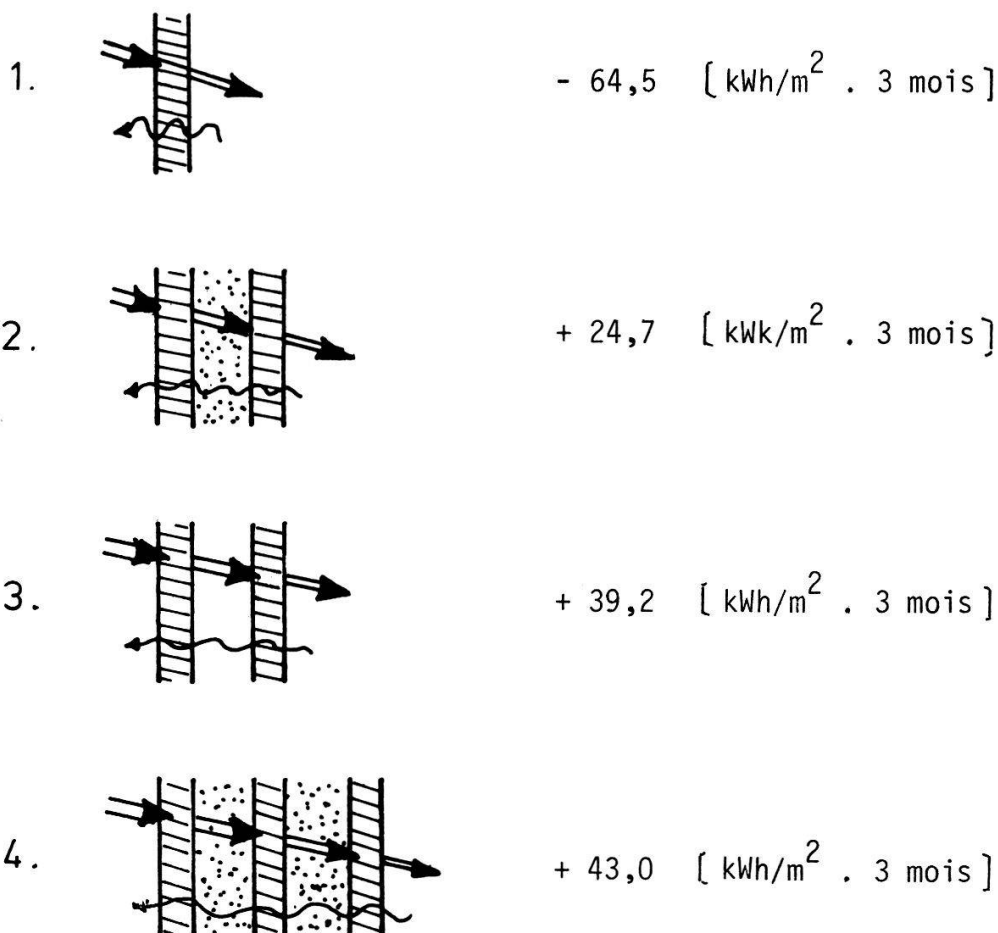


Figure 5

Une extrapolation sur un hiver nous permet de faire les estimations suivantes:

Modification	Gains sur un hiver (fenêtre orientée au Sud)
simple vitrage → double	180 [kWh/m ² an]*)
simple vitrage → double évacué	207 [kWh/m ² an]
double vitrage → triple	37 [kWh/m ² an]

*) Ces gains peuvent être comparés au chiffre de 65 [kWh/m²] qui est la quantité d'énergie nécessaire à la fabrication d'un m² de verre à vitre.

Ces calculs nous montrent qu'une politique d'économie d'énergie ne conduit par forcément à une diminution du confort: il n'est pas nécessaire de réduire la surface de vitrage, il suffit de choisir avec soin *son type et son orientation*.

La Fig. 6 nous donne finalement une vision plus pratique du phénomène: on y voit pour un type de vitrage assez particulier (triple vitrage avec un verre absorbant), la variation du k_{apparent} en fonction de l'ensoleillement journalier moyen en [kWh/m² · jour]. On notera que dès que l'énergie solaire journalière moyenne est supérieure à 2.3 [kWh/m² · jour], le k devient *négatif*, c'est à dire que les apports deviennent supérieurs aux pertes.

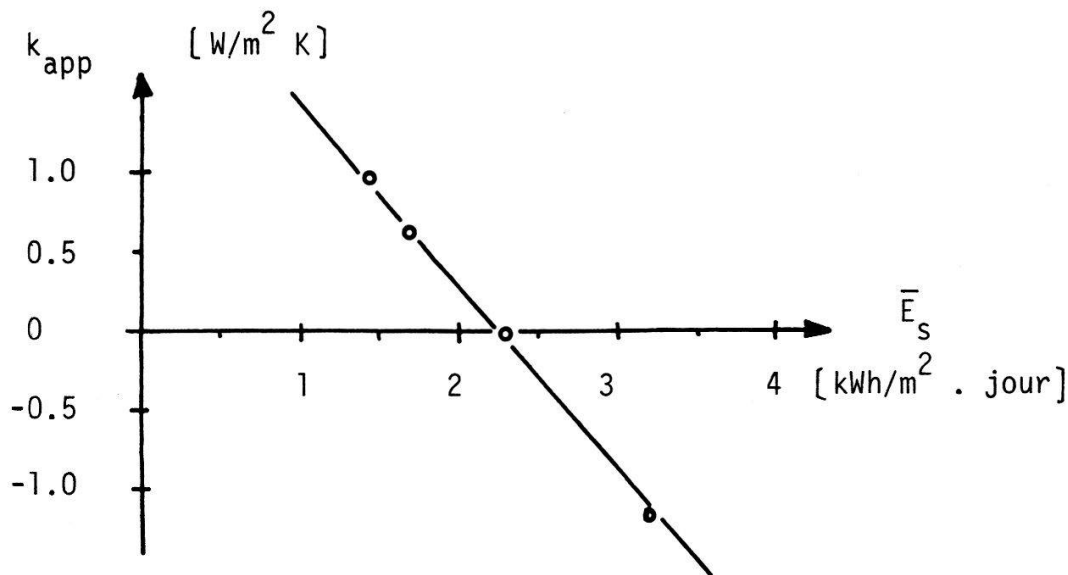


Figure 6

Pour conclure le paragraphe relatif aux vitrages, rappelons que les pertes par rayonnement, jouent un rôle important dans le comportement thermique des vitrages. Aussi, si l'on veut augmenter le rendement de notre 'capteur fenêtre', c'est dans ce sens qu'il faut agir, c'est dans ce sens également que nous allons diriger nos prochains travaux.

2. Apports solaires au travers d'un mur opaque

Passons au deuxième élément important dans les déperditions thermiques d'un bâtiment: il s'agit des pertes thermiques au travers des parties pleines de la construction. Des études dans cette direction ont été effectuées par Carrier il y a fort longtemps, alors que l'on ne parlait pas encore d'économie d'énergie.

En régime stationnaire, la résistance thermique d'un mur se calcule en faisant la somme des résistances thermiques des différents éléments qui le constituent:

$$R_{\text{tot}} = \sum R_j = \frac{1}{\alpha_{\text{ext}}} + \sum_{j=1}^n \frac{d_j}{\lambda_j} + \frac{1}{\alpha_{\text{int}}}$$

avec

$$\alpha_{\text{ext}} = 25 \text{ [W/m}^2 \text{ K]}$$

$$\alpha_{\text{int}} = 8 \text{ [W/m}^2 \text{ K]}$$

Considérons à titre d'exemple, un mur standard constitué de 17 cm de brique, de 6 cm de laine de verre et de 6 cm de brique intérieure.

On aura:

$$k_{\text{mur}} = \frac{1}{R_{\text{tot}}} = 0.54 \text{ [W/m}^2 \text{ K]}$$

Lorsque ce mur est exposé au rayonnement solaire, il en capte et en stocke une partie, ce qui provoque une variation de sa résistance thermique apparente.

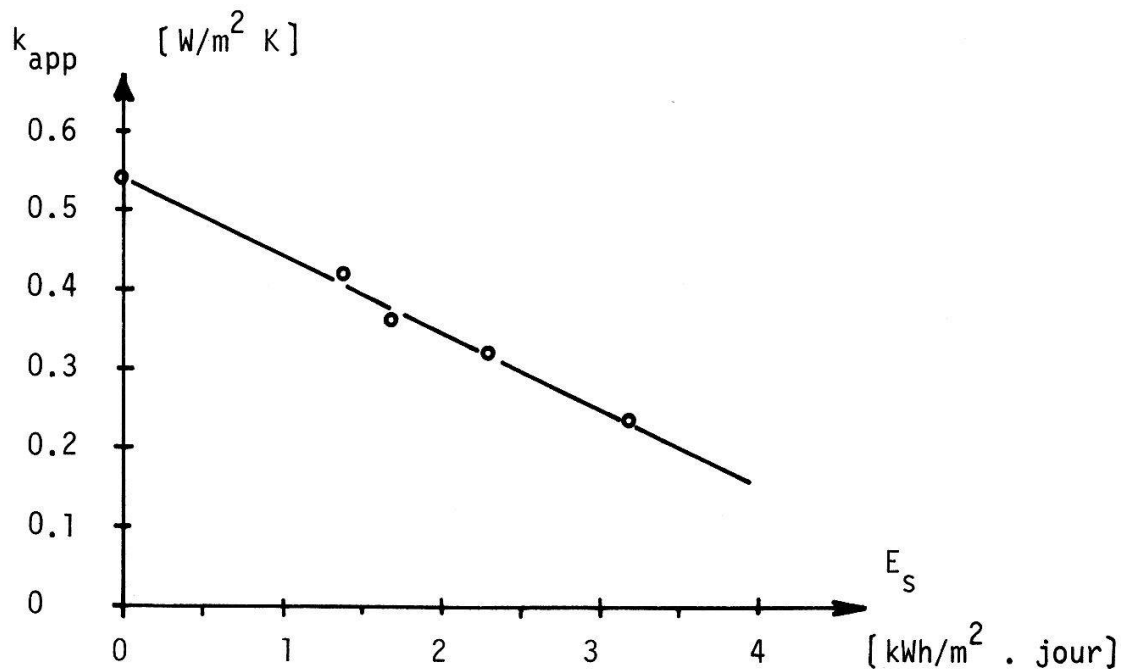


Figure 7

Etant donné l'amortissement et le déphasage provoqués par le mur, seul un modèle dynamique permet d'approcher le phénomène.

Durant l'hiver 1977-1978, des mesures ont porté sur le comportement thermique d'un mur standard tel que celui donné ci-dessus à titre d'exemple. Les mesures ont été effectuées de la manière suivante: une cellule soigneusement calorifugée a été accolée au mur test, une température de 20°C a été maintenue de manière constante à l'intérieur de la cellule. On a mesuré en permanence l'énergie nécessaire au maintien de cette température, la température en divers points du mur test, ainsi que les paramètres météorologiques extérieurs (ensoleillement, température extérieure, vitesse et direction du vent).

Un premier résultat intéressant de ces mesures est représenté sur la Fig. 7, celle-ci montre la variation de la résistance thermique apparente du mur en fonction de l'ensoleillement journalier moyen donné en [kWh/m² jour]. On notera que la résistance apparente d'un mur standard varie d'un facteur deux lorsque l'insolation journalière moyenne passe de 0 à 3 [kWh/m² jour].

Ces mesures effectuées sur un mur standard non optimisé du point de vue solaire montrent que mes mesures simples:

- (a) limitation des pertes (enveloppe transparente, couche avec faible coefficient d'émissivité dans l'infra-rouge, etc. . .)
- (b) modification du coefficient d'absorption dans le visible (couleur, etc. . .)
- (c) modification de la capacité thermique du mur (masse, position de l'isolation, etc. . .)

peuvent permettre de passer d'un mur qui perd de l'énergie à un mur qui en capte (dont le mur Trombe est un exemple).

En conclusion, une analyse plus détaillée de tous les constituants d'un bâtiment conduit tout naturellement à la réalisation de systèmes passifs de captage de l'énergie solaire. Dans de telles réalisations, ce n'est plus le système solaire qui est ajouté au bâtiment, mais c'est la construction elle-même qui devient un système de captage de l'énergie solaire.

Über den Energieverbrauch von Gebäuden durch Wärmestrahlung

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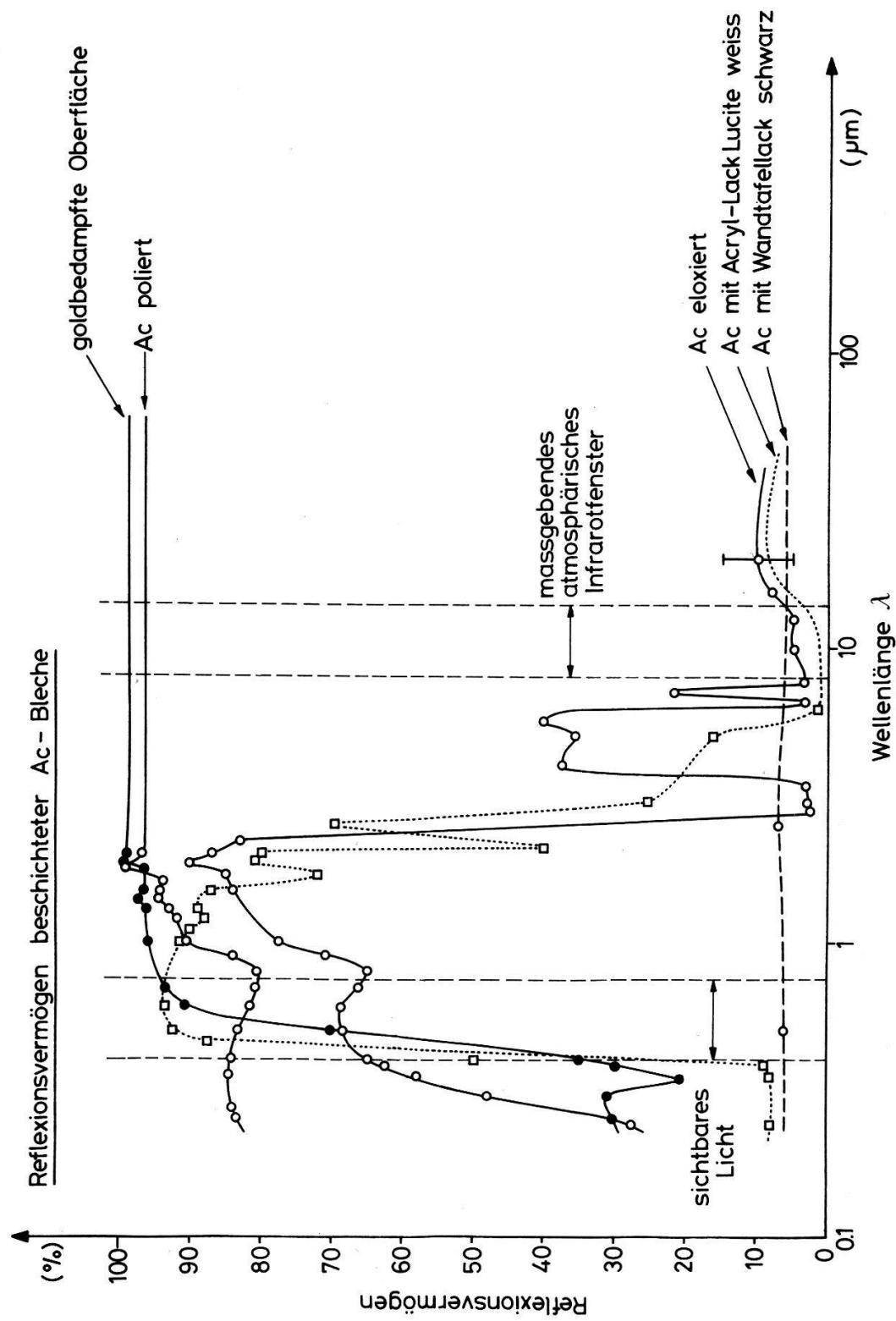
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Der Energiebedarf in der Schweiz auf Primärstufe in den Jahren 1974–1976 betrug durchschnittlich 24 GW. 1 GW entspricht 8765 GWh pro Jahr. Eine riesige Menge, wenn man bedenkt, dass ca. 80% dieser Energie importiert werden und nur ungefähr 12 GW, d.h.: rund die Hälfte auf Stufe Nutzenergie Anwendung findet: Licht, Chemie, mechanische Arbeit oder thermische Verwendung [1]. Die Schätzungen über die Entwicklung des Energiebedarfs gehen stark auseinander, trotzdem dürfen wir annehmen, dass die Schweizer Bevölkerung zu Beginn des 21. Jhdt. ca. doppelt soviel Energie verbrauchen wird wie heute. Daher müssen einerseits Alternativen Energien gesucht, andererseits muss alles unternommen werden, um Energieverluste zu verringern. Im Auftrag des Nationalen Forschungsprogramms Energie untersuchen wir den Einfluss der Wärmeabstrahlung auf den Energiehaushalt von Gebäuden.

Um Aussagen über mögliche Energieeinsparungen machen zu können, muss man sich zuvor aber Klarheit über die eingestrahlte Energie und deren Wirkung auf die Energiebilanz von Wärmetransportvorgängen an Gebäudeoberflächen verschaffen.

Figur 1 zeigt sowohl die *Sonneneinstrahlung* als auch die *atmosphärische Gegenstrahlung* auf eine horizontale Fläche auf Meereshöhe. Der spektrale Verlauf der auf der Erdoberfläche auftreffenden Sonnenstrahlung wird durch die Absorptionsbanden von O_3 , O_2 , H_2O und CO_2 charakterisiert. Die umhüllende Kurve (gestrichelt) entspricht der einfallenden Sonnenstrahlung inklusive Molekülstreuung, aber ohne Molekülabsorption. Vergleicht man die Wärmeabstrahlung einer 1 m^2 grossen, schwarzen Fläche auf Lufttemperatur (25°C) (rechte Seite, gestrichelt) mit der atmosphärischen thermischen Gegenstrahlung, so findet man zwischen $8\text{--}14\text{ }\mu\text{m}$ ein Loch, d.h.: einen Bereich, in dem die Atmosphäre nicht zurückstrahlt. Die von der Erde abgestrahlte Energie wird daher nur z.T. kompensiert. Ein Vergleich zwischen Sonneneinstrahlung und atm. Gegenstrahlung zeigt, dass die Flächen unter beiden Kurven gleich gross sind. Die eingestrahlte Energie von der Sonne und der Atmosphäre sind somit ungefähr gleich gross. Weiter ist zu bemerken, dass mit Solarzellen nur Energien aus dem Bereich der Sonneneinstrahlung ausgenutzt werden können. Mit einer IR-Verspiegelung hingegen lassen sich mit einfachen Mitteln auch Energien der gleichen Grössenordnung im Bereich der Infrarotabstrahlung einsparen, d.h. eine merkliche Verbesserung der Energiebilanz erzielen.

Wie seit langem bekannt, ist die Atmosphäre in gewissen IR-Spektralbereichen durchsichtig. Ein wichtiges derartiges *atmosphärisches Fenster* befindet sich bei $8\text{--}14\text{ }\mu\text{m}$, wie z.B. anhand von Berechnungen der Transmission mittels LOWTRAN-Programm [2] aufgezeigt wurde. Die Transparenz der gesamten Atmosphäre in diesem Fenster wird umso grösser, je mehr sich die Beobachtungsrichtung dem Zenith nähert. Dies hat zur Folge, dass die Aussenwandtemperatur für horizontale Flächen bei klaren Nächten stärker unter die Lufttemperatur sinkt als vertikale Wände [4].



Figur 2

Bei der Gebäudehülle spielen die Infraroteigenschaften der Baumaterialien eine wichtige Rolle. *Aluminium* als Fassadenmaterial der modernen Architektur nimmt sicher eine Vorrangstellung ein. Im Gegensatz zu der weitverbreiteten Meinung, hat eine Untersuchung des optischen Reflexionsvermögens gezeigt, dass die heute verwendeten Al-Bleche zwar im Sichtbaren gut reflektieren, im IR aber wegen der Schutzschichten praktisch schwarz sind. (Fig. 2). Reines Anticorodal (Ac) weist im Bereich des atm. Fensters eine Reflexion von ca. 95% auf, eloxiertes zeigt aber ausgerechnet zwischen 8–14 μm eine schwache Reflexion, was gleichbedeutend ist mit einem hohen Emissionsvermögen. Der Grund für das schlechte Reflexionsvermögen liegt in der Aluminiumoxidschicht, welche beim Eloxieren von Ac entsteht. Al_2O_3 absorbiert ab 6.5 μm praktisch vollständig.

Nicht nur Aluminium, sondern in zunehmendem Masse auch Glas spielt im modernen Fassadenbau eine wichtige Rolle. Ausgerechnet das *Fenster* aber ist zum grossen Teil verantwortlich für den Wärmefluss durch die Hauswand. Normales Fensterglas zeigt zwischen 8–14 μm eine niedrige Reflexion, hervorgerufen durch die starke Absorption von Glas in diesem Spektralbereich. Eine Verspiegelung der Glasoberfläche mit spektral selektiven Schichten wie $\text{TiO}_2/\text{Ag}/\text{TiO}_2$ oder $\text{SiO}_2/\text{Au}/\text{SiO}_2$ erhöht die Reflexion auf 85–90% ($\lambda > 3 \mu\text{m}$) je nach Zusammensetzung und Schichtdicke. Zusätzlich kann die Wärmedurchgangszahl (k -Wert) durch Innerverspiegelung eines Doppelglasfensters im Vergleich zu einer normalen Klarglas-Doppelscheibe etwa halbiert werden [3].

Zusammenfassend stellen wir fest, dass eine IR-Verspiegelung der Fassadenelemente sicher eine Verminderung der Energieverluste einbringt. Die mögliche Ersparnis für Gebäude im Mittelland dürfte ungefähr im Bereich von 5–15% des ursprünglichen Energieverbrauches liegen [4].

Die Autoren möchten den Herren W. Borer, A. Kunz und M. Rohr für die Konstruktion des Abtastgerätes und die Entwicklung elektronischer Steuergeräte, Herrn W. Herrmann für die Herstellung selektiver Schichten ihren besten Dank aussprechen. Diese Arbeit wurde im Rahmen des Nationalen Forschungsprogramms Energie des Schweizerischen Nationalfonds finanziert und von der GRD des EMD und der ETHZ mit unterstützt.

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Messung des Sonnenspektrums im fernen Infrarot

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Das Projekt, dessen Ziel die Absolutmessung der Sonnentemperatur im fernen Infrarot war, wurde im September 1978 mit einem Ballonflug abgeschlossen. Das beste bisher erzielte Resultat ist ein Wert von $4530 \pm 100/150 \text{ K}$ für das

Temperaturminimum der Strahlungstemperatur der Sonne [1]. Dieses entspricht einem Temperaturminimum von 4450 K in der Sonnenatmosphäre.

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MIS Solarzellen aus polykristallinem Silizium

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Kürzlich wurde entdeckt, dass die Einführung einer dünnen, isolierenden Schicht zwischen Metall und Halbleiter eines Schottky-Kontaktes die photovoltaische Effizienz wesentlich erhöhen kann. Damit ist die Schottky Diode, in Form eines MIS Überganges, zur Alternative zum $p-n$ Übergang der konventionellen Solarzelle geworden. Ein weiterer Faktor, der zur Verbilligung der Zellen für eine zukünftige terrestrische Anwendung führen kann, besteht in der Anwendung von polykristallinem Basismaterial.

Wir haben MIS Photovoltadioden aus ein- und polykristallinem p -Silizium mit Metallen verschiedener Austrittsarbeit präpariert und ausgemessen. Damit konnte untersucht werden, inwiefern Metalle niedriger Austrittsarbeit sich vorteilhaft auf den Wirkungsgrad auswirken.

Elektronenbeugung an aufgestäubten Tantalschichten

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Gesputterte Tantalschichten können in zwei verschiedenen Modifikationen wachsen: α -Ta besitzt die Struktur des massiven Tantals (bcc), β -Ta kommt hingegen nur in dünnen Schichten vor und wurde an Hand von Röntgendaten je nach Autor als tetragonale oder als hexagonale Struktur interpretiert. Wir haben die Struktur von Ta-Schichten, die als Ausgangsmaterial für Dünnschichtkondensatoren dienen, mit Elektronenbeugung untersucht. Die Schichten sind β -Ta, und die Beugungsbilder lassen sich eindeutig einer hexagonalen Struktur mit $\langle 100 \rangle$ -Textur zuordnen. Auf Au-Unterlagen gesputterte Ta-Schichten haben dagegen die Struktur von α -Ta mit einer $\langle 111 \rangle$ -Textur.

Constante de diffusion du bore dans le silicium épitaxial

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M. ROULET

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La diffusion d'impuretés dans des couches épitaxiales est souvent plus grande que dans des cristaux massifs. La constante de diffusion du bore a été mesurée entre 900°C et 1050°C dans des couches de silicium sur saphir (SOS) de 0.6 μm d'épaisseur implantées à 40 keV ($4 \cdot 10^{14} \text{ cm}^{-2}$ à $1.5 \cdot 10^{15} \text{ cm}^{-2}$). Des profils de B ont été obtenus par la mesure de la dose totale de B avec la réaction nucléaire $^{11}\text{B}(p, \alpha_1)^8\text{Be}$, suivie de l'ablation de couches successives. Nos résultats montrent une diffusion 1.1 à 2.4 fois plus rapide que dans du Si massif, même en considérant l'effet de concentration bien connu dans Si. Ceci est probablement lié aux défauts d'empilement dus au 'mismatch' à l'interface silicium-saphir.

Bremsstrahlung isochromat spectroscopy (BIS)

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BIS livre des informations proches de la densité des états inoccupés au-dessus du niveau de Fermi. Dans ce but un spectromètre XPS avec monochromateur (1486.6 eV) a été complété par une source d'électrons monochromatiques (canon de Pierce avec cathode imprégnée) et un détecteur de rayons X mous (photocathode en CsI et channeltron pour la détection des photoélectrons émis). La résolution déterminée sur la base d'un spectre du niveau de Fermi de Ag est meilleure que 0.43 eV. Le libre parcours moyen élastique des électrons pénétrant dans l'échantillon avec une énergie cinétique de l'ordre de 1500 eV est de 10 à 25 Å dans les métaux si bien que la surface doit rester absolument propre pendant la mesure. Un vide dans le domaine 10^{-12} Torr permet des temps d'intégration de 12 à 24 heures, ce qui est suffisant pour obtenir une bonne statistique. Les spectres des états 4f inoccupés sont en bon accord avec la théorie.

Optisches Pumpen des 1.315 μm Iodlasers mit einer Hg-Niederdrucklampe

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K. J. WITTE

(Projektgruppe für Laserforschung, Garching)

Wir haben mit einer Hg-Niederdrucklampe den 1.315 μm -Iodlaser optisch gepumpt. Die Lampe (Länge: 1.2 m, Hg-Druck: 0.1 torr, Durchmesser: 10 mm)

lieferte Pumplichtpulse von 25 msec Länge mit einer Energie von 3.1 J in der 253.7 nm Linie. Die Energie der Laserpulse betrug 100 mJ bei einer Dauer von 22 msec. Der erreichte Wirkungsgrad des Lasers war grösser als 1%. Dieser Wert ist auch im kontinuierlichen Betrieb oder bei hohen Repetitionsraten erreichbar.

Modelling and experiments on laser radiation absorption in laser generated plasma

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For Laser-Fusion research it is important that the laser radiation absorption properties of its self-generated plasma be well understood. This paper describes experiments and a numerical simulation code, ZWERG.

The experiments show that efficient absorption can be accomplished by utilising plasma wave resonance.

Most of the energy absorbed by this mechanism is thermalised and the rest is lost to non-thermal particles. The computer code, ZWERG, which models plasma wave resonance, is able to simulate the experimental results within the experimental errors.

Predictions are made for a range of laser parameters (intensity, wavelength and pulse duration).

Spurenanalyse in Gasen mit laserinduzierter Schlierentechnik

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Bei der Spurenanalyse in Gasen mit optischen Methoden hat sich die direkte Absorptionsspektroskopie aufgrund der beschränkten Empfindlichkeit als nur bedingt geeignet erwiesen. Günstiger ist es, die Erwärmung des Gases bei Absorption von Licht zu messen, wie dies indirekt beim Spektrophon geschieht.

Weitere Vorteile erzielt man, indem man die Aufheizung eines Gases aufgrund einer Absorption von Laserstrahlung durch den im Bereich des Strahlengangs veränderten Brechungsindex nachweist: Ein weiterer Lichtstrahl, der durch diese Zone läuft, erfährt dann eine Ablenkung.

Eine Anordnung, die dieser Effekt ausnutzt, wird beschrieben. Die experimentellen Ergebnisse werden mit denen anderer Techniken, insbesondere dem Spektrophon, verglichen. Als Vorteile ergeben sich eine hohe räumliche Auflösung und die absolute Kontaktfreiheit der Methode, die einen Einsatz in aggressiven Medien erlaubt.

Physique nucléaire et corpusculaire

Sur le caractère périphérique de la diffusion quasi-libre

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On montre que la diffusion quasi-libre (DQL) N-N dans la réaction de fracture du deuteron fait intervenir des moments relatifs (N-deuteron) grands; le modèle du 'sharp cut off' [1] modifié et adapté à cette réaction [2] la décrit de manière satisfaisante. Les mêmes calculs sont appliqués à la DQL α - α dans la réaction ${}^6\text{Li}(\alpha, \alpha\alpha)\text{d}$; les résultats sont discutés.

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Étude des pouvoirs d'analyse de la réaction ${}^{92}\text{Zr}(\vec{p}, \alpha){}^{89}\text{Y}$

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Abstract. On a mesuré les pouvoirs d'analyse conduisant aux quatre premiers niveaux de ${}^{89}\text{Y}$, lors de la réaction ${}^{92}\text{Zr}(\vec{p}, \alpha)$, à une énergie de 35 MeV. On a étudié la dépendance des pouvoirs d'analyse en fonction des paramètres du potentiel optique pour les voies d'entrée et de sortie. L'indépendance en J du facteur de forme est précisé. Les distributions angulaires des pouvoirs d'analyse sont bien reproduites par des calculs en DWBA utilisant un facteur de forme microscopique pour décrire le processus de transfert des trois nucléons.

Nous présentons dans ce rapport quelques résultats obtenus lors de l'étude du pouvoir d'analyse de la réaction $(\vec{p}, \alpha)$ sur le ${}^{92}\text{Zr}$. Le pouvoir d'analyse est défini par la relation

$$A_y = \frac{\sigma_+(\theta) - \sigma_-(\theta)}{P_{y-}\sigma_+(\theta) + P_{y+}\sigma_-(\theta)} \quad (1)$$

où $\sigma_-(\theta)$ et $\sigma_+(\theta)$ sont les sections efficaces de la réaction et P_{y-} et P_{y+} les polarisations du faisceau pour des protons de spins 'down' et 'up' respectivement.

Nous insisterons principalement sur la forte dépendance de ces grandeurs en fonction des paramètres du modèle optique et sur l'indépendance en J du facteur de forme. Lors d'une précédente étude [1, 2] les distributions angulaires des sections efficaces différentielles de cette réaction ont été reproduites d'une manière satisfaisante par des calculs effectués dans la théorie des ondes distordues

(DWBA) utilisant le formalisme microscopique développé par Falk [3]. Nous avons utilisé les mêmes paramètres pour les voies d'entrée et de sortie et pour les états liés des particules que lors de l'étude précédemment citée [1, 2].

Dans une publication antérieure [4] nous indiquons que les pouvoirs d'analyse sont dûs principalement – contrairement aux sections efficaces différentielles qui sont fortement influencées par le potentiel spin-orbite – aux termes du potentiel optique indépendants du spin. Ceci apparaît clairement sur la Fig. 1 où nous remarquons que les calculs effectués sans termes spin-orbite permettent de restituer dans les grandes lignes les pouvoirs d'analyse. Ce résultat est à rapprocher de ceux obtenus précédemment lors des réactions de transfert à un nucléon (d, p) par exemple. Toutefois nous pouvons préciser d'avantage l'origine de la structure des pouvoirs d'analyse. Pour ce faire nous avons réalisé des calculs sans termes d'absorption dans les voies d'entrée et de sortie. Nous présentons les résultats pour le niveau fondamental $J = \frac{1}{2}^-$ de ^{89}Y sur les Figs. 2 et 3 respectivement. Des résultats analogues seraient obtenus pour les niveaux excités. Nous constatons que lorsque nous posons $W_\alpha = 0$ les structures des distributions angulaires des sections efficaces différentielles et des pouvoirs d'analyse sont fondamentalement détériorés, l'effet étant plus marqué pour le pouvoir d'analyse. Par contre, lorsque similairement, nous posons l'absorption dans la voie d'entrée nulle les deux distributions angulaires quoique dégradées quant à l'amplitude conservent la phase des données expérimentales. Nous pouvons conclure que le terme d'absorption du potentiel optique dans la voie de sortie joue un rôle prépondérant dans la restitution des pouvoirs d'analyse. Cela donne du poids à un modèle classique comme celui de Newns [5] donnant à l'absorption le rôle principal pour l'obtention du pouvoir d'analyse. Satchler a montré [6] que lorsque le facteur de forme est presque indépendant de J et en absence d'interaction spin-orbite les pouvoirs d'analyse pour les niveaux $J = L + \frac{1}{2}$ et $L - \frac{1}{2}$ sont liés par la relation

$$A_y(J = L + \frac{1}{2}) = -\frac{L}{L+1} A_y(J = L - \frac{1}{2}) \quad (2)$$

avec L moment cinétique orbital transféré.

Cette relation est excellemment vérifiée pour les niveaux $\frac{1}{2}^-$ et $\frac{3}{2}^-$ de ^{89}Y comme ceci est présenté sur la Fig. 4. Dans ce cas le facteur de proportionnalité est égal à $\frac{1}{2}$.

La 'quasi-indépendance' en J du facteur de forme peut être mise en évidence simplement lorsque nous considérons l'expression de ce dernier fournie par la théorie microscopique de Falk [3].

$$F(R) = \sum_{p_1 p_2 p_3 N' n' N n}^{[n_1 l_1 j_1][n_2 l_2 j_2]} J_{AB}([n_1 = n, l_1 = l, j_1 = j][n_2 = n, l_2 = l, j_2 = j]; 000) \\ \times (2l_n + 1)^{1/2} a_{p_1} a_{p_2} a_{p_3} \begin{pmatrix} p_1 l_n 0 \\ p_2 l_n 0 \end{pmatrix} \mu, \mu \begin{pmatrix} N' 00 \\ n' 00 \end{pmatrix} \begin{pmatrix} N' 00 \\ p_3 l_3 0 \end{pmatrix} 2\mu, \mu \begin{pmatrix} N l_3 0 \\ n 00 \end{pmatrix} \\ \times I_{nn'} \left[\frac{H_{Nl_3}(3\nu R^2)}{R} \right] \quad (3)$$

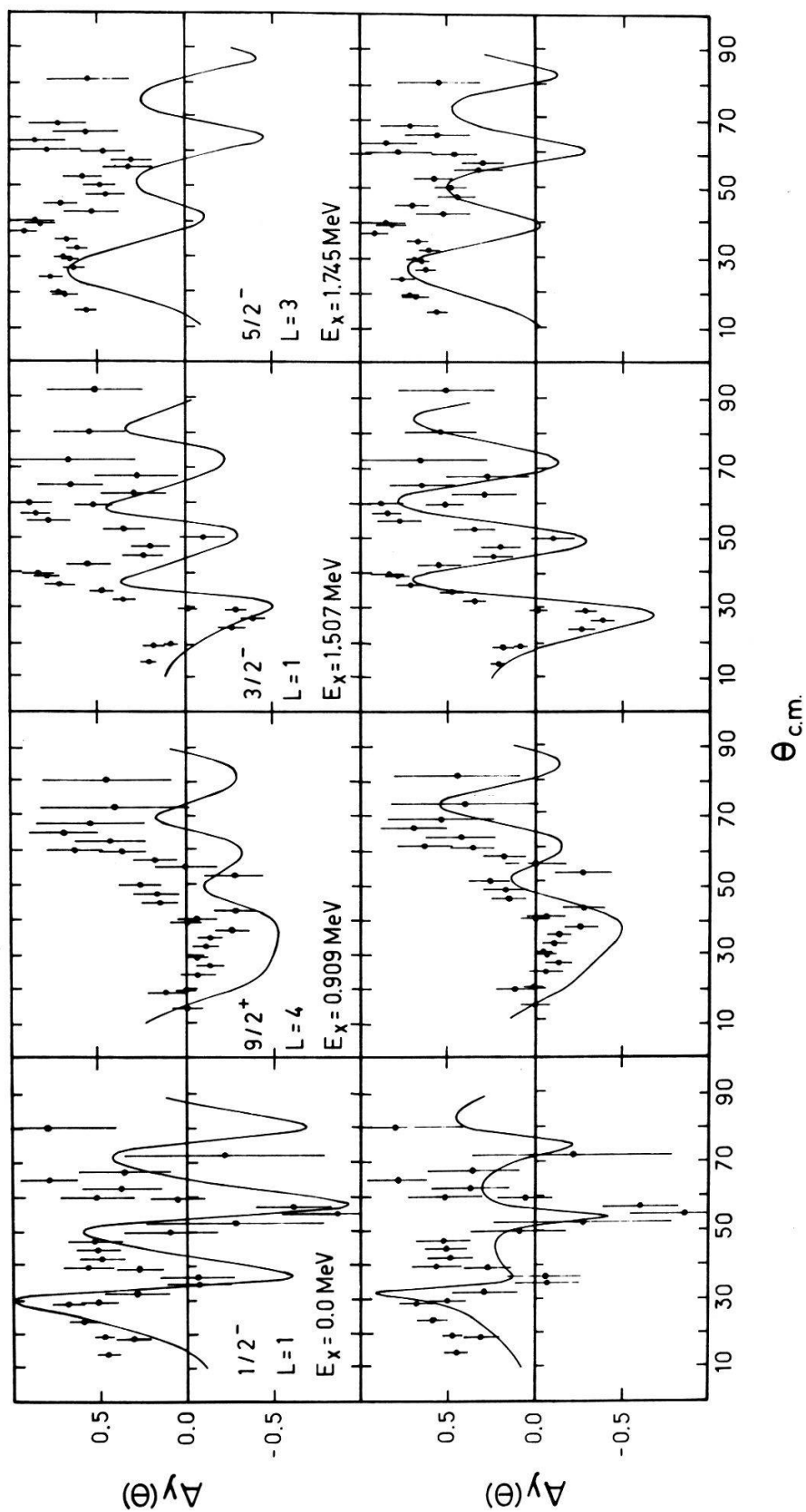


Figure 1

Distribution angulaire des pouvoirs d'analyse pour la réaction $^{92}\text{Zr}(\bar{p}, \alpha)^{89}\text{Y}$ à 35 MeV.

Les courbes sont les résultats de calculs dans la théorie DWBA microscopique sans interaction spin-orbite dans la voie d'entrée pour la partie supérieure, avec une interaction spin-orbite $V_{so} = 7$ MeV pour la partie inférieure.

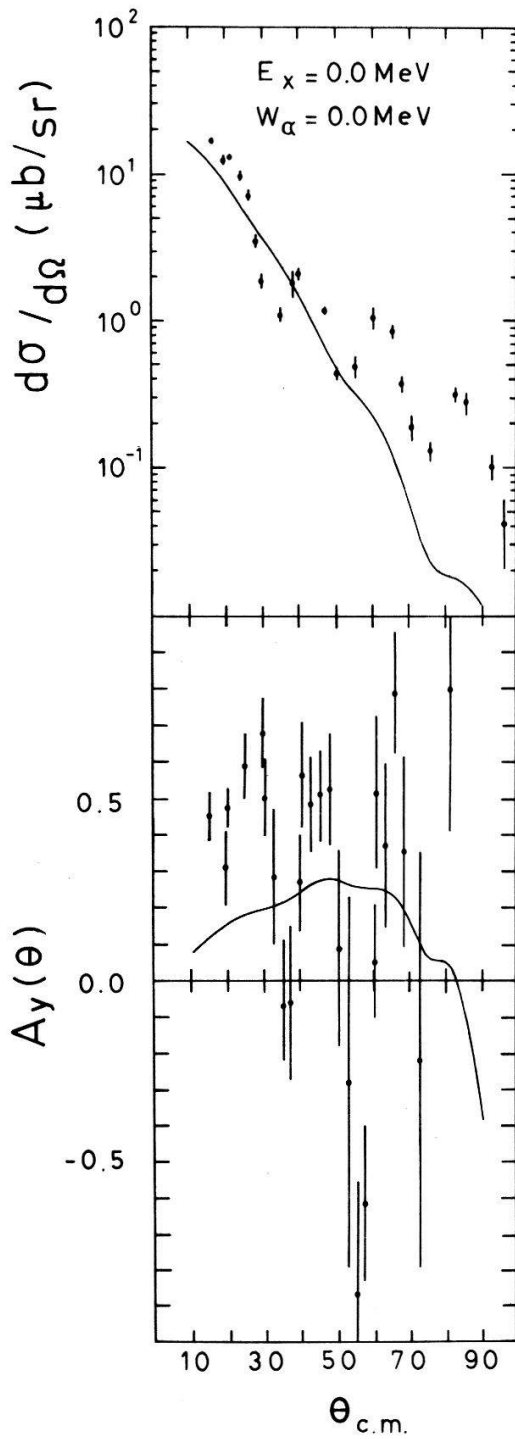


Figure 2

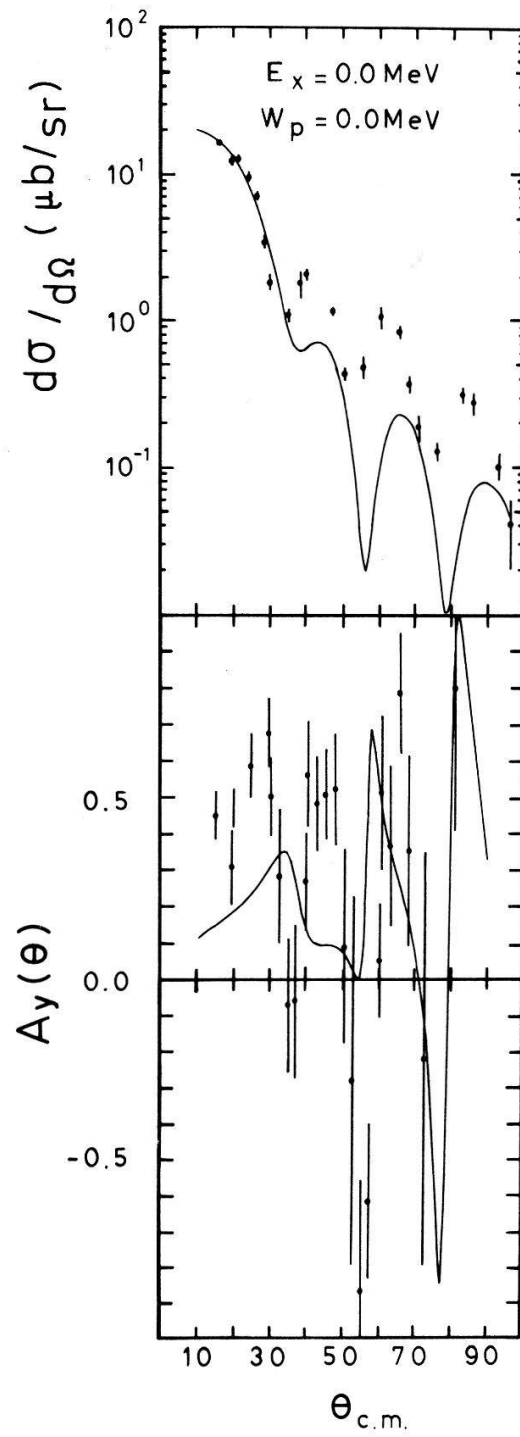


Figure 3

Figure 2

Influence du terme d'absorption du modèle optique dans la voie de sortie. Distributions angulaires du pouvoir d'analyse et de la section efficace différentielle de la réaction $^{92}\text{Zr}(\vec{p}, \alpha)^{89}\text{Y}$ à 35 MeV pour le niveau fondamental $\frac{1}{2}^-$ de ^{89}Y .

Figure 3

Influence du terme d'absorption du modèle optique dans la voie d'entrée. Distributions angulaires du pouvoir d'analyse et de la section efficace différentielle de la réaction $^{92}\text{Zr}(\vec{p}, \alpha)^{89}\text{Y}$ à 35 MeV pour le niveau fondamental $\frac{1}{2}^-$ de ^{89}Y .

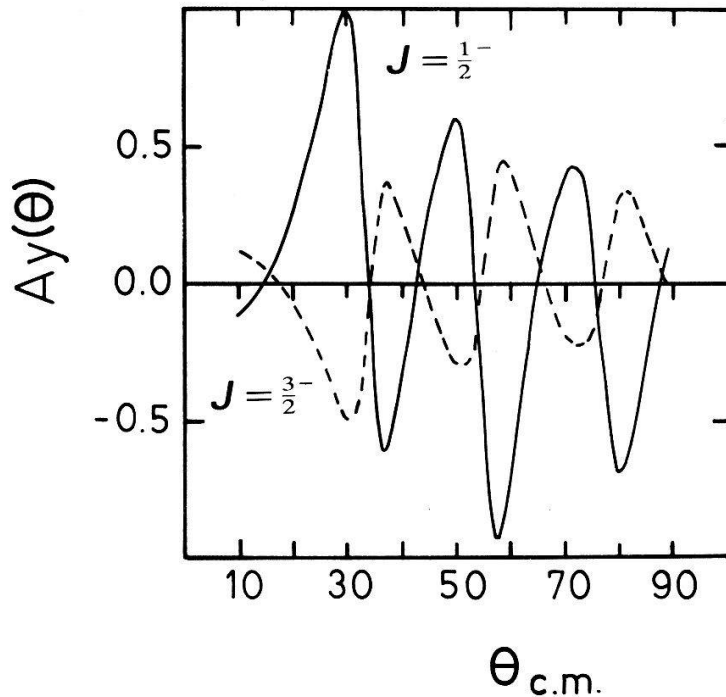


Figure 4

Distributions angulaires des pouvoirs d'analyse pour les transitions $L = 1$ de la réaction $^{92}\text{Zr}(\vec{p}, \alpha)^{89}\text{Y}$ à 35 MeV conduisant aux états finaux $\frac{1}{2}^-$ et $\frac{3}{2}^-$. Les courbes sont les résultats de calculs dans la théorie DWBA microscopique sans interaction spin-orbite pour le proton incident.

Les termes $\langle |\mu, \mu| \rangle$ et $\langle |2\mu, \mu| \rangle$ sont les coefficients de la transformation de Brody-Moshinsky permettant de séparer les coordonnées internes et relatives des nucléons transférés.

$I_{nn'}$ est une intégrale de recouvrement provenant de l'intégration sur les coordonnées internes.

$[n_1 l_1 j_1]$ et $[n_2 l_2 j_2]$ indiquent les configurations des neutrons transférés. Les différents indices de sommation sont liés par les lois de conservation de l'énergie

$$2p_1 + l_1 + 2p_2 + l_2 = 2N' + L' + 2n' + l'$$

$$2N' + L' + 2p_3 + l_3 = 2N + L + 2n + l$$

et du moment angulaire

$$\vec{l}_1 + \vec{l}_2 = \vec{L}' + \vec{l}'$$

$$\vec{L}' + \vec{l}_3 = \vec{L} + \vec{l}$$

Dans l'hypothèse où les moments cinétiques des deux neutrons transférés sont couplés à 0 le facteur spectroscopique J_{AB} se réduit au facteur spectroscopique du proton transféré, qui ne dépend que du moment cinétique de ce dernier l_3 , et les nombres quantiques principaux N sont les mêmes pour les niveaux $J = \frac{3}{2}$ et $J = \frac{1}{2}$. Les autres termes sont indépendants du moment cinétique total J à l'exception des coefficients a_p de développement des fonctions d'onde de Saxon-Woods sur les fonctions d'onde de l'oscillateur harmonique. Ceux-ci ne peuvent toutefois influencer que sur l'amplitude des oscillations du facteur de forme car le terme radial $H_{Nl_3}(2\nu R^2)/R$ est identique pour les deux états. De plus les différences entre ces coefficients [7] pour les configurations $\pi(2p_{3/2})$ et $\pi(2p_{1/2})$ sont si faibles que les deux facteurs de forme sont tout à fait semblables, Fig. 5.

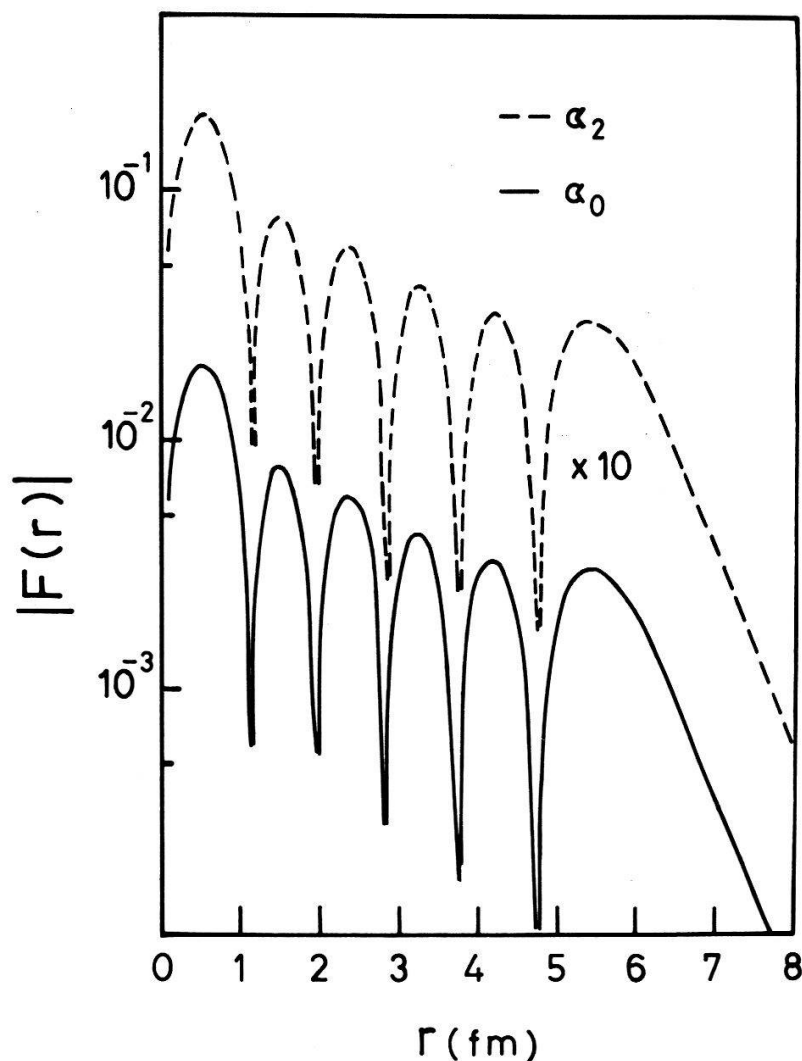


Figure 5

Comparaison des facteurs de forme calculés dans la théorie DWBA microscopique pour les transitions $L = 1$ de la réaction $^{92}\text{Zr}(\bar{p}, \alpha)^{89}\text{Y}$ à MeV conduisant aux états finaux $\frac{1}{2}^-(\alpha_0)$ et $\frac{3}{2}^-(\alpha_2)$ de ^{89}Y .

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Proton-induzierte Präequilibriums- α -Emission bei $E_p = 72$ MeVZ. LEWANDOWSKI,¹⁾ E. LÖFFLER und R. WAGNER

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Mit einem 72 MeV Protonenstrahl des SIN-Injektor-Zyklotrons werden α -Spektren aus der $^{27}\text{Al}(p, \alpha x)$ - und der $^{197}\text{Au}(p, \alpha x)$ -Reaktion bei verschiedenen Winkeln mit Hilfe von Si-Teleskopen gemessen. Die Analyse der winkelintegrierten Spektren erfolgt im Rahmen des Exziton-Modells. Die spektrale Verteilung und der Preformations-Faktor werden beim ^{197}Au mit $(\pi^-, \alpha x)$ -Daten verglichen.

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Cluster-Effekte in Transferreaktionen im ^9Be - ^{12}C System

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Die Struktur von ^9Be lässt erwarten, dass bei Reaktionen mit diesem Kern Cluster-Transferprozesse eine wichtige Rolle spielen. Ausführliche Untersuchungen wurden am $^9\text{Be} + ^{12}\text{C}$ -System durchgeführt. Es wurden u.a. die folgenden Ausgangskanäle beobachtet: Elastische Streuung und Reaktionen mit ^8Be und α -Teilchen als Reaktionsprodukte. Die Messungen wurden am Tandem-Beschleuniger der ETH Zürich durchgeführt. Für die theoretische Interpretation wurden Transferprozesse mittels des 'finite range DWBA'-Programmes MARS-SATURN [1] berechnet; der Compound-Anteil wurde nach der Hauser-Feshbach-Theorie auf Grund der Wirkungsquerschnitte für die Emission leichter Partikel berücksichtigt [2].

Bei der elastischen Streuung (Fig. 1) fällt der Wiederanstieg bei Rückwärtswinkeln auf, welcher weder durch die Streuung am optischen Potential noch durch Compoundprozesse erklärt werden kann. Dagegen liefert der Austausch eines ^3He -Clusters in diesem Winkelbereich einen Beitrag von der gewünschten Grösse.

Bei den untersuchten $(^9\text{Be}, ^8\text{Be})$ - und $(^9\text{Be}, \alpha)$ -Reaktionen ergab sich, dass jeweils zwei Reaktionsmechanismen mit Transfer von verschiedenen Clustern beteiligt sein müssen. Im Falle der $(^9\text{Be}, ^8\text{Be})$ -Reaktion (Fig. 2) ist bei Vorwärtswinkeln der Neutrontransfer, bei Rückwärtswinkeln der α -Transfer dominant. Bei der $(^9\text{Be}, \alpha)$ -Reaktion (Fig. 3) sind je nach Winkelbereich Prozesse mit ^5He - und ^8Be -Transfer vorherrschend. Die theoretische Erklärung ist jedoch

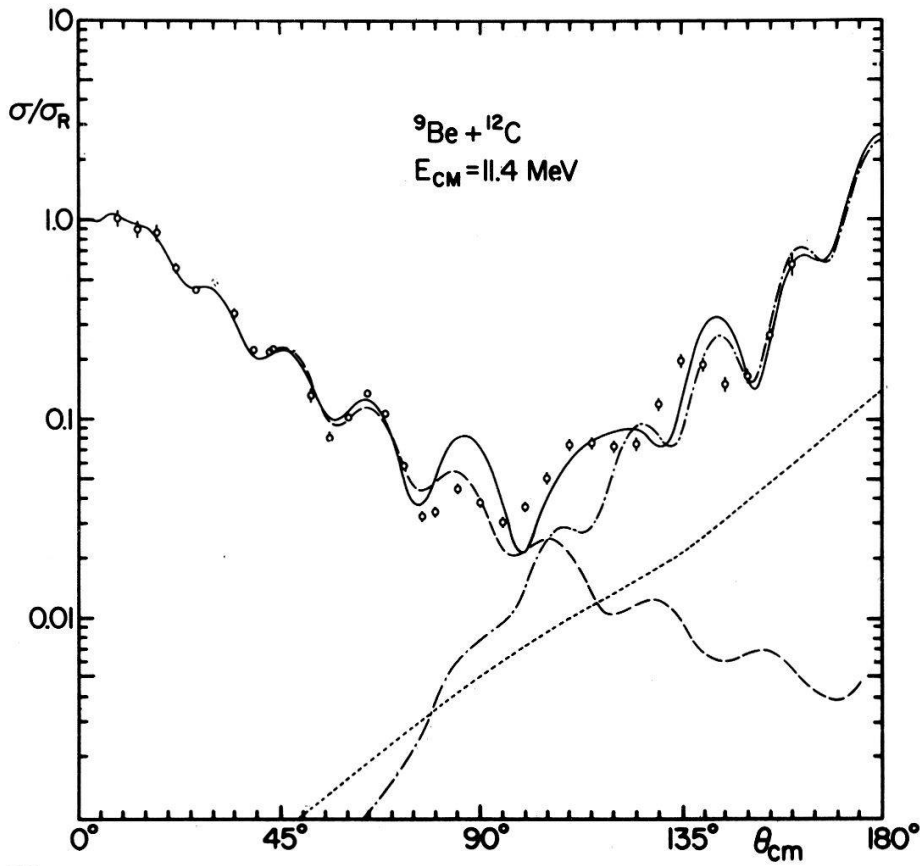


Figure 1

Winkelverteilung für die elastische Streuung von ${}^9\text{Be}$ an ${}^{12}\text{C}$ Kernen. Potential-Streuung: ---; Elastischer Transfer eines ${}^3\text{He}$ -Clusters: - · - · -; Compoundanteil: · · · · ·; Resultante aller drei Prozesses: ———.

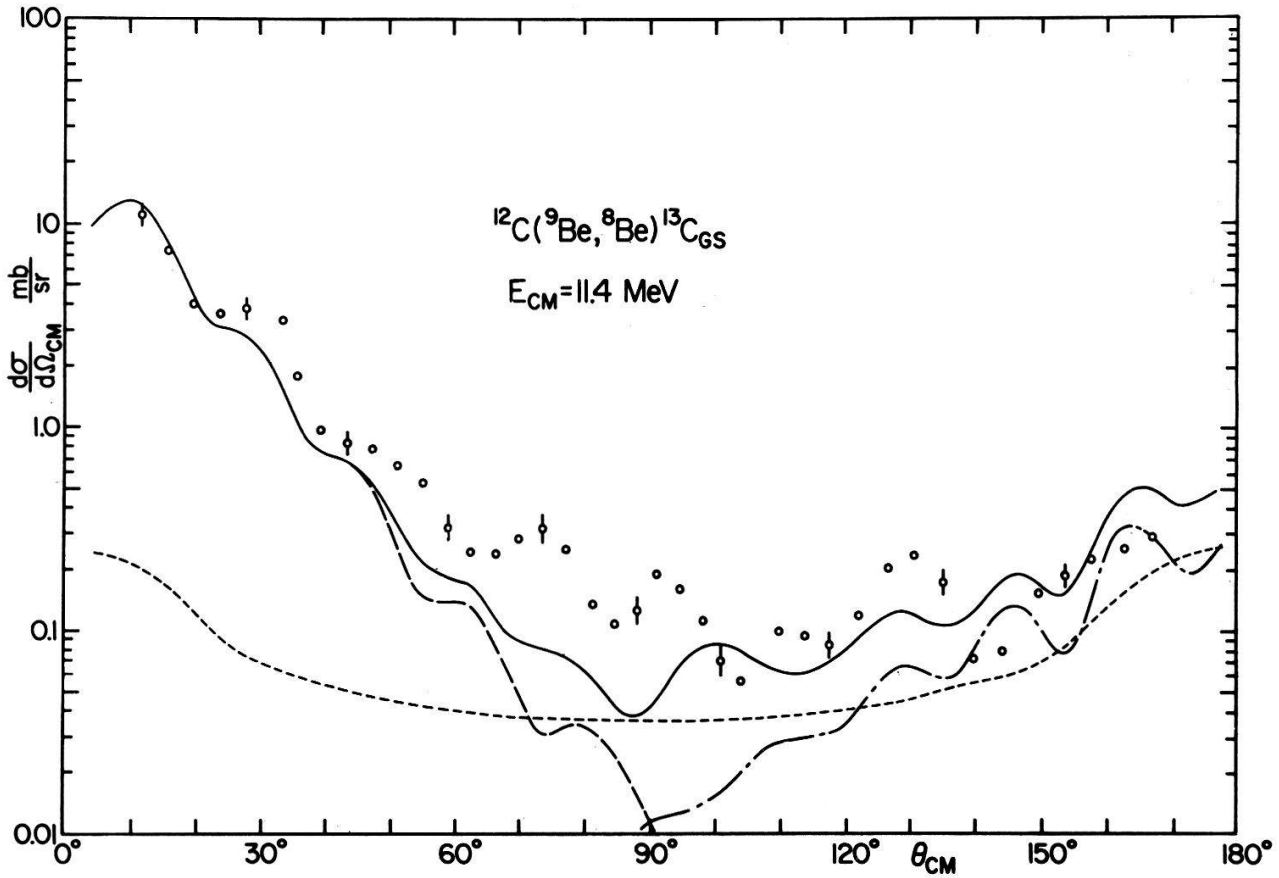


Figure 2

Winkelverteilung der Reaktion ${}^{12}\text{C}({}^9\text{Be}, {}^8\text{Be}){}^{13}\text{C}$. Neutronentransferanteil: ---; α -Transferanteil: - · - · -; Compoundanteil: · · · · ·; Resultante aller drei Prozesses: ———.

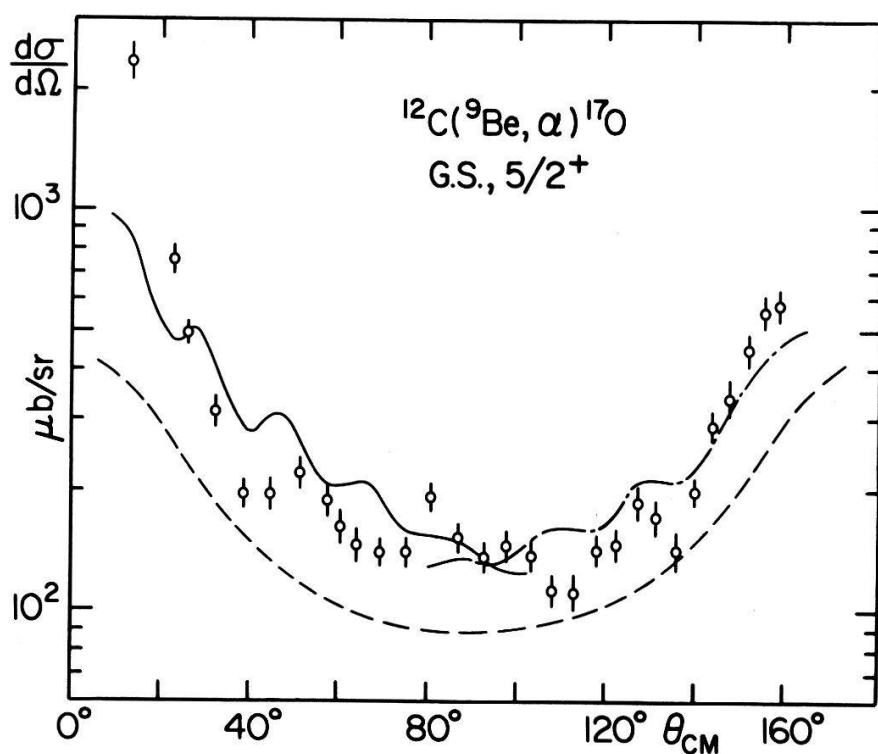


Figure 3

Winkelverteilung der Reaktion $^{12}\text{C}(^9\text{Be}, \alpha)^{17}\text{O}$. Compoundanteil: ---; Summe von Compound- und ^5He -Transferanteil: —; Summe von Compound- und ^8Be -Transferanteil: - · - · -.

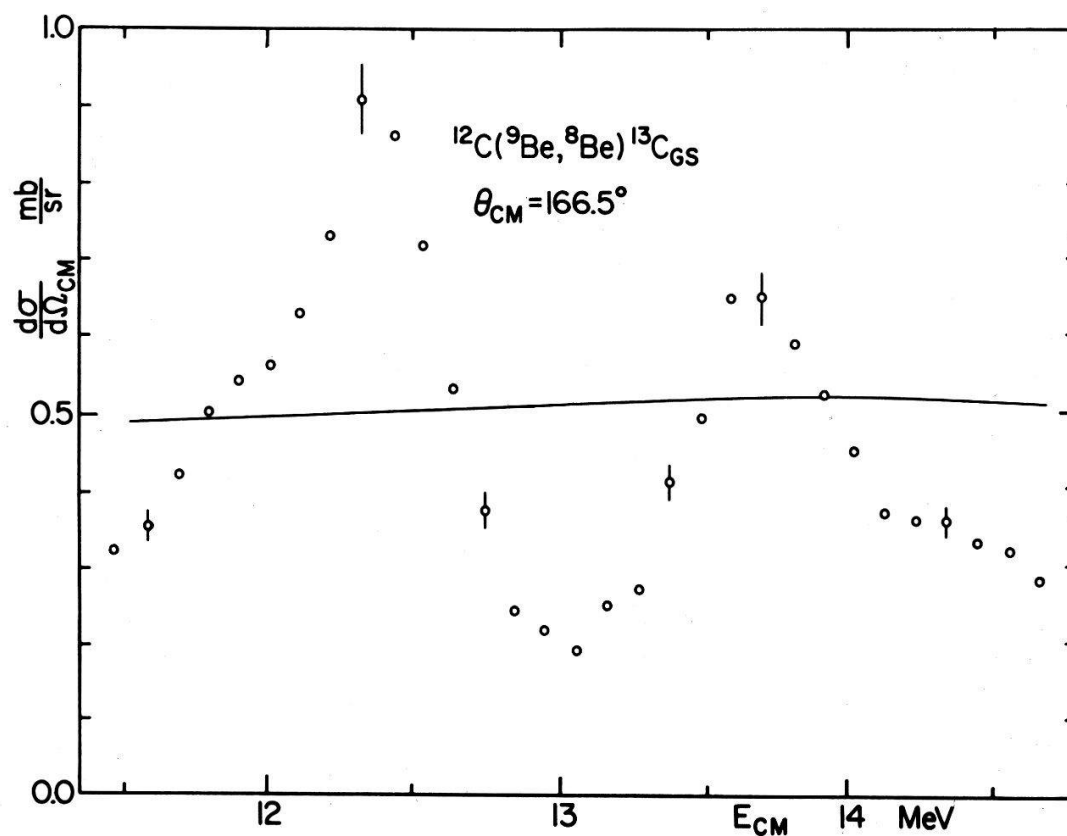


Figure 4

Die Energieabhängigkeit des $(^9\text{Be}, ^8\text{Be})$ -Prozesses an ^{12}C Kernen, Summe von α -Transfer- und Compoundanteil: —.

nicht voll befriedigend. Diese Feststellung wird noch unterstrichen, wenn man die Anregungskurven der (^9Be , ^8Be)-Reaktion betrachtet, welche bei verschiedenen Winkeln im Energiebereich zwischen $E_{cm} = 11.5$ und 14.5 MW aufgenommen wurden. Beim extremen Rückwärtswinkel $\theta_{cm} = 166.5^\circ$ zeigte sich eine stark ausgeprägte Struktur, welche durch einen einfachen α -Transfer nicht erklärt werden kann. Ob sie durch Interferenz des berücksichtigten Einstufenprozesses mit vernachlässigten Zweistufenprozessen oder Zwischenkernreaktionen zustande kommen kann, bleibt noch abzuklären.

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Theoretical comparison of the accuracy between direct and polarity correlation techniques for a projected Gauss–Markovian process

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The display variance of an on-line subcritical reactivity meter based on reactor neutron noise analysis in the time domain has been investigated theoretically. The device uses the so-called 'zero-crossing correlation method' and polarity correlation techniques. An algorithm is given which enables computation of the variance function of a polarity correlation function if the conditioned detector signal fluctuations are Gauss–Markovian. A comparison shows that the RMS display deviations due to the polarity correlation techniques (one-bit quantization) are about 25% larger than those expected from direct correlation techniques (multi-bit quantization). This is in good agreement with results obtained from experimental investigations.

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Kristallspektromettermessung des $3d^{5/2}-2p^{3/2}$ Überganges in myonischem Phosphor

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Das Verhältnis der Wellenlängen des $3d^{5/2}-2p^{3/2}$ -Röntgenüberganges in myonischem ^{31}P und der 84 keV Kerngammalinie von ^{170}Tm wurde zu

$$\lambda^{\text{P}}/\lambda^{\text{Tm}} = 0.957257(30)$$

bestimmt. Das Experiment am Myonenkanal des SIN, sowie die Bestimmung des theoretischen Wertes $\lambda_{\text{th}}^{\text{P}}$ des Röntgenüberganges sind durchgeführt worden wie in Ref. [1] beschrieben. Der Vergleich zwischen experimentellem und theoretischem Wert ergibt

$$(\lambda_{\text{exp}}^{\text{P}} - \lambda_{\text{th}}^{\text{P}}) / \lambda_{\text{th}}^{\text{P}} = (-16 \pm 31) \times 10^{-6}$$

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Stoboscopic measurements of the μ^+ magnetic moment; statistical analysis

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A determination of the positive muon magnetic moment (in units of the magnetic moment of the proton, i.e. μ_{μ}/μ_p), completed recently at SIN, has yielded in a first analysis the ratio μ_{μ}/μ_p with the best precision currently available of ± 0.9 ppm [1]. The experiment has been performed by stopping muons in a liquid target and observing their Larmor precession frequency in an externally applied magnetic field. For that purpose a stroboscopic method has specially been developed. In this paper we focus on that method, the data reduction and the statistical evaluation procedures applied for the μ_{μ}/μ_p determination. The last result is presented.

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$\mu^- \rightarrow e^+$ -Konversion an Schwefel

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Am SIN wurde mit gestoppten Müonen nach Positronen aus der Reaktion $\mu^- + {}^{32}\text{S} \rightarrow e^+ + {}^{32}\text{Si}^*$ gesucht. Dabei wurde eine neue Grenze für das Verzweungsverhältnis der $\mu^- \rightarrow e^+$ -Konversion am Atomkern, bezüglich des normalen Müon-Einfangs, gefunden. Nach Konopinski-Mahmoud ist diese Umwandlung erlaubt, im gewöhnlichen additiven Leptonschema jedoch verboten. Der Prozess bietet deshalb die Möglichkeit zur Unterscheidung zwischen den beiden bisher als äquivalent betrachteten Leptonschemata, falls ein Mechanismus für den doppelten Ladungsaustausch zwischen Leptonen und Hadronen im Kern existiert.

Myon-Strahlungseinfang in ^{16}O

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Der von der Emission eines hochenergetischen Photons ($E_\gamma > m_\mu/2$) begleitete Einfang eines Myons wurde zum ersten Mal in einem leichten Kern beobachtet. Ca. 1200 Ereignisse der Reaktion $^{16}\text{O}(\mu^-, \nu_\mu \gamma)^{16}\text{N}$ wurden mit einem hochauflösenden Paarspektrometer registriert. Die Messungen wurden am SIN im μ^- -Strahl mit Wasser- und schweren Wassertargets durchgeführt. Die Reduktion der Daten, die Elimination des Pion induzierten Untergrundes sowie eine erste Analyse des Spektrums werden diskutiert.

Pion-calcium scattering

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π^+ and π^- elastic scattering off ^{40}Ca and ^{48}Ca was measured at three energies around the πN (3, 3) resonance: 130, 180 and 230 MeV. One of the primary hopes of this experiment is to gather information on the neutron distribution near the surface of the nucleus, because in the (3, 3) resonance region the elastic scattering of a π^+ from a proton is much stronger than from a neutron (and vice-versa for π^-). The results will be presented and discussed.

Production d'un pion et double échange de charge sur ^4He à 1.7 GeV/c

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Nous avons étudié les réactions $\pi^+{}^4\text{He} \rightarrow \pi^+\pi^-3pn$ (3.07 ± 0.22 mb), $\pi^+{}^4\text{He} \rightarrow \pi^+\pi^-2pd$ (1.22 ± 0.16 mb) et $\pi^+{}^4\text{He} \rightarrow \pi^-4p$ (0.25 ± 0.05 mb) produites dans une chambre à bulles à hélium.

La production d'un pion est caractérisée par une forte interaction dans l'état final et une très faible présence de la résonance ρ^0 , contrairement au même processus observé sur un nucléon libre.

Nous proposons un modèle classique pour le double échange de charge: production d'un π^- et absorption du π^+ sur une paire $p-n$. Ce modèle reproduit correctement la section efficace et les spectres différentiels. Il explique d'autre part la faible présence de protons spectateurs dans cette réaction.

D , R , A and P for small angle pp elastic scattering at 312, 392, 493 and 575 MeV

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The Wolfenstein parameters D , R , A and the polarization parameter P have been measured for elastic p - p scattering in the Coulomb-nuclear interference region between $\approx 3_{cm}^0$ and 33_{cm}^0 . The experiment was performed at SIN using the accelerated polarized proton beam when available (i.e. at 575 MeV only with $P_B = 63\%$) and a polarized beam obtained through scattering at 8° on a thin Be target at other times (i.e. at 312, 392 and 493 MeV with $P_B = 41.63\%$). The statistical errors are typically $\approx \pm 0.08$ on D , R and A and < 0.02 on P . A good agreement with phase shift predictions is found.

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Measurement of the A_{00NN} parameter for elastic p - p scattering between 400 and 600 MeV

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Results for the spin-spin correlation parameter A_{00NN} for elastic p - p scattering at CMS angles between 30° and 90° are presented. Measurements using the SIN polarized proton beam and a polarized butanol target were made at 8 different energies uniformly covering the region between 400 and 600 MeV. The p - p events were detected by two MWPC telescopes and were reconstructed using a novel on-line reconstruction technique. This new method enabled a relatively quick and simple data analysis.

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Dépendance en énergie de la production de K^* par échange de parité naturelle dans la réaction $K^\pm p \rightarrow K^0 \pi^\pm p$

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(Universités de Genève et Lausanne)

Nous présentons une analyse préliminaire des amplitudes d'échange de parité naturelle dans la voie t pour la production du $K^*(890)$ et du $K^*(1420)$ à 50 GeV/c.

La dépendance en t de la section efficace d'échange de parité naturelle à 10 GeV/c (déterminée par notre groupe lors d'une expérience précédente au PS du CERN) a été paramétrisée par un simple modèle de Regge. Nous comparons ici l'extrapolation de ce modèle à 50 GeV/c aux données acquises à cette énergie.

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Étude de la réaction $\pi^\pm \rightarrow K^0 K^\pm p$ à 50 GeV/c

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Le spectromètre des universités de Genève et Lausanne est actuellement en opération dans un faisceau hadronique du SPS au CERN.

Nous présentons des résultats préliminaires de l'analyse de la réaction $\pi^\pm p \rightarrow K^0 K^\pm p$ à 50 GeV/c: les moments de la distribution angulaire du système $K^0 K^\pm$ ont été calculés en fonction du transfert d'impulsion et de la masse effective $K^0 K^\pm$, confirmant l'existence du $A_2(1950)$ de $J^P = 4^+$, $I^G = 1^-$.

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Invariance des interactions fortes sous l'isoparité-G

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Les principes de symétries des interactions fortes conduisent à des prédictions qui peuvent faire l'objet, dans certains cas, de tests quantitatifs. Ainsi, la conservation de l'isospin I et celle de la conjugaison de charge C ont été testées aux

basses et aux hautes énergies. Par contre, la conservation de l'isoparité G (où $G = C \exp i\pi I_1$) n'a que peu de support expérimental, particulièrement aux hautes énergies. Les annihilations pioniques $\bar{p}n$ se prêtent à ce genre de mesure quantitative; nous avons utilisé dans ce but les réactions $\bar{p}n \rightarrow k\pi$ ($5 \leq k \leq 8$) engendrées dans le deutérium par des antiprotons de 4.3 et 5.3 GeV/c.

Study of nuclear structure by means of the (p, α) -reaction in the Fe-region

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Abstract. Measurements of the $^{55}\text{Mn}(p, \alpha)^{52}\text{Cr}$, $^{56}\text{Fe}(p, \alpha)^{53}\text{Mn}$ and $^{54}\text{Fe}(p, \alpha)^{51}\text{Mn}$ reactions at $E_p = 35$ MeV have been carried out. A microscopic analysis of the three particle pickup process leading to low-lying states in the final nuclei points to seniority forbidden transitions. However, the transition strength indicate contributions of two step processes in the reaction mechanism.

1. Introduction

In the last years several publications [1, 2, 3] have shown that the microscopic description of (p, α) -reactions provides information on shell model wave functions. Although it is not possible to deduce exact wave functions it is possible to test not only the amplitudes but also the relative signs of the components of different configurations by means of the coherence properties of the (p, α) -reaction [4].

The aim of this work is to apply the microscopic model for (p, α) -reactions performed on such target nuclei for which shell model calculations have been carried out and wave functions are available. We have studied the reactions $^{56}\text{Fe}(p, \alpha)^{53}\text{Mn}$, $^{54}\text{Fe}(p, \alpha)^{51}\text{Mn}$ and $^{55}\text{Mn}(p, \alpha)^{52}\text{Cr}$ induced by 35 MeV protons. The nuclei investigated in these measurements have shell structures characterized by nearly closed $1f_{7/2}$ proton or neutron shells. The first and third of these reactions produce residual nuclei with $N = 28$ whereas the second reaction starts from a nucleus with a filled $1f_{7/2}$ neutron shell.

2. Experiment and analysis

The experiments were performed with the SIN injector cyclotron using an energy-analysed proton beam of 12 keV resolution at an energy of 35 MeV. This

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²⁾ Work supported by the Swiss National Science Foundation.

Table I
Optical and bound-state potential parameters (Saxon-Woods type)

Reaction	V_0 (MeV)	r_0 (fm)	a_0 (fm)	W (MeV)	r_i (fm)	a_i (fm)	V_{s0} (MeV)	r_{s0} (fm)	a_{s0} (fm)	r_c (fm)	β (fm)
(p, p)	43.6	1.250	0.60	3.13 17.96*)	1.375 1.375*)	0.593 0.593*)	8.80	0.957	0.672	1.17	
(α , α)	198.4	1.427	0.53	29.0	1.427	0.530				1.40	
Bound-state (non-local)											
p	73.14	1.245	0.520				13.0	1.245	0.520	1.334	-0.88
n	64.54	1.274	0.519				13.0	1.274	0.519		-0.88

*) surface absorption: derivative of Saxon-Woods form factor.

energy was chosen to keep compound nucleus contributions as low as possible and to guarantee measurable cross sections. Self-supporting targets with a thickness between 200 and 250 $\mu\text{g}/\text{cm}^2$ were used. The Fe-targets consisted of 99.9% ^{56}Fe and of about 96% ^{54}Fe , respectively.

For a quantitative analysis of the present results DWBA calculations were carried out using the code DWUCK [5] in the zero range approximation. The spectroscopic amplitudes have been calculated by the methods of Glendenning [6] and Towner and Hardy [7]. More details regarding the description of the microscopic form factor can be found in Refs. 1 and 3.

For the proton and alpha optical potential we used the same parameter sets for all three reactions. For the proton potential we used a new universal proton optical potential fitted on a large number of nuclei at various energies [8]. For the alpha optical potential we generated three equivalent potentials with well depths of 108, 153 and 198 MeV starting from alpha elastic scattering data at 41.96 MeV on ^{52}Cr of Ref. 9. In the analysis the deepest alpha potential proved to fit the (p, α)-data best. The parameters for the proton and neutron bound state potential were taken from an investigation in which an universal single particle potential for spherical nuclei is generated fitting not only the measured charge distributions but also reproducing the separation energies for the last nucleons [10]. The bound state and optical model parameters finally used are listed in Table I.

The wave functions for the ^{56}Fe - and ^{55}Mn -ground state have been calculated by K. Ogawa [11]. In order to make the analysis tractable we have taken into account only the main components of these extended shell model wave functions which are tabulated in Table II. For the ^{54}Fe ground state and for the ground and

Table II
Main components of the ^{56}Fe - and ^{55}Mn - and ^{54}Fe -wave function

$ ^{55}\text{Mn}\rangle_{5/2^-} = \pi[(1f_{7/2})^5 v = 1]_{7/2} \otimes \nu[-0.32787(2p_{1/2})(2p_{3/2})_2 - 0.19947(2p_{1/2})(1f_{5/2})_2 - 0.30252(2p_{3/2})_2^2]$ $+ \pi[(1f_{7/2})^5 v = 3]_{5/2} \otimes \nu[-0.30833(2p_{1/2})(2p_{3/2})_2 - 0.18434(2p_{1/2})(1f_{5/2})_2 - 0.26577(2p_{3/2})_2^2]$ $+ \pi[(1f_{7/2})^5 v = 3]_{5/2} \otimes \nu[+0.27476(2p_{1/2})_0^2 + 0.56428(2p_{3/2})_0^2 + 0.24067(1f_{5/2})_0^2]$
$ ^{56}\text{Fe}\rangle_{0^+} = \pi[(1f_{7/2})^6 v = 0]_0 \otimes \nu[+0.32092(2p_{1/2})_0^2 + 0.69275(2p_{3/2})_0^2 + 0.33585(1f_{5/2})_0^2]$ $+ \pi[(1f_{7/2})^6 v = 2]_2 \otimes \nu[-0.33240(2p_{1/2})(2p_{3/2})_2 - 0.23477(2p_{1/2})(1f_{5/2})_2 - 0.30294(2p_{3/2})_2^2]$
$ ^{54}\text{Fe}\rangle_{0^+} = \pi[(1f_{7/2})^6 v = 0]_0 \otimes \nu[+1.0(1f_{7/2})_0^8]$

low-lying states in the final nuclei ^{53}Mn , ^{52}Cr and ^{51}Mn we used the wave functions calculated by W. Kutschera et al. [12]. The amplitudes of these wave functions are consistent with those deduced by J. D. McCullen et al. [13] in an analogous shell model calculation for $1f_{7/2}$ -shell nuclei.

3. Results and discussion

In Figs. 1, 2 and 3 the angular distributions for the transitions leading to the ground and lowest excited states in the final nuclei ^{53}Mn , ^{52}Cr and ^{51}Mn are shown. It is generally observed that the fits obtained with the microscopic model are satisfactory. On the other hand the large differences in the transition strength between the ground and first excited state for each reaction shown in these figures is striking. This can be understood according to Sherr [14] because the (p, α) -reaction can alter the seniority in the proton configuration only by one unit. Therefore the transitions leading to one unpaired proton (seniority 1) in the $1f_{7/2}$ -shell in the final nucleus (the reversed case is $^{55}\text{Mn}(p, \alpha)^{52}\text{Cr}$) with a j -transfer of $7/2$ are strongest. In all cases where the final state is a $5/2^-$ -state (in $^{55}\text{Mn}(p, \alpha)^{52}\text{Cr}$ the initial state) three unpaired protons having seniority three are required to form these states. The (p, α) -reaction can reach such states only through proton configurations having seniority two and in these cases low transition strengths are to be expected. The same behaviour shows up in one proton-pick up reactions, e.g. $^{54}\text{Fe}(d, ^3\text{He})^{53}\text{Mn}$ measured by E. Newman and J. C. Hiebert [15] or by G. Mairle et al. [16]. Analogous cases are the weak transitions to the $3/2^-$ -state in ^{53}Mn and ^{51}Mn and the transition to the $9/2^-$ -state in ^{51}Mn .

We relate the experimental to the theoretical cross section as follows:

$$(d\sigma/d\Omega)_{\text{exp}} = \varepsilon (d\sigma/d\Omega)_{\text{DWBA}}.$$

The zero range approximation which is used in our calculation introduces a normalizing factor. It is chosen in such a way that the enhancement factor ε is unity for the strongest observed transition $J^\pi = 7/2^-$ in each individual reaction. The enhancement factors ε for the other transitions will then be a measure of how well the experimental data are described by the theory. A value of $\varepsilon = 1$ would indicate a perfect description.

In Table III the enhancement factors ε for the considered transitions are shown. Although in our analysis we are using extended shell model wave functions including components having seniority quantum number up to $v = 3$ in the proton configurations it is surprising that the enhancement factors ε deviate significantly from unity in all transitions considered. Such a disagreement of the DWBA-theory using the microscopic formalism is contrary to our previous experience (Refs. 2, 3, 4). However, it may be possible to explain this discrepancy by either incomplete wave functions and/or an inadequate description of the reaction mechanism. In the first case core-excitations of the $1f_{7/2}$ -shell, where the protons are distributed over the $1f_{5/2}$ - or $2p_{3/2}$ -shell may contribute to the $J^\pi = 5/2^-$ and $3/2^-$ transitions. Some indications in this direction are also given in Refs. 14, 15, 16, 17. In the second case, since the one-step three-nucleon pick up process gives cross sections which do not agree with the experiment, coherent contributions of the two step mechanism, e.g. (p, p') (p', α) , may be important.

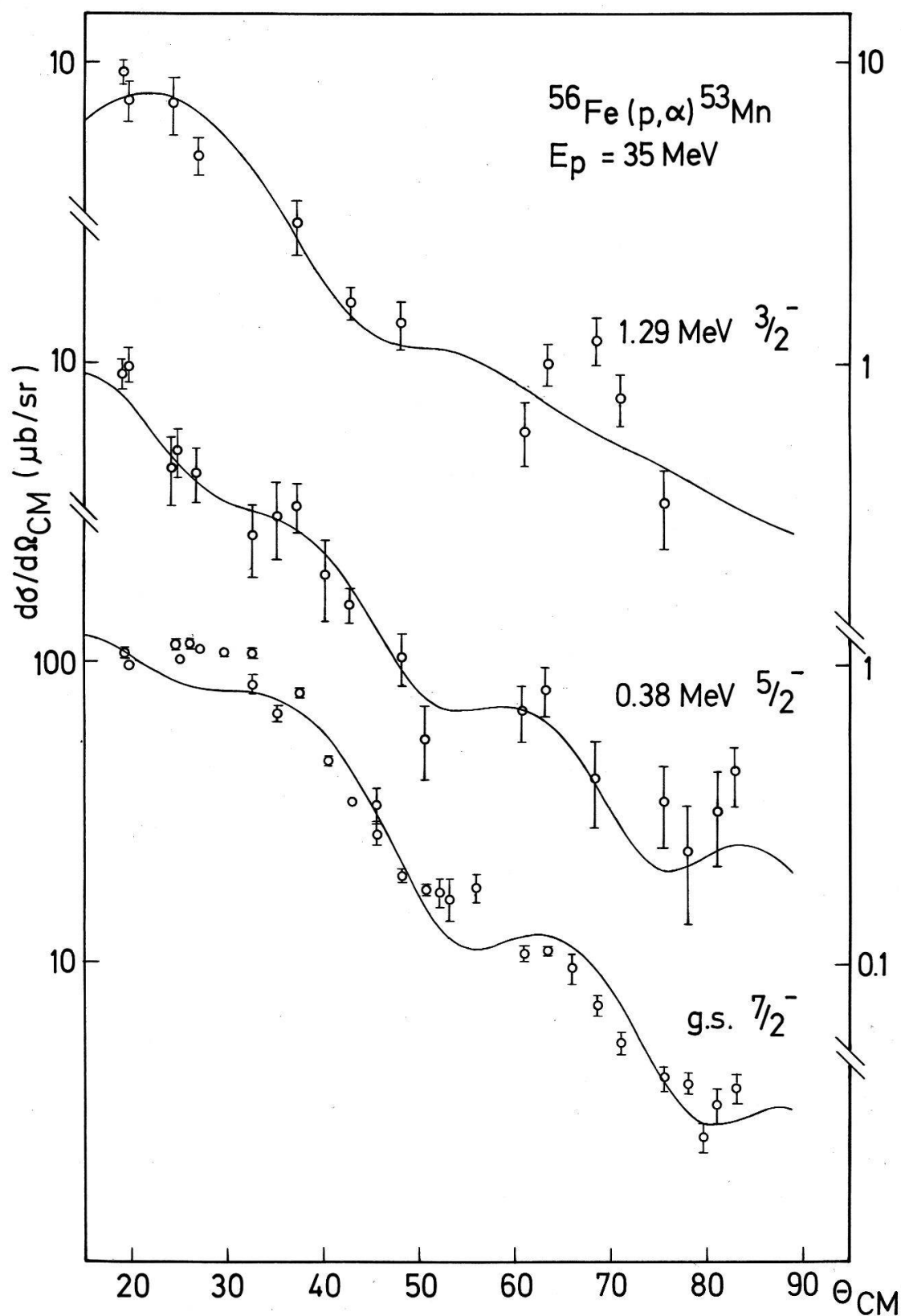


Figure 1

Angular distributions of the reaction $^{56}\text{Fe}(p, \alpha)^{53}\text{Mn}$ leading to the ground state and to the first two excited states of ^{53}Mn .

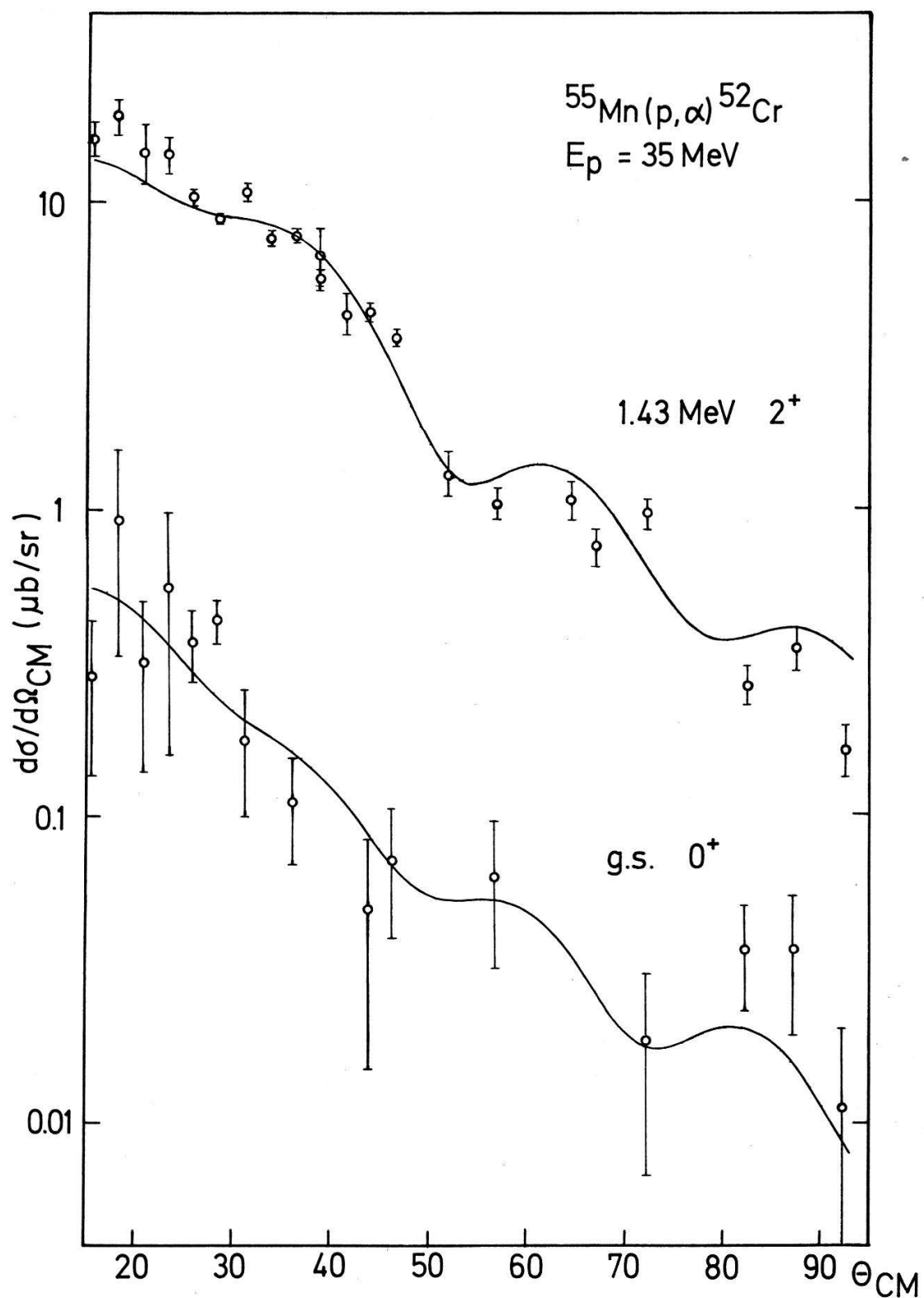


Figure 2
Angular distributions of the reaction $^{55}\text{Mn}(p, \alpha)^{52}\text{Cr}$ leading to the ground state and to the first excited state of ^{52}Cr .



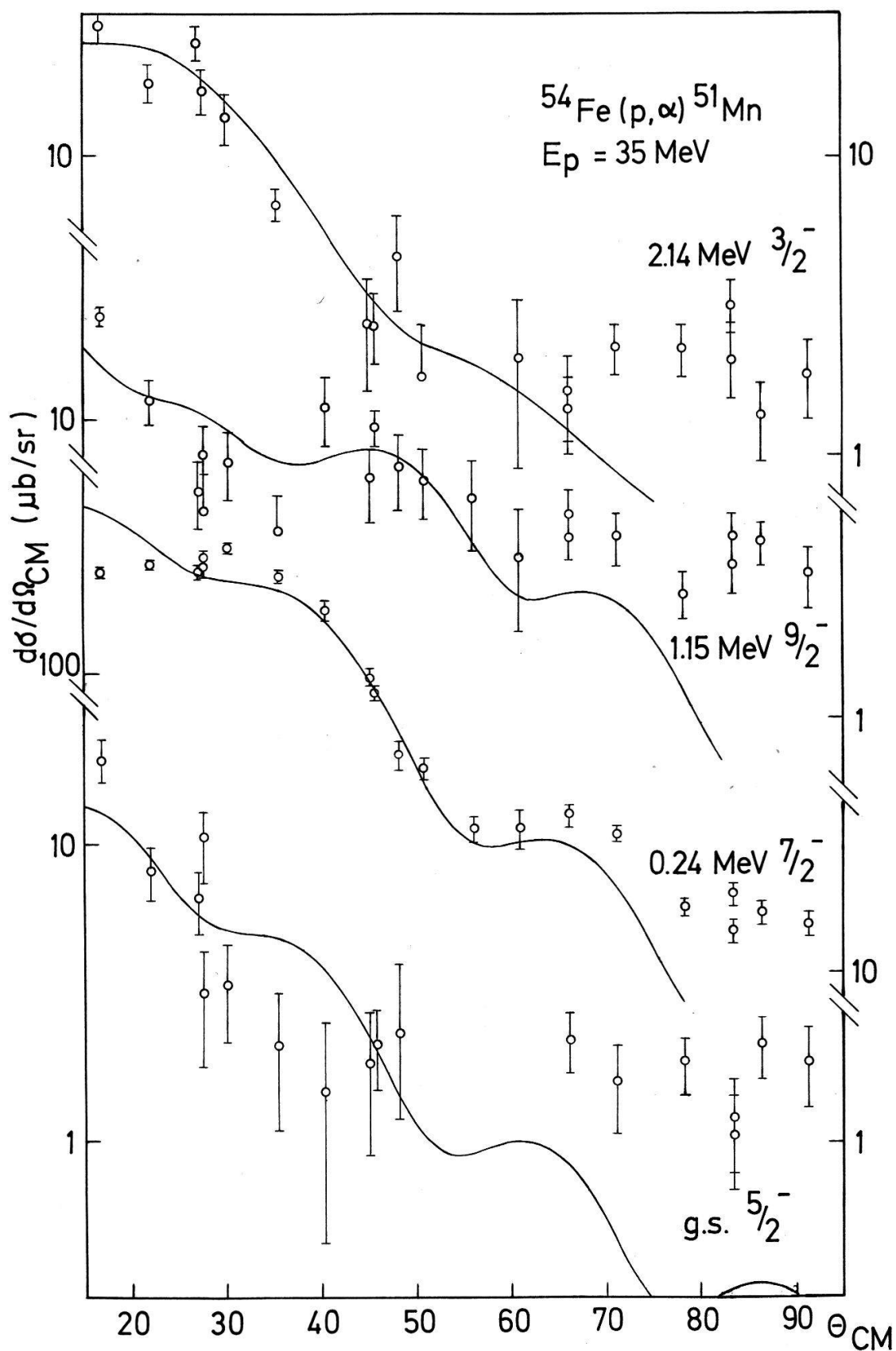


Figure 3
Angular distributions of the reaction $^{54}\text{Fe}(p, \alpha)^{51}\text{Mn}$ leading to the ground state and to some excited states of ^{51}Mn .

Table III
Enhancement factors

Final nucleus	J^π	Final states E_x (MeV)	ε
^{53}Mn	$7/2^-$	0.0	1 ^{a)}
	$5/2^-$	0.38	0.15
	$3/2^-$	1.29	0.02
^{52}Cr	$0^+(5/2)^{\text{b)}}$	0.0	10.6
	$2^+(7/2)^{\text{c)}}$	1.43	1 ^{a)}
^{51}Mn	$5/2^-$	0.0	0.25
	$7/2^-$	0.24	1 ^{a)}
	$9/2^-$	1.15	8.0
	$3/2^-$	2.14	0.03

^{a)} normalized to unity.

^{b)} J -transfer.

^{c)} main J -transfer.

Investigations of the possible core-excitations and two-step processes for these transitions are now underway.

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Measurements of pre- and postfission neutrons of the $^{238}\text{U}(\alpha, \text{xf})$ -reaction at $E_\alpha = 50 \text{ MeV}$

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Abstract. Neutron time-of-flight measurements in 0° and 90° direction with respect to the fission fragments for alpha induced fission of ^{238}U have been performed. Pre- and postfission neutrons could be separated by an iterative procedure. Numbers and average kinetic energies of these neutrons as a function of the mass partition and the total kinetic energy of the fragments are given.

1. Introduction

In the last years techniques of direct measurements of pre- and postfission neutrons in low and high energy fission became more and more useful [1–5]. The neutron energy spectra are measured in coincidence with the two fission fragments at two angles (normally at 0° and 90°) with respect to the direction of the fission axis. The average number and energy spectrum of the prefission neutrons and the postfission neutrons can then be determined by an iteration process based on two assumptions:

- (1) The prefission neutrons are emitted isotropically in the center of mass (c.m.) system of the fissioning nucleus.
- (2) The postfission neutrons are emitted isotropically in the c.m. system of the fully accelerated fragment.

Both assumptions are not completely justified because of the angular momenta of the fissioning system and of the fission fragments. For a thorough discussion see the paper of Cheifetz et al. [2]. The results for the prefission neutrons also include a contribution due to 'scission' neutrons which are emitted during the transition of the fissioning nucleus from the saddle to the scission point and during the scission process. It is generally assumed that these neutrons will be emitted isotropically in the c.m. system of the fissioning nucleus and hence cannot be separated from the prefission neutrons which are emitted prior to the saddle-to-scission transition. Evidence for the existence of scission neutrons was found in the spontaneous fission of ^{252}Cf [6] and in the thermal-neutron fission of ^{235}U [7].

The aim of this work was to measure the number and energy spectra of the prefission neutrons as a function of the fragment mass partition and the total kinetic energy of the fragments. As a by-product one obtains also the number and kinetic energy of the postfission neutrons. The prefission neutron distributions may give some hints concerning the correctness for the common compound-nucleus picture of fission. A part of the prefission neutrons seems to be emitted not only as scission neutrons but also as precompound-neutrons [8].

2. Experiment and data analysis

The experimental arrangement is shown schematically in Fig. 1. The fission fragment energies are measured by two solid state detectors inside a 40 cm

ARRANGEMENT

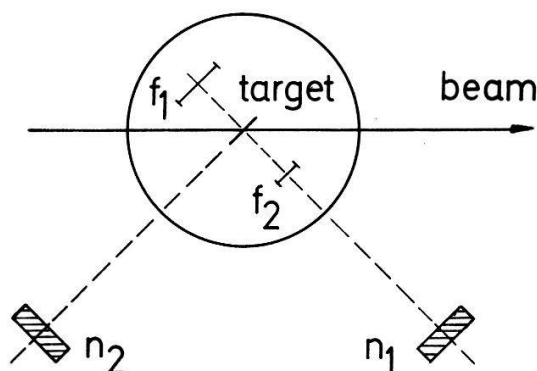
 f_i ... fission detectors n_i ... neutron detectors

Figure 1

Schematical representation of the experimental arrangement.

diameter spherical scattering chamber. One of these detectors has an effective surface of 900 mm^2 and the other one of 300 mm^2 . The distance between the scattering centre and the detector surface is 85 mm. Different detector diameters were chosen in order to increase the coincidence rate upset by the reaction kinematics. The neutrons are detected outside the 3 mm thick Al-scattering chamber wall in a distance of 75 cm from the target by two NE 213 liquid scintillators mounted on XP 2040 photomultipliers. The scintillators which have good pulse shape discrimination properties have a length of 5.1 cm and a diameter of 12.7 cm. The neutron detectors are shielded by 5 cm thick lead layers on its circumference to reduce the number of random events due to γ -rays emitted from the collimators and slits in the beam transport system and the scattering chamber walls.

The experiment described in this paper was performed by means of a 50 MeV α -beam accelerated by the injector cyclotron of the Swiss Institute of Nuclear Research (SIN), Villigen, Switzerland. We used a $100 \mu\text{g}/\text{cm}^2$ thick target of enriched uranium (99.7% ^{238}U) evaporated on a $110 \mu\text{g}/\text{cm}^2$ Ni backing.

The electronic system was designed to measure either binary events coming from two fission fragments or triple events consisting of two fission fragments and a neutron detected by the 0° or 90° detector. The electronic system consisted of standard fast-slow techniques. Not only the analog pulses of the fission detectors and the time-of-flight of the neutrons (started by the smaller fission detector) but also the analog pulses of the photomultipliers and a pulse shape discrimination signal were fed to eight ADC's of a PDP 11/45. The signals were recorded event-by-event on magtape and analysed off-line. For the liquid scintillators the discrimination level was set at half the Compton edge of ^{241}Am , which is equivalent to a neutron energy of 200 keV. Calibration measurements with a thin ^{252}Cf source were performed with the same experimental settings between the experimental runs. The detection efficiency of the neutron detectors was obtained by measuring the neutron spectrum of the ^{252}Cf source and by comparing the results with the accurate measurements of Bowman et al. [6].

The masses and kinetic energies of the fragments were determined by an iterative procedure using the calibration formula of Schmitt et al. [9]. The average number of neutrons emitted from the fragments used for the mass and energy correction of the fragments was taken in the first step from a similar experiment carried out by Fraenkel et al. [4]. Analogously to Fraenkel et al. we made a

correction to the fragment kinetic energy as the result of the recoil momentum imparted to the fragment by the neutron which is detected in coincidence in the 0° detector. The neutron time-of-flight was obtained by a procedure similar to [4], which includes corrections for the time-of-flight of the fission fragment and for pulse-height dependence of the signals in the solid state detector and in the scintillators.

Some problems arose in the determination of the efficiency of the neutron detectors. Although Bowman's results were corrected for the finite size of the detectors and extrapolated to the angles in our experiment, the experimental efficiency differs largely from the theoretical prediction and shows some bumps similar to the results of Gayer and Fraenkel [5]. This is presumably due to contributions of scattered neutrons from the surrounding materials especially from inelastic reactions in the scattering chamber walls. But as the results for the Cf-source were satisfactory we have as well confidence in the results of the uranium reaction since these are comparable to those obtained by Fraenkel et al. [4].

The number and energy distribution of the pre- and postfission neutrons were obtained from the experimental angular and energy distribution on the basis of the two assumptions mentioned in the introduction. The neutron energy spectra were restricted experimentally to the energy range of 0.5–10.0 MeV in the laboratory system. Since 99% of the pre- and postfission neutrons are detected in this window accurate distributions can be expected. The number and energy distributions of the prefission neutrons and the corresponding distributions for the postfission neutrons were determined by an iterative procedure similar to that of Cheifetz et al. [3] and Fraenkel et al. [4]. A detailed description of the iteration method is given in [4]. By this method we obtained upper and lower limits to the values ν_0 and ν_1 the number of pre- and postfission neutrons and the results reported below are averages of those limits obtained after one iteration.

Random events arose due to γ -rays and neutrons emitted from the target backing, collimators and the beam stop. The beam stop was in a distance of 5 m from the target and was shielded carefully by concrete and a paraffin wall to reduce the number of random events. The random spectrum was obtained by detecting those events in which the 'stop' signal preceded the 'start' signal of the fission fragment. The random spectrum was nearly constant in time and amounted to few percents of the total number of events. They were subtracted during the analysis from the 0° and 90° neutron spectra.

3. Results and discussion

The fission yield is reproduced in Fig. 2a as a function of the fragment mass and in Fig. 3a as a function of the total kinetic energy of the fragments before neutron emission. As expected the mass distribution is still mainly asymmetric though the valley between the two maxima is fairly high. The fission yield distribution versus total fragment kinetic energy is as usual bell shaped with a width of more than 30 MeV. In Figs. 2b and 3b the corresponding distributions of the postfission neutrons ν_1 per fission event are shown. The diagram ν_1 versus fragment mass does no longer exhibit the 'saw-tooth' picture as in low energy fission. Shell effects are washed out and the yield ν_1 increases monotonically with

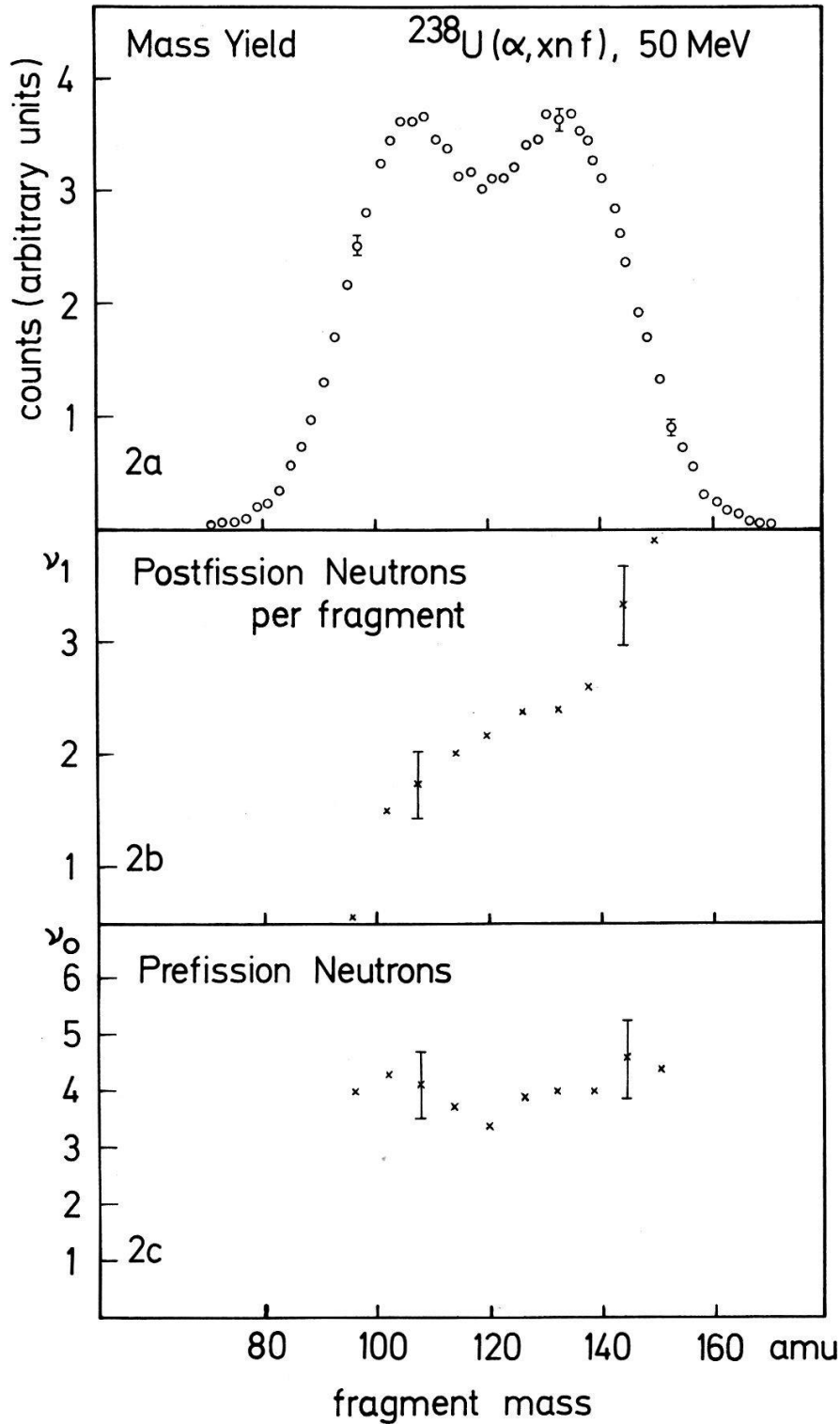


Figure 2

Mass yield (2a), number of postfission neutrons per fragment (2b) and number of prefission neutrons (2c) as a function of the fragment mass for the $^{238}\text{U}(\alpha, xn f)$ -reaction.

the fragment mass. Only a flat shape survives near the mass $A = 132$ which is dominated by magic numbers $Z = 50$ or $N = 82$. The increase of ν_1 is due to the neutron excess of the heavier fragments. Figure 3b shows a decrease of ν_1 with increasing total fragment kinetic energy. This is mainly because at higher fragments kinetic energy asymmetric fission dominates. This means that less deformation energy is available in the fragments and therefore fewer postfission neutrons

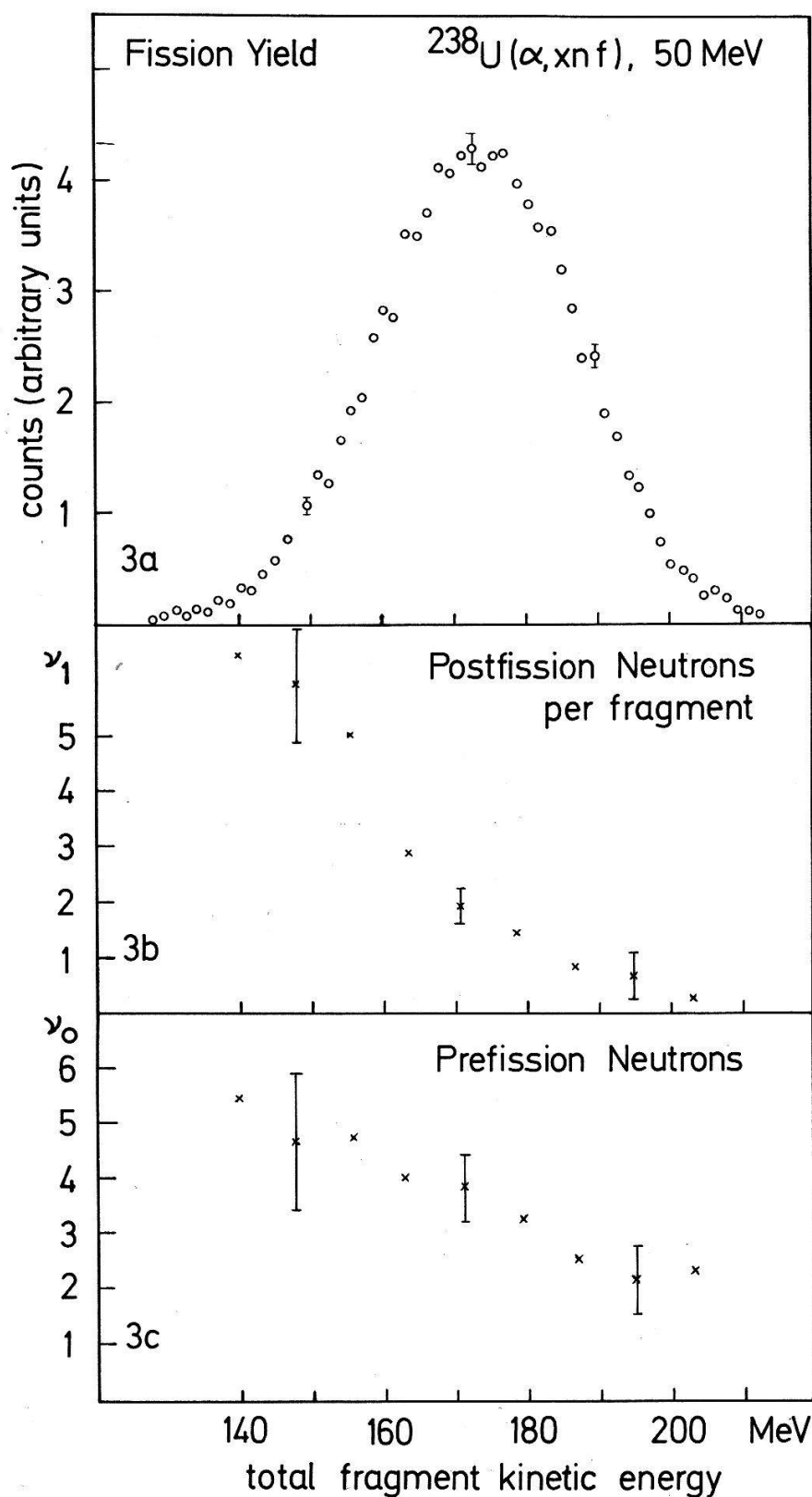


Figure 3
Fission yield (3a), number of postfission neutrons per fragment (3b) and number of prefission neutrons (3c) as a function of the total fragment kinetic energy.

ν_1 will be emitted. The average number of postfission neutrons is 5.5 ± 1.2 and their average kinetic energy is 1.45 ± 0.17 MeV. Within our experimental accuracy we do not see any distinct dependence of the average kinetic energy of the postfission neutrons on the fragment mass or the total kinetic energy of the fragments.

In Figs. 2c and 3c the distributions of the prefission neutrons per fissioning event ν_0 as a function of the fragment mass and the total fragment kinetic energy are shown. As expected ν_0 is nearly independent on fission properties such as the mass splitting and the fragment kinetic energy. The observed slow decrease in the number of prefission neutrons with respect to the total fragment kinetic energy might be due to such an energy partition in the fission process whereby a greater part of the available energy is imparted to the fragments as kinetic energy and therefore neutron emission is less probable. This could indicate that the mechanism of the prefission (and scission-) neutron emission is not completely independent of the fission channel. Additional measurements are desirable to cast more light on these questions. We found an average value of 2.9 ± 0.5 prefission neutrons per fission event, in agreement within the experimental errors of the value 3.6 ± 1.6 found by Fraenkel et al. [4] in the same reaction induced by 45 MeV alphas. For the average kinetic energy of the prefission neutrons we obtained a value of 2.2 ± 0.4 MeV which is higher than the corresponding value of postfission neutrons. An analogous result was found in other reactions [2, 5]. Our results for the postfission neutron distributions as well as the absolute value are in good agreement with the data of Fraenkel et al. [4]. Unfortunately these authors did not publish any prefission neutron distributions and values of average kinetic energies for pre- and postfission neutrons.

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We are obliged to S. Steiner for his assistance and we wish to express our thanks to the staff of the SIN cyclotron laboratory. The authors of the Atominstitut der Oesterreichischen Universitaeten, Vienna, are grateful to the Fonds zur Foerderung der wissenschaftlichen Forschung and the authors of the Universitaet Zuerich wish to thank the Schweizerischen Nationalfonds for financial support.

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Microscopic description of relativistic heavy-ion scattering within the multiple scattering framework

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Based on a microscopic description of the elastic scattering of relativistic heavy ions within the Glauber multiple scattering framework, we have analyzed the Saclay data on the elastic scattering of alpha-particles by p , ^4He , ^{12}C , and $^{40,42,44,48}\text{Ca}$ in the energy range between $T_\alpha^{\text{lab}} = 1.37$ and 2.55 GeV. This study is primarily devoted to the test of the reaction mechanism in a parameterfree analysis, and therefore all available experimental information on elastic nucleon-nucleon scattering and nuclear one-body formfactors has been introduced as an input. Even when two-body correlations and the spin dependence of the nucleon-nucleon amplitude are neglected, the theoretical differential cross sections fit very nicely most of the experimental data at low momentum transfers.

First observation of the reaction $p(\uparrow)p(\uparrow) \rightarrow \pi^+d$ at 580 MeV

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The polarization parameter $A_{NN} = \sigma_{yy}/\sigma_{00}$ of the reaction $pp \rightarrow \pi^+d$ has been observed for the first time, using the SIN accelerated polarized proton beam at 580 MeV and a polarized butanol target. The particle trajectories have been detected with the aid of MWPC's. The results $A_{NN} = -0.93 \pm 0.05$, -0.92 ± 0.05 and -0.96 ± 0.05 at $\theta_{CM}^\pi = 87^\circ$, 80° and 74° respectively are in good agreement with recent predictions [1] based on the $N-\Delta$ interaction. A systematic error of $\Delta A/A \approx 15\%$ in the evaluation of the data is still possible at the present time.

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Production de résonances pioniques à 50 GeV/c

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Une quantité considérable de données a été prise dans les canaux $\pi^\pm p \rightarrow \pi^\pm \pi^0 p$ et $\pi^\pm p \rightarrow \pi^\pm \pi^+ \pi^- \pi^0 p$ dans le cadre d'une expérience au Super Synchrotron à Protons (SPS) du CERN. Les pions neutres ont été détectés avec une haute résolution dans un grand détecteur à argon liquide. La production de résonances est présentée en termes de sections efficaces.

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Théorie

The sine-Gordon chain: mass diffusion

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We present and discuss molecular-dynamics results aimed at studying the response on a small static external field of a sine-Gordon chain in the presence of damping, and subject to a random force. On the basis of these results, we clarify the relevance of thermalized sine-Gordon solitons in the diffusion process.

Surface tension and phase transition for lattice systems

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We introduce the surface tension for arbitrary spin systems and study its general properties. In particular we show that for a large class of systems the surface tension is zero at high temperature. We also derive a geometrical condition for the surface tension to be zero at all temperature. For discrete spin system this condition becomes a criteria to establish the existence of a phase transition associated with surface tension. This criteria is illustrated on several examples.

Transport and thermodynamic properties of disordered one-dimensional lattices

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For one-dimensional lattices with random nearest-neighbor interactions we determine the low energy limit for the density of states, calculate the low temperature specific heat, and investigate certain transport properties. Our results are applicable to lattice vibrations of a chain with random force constants, diffusion of classical particles with random transfer rates, low-energy spin-wave excitations in random ferromagnetic Heisenberg chains, and tight-binding electron bands with correlated diagonal and off-diagonal disorder.

Effets de la géométrie sur les propriétés du cristal de Wigner bidimensionnel

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On caractérise le cristal de Wigner bidimensionnel constitué par un réseau mono-atomique parfait d'ions immergés dans un bain homogène neutralisant, par trois paramètres, pour toute densité donnée. Ces paramètres sont: le rapport α des côtés de la maille primitive, l'angle φ entre les côtés de la maille et le rapport $\nu = \lim_{N_1, N_2 \rightarrow \infty} N_2/N_1$ où N_1 et N_2 représentent le nombre de mailles du cristal dans les 2 directions du parallélogramme formé par l'union des mailles primitives.

Par une méthode analytique et numérique qui sera décrite ailleurs, on a examiné l'énergie de Madelung, la pression mécanique¹⁾ et la matrice dynamique du modèle. L'énergie de Madelung ε dépend de α et φ mais pas de ν , si les ions sont situés aux centres des mailles. Pour α fixé l'énergie par particule a un minimum en $\varphi_{\min}(\alpha)$ et l'on a constaté que $\alpha \cdot \varphi_{\min}(\alpha) = \pi/3$. Le minimum minimorum est bien obtenu pour $\alpha = 1$ et $\varphi = \pi/3$, c'est à dire pour le réseau triangulaire et l'on trouve:

$$\varepsilon = -0.374 > -\frac{3}{8}$$

Pour ce réseau, on a calculé la pression mécanique qui dépend encore de ν et trouvé que pour $\nu = 3.14106$, cette pression était nulle. Pour un réseau rectangulaire, en revanche, cette pression est indépendante de ν et positive.

¹⁾ Ph. Choquard – Réunion de la SSP-Neuchâtel 1978.

Enfin, l'analyse de la matrice dynamique effectuée dans le cas des conditions aux bords périodiques a révélé que les fréquences propres $\omega_j(0)$ ($j = 1, 2$) du centre de masse (vecteur d'onde $q = 0$) dépendaient de ν et que $\lim_{q \rightarrow 0} \omega_j(q) \neq \omega_j(0)$ contrairement à ce qui est communément admis. L'erreur usuelle vient d'un traitement incorrect de l'interaction particule-bain qui dépend de la forme microscopique et macroscopique du cristal considéré.

Fluctuations de charge dans un plasma unidimensionnel

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Pour le plasma à deux composantes unidimensionnel on calcule la distribution de probabilité d'une observable générale à une particule.

On met en évidence la différence entre les fluctuations de charges et celles du nombre des particules. Alors que la fluctuation du nombre de particules $\langle N^2 \rangle_\Lambda = 0(|\Lambda|)$ se comporte de façon normale lorsque $|\Lambda| \rightarrow \infty$, la fluctuation de charge $\langle Q^2 \rangle_\Lambda$ est de l'ordre de $0(1)$ et sa distribution de probabilité $P_\Lambda(Q)$ converge lorsque $|\Lambda| \rightarrow \infty$.

Ce dernier fait nous permet d'établir une relation intégrale entre les fonctions de corrélation.

En dimension $\nu > 1$, cette relation entraîne que la fluctuation de charge $\langle Q^2 \rangle_\Lambda$ est de l'ordre de la surface de Λ .

Generalized Frenkel-Kontorowa model for disordered systems

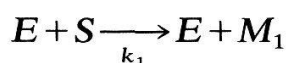
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We study a generalized Frenkel-Kontorowa model to describe a one-dimensional disordered system. We show that the problem of the equilibrium configurations of such a model is exactly equivalent to an Ising model with exponential interaction. We compute the configurational density of states and discuss the possibility of having a linear specific heat at low temperature. Conductivity is also computed within a master equation framework.

An exactly solvable model for enzyme-triggered polymerization

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A given substrate molecule reacts with an enzyme:



where M_1 is a monomer unit capable of polymerizing according to:



where M_n denotes an n -mer. Both reactions are taken to be irreversible. The kinetic equations for the system are an infinite set of coupled non-linear differential equations. A formal solution and analytical expressions for some relevant quantities are obtained.

Continuous symmetry breaking in closed intervals of the temperature axis and the Ising-, XY- and Heisenberg models

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Abstract. Performing a new transformation on the partition function of the Ising-, anisotropic XY- and Heisenberg models, the existence of continuous symmetry breaking is proved on intervals of the temperature axis below the exact, maximal critical temperature T_{cm} . In the anisotropic case the exact, maximal critical temperature does depend on the anisotropic parameter of the coupling constant. The continuous symmetry breaking occurs in the presence of homogeneous or inhomogeneous, external, magnetic fields. It is shown for the XY-model with inhomogeneous, external field in the z -direction that this model also possesses continuous symmetry breaking on intervals of the temperature axis below the exact, maximal critical temperature. The relation of this model to the BCS-model is apparent, therefore the isothermal, local resistivity is discussed for the model. It is proved that the isothermal, local resistivity is zero in the associated superconducting state.

1. Introduction

The interesting fact that Ising model has continuous phase transition in the presence of an external magnetic field [1] announces the possibility of continuous phase transition if the order parameter is different from zero below the transition temperature. Therefore it is necessary to introduce a notion to make a difference between two possible continuous symmetry breaking at two different transition points.

Let us recall that with the high temperature expansion method or with Padé approximants for polynomials one could fairly well locate a singularity of the susceptibility or of the specific heat of the Ising and Heisenberg models, see for instance Ref. 2. Because one used the temperature to the power -1 , T^{-1} , as expansion parameter, the obtained convergence radius is just associated to a maximal transition temperature of continuous symmetry breaking. These methods could not clear up what happens 'below that convergence radius'. Suppose that we know exactly this convergence radius, then we call to this exact value associated transition temperature as the exact, maximal critical temperature T_{cm} .

Our concern is to show that below that exact, maximal critical temperature T_{cm} , intervals of critical temperature points i_c do exist and they are dense for all $T \in i_c$ and $T < T_{cm}$. In the case of the Ising model this fact is achieved by generalizing the transformation which leads to the existence of continuous symmetry breaking in the Ising model if the external magnetic field is incorporated

into the model [1]. Combining this transformation with a new one, it results the appropriate transformation on the partition function, which allows to prove the existence of continuous symmetry breaking for temperatures $T < T_{cm}$ and for all $T \in i_c$. To establish the proof we use the monotone increasing property of the partition function in the off-diagonal entries [3, 4], which allowed to construct lower and upper cumulant bounds of smaller dimensionality to the susceptibility, specific heat of the Ising and Heisenberg models [3, 4].

This method is generalized to the isotropic or anisotropic XY- and Heisenberg models. For these models it is shown again that one can find closed, dense intervals $i_{c\alpha}$ on the temperature axis and that below the exact, maximal critical temperatures $T_{cm\alpha}$, $T < T_{cm\alpha}$, where α is the anisotropy index of the spin interaction matrices, $\alpha = 1, 2, 3$ after the three different directions of spin quantization. Again it is shown that the susceptibility, specific heat of the models etc. are divergent and that by cumulant inequalities [3, 4].

It is of course a suggestive question what applications can be made with these new results or how consistent are these results with some facts in the nature. Now let us point out that if the exact, maximal transition temperature is about 1500 K, that means the off-diagonal entries of the Ising model with nearest neighbour interaction are of order 1500 K, then we do not expect any spectacular thing as it is in the nature (iron). But if the coupling matrix element becomes of the order of the Fermi temperature $T_{cm} > 10^4$ K, then we expect to find a closed dense interval i_c of continuous phase transition points on the temperature axis $T < T_{cm}$. This latter case corresponds to the superconducting state of a piece of metal if one would make a lattice gas model of superconductivity. This latter model would be a crude approximation but upper and lower bounds, given by this crude model, to the usual electron phonon model would support superconductivity.

Therefore in the 3rd section we looked to another related description of superconductivity. This is the isotropic XY-model with inhomogeneous external field in the z -direction. This inhomogeneous external field term describes the band structure in the rigid ion model. The isotropic spin-spin interaction contains the electron-electron and electron-phonon interaction on an appropriate way. These both interaction sum up to a value of order 10^4 K. This value is a result of the BCS-theory [5], which has been formulated also in the space of Pauli-spin operators [6]. Our formulation is slightly different from Ref. 6, because our commutation rules of spin operators are different. However, we show that continuous symmetry breaking in the model occurs in an interval i_c of densely defined critical temperature points $T < T_{cm}$ and if the band energy $\hat{\epsilon}(q)$ does not exceed a maximal value $\epsilon_{\max}$ for all wave vectors q in the Brillouin zone $Z_B^d(a)$, $\hat{\epsilon}(q) < \epsilon_{\max}$ for $q \in Z_B^d(a)$. Furthermore it follows that for $T \in i_c$ and $\hat{\epsilon}(q) < \epsilon_{\max}$ the isothermal, local resistivity [7, 8] is zero as it should be for weak coupling superconductors. This fact demonstrates again the power of the method in section 2.

2. Phase transition in the Ising and Heisenberg models

Let us define a finite d -dimensional volume Λ_d by

$$\Lambda_d = \left\{ (a, n) = \sum_{i=1}^d a_i n_i, n_i \in \mathbf{Z} \right\}$$

of the infinite, d -dimensional volume $Z^d(a)$, $\Lambda_d \subset Z^d(a)$. Further, associate with the points $l = \{l_i, \dots, l_d\}$, $l_i = a_i n_i$, random variables or fields φ_l and Pauli-spin operators σ_l^α , $\alpha = 1, 2, 3$. The Pauli-spin operators fulfil the commutation relations $[\sigma_k^\alpha, \sigma_l^\beta] = 2i\varepsilon_{\alpha\beta\gamma}\sigma_k^\gamma\delta_{k,l}$ with $k \in Z^d(a)$.

Definition 2.1. Let us define the scalar products

$$(\phi, I\phi) = \sum_{\substack{k, l \in \Lambda_d \\ \alpha = 1, 2, 3}} \phi_k^\alpha (I^\alpha)_{kl} \phi_l^\alpha \quad (2.1)$$

and

$$(\phi, A\phi)_k = \sum_{\alpha = 1, 2, 3} \phi_k^\alpha A_{kk}^\alpha \phi_k^\alpha, \quad (2.2)$$

in general the matrices I^α are different.

Further, let

$$V(\{\phi^\alpha\})_d = - \sum_{k \in \Lambda_d} \ln 2 \operatorname{ch} \sqrt{(\phi, \phi)_k} \quad (2.3)$$

be, then the configurational partition function Q_{Λ_d} of the $V(\{\phi^\alpha\})_d$ -lattice theory is given by the perturbed Gaussian measure

$$d\mu = \exp[-V(\{\phi^\alpha\})_d] d\mu_0 \quad (2.4)$$

and

$$d\mu_0 = \prod_{\beta=1}^3 \det^{-1/2}(I^\beta) \exp[-\frac{1}{2}(\phi, I^{-1}\phi)] \prod_{\substack{k \in \Lambda_d \\ \alpha = 1, 2, 3}} (2\pi)^{-1/2} d\phi_k^\alpha \quad (2.5)$$

One has for the configurational partition function $Q_{\Lambda_d} = \int d\mu$, which we call configurational measure. The matrices I and I^{-1} are positive definite and fulfil the relation $I \cdot I^{-1} = 1$.

After giving these definitions, one can make the relation between the configuration measure of $d\mu$ and the partition function of the Heisenberg model:

Lemma 2.2. Let $H(I^\alpha, h^\alpha)$ be the Heisenberg model Hamiltonian with inhomogeneous, external magnetic fields h_l^α at each lattice site $l \in \Lambda_d$:

$$H(I^\alpha, h^\alpha) = \frac{1}{2}(\sigma, I\sigma) - (h, \sigma), \quad (2.6)$$

then the configurational measure $Q_{\Lambda_d} = \int d\mu$, given by (2.4), and the partition function of the Heisenberg model (2.6) fulfil the relation

$$\operatorname{Tr} \{\exp[-H(I^\alpha, h^\alpha)]\} = \int \exp[-V(\{\phi^\alpha + h^\alpha\})] d\mu_0. \quad (2.7)$$

We omit the proof of this lemma here. But one should notice that $V(\{\phi^\alpha + h^\alpha\}) = -\sum_{k \in \Lambda_d} \ln 2 \operatorname{ch} \sqrt{(\phi + h, \phi + h)_k}$ is with

$$(\phi + h, \phi + h)_k = \sum_{\alpha=1,2,3} (\phi_k^\alpha + h_k^\alpha)^2.$$

At first, let our concern be the Ising model, then the Definition 2.1 reduces to one component lattice fields ϕ_i . Further only the 3rd component of the Pauli-spin operator occurs in Lemma 2.2.

Theorem 2.3. *Let T_{cm} be the so-called exact, maximal critical-temperature defined by high temperature expansion or by other mathematical methods for the d -dimensional Ising model, $d > 1$. Then the Ising model,*

$$H_{\Lambda_d}(I) = \frac{1}{2}(\sigma, I\sigma) = \frac{1}{2} \sum_{k,l \in \Lambda_d} \sigma_k I_{kl} \sigma_l, \quad \sigma_k = \{\pm 1\}_k \quad (2.8)$$

possesses continuous symmetry breaking below the maximal critical temperature T_{cm} , where finite magnetization $m_k = \langle \sigma_k \rangle \neq 0$ occurs for every lattice site $k \in Z^d(a)$

Proof. Let I_1 be the coupling matrix for temperature $T_1 < T_{cm}$ and I_2 the coupling matrix for temperature $T_2 > T_{cm}$, where T_{cm} is the maximal critical temperature in the above sense. We choose T_1 and T_2 such that $T_1 = xT_2$, $T_1 < T_2$, $x^{-1} = 1 + y$ and $y^{-1}T_2 < T_1$, then $I_1 = I_2 + yI_2$. To the yI_2 -matrix associated Ising-model possesses symmetry breaking of continuous type, because is $y^{-1}T_2 < T_1$. The Ising-model Hamiltonian can be written in the form $H_{\Lambda_d}(I_2) + H_{\Lambda_d}(yI_2)$, where the Hamiltonian $H_{\Lambda_d}(yI_2)$ is responsible for the continuous symmetry breaking. One has for the partition function

$$Q_{\Lambda_d}^{I_1} = \operatorname{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_1)] \} = \operatorname{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(yI_2)] \exp [-H_{\Lambda_d}(I_2)] \}, \quad (1.9)$$

where we consider $H_{\Lambda_d}(I_2)$ as perturbation and the temperature dependence is incorporated into the coupling constants I_i . The spin operators σ_k of $H_{\Lambda_d}(I_2)$ have from zero different expectation values with respect to the density operator of $H_{\Lambda_d}(yI_2)$. Therefore to take into account the singular spectrum part of $H_{\Lambda_d}(I_2)$ with respect to the normalized eigenvectors of $\exp [-H_{\Lambda_d}(yI_2)]$, we write $H_{\Lambda_d}(I_2)$ in the form

$$H_{\Lambda_d}(I_2) = \frac{1}{2}(\delta\sigma, I_2 \delta\sigma) + (h, \delta\sigma) + \frac{1}{2}(m, I_2 m), \quad h = I_2 m, \quad (2.10)$$

where $m_k = \langle \sigma_k \rangle_y \neq 0$ and the expectation in $\langle \sigma_k \rangle_y$ is taken with the density operator of $H_{\Lambda_d}(yI_2)$, $\delta\sigma_k = \sigma_k - m_k$. After Lemma 2.2 the operators $\exp [-H_{\Lambda_d}(I_2)]$ and $\exp [-H_{\Lambda_d}(yI_2)]$ can be represented by perturbed Gaussian measures, see Definition 2.1,

$$\exp [-H_{\Lambda_d}(I_2)] = \int \exp [-\frac{1}{2}(m, I_2 m) + (\varphi - h, \delta\sigma)] d\mu_0(I_2) \quad (2.11)$$

and

$$\exp [-H_{\Lambda_d}(yI_2)] = \int \exp [(\varphi, \sigma)] d\mu_0(yI_2), \quad (2.12)$$

where we indicate the matrix dependence of the Gaussian measures. To prove the assertion of the theorem we must consider the expression $\operatorname{Tr} \{ \exp [-H_{\Lambda_d}(I_2) + (\phi, \sigma)] \}$, which is the configuration measure of the Ising model $H_{\Lambda_d}(I_2)$ with

external field term (ϕ, σ) . It holds:

$$\begin{aligned} \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_2) + (\phi, \sigma)] \} \\ = \int \exp [-\tfrac{1}{2}(m, I_2 m) - (\phi' - h, m) - V(\{\phi' + \phi - h\})] d\mu_0(I_2). \end{aligned} \quad (2.13)$$

Performing the scale transformations

$$\phi_k \rightarrow \phi_k \cdot m_k^{-1} \quad \text{and} \quad \phi_k \rightarrow \phi_k + x_k \quad (2.14)$$

with constraint

$$x_k = m_k \sum_{l \in \Lambda_d} (I_2)_{kl} [1_l - m_l], \quad (2.15)$$

the configuration measure (2.13) takes the form

$$\begin{aligned} \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_2) + (\phi, \sigma)] \} = \text{Tr}_\sigma \{ \exp [-\tfrac{1}{2}(m, I_2 m) - \tfrac{1}{2}(x, \bar{I}_2^{-1} x) \\ + (1, \beta) + (h, m)] \int d\mu_0(I_2) \exp [2(n, \phi + \beta)] \}, \end{aligned}$$

where $(\bar{I}_2)_{kl} = m_k (I_2)_{kl} m_l$, $n_k = \{0, 1\}_{f_k} = \frac{1}{2}(1_k + \sigma_k)$ and $\beta_k = m_k^{-1} \cdot x_k - h_k - \phi_k = \sum_{l \in \Lambda_d} (I_2)_{kl} [1_l - 2m_l] - \phi_k$. Performing the ϕ -integrations one gains the expression

$$\begin{aligned} \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_2) + (\phi, \sigma)] \} \\ = \exp [-\tfrac{1}{2}(m, I_2 m) - \tfrac{1}{2}(x, \bar{I}_2^{-1} x) + (h, m)] \cdot \text{Tr}_\sigma \{ \exp [-2(n, I_2 n) + (\beta, \sigma)] \}, \end{aligned}$$

which results for the Ising configuration measure $Q_{\Lambda_d}^I$ the following:

$$Q_{\Lambda_d}^{I_1} = \exp [A(I_2)] \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_1) + (f, \sigma)] \}, \quad (2.16)$$

where we defined

$$\begin{aligned} A(I_2) = -(1, I_2 1) + (1, I_2 m), \\ f_k = 2 \sum_{l \in \Lambda_d} (I_2)_{kl} [m_l - 1_l]. \end{aligned} \quad (2.17)$$

Applying the above transformation to the Ising configuration measure several times, one gets

$$Q_{\Lambda_d}^{I_1} = \exp [A^{(n)}(I_2)] \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_1) + (f^{(n)}, \sigma)] \} \quad (2.18)$$

where

$$f_k^{(n)} = 2n \sum_{l \in \Lambda_d} (I_2)_{kl} (m_l - 1_l), \quad n = \pm 1, \pm 2, \dots, \pm N, \dots \quad (2.19)$$

From the work of the author [1] it follows that the Ising model with interaction matrix I and external field in the Hamiltonian possesses continuous symmetry breaking if the external field coincides with the values $2\alpha \sum_l I_{kl}$, $\alpha = 0, \pm 1, \pm 2, \dots, M, \dots$, at each lattice site $k \in \mathbb{Z}^d(a)$. In (2.18) we have chosen the coupling matrix I_1 such that we are below the maximal transition temperature

T_{cm} . Applying in this case the procedure of the above reference, one gains the condition

$$2\alpha \sum_{l \in \Lambda_d} (I_1)_{kl} = 2n \sum_{l \in \Lambda_d} (I_2)_{kl} (m_l - 1) \quad (2.20)$$

to eliminate the external field term in (2.18).

Notice that $m_l = \langle \sigma_l \rangle_y$ is defined on a way that the symmetry breaking is present in the I_1 -Ising model: $yI_2 > I_1 > I_{cm}$ where the I_{cm} -matrix corresponds to the exact, maximal critical temperature T_{cm} , that means I_1 and yI_2 belong to the broken symmetry region.

To show that the continuous symmetry breaking exists for temperatures $T < T_{cm}$, that means the susceptibility, specific heat etc. of the Ising model are divergent in the temperature region $T < T_{cm}$, it is necessary to express the right hand side of (2.18) in a way that the trace is just described by an Ising Hamiltonian of coupling matrix I_2 and an external field term. This transformation can be gained from (2.13) if the lattice field representation is used in the Ising configuration measure $Q_{\Lambda_d}^{I_1}$. It follows

$$\text{Tr}_{\sigma} \{ \exp [-H_{\Lambda_d}(I_1)] \} = \left(\frac{1+y}{1+2y} \right)^{\frac{\Lambda_d}{2}} \exp [A(I_2)] \text{Tr}_{\sigma} \{ \exp [-\frac{1}{2}(\sigma, I_y \sigma) + (b, \sigma)] \} \quad (2.21)$$

by using (2.11–12) and the transformations

$$\phi'_k + \phi_k \rightarrow \phi'_k \rightarrow \phi'_k - \frac{1+y}{1+2y} \sum_{l \in \Lambda_d} (I_2)_{kl}. \quad (2.22)$$

The quantities b_k and I_y are given by

$$b_k = \sum_{l \in \Lambda_d} (I_2)_{kl} \left[2m_l - \frac{y}{1+2y} 1_l \right], \quad I_y = \frac{y}{1+2y} \cdot I. \quad (2.23)$$

This transformation can be applied several times again, it holds for the gained, external field term:

$$b_k^{(n)} = n b_k, \quad n = \pm 1, \pm 2, \dots, \pm N, \dots \quad (2.24)$$

In this case again, one can transform away the $b_k^{(n)}$ as the $f_k^{(n)}$ and that under the condition

$$2\alpha \frac{y}{1+2y} \sum_{l \in \Lambda_d} (I_2)_{kl} = b_k^{(n)} \quad (2.25)$$

which assures that the result

$$Q_{\Lambda_d}^{I_1} = \left(\frac{1+y}{1+2y} \right)^{\frac{\Lambda_d}{2}} F(I_2, y) \cdot \text{Tr}_{\sigma} \{ \exp [-\frac{1}{2}(\sigma, I_y \sigma)] \} \quad (2.26)$$

holds if (2.25) is satisfied. F is brave as one can show.

Note that it is allowed to choose $I_1 > I_2 > I_y = I_{cm}$ and therefore the right hand side of (2.26) describes the I_1 -Ising system at its exact maximal critical point where the corresponding susceptibility, specific heat, etc. of the Ising model are divergent, which can be shown by using the monotone increasing property of the

Ising configuration measure in the off-diagonal couplings of ferromagnetic type [3, 4]. These facts and results prove the theorem. Q.E.D.

From the proof of the above theorems one has as consequence:

Corollary 2.4. *Let $H_{\Lambda_d}(I_1)$ and $H_{\Lambda_d}(I_2)$ be two Ising-Hamiltonians with constraints $I_1 > I_2 > I_{cm} = y[1+2y]^{-1} \cdot I_2 > 0$ and $I_1 = I_2[1+y]$, $y > 0$, then the Ising configuration measure and the matrices I_1 and I_2 fulfil the relations*

$$Q_{\Lambda_d}^{I_1} = \left(\frac{1+y}{1+2y} \right)^{\frac{\Lambda_d}{2}} F(I_2, y) \cdot \text{Tr}_{\sigma} \{ \exp [-\frac{1}{2}(\sigma, I_y \sigma)] \},$$

$$2\alpha \sum_{l \in \Lambda_d} (I_1)_{kl} = 2n \sum_{l \in \Lambda_d} (I_2)_{kl} [m_l - 1_l],$$

and

$$2\alpha \sum_{l \in \Lambda_d} (I_2)_{kl} \frac{y}{1+2y} = 2n \sum_{l \in \Lambda_d} (I_2)_{kl} [m_l - 1_l]$$

with definition $m_l = \langle \sigma_l \rangle_y = [Q_{\Lambda_d}^{I_y}]^{-1} \cdot \text{Tr}_{\sigma} \{ \exp [-H_{\Lambda_d}(yI_2)] \sigma_l \}$.

To extend Theorem 2.3 with external magnetic field in arbitrary direction, one can use Lemma 2.2 and especially the representation (2.7) of the Heisenberg model Hamiltonian $H(I^{\alpha}, h^{\alpha})$ (2.6). Because here one is concerned with an anisotropic problem, it is necessary to introduce three different, exact, maximal critical temperatures $T_{cm\alpha}$, $\alpha = 1, 2, 3$.

Theorem 2.5. *Let $H_{\Lambda_d}(I^{\alpha}, h^{\alpha})$ be a d -dimensional Heisenberg model Hamiltonian (2.6), $d > 1$, with anisotropic coupling matrices $I^{\alpha} > 0$, $\alpha = 1, 2, 3$, for ferro- or antiferro- off-diagonal entries, then to the d -dimensional Heisenberg model associated quantities as susceptibility, specific heat, etc. possess continuous symmetry breaking below the exact, maximal critical temperatures $T_{cm\alpha}$, where finite magnetizations $m_k^{\alpha} = \langle \sigma^{\alpha} \rangle \neq 0$, $k \in Z^d(a)$, occur on every lattice site k . The matrix elements $(I^{\alpha})_{kl}$ should further not depend necessarily on the difference of two sites $k-l$.*

Let us pronounce again that continuous symmetry breaking means together singular and divergent behaviours of the physical quantities as susceptibility etc. To establish the above Theorem 2.5 one needs two steps again: at first one derives to Corollary 2.4 equivalent conditions and secondly one shows that continuous symmetry breaking below the exact, maximal transition temperature $T_{cm\alpha}$ occurs for $m_k^{\alpha} \neq 0$.

Proof. Notice one can apply the scale transformation

$$\phi_k^{\alpha} \rightarrow \phi_k^{\alpha} - \sum_{l \in \Lambda_d} (I^{\alpha})_{kl} \quad (2.27)$$

to the configuration measure (2.7). One obtains

$$Q_{\Lambda_d} = \text{Tr}_{\sigma} \left\{ \int d\mu_0 \exp [-(1, \phi) + (\sigma, \phi - I \cdot 1 + h)] \right\} \\ = \text{Tr}_{\sigma} \{ \exp [-\frac{1}{2}(1, I1) - \frac{1}{2}(1 + \sigma, I[1 + \sigma]) + (h - 1 \cdot I, \sigma)] \} \quad (2.28)$$

from which it follows that the components of the magnetic field are cancelled out if the relations

$$h_k^{\alpha} = 2 \sum_{l \in \Lambda_d} (I^{\alpha})_{kl} \quad (2.29)$$

are satisfied. One can apply the above transformations (2.27) several times, then the constraint (2.29) is generalized to

$$h_k^{\alpha} = 2w^{\alpha} \sum_{l \in \Lambda_d} (I^{\alpha})_{kl}, \quad w^{\alpha} = 0, \pm 1, \pm 2, \dots, \pm W, \dots \quad (2.30)$$

This result already demonstrates that the transformations, which lead to the proof of the Theorem 2.3 and especially to formula (2.26) will work in this case also and physical quantities associated to the Heisenberg model (2.6) possess continuous symmetry breaking. Therefore we mimic the notation of the proof of Theorem 2.3, i.e. the notation of the Ising case.

Now, let I_1^{α} be coupling matrices for temperatures $T_1 < T_{cm\alpha}$ and I_2 the matrices for temperatures $T_2 > T_{cm}$. Choose T_1 and T_2 so that $T_1 = [1 + y]^{-1} T_2$ then $T_1 > y^{-1} T_2$ and therefore to the matrices $yI_2^{\alpha} > I_1^{\alpha}$ associated Heisenberg models possess symmetry breaking of continuous type. Let us split the Hamiltonian $H_{\Lambda_d}(I_1^{\alpha}, h^{\alpha})$ (2.6) as follows

$$H_{\Lambda_d}(I_1^{\alpha}, h^{\alpha}) = H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha}) + H_{\Lambda_d}(yI_2^{\alpha}, y h_2^{\alpha}), \quad (2.31a)$$

$$H_{\Lambda_d}(yI_2^{\alpha}, y h_2^{\alpha}) = y H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha}). \quad (2.31b)$$

The Hamiltonian (2.31b) is responsible for the continuous symmetry breaking. It holds

$$\text{Tr}_{\sigma} \{ \exp [-H_{\Lambda_d}(I_1^{\alpha}, h^{\alpha})] \} = \text{Tr}_{\sigma} \{ \exp [-H_{\Lambda_d}(yI_2^{\alpha}, y h_2^{\alpha})] \exp [-H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha})] \} \quad (2.32)$$

where we consider $H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha})$ as a perturbing part of a Hamiltonian. Thank to the results (2.28–30) and the choice of I_1^{α} , the Pauli spin operators σ_k^{α} of $H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha})$ will always have from zero different expectation values according to the density operator of $H_{\Lambda_d}(yI_2^{\alpha}, y h_2^{\alpha})$ and that also for $h^{\alpha} = 0$. Therefore we take again into account the singular spectrum part of $H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha})$ with respect to the eigenvectors of the density operator of $H_{\Lambda_d}(yI_2^{\alpha}, y h_2^{\alpha})$. We define:

$$H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha}) = \frac{1}{2}(\delta\sigma, I_2 \delta\sigma) + (I_2 m - h_2, \delta\sigma) + \frac{1}{2}(m, I_2 m) - (h_2, m) \quad (2.33)$$

where $\delta\sigma_k^{\alpha} = \sigma_k^{\alpha} - m_k^{\alpha}$, $m_k^{\alpha} = \langle \sigma_k^{\alpha} \rangle_y \neq 0$ and the expectation value $\langle \rangle_y$ is taken with the density operator of $H_{\Lambda_d}(yI_2^{\alpha}, y h_2^{\alpha})$. Using the lattice field representations (2.7)

for the two factors m (2.32) as in (2.11–12), one observes that the relation

$$\begin{aligned} \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_2^\alpha, h^\alpha) + (\phi + h, \sigma)] \} &= \exp [-\tfrac{1}{2}(m, I_2 m) + (h, m)] \\ &\quad * \int d\mu_0 \exp [-V(\{\phi^{\alpha'} + \phi^\alpha + h^\alpha - I_2^\alpha m^\alpha\}_d - (\phi' + h - I_2 m, m))] \end{aligned} \quad (2.34)$$

holds.

Applying the scale transformations

$$\phi_k^\alpha \rightarrow \phi_k^\alpha (m_k^\alpha)^{-1} \quad \text{and} \quad \phi_k^\alpha \rightarrow \phi_k^\alpha + m_k^\alpha \sum_{l \in \Lambda_d} (I_2^\alpha)_{kl} (1_l^\alpha - m_l^\alpha) \quad (2.35)$$

to (2.34) it results

$$\begin{aligned} \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_2^\alpha, h^\alpha)] \} \\ = \exp [-\tfrac{1}{2}(m, I_2 m) - \tfrac{1}{2}(1 - m_1 I_2 [1 - m]) - (h - I_2 m, m)] \\ \quad * \text{Tr}_\sigma \{ \exp [-2(n, I_2 n) - (I_2 \cdot 1 - 2I_2 m + h, \sigma)] \} \end{aligned} \quad (2.36)$$

where the scalar products are defined as in Definition 2.1 and $n_k^\alpha = \frac{1}{2}(1_k^\alpha + \sigma_k^\alpha)$. This transformation (2.35) can be performed several times again, which results for the configuration measure $Q_{\Lambda_d} = Q_{\Lambda_d}(I_1^\alpha, h^\alpha)$ the following:

$$\begin{aligned} Q_{\Lambda_d}(I_1^\alpha, h^\alpha) &= \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_1^\alpha, h^\alpha)] \} \\ &= \exp [A^{(n)}(I_2^\alpha, h^\alpha)] \cdot \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_1^\alpha, 0) + (f^{(n)}, \sigma)] \} \end{aligned} \quad (2.37)$$

with

$$f_k^{(n)} = \{f_k^{1,(n)}, f_k^{2,(n)}, f_k^{3,(n)}\}$$

and

$$f_k^{\alpha,(n)} = h_k^\alpha + 2n^\alpha \sum_{l \in \Lambda_d} (I_2^\alpha)_{kl} [1_l^\alpha - m_l^\alpha] \quad (2.38)$$

and $n^\alpha = \pm 1, \pm 2, \dots, \pm N, \dots$. From (2.30–38) it is clear that one can eliminate $f^{(n)}$ in (2.37) under the condition

$$2w^\alpha \sum_{l \in \Lambda_d} (I_1^\alpha)_{kl} = h_k^\alpha + 2n^\alpha \sum_{l \in \Lambda_d} (I_2^\alpha)_{kl} [1_l^\alpha - m_l^\alpha] \quad (2.39)$$

and continuous symmetry breaking, analogously as in the physical quantities of the Ising-model, can be present in the 'broken symmetry region' of the Heisenberg model (2.6) because it holds $yI_2^\alpha > I_1^\alpha > I_{cm}^\alpha$. I_{cm}^α are the matrices which correspond the exact, maximal critical-temperatures $T_{cm\alpha}$.

It is again necessary to show that the susceptibility, specific heat, etc. are divergent in the temperature region $T \leq T_{cm\alpha}$. Therefore we transform (2.37) into a form where the coupling matrices I_1 are entirely replaced by the coupling matrices I_2 . Using the representation (2.7) on the right hand side of (2.32) one obtains:

$$Q_{\Lambda_d}(I_1^\alpha) = \left(\frac{1+y}{1+2y} \right)^{\frac{\Lambda_d}{2}} \exp [C(I_2^\alpha, h^\alpha)] \text{Tr}_\sigma \{ \exp [-\tfrac{1}{2}(\sigma, I_y \sigma) + (B, \sigma)] \} \quad (2.40)$$

with help of the transformations

$$\phi_k^{\alpha'} + \phi_k^{\alpha} \rightarrow \phi_k^{\alpha'} \rightarrow \phi_k^{\alpha'} - \frac{1+y}{1+2y} \sum_{l \in \Lambda_d} (I_2)_{kl}. \quad (2.41)$$

B_k^{α} and I_y^{α} are

$$B_k^{\alpha} = h_k^{\alpha} - \sum_{l \in \Lambda_d} (I_2^{\alpha})_{kl} \left[\frac{y}{1+2y} 1_l^{\alpha} - 2m_l^{\alpha} \right], \quad I_y^{\alpha} = \frac{y}{1+2y} I_2^{\alpha}. \quad (2.42)$$

One can apply this transformation several times again. This results an effective field $B^{(n)}$ with components

$$B_k^{\alpha, (n)} = h_k^{\alpha} + 2n^{\alpha} (B_k^{\alpha} - h_k^{\alpha}), \quad n^{\alpha} = \pm 1, \pm 2, \dots, \pm N, \dots \quad (2.43)$$

on the lattice $Z^d(a)$. Transforming the effective fields $B^{(n)}$ under the condition

$$2w^{\alpha} \sum_{l \in \Lambda_d} (I_2^{\alpha})_{kl} \cdot \frac{y}{1+2y} = B_k^{\alpha, (n)}, \quad w^{\alpha} = 0, \pm 1, \dots, \pm W, \dots \quad (2.44)$$

away, one gains from (2.40) the result

$$\text{Tr}_{\sigma} \{ \exp [-H_{\Lambda_d}(I_1^{\alpha}, h^{\alpha})] \} = \left(\frac{1+y}{1+2y} \right)^{\frac{\Lambda_d}{2}} f(I^{\alpha}, h^{\alpha}, y) \text{Tr}_{\sigma} \{ \exp [-\frac{1}{2}(\sigma, I_y \sigma)] \} \quad (2.45)$$

The function f is brave again.

The fact that it is allowed to choose $I_1^{\alpha} > I_2^{\alpha} > I_y^{\alpha} = I_{cm}^{\alpha}$, allows to work at the exact, maximal critical point I_{cm}^{α} , where the corresponding susceptibility, etc. are divergent and $m_k^{\alpha} \equiv 0$ for $h_k^{\alpha} \equiv 0$. These properties of the configurational measure $Q_{\Lambda_d}(I^{\alpha})$, susceptibility etc. can be shown by using the monoton increasing property of the configuration measure in the off-diagonal couplings of ferromagnetic type [3, 4] for instance. These results prove the theorem again and will not be reproduced here. Q.E.D.

As a consequence of the proof of the Theorem 2.5 one has the

Corollary 2.6. *If $H_{\Lambda_d}(I_1^{\alpha}, h^{\alpha})$ and $H_{\Lambda_d}(I_2^{\alpha}, h_2^{\alpha})$ are two Heisenberg Hamiltonian with constraints*

$$I_1^{\alpha} > I_2^{\alpha} > I_{cm}^{\alpha} = \frac{y}{1+2y} I_2^{\alpha} > 0$$

and $I_1^{\alpha} = I_2^{\alpha}[1+y]$, y a real number $0 < y_{\max}$, then the configuration measures $Q_{\Lambda_d}(I_1^{\alpha}, h^{\alpha})$ and $Q_{\Lambda_d}(I_y^{\alpha})$ and the matrices I_1^{α} and I_2^{α} fulfil the relations

$$\begin{aligned} Q_{\Lambda_d}(I_1^{\alpha}) &= \text{Tr}_{\sigma} \{ \exp [-H_{\Lambda_d}(I_1^{\alpha}, h^{\alpha})] \} \\ &= \left(\frac{1+y}{1+2y} \right)^{\frac{\Lambda_d}{2}} f(I^{\alpha}, h^{\alpha}, y) \text{Tr}_{\sigma} \{ \exp [-\frac{1}{2}(\sigma, I_y \sigma)] \} \end{aligned} \quad (2.45)$$

and

$$2w^{\alpha} \sum_{l \in \Lambda_d} (I_2^{\alpha})_{kl} \cdot \frac{y}{1+2y} = h_k^{\alpha} - 2n^{\alpha} \sum_{l \in \Lambda_d} (I_2^{\alpha})_{kl} \left[\frac{y}{1+2y} \cdot 1_l^{\alpha} - 2m_l^{\alpha} \right] \quad (2.44)$$

with definition

$$m_l^\alpha = [Q_{\Lambda_d}(I_y^\alpha, h_2^\alpha)]^{-1} \cdot \text{Tr}_\sigma \{ \exp [-H_{\Lambda_d}(I_y^\alpha, y h_2^\alpha)] \sigma_l^\alpha \}.$$

These results, especially the Theorems 2.3 and 2.5 with Corollary 2.6, admit the following:

Theorem 2.7. *Let $H_{\Lambda_d}(I_1^\alpha, h^\alpha)$ and $H_{\Lambda_d}(I_2^\alpha, h_2^\alpha)$ be two d -dimensional, anisotropic Heisenberg Hamiltonian of type (2.6), then the physical quantities as free energy, susceptibility, specific heat etc. have singular or divergent behaviour for closed temperature intervals below the exact, maximal critical temperatures T_{cm} and that if the relations*

$$2w^\alpha \sum_{l \in \Lambda_d} (I_1^\alpha)_{kl} = h_k^\alpha + 2n^\alpha \sum_{l \in \Lambda_d} (I_2^\alpha)_{kl} [1_l^\alpha - m_l^\alpha]$$

under the constraint $I_1^\alpha > I_2^\alpha > I_{cm}^\alpha$, $I_1^\alpha = I_2^\alpha [1 + y]$, y real and $y > 0$ are fulfilled for continuous change of the parameters in I_1^α and I_2^α .

The proof of this theorem follows immediately from the considerations made to the Ising and Heisenberg models in this section. Let us turn to the applications of these results.

3. XY-model with external field in the z -direction and superconductivity

A better understanding can be gained in the case of the isotropic XY-model with transverse field in the z -direction by constructing at first upper and lower bounds to the thermodynamic functions. The Hamiltonian can be written as

$$\begin{aligned} H_{\Lambda_d}(v, \varepsilon) &= H_{\Lambda_d}(0, \varepsilon) + V_{\Lambda_d}(v, 0), \\ H_{\Lambda_d}(v, \varepsilon) &= -\frac{1}{2} \sum_{k \in \Lambda_d} [\sigma_k^3 + \varepsilon_k^3]^2 - \frac{1}{2} \sum_{\substack{k, l \\ \alpha=1,2}} v_{k-l} \sigma_k^\alpha \sigma_l^\alpha, \end{aligned} \quad (3.1)$$

the ε_j correspond to the inhomogeneous magnetic field, the matrix (v_{k-l}) is positive definite and $v_0 > 3 \sum_{l \in \Lambda_d, l \neq k} v_{k-l}$. $V_{\Lambda_d}(v, 0)$ is just the interaction part of (3.1).

For the construction of the bounds we use the Golden-Thomson-theorem [9, 10]. Because we make the construction in a finite volume and then we take the thermodynamic limit, it is enough to work at first with finite matrices and therefore to use the

Theorem 3.1. *Let A and B two hermitian square matrices with bounded traces, then*

$$\text{Tr} \{ \exp [A + B] \} \leq \text{Tr} \{ \exp [\tfrac{1}{2}B] \exp [A] \exp [\tfrac{1}{2}B] \} \quad (3.2)$$

holds.

This theorem can be extended to infinite lattice systems [11, 12] which is related to the work of Segal [13].

The proof of phase transition in the model system (3.1) can be gained by using positive definitivity of operators $-H_{\Lambda_d}(v, \varepsilon)$, $-V_{\Lambda_d}(v, 0)$ and $-H_{\Lambda_d}(0, \varepsilon)$ and by using the relation

$$\text{Tr} \{ \exp [A + B] \} \leq [\text{Tr} \{ \exp [2A] \}]^{1/2} [\text{Tr} \{ \exp [2B] \}]^{1/2} \quad (3.3)$$

for bounded and symmetric A and B . The inequality (3.3) follows by Schwarz inequality and by the properties of A and B . To proceed to the construction, we work in the spirit of the Refs. [3, 4, 14].

Theorem 3.2. Let $\hat{\sigma}_q^\alpha$ be the Fourier-transformation of the Pauli-spin operators σ_k^α , $k \in Z^d(a)$, $\alpha = 1, 2$ and q is the d -dimensional wave vector in the Brillouin-zone $Z_B^d(a)$. Further, let

$$\hat{\chi}(v | q) = \lim_{\Lambda_d \rightarrow \infty} [\text{Tr} \{ \exp [-H_{\Lambda_d}(v | \varepsilon)] \}]^{-1} \cdot \text{Tr} \left\{ \exp [-H_{\Lambda_d}(v | \varepsilon)] \sum_{\alpha=1,2} \hat{\sigma}_q^\alpha \hat{\sigma}_q^\alpha \right\} \quad (3.4)$$

define as the XY-correlation function and $\hat{\chi}_I(v/4 | q)$ those of the Ising model. Then these correlation functions $\hat{\chi}_I$ and $\hat{\chi}$ fulfil the inequality

$$\hat{\chi}_I\left(\frac{v}{4} \middle| q\right) \leq \hat{\chi}(v | q) \quad (3.5)$$

under the constraint

$$-\lim_{\Lambda_d \rightarrow \infty} \left[\frac{1}{2\Lambda_d} \ln \text{Tr} \{ \exp [-\frac{1}{2}(\sigma^1, v\sigma^1)] \} + \frac{1}{\Lambda_d} \sum_{k \in \Lambda_d} \ln \text{ch } \varepsilon_k \right] \geq 0 \quad (3.6)$$

with

$$(\sigma^1, v\sigma^1) = \sum_{k,l \in \Lambda_d} \sigma_k^1 v_{k-l} \sigma_l^1.$$

Proof. Choosing A and B in (3.3) as

$$A = -\frac{1}{2}H_{\Lambda_d}(v, \varepsilon), \quad A + B = -\frac{1}{2}V_{\Lambda_d}(v, 0)$$

one gets the inequality

$$\begin{aligned} \lim_{\Lambda_d \rightarrow \infty} \left[\frac{1}{\Lambda_d} \ln \text{Tr} \{ \exp [-\frac{1}{2}V_{\Lambda_d}(v, 0)] \} - \frac{1}{2\Lambda_d} \ln \text{Tr} \{ \exp [H_{\Lambda_d}(0, \varepsilon)] \} \right] \\ \leq \lim_{\Lambda_d \rightarrow \infty} \frac{1}{2\Lambda_d} \ln \text{Tr} \{ \exp [-H_{\Lambda_d}(v, \varepsilon)] \}. \end{aligned} \quad (3.7)$$

Further using

$$\begin{aligned} \frac{1}{\Lambda_d} \ln \text{Tr} \{ \exp [\frac{1}{4}(\sigma^1, v\sigma^1)] \} \leq \frac{1}{2\Lambda_d} [\ln \text{Tr} \{ \exp [-V_{\Lambda_d}(v, 0)] \} \\ + \ln \text{Tr} \{ \exp [-\frac{1}{2}(\sigma^1, v\sigma^1)] \}] \end{aligned}$$

and the definition

$$\frac{1}{\Lambda_d} \ln \text{Tr} \{ \exp [-V_{\Lambda_d}(v, 0)] \} = - \int_0^1 d\lambda \frac{1}{\Lambda_d} \text{Tr} \{ \rho_{\Lambda_d}(\lambda v) \frac{\partial}{\partial \lambda} V_{\Lambda_d}(\lambda v, 0) \} \\ + \frac{1}{\Lambda_d} \ln \text{Tr} \{ \exp [-V_{\Lambda_d}(0, 0)] \}$$

in the inequality (3.7), then the inequality (3.5) of the theorem follows under the constraint (3.6). Q.E.D.

Corollary 3.3. *Under the constraint (3.6) it holds*

$$\chi_I \left(\frac{v}{4} \mid k-l \right) \leq \chi(v \mid k-l) \quad (3.8)$$

by the Fourier-transformation of (3.5).

From the works [3, 4, 14] it follows that cumulant inequalities can be derived for the model (3.1). Let us denote the two point cumulant, associated to the model (3.1), by

$$\chi_\alpha^c(v \mid k-l) = \chi_\alpha(v \mid k-l) - \langle \sigma_k^\alpha \rangle \langle \sigma_l^\alpha \rangle \quad (3.9)$$

with $\chi_\alpha(v \mid k-l) = \langle \sigma_k^\alpha \sigma_l^\alpha \rangle$ and $\langle A \rangle$ denotes the expectation value of an operator with respect to the density operator of (3.1). The two point cumulant of the Ising model is

$$\chi_I^c(v \mid k-l) = \chi_I(v \mid k-l) - \langle \sigma_k^3 \rangle_I \langle \sigma_l^3 \rangle_I \quad (3.10)$$

with an expectation value of an operator $\langle A \rangle_I$ belonging to the Ising-model. Let us note the

Theorem 3.4. *Under the condition (3.6) the d -dimensional two point cumulants of the XY-model with external, inhomogeneous field in the z -direction fulfil the cumulant inequalities*

$$\chi_I^c(3v \mid k-l) \geq \chi_\alpha^c(v \mid k-l) \geq \chi_I^c\left(\frac{1}{4}v \mid k-l\right) \quad (3.11)$$

which has the consequence that it holds

$$\lim_{k-l \rightarrow \infty} \langle \sigma_k^\alpha \sigma_l^\alpha \rangle = \langle \sigma_m^\alpha \rangle \langle \sigma_n^\alpha \rangle \quad (3.12)$$

in the thermodynamic limit and for $v > v_{cm}$, where χ_I^c is the two point cumulant of the Ising model and v_{cm} corresponds to the exact, maximal critical temperature.

The proof of this theorem is essentially in Refs. [4, 14] and we shall not present it here.

The Theorems 3.2 and 3.4 are the basis of the existence of continuous symmetry breaking in the model (3.1). Further, the application of the Theorems

(2.3), (2.5) and (2.7) to the physical quantities of the model (3.1) leads to the statement:

Theorem 3.5. *The XY-model with inhomogeneous, external field ε_k in the z -direction has continuous symmetry breaking in the points of a closed interval of temperature axis below the exact, maximal critical temperature T_{cm} and in the case $\varepsilon_k < \varepsilon_{\max}$ for all $k \in Z^d(a)$, where the static susceptibility $\hat{\chi}_\alpha^c(v | q=0)$ does diverge with critical point exponent γ .*

Proof. Because the cumulant inequalities (3.11) are valid for all $k, l \in Z^d(a)$ we may sum over the index l in (3.11) and the inequalities remain valid. Applying the Theorems 2.3, 2.5 and 2.7 to the lower and upper bounds of the gained result, one obtains the proof of the theorem if one takes $h_k^1 = h_k^2 = 0$, $(I^3)_{kl} = 0$ and $\varepsilon_k < \varepsilon_{\max}$ for all $k, l \in Z^d(a)$. The condition $\varepsilon_k < \varepsilon_{\max}$ is known from high temperature expansions. Q.E.D.

To come to the interesting point of the XY-model with inhomogeneous, external field in the z -direction (3.1) we note that the model (3.1) is in a well defined relation to the BCS-model of superconductivity [5, 6] and to a generalized Dicke model of lasers. In these two cases it is interesting to study the resistivity. In the superconducting state of matter the isothermal resistivity is zero. The relation of (3.1) to the original electron-phonon or electron-photon system is approximative but can be controlled and will not be studied here.

Let us define the scalar product

$$(X, Y) = \text{Tr} \{ X^+ \delta \int_0^1 d\lambda Y(-i\lambda) \} \quad (3.13)$$

where $Y(-i\lambda) = \exp[\lambda H] Y \exp[-\lambda H]$, ρ denotes the density operator of the model with local Hamiltonian $H \sim \Lambda_d^0$, i.e. the spectrum of H is of order Λ_d^0 [11, 12], the resolvent operator $R(z)$ is given by

$$R(z) = [z - L]^{-1}, \quad LX = HX - XH \quad \text{and} \quad z \in \mathbb{C}. \quad (3.14)$$

Theorem 3.6. *Let F_α be the α th component of the force operator*

$$F_\alpha = iLj_\alpha = - \int \frac{dq^d}{(2\pi)^d} \frac{\partial \hat{\varepsilon}(q)}{\partial q_\alpha} \int \frac{dp^d}{(2\pi)^d} \times [\hat{v}(p) - \hat{v}(p+q)] [\hat{\sigma}_{-p}^1 \hat{\sigma}_{p+q}^2 + \hat{\sigma}_{p+q}^2 \hat{\sigma}_{-p}^1] \quad (3.15)$$

with Fourier transformations $\hat{\varepsilon}(q)$, $\hat{v}(q)$ and $\hat{\sigma}_q$ of ε_k , v_{kl} and the spin operators σ_k^α . The integrations in (3.15) are taken over the Brillouin zone $Z_B^d(a)$, p and $q \in Z_B^d(a)$. Then the isothermal, local resistivity,

$$(R_i^l)_{\alpha\alpha} = i(en)^{-2} (F_\alpha, R(i0)F_\alpha), \quad (3.16)$$

is zero for the model (3.1) in a finite, closed interval of the temperature axis and that below the exact, maximal critical temperature T_{cm} and $\varepsilon < \varepsilon_{\max}$ for all $k \in Z^d(a)$.

Proof. Note that the force operator F_α (3.15) is constructed with help of the current operator

$$j_\alpha = \int \frac{dq^d}{(2\pi)^d} \frac{\partial \hat{\varepsilon}(q)}{\partial q_\alpha} [\hat{\sigma}_q^3 + 1] \quad (3.17)$$

but the spin operators $\hat{\sigma}_q^\gamma$ fulfil the commutation relations

$$[\hat{\sigma}_q^\alpha, \hat{\sigma}_p^\beta] = i \epsilon_{\alpha\beta\gamma} \sigma_{p+q}^\gamma \quad (3.18)$$

which are different from those used in Ref. [6].

To evaluate exactly the isothermal, local resistivity (3.16) below the exact, maximal critical temperature T_{cm} and $\varepsilon_k < \varepsilon_{max}$ for all $k \in Z^d(a)$, we use the relation

$$\begin{aligned} (R_i^l)_{\alpha\alpha} &= i(en)^{-2} (F_\alpha, R(i0)F_\alpha) \\ &= (en)^{-2} \frac{\beta}{2} \int_{-\infty}^{\infty} dt \operatorname{Tr} \{ \rho [F_\alpha, F_\alpha(t)]_+ \}, \end{aligned} \quad (3.19)$$

which can be gained by inequalities [15] or by other methods [16]. In (3.19) we have written explicitly the temperature factor $\beta = (k_B T)^{-1}$.

Let us choose the band energy $\hat{\varepsilon}(q)$ in (3.15–16) so that our working points are always in the critical region of the critical temperature T_{cm} . Notice, this choice of parameter values does not affect the fact that the adiabatic conductivity is zero, i.e.

$$\lim_{\omega \rightarrow 0} \sigma_{\alpha\alpha}(0, \omega) = \lim_{\omega \rightarrow 0} a \cdot \omega^\lambda = 0, \quad \lambda > 0 \quad (3.20)$$

and therefore the dynamical critical point exponent λ must fulfill the relation $\lambda > 0$ and a must be greater or equal to zero, $a \geq 0$. To evaluate the isothermal, local resistivity (3.16) or (3.19) on the critical temperature line, we make the scale transformation

$$\hat{\sigma}_q^\alpha = \zeta \hat{s}_{q\xi}^\alpha \quad (\hat{\varepsilon}_q > \varepsilon_{max} \text{ at first}) \quad (3.21)$$

with constraint that ξ is the correlation length associated to the symmetry breaking and ζ is given by the relation that the two susceptibilities given by (3.21) are identical. It holds

$$\zeta = \xi^{(d/2+1-\eta/2)}, \quad (3.22)$$

where d is the dimension of the lattice $Z^d(a)$ and η is the anomalous dimension. $\langle \hat{\sigma}_q^\alpha \hat{\sigma}_{-q}^\alpha \rangle$ can be represented as

$$\langle \hat{\sigma}_q^\alpha \hat{\sigma}_q^\alpha \rangle = \zeta^2 \xi^{-d} \langle \hat{s}_{q\xi}^\alpha \hat{s}_{q\xi}^\alpha \rangle = \xi^{2-\eta} \langle \hat{s}_{q\xi}^\alpha \hat{s}_{q\xi}^\alpha \rangle, \quad (3.23)$$

i.e. in scaling form. ξ^{-d} in the 1st equality comes from the δ -function (gained by averaging).

Using the inequality

$$\begin{aligned} \rho &\leq \rho(v) = [\operatorname{Tr} \{ \exp [-H(v, \varepsilon)] \}]^{-1} \prod_{\alpha=1,2,3} \exp [V(\varepsilon^\alpha)], \\ V(\varepsilon^\alpha) &= \int_{\frac{d}{B}} \frac{dx^d}{(2\pi)^d} [\hat{s}_x^\alpha + \hat{\varepsilon}^\alpha(x)]^2, \quad \hat{\varepsilon}^3(x) = \hat{\varepsilon}(x), \end{aligned} \quad (3.24)$$

one can construct upper bounds to the isothermal, local resistivity. We choose the ε_k^α such that the $V_{\Lambda_d}(\varepsilon^\alpha)$ -models do not exhibit continuous symmetry breaking and the expectation values do exist. Therefore it holds after the scale transformations:

$$(R_i^l)_{\alpha\alpha} \leq (en)^{-2} \frac{\beta}{2} \int_{-\infty}^{\infty} dt \operatorname{Tr} \left\{ \rho(v) \left[F_\alpha \left(\frac{t}{2} \right), F_\alpha \left(\frac{t}{2} \right) \right]_+ \right\} \leq \xi^{2-2d-2\eta} \cdot C(\xi). \quad (3.25)$$

Using the scaling transform (3.21) in the force operator,

$$F_\alpha = -\xi^{-d-1} \int_{\frac{d}{B}} \frac{dx^d}{(2\pi)^d} \frac{\partial \hat{\varepsilon}^3(x/\xi)}{\partial x_\alpha} \int \frac{dy^d}{(2\pi)^d} [\hat{v}(y/\xi) - \hat{v}(y/\xi + x/\xi)] [\hat{s}_y^1, \hat{s}_{y+x}^2]_+, \quad (3.26)$$

it allows to evaluate the upper bound (3.25) of $(R_i^l)_{\alpha\alpha}$. In (3.26) the integration boundaries do depend on ξ ,

$$\frac{\partial \hat{\varepsilon}^3(x/\xi)}{\partial x} \rightarrow 0$$

for $\xi \rightarrow \infty$ if $d + \eta > 1$ therefore $C(\xi)$ goes to zero thanks the derivative of $\hat{\varepsilon}^3(x/\xi)$. But ξ goes to infinity if we approach the critical interval of temperature axis below the exact, maximal critical temperature for $\hat{\varepsilon}^3(q) = \hat{\varepsilon}^3(q) < \varepsilon_{\max} = \text{constant}$, which proves the Theorem 3.6. Note this is consistent with the assumption of dynamical scaling and the definition of adiabatic conductivity or resistivity (3.20).

Q.E.D.

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Dynamics of the $S = \frac{1}{2}$ linear Heisenberg antiferromagnet at zero temperature

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We present an analytical expression for the dynamical spin correlation function of the $S = \frac{1}{2}$ linear Heisenberg antiferromagnet in (q, ω) -space at $T = 0$. Our approach is based on the fact that the spectrum is dominated by a continuum of spin-wave excitations. Using sum rules we obtain the susceptibility and the static correlation function. In the presence of a uniform magnetic field the spectrum is expected to have a double-peaked structure.

**Sur les équations d'équilibre des systèmes classiques
avec forces de portée quelconque**

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On étudie les systèmes classiques de particules ponctuelles interagissant par potentiels de portée quelconque.

En définissant les états d'équilibre par une généralisation de la condition KMS, on montre que les mesures de corrélation sont maxwelliennes dans les vitesses et satisfont les équations de BBGKY au sens des distributions.

On établit que les mesures de corrélation sont des fonctions de classe C' , si les forces sont elles-mêmes régulières et de portée finie.

Le cas des forces à longue portée est illustré par les systèmes coulombiens à une dimension.

**Paramagnons and magnons of the quantum Heisenberg model
and the modular Hilbert algebras**

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Abstract. The problem of the Fourier transform of generalized operators is considered for the case where the operators grow with respect to the transforming parameter n as $O(n^N)$. These considerations allow to discuss linear response theory of the quantum Heisenberg model by modular Hilbert algebras. The response and relaxation functions are defined for any vectorstate to discuss them by the perturbation theory for nearly degenerate spectra. It is shown for the quantum Heisenberg model that the dynamical longitudinal and transversal magnetic susceptibilities possess at least a two pole structure for temperatures T above and below the transition temperature T_c . The longitudinal ones are overdamped for all temperatures; on the contrary the transversal ones are not for $T < T_c$; that is the longitudinal and transverse paramagnons and the longitudinal magnons are overdamped, but the transverse magnons are not and they possess a gap at the center of the Brillouin zone.

1. Introduction

The conventional statistical mechanics is described by the equilibrium state of a finite system which is a Gibbs-state. The state of an infinite continuous system can be also a Gibbs-state [1]: a generalized Gibbs-state. Further, one can show for a certain class of operators that these Gibbs-states [1] and the KMS-condition or detailed balance are equivalent because the latter can be generated from the first one. This will not be shown here, but just used in the KMS-condition. If one would like to consider a lattice system in the thermodynamic limit, one must transform it to a continuous one to gain its Gibbs-state. To perform this transformation, generalized operators and their Fourier transforms are introduced in section 2, where some results on Fourier transform of generalized functions [2, 3] is generalized to operators [4]. These conditions allow to transform the lattice Heisenberg model described by discrete spin observables into those Heisenberg models represented by continuous spin observables and to work in the thermodynamic limit.

To formulate linear response theory by modular Hilbert algebras [5], one must introduce a new scalar product on the set of observables and define a new Hilbert space $\mathcal{H}^\Delta$ [6].

Giving the operator representation of the response and the relaxation function, the perturbation theory for nearly degenerate spectra [7] is applied to these functions. This application of perturbation theory of nearly degenerate spectra to linear response theory allows to make contact with the theory of hydrodynamics as Navier-Stokes equation, etc. or with transport equations as the Boltzmann equation [8, 9].

In the section 4 these theories have been applied to the quantum Heisenberg model. For this model it is shown that the longitudinal and transverse dynamical, magnetic susceptibilities possess at least a two pole structure which can be interpreted as paramagnons above the transition temperature T_c and magnons for temperatures $T < T_c$. The paramagnons and the longitudinal magnons are overdamped; on the contrary the transversal magnons are not overdamped near the Brillouin zone center. Further the transverse magnons have a gap at the center of the Brillouin zone for magnetic field $h = 0$ [10]. These results clear up ambiguities in the present literature about paramagnons [11] and about the gap in the magnon spectrum of the quantum Heisenberg model.

2. Generalized operators

In this section, generalized operators will shortly be explored to develop the Fourier transform of them. Some of these generalized operators are in themselves interesting and have a great advantage to describe the Fourier transform of operators. Let us start with the introduction of some definitions.

2.1. Definition. Let D_0 be a fundamental space of a class of fundamental functions $\phi \in D_0$ with support ϕ in the set $0 = 0_1 \times 0_2 : 0_1 \subseteq \mathbf{R}^d, \text{supp } \phi \subset 0$. A continuous linear functional (f, ϕ) in some fundamental space D_0 is called a

generalized function:

$$(f, \phi) = \int_{0_1} d^d x \langle f, \phi \rangle(x) = \int_{0_1} d^d x \langle f(x), \phi(x) \rangle \quad (2.1)$$

where $\langle \ , \ \rangle$ denotes traces or integrals associated to the set 0_2 . Further, let A_n be an operator depending on the parameter n . The norm of A_n is defined by the conjugate operator A_n^* as

$$\|A_n^*\| = \sup_{\phi \in D_0} \frac{\|A_n^* \phi\|}{\|\phi\|} \quad (2.2)$$

Let $\|A_n^*\|$ be of order n^α : $A_n = O(n^\alpha)$ for $|n| \rightarrow \infty$. The operator A_n maps a space D'_0 into a space $\mathcal{E}'_0$ and fulfills the relation

$$T_m A_n T_m^{-1} = A_{n+m}, \quad (2.3)$$

where T_m is the translation operator and

$$m, n \in \Lambda_d \subset \mathbf{Z}^d = \left\{ n = \sum_{i=1}^d 1_i n_i \mid n^i = 0, \pm 1, \pm 2, \dots \right\}.$$

2.2. Theorem. The Fourier series

$$\sum_{n \in \Lambda_d} A_n \exp(inx) \quad (2.4)$$

of the operators A_n converges then and only then to a generalized operator $A(x)$, if there is an α such that $\|A_n^*\| = O(n^\alpha)$ for $|n| \rightarrow \infty$. In the case of convergence and if $[A_n, x] = A_n x - x A_n = 0$ holds for all $n \in \Lambda_d$, then the Fourier transform of the generalized operator $A(x)$ can be written as

$$\hat{A}(y) = \sum_{n \in \Lambda_d} A_n \delta(y - n) \quad (2.5)$$

for $[A_n, y] = 0$. $\hat{A}(y)$ is a generalized operator again.

Proof. Because the operator A_n , $n \in \Lambda_d$, maps the space D'_0 into the space $\mathcal{E}'_0$, therefore the conjugate operator A_n^* maps D_0 into $\mathcal{E}_0$ and does depend on the parameter n . Further, A_n^* is bounded for finite n , then A_n is also bounded for finite n . It holds $(\lim_{n \rightarrow n_0} A_n^*)^* = \lim_{n \rightarrow n_0} A_n$, while for any $f \in D'_0$ and $\phi \in \mathcal{E}_0$ it holds

$$(A_n f, \phi) = (f, A_n^* \phi) \rightarrow (f, A_{n_0}^* \phi) = (A_{n_0} f, \phi).$$

Because of this fact, the series (2.4) is only converging to the generalized operator $A(x)$, if the series – made by the term by term Fourier transform, towards $\hat{A}(y)$ converges, which is the Fourier transform of $A(x)$. Therefore, it is enough to consider the series (2.5). Let us consider the operator

$$\hat{A}_1(y) = \sum_{\substack{n \in \Lambda_d \\ n \geq 0}} A_n H(y - n) - \sum_{\substack{n \in \Lambda_d \\ n < 0}} A_n H(-y - n). \quad (2.6)$$

For every fundamental function ϕ , it holds

$$\begin{aligned} (\hat{A}_1 f, \phi) &= \int d^d y \langle \hat{A}_1 f, \phi \rangle(y) \\ &= \sum_{\substack{n \in \Lambda_d \\ n \geq 0}} \int d^d y \langle A_n f(y), H(y-n)\phi(y) \rangle \\ &\quad - \sum_{\substack{n \in \Lambda_d \\ n < 0}} \int d^d y \langle A_n f(y), H(-y-n)\phi(y) \rangle, \end{aligned}$$

which is convergent. Therefore the series, which can be gained by differentiation of (2.6), converges towards the generalized operator $A(x)$ with its Fourier transform $\hat{A}(y)$. Q.E.D.

This above theorem can be generalized easily to the case if the operator A_n for all $n \in \Lambda_d$ does not commute with x and y , but which we don't do here.

Let $U(x)$ be an unitary fundamental function, which is zero for x not in the elementary cell v of Λ_d . $U(x)$ fulfills

$$\sum_{n \in \Lambda_d} U\left(\frac{x}{2\pi} + n\right) = 1 \quad (2.7)$$

and its Fourier transform $\hat{U}(x)$ is zero if $x = m$, $m \neq 0$ and $\hat{U}(x) = 1$ for $x = 0$.

2.3. Theorem. Let $A(x)$ be a generalized operator of the form (2.4) and $U(x)$ an arbitrary unitary fundamental function, then it holds

$$A_m = \frac{1}{(2\pi)^d} \int A(x) U\left(\frac{x}{2\pi}\right) \exp(-imx) d^d x. \quad (2.8a)$$

Let the generalized operator $A(x)$ be periodic, $A(x) = A(x + 2\pi n)$. In this case, the equation (2.8a) reduces to

$$A_m = \frac{1}{(2\pi)^d} \int_v A(x) \exp(-imx) d^d x. \quad (2.8b)$$

Proof. One has

$$A_m = \frac{1}{(2\pi)^d} \sum_{n \in \Lambda_d} A_n \int U\left(\frac{x}{2\pi}\right) \exp(i[n-m]x) d^d x = A_m$$

because

$$\frac{1}{(2\pi)^d} \int U\left(\frac{x}{2\pi}\right) \exp(i[n-m]x) d^d x = \delta_{n,m}.$$

Further, it holds

$$\begin{aligned}
 A_m &= \frac{1}{(2\pi)^d} \int A(x) U\left(\frac{x}{2\pi}\right) \exp(-imx) d^d x \\
 &= \sum_{n \in \Lambda_d} \frac{1}{(2\pi)^d} \int_v A(x + 2\pi n) U\left(\frac{x}{2\pi}\right) \exp(-imx) d^d x \\
 &= \sum_{n \in \Lambda_d} \frac{1}{(2\pi)^d} \int_v A(x) U\left(\frac{x}{2\pi} + n\right) \exp(-imx) d^d x \\
 &= \frac{1}{(2\pi)^d} \int_v A(x) \exp(-imx) d^d x,
 \end{aligned}$$

while the relation $\sum_n U(x/2\pi + n) = 1$ holds.

Q.E.D.

It follows:

2.4. Theorem. Let $A(x)$ be a periodic generalized operator with the period 2π and let its Fourier transform be $\hat{A}(y)$, then it holds

$$A(x) = \sum_{n \in \Lambda_d} A_n \exp(inx),$$

$$\hat{A}(y) = \sum_{n \in \Lambda_d} A_n \delta(y - n)$$

and

$$A_n = \frac{1}{(2\pi)^d} \int_y A(x) \exp(-inx) d^d x,$$

if $[A_n, x] = 0$ and $[A_n, y] = 0$.

The proof of this theorem follows from the previous Theorems 2.2 and 2.3.

Let B_1 and B_2 be two generalized operator in D'_0 , i.e.

$$\lim_{\alpha} B_i[f - f_{\alpha}] = 0 \quad \text{for } f, f_{\alpha}, B_i f \quad \text{and} \quad B_i f_{\alpha} \in D'_0.$$

Then the sum and the product of two generalized operator, $B_1 + B_2$ and $B_1 B_2$, are also in D'_0 . Multiplication of a generalized operator B with a complex number λ gives again a generalized operator (λB) in D'_0 . Therefore the generalized operators in D'_0 form an algebra. An algebra is called a C^* -algebra, if the algebra contains the adjoint elements also and a norm is defined on the algebra.

As an application of generalized operators, we will consider the algebra of spin operators in section 4. To discuss physical properties of the Heisenberg model in the sense of linear response theory, let us consider the algebraic formulation of this theory.

3. Projection technique and linear response theory

The necessary mathematical material to this section has been partly developed and proved for linear response theory on an algebraic way in [5, 6]. These results will be extended to the perturbation theory of nearly degenerate spectra.

The foregoing section was devoted to introduce generalized operators which can make up the Hamiltonian H , but here H will be a bounded operator.

Let ω be any vector state on the von Neumann algebra $\mathcal{M}$ satisfying the KMS-condition at temperature $T = \beta^{-1}$, Boltzmann constant $k_B = 1$. The Hilbert space $\mathcal{H}$, on which $\mathcal{M}$ is defined, contains a cyclic element Ω which is separating and defines the vector state $\omega(x) = (\Omega, x\Omega)$ for all $x \in \mathcal{M}$.

Some results on modular Hilbert algebras can be condensed in the following lemma:

3.1. Lemma. *If Ω is separating and H is self-adjoint operator on $\mathcal{H}$, then there exists an operator $\Delta^\beta = \exp(-\beta H)$ on $\mathcal{H}$ such that*

$$\Delta^\beta \Omega = \Omega, \quad \Delta^\beta = FS \quad \text{and} \quad \Delta^{-\beta} = SF,$$

where

$$S = J\Delta^{\beta/2} = \Delta^{-\beta/2}J, \quad F = J\Delta^{-\beta/2} = \Delta^{\beta/2}J.$$

The isometric involution J in $\mathcal{H}$ satisfies $J\Delta^{it} = \Delta^{it}J$. S and F are just conjugate linear operators in $\mathcal{H}$, whose domains are dense in $\mathcal{H}$.

The proof of this lemma is given in [5].

3.2. Definitions. The state ω over $\mathcal{M}$ satisfies the KMS-boundary condition:

$$\begin{aligned} F_{xy}(t) &= \omega(x_t y) = (\Delta^{it} x \Omega, y \Omega) \\ F_{xy}(t - i\beta) &= \omega(y x_t) = (y \Omega, \Delta^{it+\beta} x \Omega) \end{aligned} \quad (3.1)$$

where $F_{xy}(z)$ is defined on the strip $-\beta < \text{Im } z < 0$ for $x, y \in \mathcal{M}$ and $x_t = \Delta^{it} z \Delta^{-it}$. With respect to the scalar product

$$(x, y) = \frac{1}{2} \int_{-\beta}^{\beta} d\alpha (\Delta^{(1/4)(\beta+\alpha)} x \Omega, \Delta^{(1/4)(\beta+\alpha)} y \Omega) \quad (3.2)$$

one can define a Hilbert space as the closure of $\mathcal{M}$.

It is of interest to note that the following results hold: The Fourier-Laplace transform of the relaxation function $\phi_{xy}(t)$ and the admittance $\hat{\chi}_{xy}(z)$ are given by

$$\begin{aligned} \hat{\phi}_{xy}(z) &= \frac{1}{2} \int_{-\beta}^{\beta} d\alpha (\Delta^{(1/4)(\beta+\alpha)} x \Omega, R(z) \Delta^{(1/4)(\beta+\alpha)} y \Omega) \\ &= (x, R(z)y), \quad z \in \mathbf{C} \end{aligned} \quad (3.3)$$

and

$$\hat{\chi}_{xy}(z) = (x, y) - z \hat{\phi}_{xy}(z) \quad (3.4)$$

for $R(z) = [z - H]^{-1}$ and $x, y \in \mathcal{M}$.

In the equations (3.1–4) the elements $x, y \in \mathcal{M}$ are chosen such that $\omega(x) = (\Omega, x\Omega) = 0$, i.e. if $\omega(x) = 0$ would not be the case then x is replaced by its invariant part $x - \omega(x)$.

Furthermore the vector state ω on $\mathcal{M}$ with separating cyclic element Ω of $\mathcal{H}$ defines the separating cyclic projection p_Ω . One has

3.3. Definitions of projections

(1) $\omega(x) = \omega(p_\Omega x) = \omega(xp_\Omega) = \omega(p_\Omega xp_\Omega)$.

(2) Let $a\Omega$ be a normed vector of $\mathcal{H}$, such that $\omega(a^*a) = 1$, $a \in \mathcal{M}$.

To $a\Omega$ associated projection is denoted by $p_{a\Omega}$.

(3) The scalar product (3.2) defines the projection P_a by

$$(x, P_a y) = (x, a)(a, y) \quad \text{and} \quad (a, P_a a) = 1 \quad (3.5)$$

with normed elements $a \in \mathcal{M}$.

The relation (3.5) just makes explicit the map from the Hilbert space associated to the scalar product (3.2) into $\mathcal{H}$. Let us denote this Hilbert space by $\mathcal{H}^\Delta$. One can define an operator U which maps $\mathcal{H}^\Delta$ into $\mathcal{H}$ by $Ux = Tx\Omega$ for all $x \in \mathcal{M}$ and relates the two scalar products (x, y) (3.2) and $\omega(x^*y)$.

The functions $\hat{\phi}_{xy}(z)$ characterize the spectrum of the Hamiltonian H . The resonances of $\hat{\phi}_{xy}(z)$ can be constructed with perturbation theory of nearly degenerate spectra. Let P be the projection on an n -dimensional orthogonal subspace of $\mathcal{H}^\Delta$:

$$P = \sum_{k=1}^n P_{a_k}, \quad Q = 1_{\mathcal{H}^\Delta} - P, \quad P_{a_k} P_{a_l} = 0 \quad (3.6)$$

for $k \neq l$ and $1 \leq k, l \leq n$. Q project on the orthogonal complement of $P\mathcal{H}^\Delta$. The P_{a_k} project on orthogonal subspaces.

3.4. Propositions. Let z be complex, $z \in \mathbf{C}$ with $\text{Im } z \neq 0$ and the Hamiltonian H bounded, then it holds

$$PR(z)P = P[z - PHP - PHQR_Q(z)QHP]^{-1}P \quad (3.7)$$

with regular resolvents

$$R(z) = [z - H]^{-1} \quad \text{and} \quad R_Q(z) = [z - QHQ]^{-1}. \quad (3.8)$$

Proof. The complex number z is a regular point of an element $x \in \mathcal{M}$ if the resolvent of x exists. The non-regular points of the resolvent are called the spectrum of x . Let $N(1_{\mathcal{H}^\Delta})$ be a neighbourhood of the unity of the von Neumann algebra, whose elements possess an inverse one: z^{-1} . Because $1_{\mathcal{H}^\Delta} - z^{-1}x$ is continuous in z^{-1} , one has $1_{\mathcal{H}^\Delta} - z^{-1}x \in N(1_{\mathcal{H}^\Delta})$ for $|z^{-1}| < \varepsilon$. Further it holds

$$\lim_{z^{-1} \rightarrow 0} [1_{\mathcal{H}^\Delta} - z^{-1}x]^{-1} = 1_{\mathcal{H}^\Delta}$$

and the resolvent is analytic, so that $R(z)$ and $R_Q(z)$ are regular.

To prove the relation (3.7) one finds from the relation $[z - H]R(z)P = P$:

$$[z - PHP]PR(z)P - PHQQR(z)P = P, \quad (3.9)$$

$$[z - QHQ]QR(z)P - QHPR(z)P = 0. \quad (3.10)$$

From (3.10):

$$QR(z)P = R_Q(z)QHP^2R(z)P.$$

Using this in (3.9), one gets

$$[z - PHP - PHQR_Q(z)QHP]PR(z)P = P,$$

which proves (3.7).

Q.E.D.

Note that the relation (3.7) is just an operator representation of the relaxation function $\hat{\phi}_{xy}(z)$ if the elements $x, y \in \mathcal{M}$ generate the subspace $P\mathcal{H}^\Delta$. Further the resolvent operator, given by the inverse of the angular bracket in (3.7), is regular and analytic for $\text{Im } z \neq 0$. The following holds:

3.5. Theorem. *The scalar product (x, y) (3.2) and the imaginary part of the relaxation function $\phi_{xy}(z)$ (3.3) are Hermitian,*

$$\phi_{xy}(z) \text{ fulfills } \phi_{xy}^+(z) = \phi_{xy}(\bar{z}).$$

Therefore to the subspace $P\mathcal{H}^\Delta$ associated relaxation matrix $\phi(z)$ satisfies the relations $\phi^+(z) = \phi(\bar{z})$ and $\text{Im } \phi(z) = \text{Im } \phi(z)^T$, where $+$ denotes hermetic conjugate and A^T the transposed matrix.

Proof. The properties of F and S , see Lemma 3.1, allow to prove the theorem. F is the adjoint of S and maps $\mathcal{H}$ to $\mathcal{H}$ or $\mathcal{H}^\Delta$ to $\mathcal{H}^\Delta$. Therefore

$$(Fx, Sy) = \overline{(x, y)}$$

for any $x \in \mathcal{D}(F)$ and any $y \in \mathcal{D}(S)$. Because the operators $S = J\Delta^{\beta/2} = \Delta^{-\beta/2}J$ and $F = J\Delta^{-\beta/2} = \Delta^{\beta/2}J$ are involutions, one has $Sy \in \mathcal{D}(S)$ and $Fx \in \mathcal{D}(F)$ for $y \in \mathcal{D}(S)$ and $x \in \mathcal{D}(F)$, so that J is a unitary linear operator from $\mathcal{H}$ to $\mathcal{H}$ or from $\mathcal{H}^\Delta$ to $\mathcal{H}^\Delta$.

It follows from (3.2):

$$\overline{(x, y)} = (y, x)$$

which proves the hermeticity of (3.2) by $(Ja, Jb) = \overline{(b, a)}$ and $a, b \in \mathcal{M}$.

To prove the hermeticity of $\text{Im } \phi_{xy}(z)$ and the relation $\phi_{xy}^+(z) = \phi_{xy}(\bar{z})$, it is necessary to consider the hermetic character of $(x, \Delta^{it}y)$.

It holds:

$$\begin{aligned} (x, \Delta^{it}y) &= \frac{1}{2} \int_{-\beta}^{\beta} d\alpha (\Delta^{(1/4)(\beta+\alpha)} Fx \Omega, \Delta^{it} \Delta^{(1/4)(\beta+\alpha)} Sy \Omega) \\ &= \frac{1}{2} \int_{-\beta}^{\beta} dx (J\Delta^{(1/4)(\beta+\alpha)} x \Omega, J\Delta^{it} \Delta^{(1/4)(\beta+\alpha)} y \Omega) = (\Delta^{it}y, x) \end{aligned}$$

by the fact $J\Delta^{it} = \Delta^{it}J$ and therefore

$$\overline{\text{Im } \phi_{xy}(z)} = -\overline{\pi(x, \delta(\omega - H)y)} = -\pi(y, \delta(\omega - H)x) = \text{Im } \phi_{yx}(z)$$

for $z = \omega + i0$. From this fact $\phi_{xy}^+(z) = \phi_{xy}(\bar{z})$ follows.

Q.E.D.

From the holomorphic property of the relaxation matrix $\phi(z)$ for $\text{Im } z \neq 0$, it follows that $\det \phi(z) \neq 0$ and therefore the inverse matrix $\phi^{-1}(z)$ is also holomorphic. In accordance to this and the relation (3.7) of Proposition 3.4, the

relaxation matrix $\phi(z)$ can be represented by

$$\phi(z) = [z - \psi + \Sigma(z)]^{-1} \chi^0 \quad (3.11)$$

with definitions

$$\psi = \gamma \chi^{0-1}, \quad \gamma_{xy} = (x, Hy), \quad \chi_{xy}^0 = (x, y) \quad (3.12)$$

and

$$\Sigma(z) = m(z) \chi^{0-1}, \quad m_{xy}(z) = -(QHx, R_Q(z)QHy), \quad (3.13)$$

for all $Ux, Uy \in \mathcal{H}$. From Theorem 3.5, it follows that γ and $\text{Im } m(z)$ are hermetic.

3.6. Corollary. *$\text{Im } m(z)$ is Hermitian and the matrix $m(z)$ satisfies the relation $m^+(z) = m(\bar{z})$.*

4. The quantum Heisenberg model and its relaxation matrix

For the sake of simplicity, we will restrict the discussion to the model defined on a d -dimensional lattice

$$\mathbf{Z}^d(a) = \left\{ \sum_{i=1}^d a_i n^i \mid n^i = 0, \pm 1, \pm 2, \dots \text{ and } a_i > 0 \right\}.$$

Here the a_i denotes the edges of the d -dimensional unit cell, called Wigner-Seitz cell. In section 2 $\mathbf{Z}^d$ denoted a lattice with $a_i = 1$ for all $i = 1, \dots, d$. Let Λ_d be here any finite volume of $\mathbf{Z}^d(a)$ with N_d as the number of Wigner-Seitz cells, $\Lambda_d \subset \mathbf{Z}^d(a)$.

Let us denote the Hilbert space, associated to the quantum Heisenberg model in a finite volume Λ_d , by $\mathcal{H}_{\Lambda_d}$. One can construct a Hilbert space by means of tensor product

$$\mathcal{H}_{\Lambda_d} = \bigotimes_{R \in \Lambda_d} \mathcal{H}_R.$$

Further the algebra of spin operators is identified with the tensor product

$$\mathcal{M}_{\Lambda_d} = \bigotimes_{R \in \Lambda_d} \mathcal{M}_R$$

where each $\mathcal{M}_R$ is isomorphic to the full matrix algebra M_2 of complex matrices in 2-dimensions. The norm closure of $\mathcal{M}_{\Lambda_d}$ is the C^* -algebra $\mathcal{M}$ of local observables, which is a von Neumann algebra if it is a dual space as a Banach space. For each $R \in \mathbf{Z}^d(a)$ $\mathcal{H}_R$ is a copy of a 2-dimensional Hilbert space. Giving an irreducible unitary representation $\text{SU}(2)$ with self-adjoint generators $s_\alpha(R)$, $\alpha = 1, 2, 3$, in $\mathcal{H}_R$, which satisfy the commutation relations

$$[s_1(R), s_2(R')] = i s_3(R) \delta_{R,R'} \quad (4.1)$$

plus cyclic permutations, then one can define

$$s_\pm(R) = 2^{-1/2} [s_1(R) \pm i s_2(R)] \quad (4.2)$$

with

$$\sum_{\alpha=1}^3 s_{\alpha}^2(R) = \{s_+(R), s_-(R)\} + s_3^2(R) = s(s+1)\mathbf{1}.$$

Then the local quantum Heisenberg Hamiltonian is defined by

$$H_{\Lambda_d} = -\frac{1}{2N_d} \sum_{\substack{R, R' \in \Lambda_d \\ \alpha=1,2,3}} J(R-R') s_{\alpha}(R) s_{\alpha}(R') - \frac{h}{N_d} \sum_{R \in \Lambda_d} s_3(R) \quad (4.3)$$

in the d -dimensional hypercube Λ_d . h is the external magnetic field and $J(R)$ fulfills $J(R) = J(-R)$. $J(0)$ is chosen such that H_{Λ_d} is positive definite for $h = 0$. Note that the Hamiltonian (4.3) for an interaction $J(R)$ with finite range is bounded for large Λ_d and Λ_d/N_d fixed. To show this, one must consider the Fourier transform of the spin operators $s_{\alpha}(R)$.

4.1. Proposition. *Let $s_{\alpha}(R)$ be the self-adjoint generators of an irreducible unitary representation $SU(2)$ in $\mathcal{H}_R$, $\alpha = 1, 2, 3$ and $R \in \Lambda_d \subseteq \mathbf{Z}^d(a)$.*

Because the spin operators $s_{\alpha}(R)$ have constant, discrete eigenvalues, they are generalized operators and their Fourier series is a generalized operator,

$$\check{s}_{\alpha}(k) = \sum_R s_{\alpha}(R) \exp(ikR) \quad (4.4)$$

with Fourier transform

$$\hat{s}_{\alpha}(x) = \sum_R s_{\alpha}(R) \delta(x - R). \quad (4.5)$$

The $s_{\alpha}(R)$ and the quantum Heisenberg model (4.3) can be represented as

$$s_{\alpha}(R) = \frac{1}{v_B} \int_{v_B} d^d k \check{s}_{\alpha}(k) \exp(-ikR), \quad (4.6)$$

$$H_{\Lambda_d} = -\frac{1}{v_B} \int_{v_B} d^d k \sum_{\alpha=1,2,3} \check{J}(k) \check{s}_{\alpha}(k) \check{s}_{\alpha}(-k) - h \check{s}_3(0), \quad (4.7)$$

where the integrals are over the Brillouin zone v_B with volume

$$v_B = \prod_{i=1}^d \left(\frac{2\pi}{a_i} \right).$$

Proof. The proof of equations (4.4–6) follow immediately from the considerations of section 2 and especially from Theorem (2.4). The representation (4.7) of the quantum Heisenberg model (4.3) follows from (4.6) and the fact that the generalized function

$$\check{f}(k) = \frac{1}{v} \sum_{R \in \mathbf{Z}^d(a)} \exp(ikR)$$

after Theorem (2.4) has the form

$$\check{f}(k) = \sum_G \delta(k - G).$$

G runs over all reciprocal lattice vectors.

(Q.E.D.)

An immediate consequence of this proposition is the following:

4.2. Corollary. *Let $\check{s}_\alpha(k)$ be the Fourier series of the spin operators $s_\alpha(R)$. Then the $\check{s}_\alpha(k)$ fulfil the commutation relation*

$$[\check{s}_1(k), \check{s}_2(k')] = i\check{s}_3(k + k') \quad (4.8)$$

with cyclic permutation of the indices 1, 2, 3 and with k and $k' \in v_B$.

We have just converted the discussion of the quantum Heisenberg model from the space $l^2[\mathbf{Z}_{(a)}^d]$ to the space $L^2[\prod_{i=1}^d [-\pi/a_i, \pi/a_i]]$. The existence of the Hamiltonian (4.3) or (4.7) for an infinite volume system has been studied elsewhere [1] and will not be considered here again. The great advantage of this definition of the Hamiltonian is that the theory of modular Hilbert algebras [5] can be taken over immediately. Therefore, the formulation of linear response theory of the section 3 remains valid and can be applied to problems related to the quantum Heisenberg model (4.7).

4.3. Theorem. *The transverse dynamical susceptibility admittance possesses at least a two-pole structure above and below the second order phase transition temperature T_c . Below T_c the magnons have a gap in the spectrum at the center of the Brillouin zone.*

Proof. In the section 3, it has been used that ω is a time invariant state on Ω . Let (Π, Ω, U_t) be its GNS representation, $\omega(x) = (\Omega, \Pi(x)\Omega)$ where x is in the algebra $\mathcal{M}$ of the observables. Ω is the cyclic vector of $\mathcal{H}$ for $\Pi(\mathcal{M})$, $\Pi(\alpha_t(x)) = U_t \Pi(x) U_t^+$. Let us consider the extension of ω to $\Pi(\mathcal{M})''$ and drop the notation Π . To prove the theorem we use the results of the section 3 and the representation of the relaxation matrix (3.11) with Definitions (3.12–13).

Let us choose the observables:

$$\bar{s}_3(k) = \sum_R [s_3(R) - M] \exp(ikR), \quad \bar{s}_-(k) = \check{s}_-(k) - [H_{\Lambda_d}, \check{s}(k)] R_\perp M \quad (4.9a)$$

$$[H_{\Lambda_d}, \bar{s}_3(k)], \quad [H_{\Lambda_d}, \bar{s}_-(k)] \quad (4.9b)$$

with their GNS representation

$$\Pi(\bar{s}_3(k)) = s_3, \quad \Pi(\bar{s}_-(k)) = s_- \quad (4.10a)$$

$$\Pi([H_{\Lambda_d}, \bar{s}_3(k)]) = Hs_3, \quad \Pi([H_{\Lambda_d}, \bar{s}_-(k)]) = Hs_- \quad (4.10b)$$

where $R_\perp^{-1} = (Hs_-, Hs_-)$ and $M = (s_-, Hs_-) = (\Omega, s_3\Omega)$. M is the magnetization and H the GNS representation of H_{Λ_d} . To show that the transverse, dynamical

susceptibility $\phi_{s_-, Hs_-}(z) = -\hat{\chi}_{s_-, s_-}(z)$ has at least a two pole structure, we make the above choice of observables. With this choice (4.10) of the observables, the matrices χ^0 , ψ and $\Sigma(z)$ have the form

$$\chi^0 = \left(\begin{array}{cc|cc} D_{\parallel}^{-1} & 0 & & 0 \\ 0 & D_{\perp}^{-1} & & \\ \hline & & R_{\parallel}^{-1} & 0 \\ 0 & & 0 & R_{\perp}^{-1} \end{array} \right), \quad (4.11)$$

$$\psi = \left(\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ 0 & MD_{\perp} & 0 & 1 \\ \hline R_{\parallel}^{-1}D_{\parallel} & 0 & 0 & 0 \\ 0 & R_{\perp}^{-1}D_{\perp} & 0 & 0 \end{array} \right), \quad (4.12)$$

$$\Sigma(k, z) = \left(\begin{array}{c|cc} 0 & & 0 \\ \hline 0 & \Sigma_{\parallel}(k, z) & 0 \\ & 0 & \Sigma_{\perp}(k, z) \end{array} \right) \quad (4.13)$$

with definitions

$$\begin{aligned} D_{\parallel}^{-1} &= (s_3, s_3), & D_{\perp}^{-1} &= (s_-, s_-) \\ R_{\parallel}^{-1} &= (Hs_3, Hs_3), & R_{\perp}^{-1} &= (Hs_-, Hs_-) \end{aligned} \quad (4.14)$$

and

$$\begin{aligned} \Sigma_{\parallel}(k, z) &= -R_{\parallel}(QHs_3, R_Q(z)QHs_3), \\ \Sigma_{\perp}(k, z) &= -R_{\perp}(QHs_-, R_Q(z)QHs_-), \end{aligned} \quad (4.15)$$

where Q projects on the orthogonal complement of the vectors (4.10b–10c) in the Hilbert space. The $\phi(z)$ -matrix has the form

$$\phi(k, z) = \left(\begin{array}{cc|cc} \phi_{s_3, s_3} & 0 & \phi_{s_3, Hs_3} & 0 \\ 0 & \phi_{s_-, s_-} & 0 & \phi_{s_-, Hs_-} \\ \hline \phi_{Hs_3, s_3} & 0 & \phi_{Hs_3, Hs_3} & 0 \\ 0 & \phi_{Hs_-, s_-} & 0 & \phi_{Hs_-, Hs_-} \end{array} \right) \quad (4.16)$$

Using equations (4.11–16) in (3.11), one gets for instance the coupled equations

$$[z - MD_{\perp}] \phi_{s_-, Hs_-} - \phi_{Hs_-, Hs_-} = 0 \quad (4.17a)$$

$$-R_{\perp}^{-1}D_{\perp} \phi_{s_-, Hs_-} + [z + \Sigma_{\perp}(k, z)] \phi_{Hs_-, Hs_-} = R_{\perp}^{-1} \quad (4.17b)$$

and

$$z \phi_{s_3, Hs_3} - \phi_{Hs_3, Hs_3} = 0 \quad (4.18a)$$

$$-R_{\parallel}^{-1}D_{\parallel} \phi_{s_3, Hs_3} + [z + \Sigma_{\parallel}(k, z)] \phi_{Hs_3, Hs_3} = R_{\parallel}^{-1} \quad (4.18b)$$

From (4.17) and (4.18) it follows

$$[z^2 - zMD_{\perp} - R_{\perp}^{-1}D_{\perp} + \Sigma_{\perp}(k, z)]\phi_{s_{\perp}, Hs_{\perp}} = R_{\perp}^{-1} \quad (4.19)$$

$$[z^2 - R_{\parallel}^{-1}D_{\parallel} + \Sigma_{\parallel}(k, z)]\phi_{s_{\parallel}, Hs_{\parallel}} = R_{\parallel}^{-1} \quad (4.20)$$

Let us now consider the quantum Heisenberg model with constant nearest neighbour coupling and with external magnetic field h . In this case, the quantities $D_{\parallel}^{-1}$, $D_{\perp}^{-1}$, $R_{\parallel}^{-1}$ and $R_{\perp}^{-1}$ fulfill the relations

$$D_{\parallel} \geq \sum_{i=1}^d 2 \sin^2(a_i k^i) C_{\parallel} + C_T, \quad C_T \geq 0 \quad \text{for } T \neq T_c \quad (4.21a)$$

$$D_{\perp} \geq \sum_{i=1}^d 2 \sin^2(a_i k^i) C_{\perp} + C_T, \quad C_T \geq 0 \quad \text{for } T \neq T_c \quad (4.21b)$$

$$R_{\parallel}^{-1} = \sum_{i=1}^d 2 \sin^2(a_i k^i) F_{\parallel}(\beta, h) \quad (4.21c)$$

$$R_{\perp}^{-1} = \sum_{i=1}^d 2 \sin^2(a_i k^i) F_{\perp}(\beta, h) + hM + zJM^2 \quad (4.21d)$$

for positive and bounded $C_{\parallel}$, C_T , $F_{\parallel}$ and $F_{\perp}$. C_T depends essentially on the temperature T and the coupling constant. The results (4.21a-b) are gained by constructing an upper bound to the Duhamel functions $D_{\parallel}^{-1}$ and $D_{\perp}^{-1}$, which are given by the Ising susceptibility [12]. $R_{\parallel}^{-1}$ and $R_{\perp}^{-1}$ (4.21c-d) have been calculated explicitly [10]. Further, it has been proved for the isotropic Heisenberg model, that the magnetization is different from zero for temperatures $T < T_c$ and external magnetic field $h = 0$ and that in $d \geq 2$ dimensions [13]. From these facts follow the proof of the theorem by taking $z = 0 + i0$ in $m_{\parallel}$ and $m_{\perp}$ of (4.19) and (4.20).

Q.E.D.

5. Conclusions

The main interest was to formulate linear response theory for infinite systems by the method of modular Hilbert algebras and to apply this method to the quantum Heisenberg model. To do so, it was necessary to introduce the Fourier transform of generalized operators to be able to work in the infinite volume limit for the Heisenberg model.

The results of physical interest are on one side surprising and on the other side are not.

They are surprising because one had not expected paramagnons in the quantum Heisenberg model. The paramagnons in the longitudinal and transverse direction are overdamped for $T > T_c$ and $h = 0$, as it is clear from equations (4.15-21):

$$\begin{aligned} \Sigma_{\parallel}(k, i\omega) &\sim 0(1), \\ \Sigma_{\perp}(k, i\omega) &\sim 0(1). \end{aligned} \quad (5.1)$$

In the case $T > T_c$ and $h \neq 0$, one has

$$\Sigma_{\parallel}(k, i\omega) \sim 0(1), \quad \Sigma_{\perp}(k, i\omega) \sim k^2 a_{\perp} \quad (5.2)$$

what means the longitudinal paramagnons are still overdamped, but the transverse paramagnons are well defined because $R_{\perp}^{-1} > 0$ for $h \neq 0$, see equation (4.21) and $m_{\perp}(io) \sim k^2 b_{\perp}$.

Below the transition temperature, $T < T_c$, the situation for $h = 0$ is very similar as in the last case, $T > T_c$ and $h \neq 0$. The longitudinal magnon is overdamped because $\Sigma_{\parallel}(io)$ remain of order 1. The transverse magnon will be not overdamped thanks to the terms $zMD_{\perp}$, $R_{\perp}^{-1}D_{\perp}$ in (4.19) and the fact that $\Sigma_{\perp}(io)$ behaves as $k^2 a_{\perp}$ for temperatures $T < T_c$. This last fact comes around by the last contribution zJM^2 of $R_{\perp}^{-1}$ (4.21d) for $h = 0$.

Further, as one sees from (4.19), the scattering amplitude in presence of external magnetic field h or in the case $M \neq 0$ for $T < T_c$ and $h = 0$, is enhanced for the transverse dynamical susceptibility, thanks to the existence of the terms $hM + zJM^2$, or the term αM^2 , on the right hand side of equation (4.19). In the case of the longitudinal susceptibility, these terms are missing and therefore one gets less contribution to the scattering amplitude (of neutrons).

On the other hand, these conclusions are not surprising because one should think over how one had gained the quantum Heisenberg model Hamiltonian: one usually considers N_d electrons localized on N_d lattice sites. The Hamiltonian for such a system is given by the kinetic and Coulomb energy of the electrons and electron-ion interaction. The ions are assumed to be rigid. To represent the electrons, the appropriate set of functions are the Wannier functions. The exchange interaction energy of the model Hamiltonian can be transformed into the quantum Heisenberg model by the relations.

$$\begin{aligned} s_3(R) &\triangleq \frac{1}{2}[c_{n\uparrow}^+(R)C_{n\uparrow}(R) - C_{n\downarrow}^+(R)C_{n\downarrow}(R)], \\ s_+(R) &\triangleq C_{n\uparrow}^+(R)C_{n\downarrow}(R), \quad s_-(R) \triangleq C_{n\downarrow}^+(R)C_{n\uparrow}(R), \end{aligned} \quad (5.3)$$

where $C_{n\lambda}(R)$ annihilates an electron in the orbital state n and spin state λ at the lattice site $R \in \mathbb{Z}^d(a)$. It is clear from (5.3) that the quantum Heisenberg model can be related to the original electron Hamiltonian, from which the quantum Heisenberg model has been deduced. But for the rest, original Hamiltonian, given by the Heisenberg model and the transformation (5.3), one can construct after the paramagnon theory [11] paramagnons. This is the reason why the presence of paramagnons in the quantum Heisenberg model is not surprising.

As a last remark, we would like to mention that a three pole structure can be constructed for the quantum Heisenberg model by keeping the orthogonalized energy also as a dynamical variable. This variable is responsible for the third pole located at $z = 0 + io$, whose width is given by the heat diffusion coefficient similarly as in liquids.

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Truncation error bounds of continued fractions for complex transport coefficients and spectral functions

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We study the calculation of complex transport coefficients $\chi(\omega)$ and power spectra in terms of complex continued fractions. Classes of equilibrium and nonequilibrium systems are investigated for which we can obtain a posteriori bounds for the truncation error $|\chi(\omega) - \chi_{(\omega)}^{(n)}| \leq c(\omega) |\chi_{(\omega)}^{(n)} - \chi_{(\omega)}^{(n-1)}|$ when the transport coefficient is approximated by its n th continued fraction approximant $\chi_{(\omega)}^{(n)}$. For example, such a class consists of the Markovian statistical systems which obey a strong detailed balance condition (i.e. the stochastic operator can be cast in symmetric form).

Exact linearization of the first equation of the B.B.G.K.Y. hierarchy

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This note reports an apparently unnoticed relation between the Kirkwood liquid-‘solid’ and the Ornstein-Zernicke phase instability criteria.

Consider an infinite classical system of particles interacting via two-body central forces of short range, $F(|x_1 - x_2|)$. Assume that, at some natural temperature β , the one-particle correlation function $\rho_1(x)$ is non-trivially periodic in R^v , that it satisfies the first equation of the B.B.G.K.Y. hierarchy, namely

$$\text{grad } \rho_1(x_1) = \int dx_2 \beta F(|x_1 - x_2|) \rho_2(x_1, x_2, \{\rho_1(x)\})$$

where $\rho_2(x_1, x_2, \{\rho_1(x)\})$ is the two-particles correlation function of the inhomogeneous system and that a small amplitude analysis of this equation is legitimate, i.e. its linearization in terms of $\rho_1(x) - \rho = \epsilon f(x)$, where ρ is the homogenous equilibrium density and where ϵ is $\ll 1$. It is then readily shown that:

(i) in expressing the exact linear functional derivative of the pair correlation function $\rho_2(x_1, x_2, \{\rho_1(x)\})$ with respect to the density $\rho_1(x_4)$ by means of the

internal field $\psi(x_2)$ conjugated to $\epsilon f(x_4)$, namely

$$\begin{aligned} (\delta\rho_2(x_1, x_2, \{\rho_1(x)\})/\delta\rho_1(x_4))|_{\epsilon=0} \\ = \int dx_3 (\delta\rho_2(x_1, x_2, \{\psi(x)\})/\delta\psi(x_3))(\delta\psi(x_3)/\delta\rho_1(x_4))|_{\psi=0} \end{aligned}$$

an operation which introduces the three particle correlation function $\rho_3(x_1, x_2, x_3, \rho)$ of the homogeneous system and the linear field-density response function

$$(\delta\psi(x_1)/\delta\rho_1(x_2))|_{\psi=0} \equiv \chi(|x_1 - x_2|) = \rho^{-1} \delta(x_1 - x_2) - c(|x_1 - x_2|)$$

where $c(|x_1 - x_2|)$ is the direct correlation function;

(ii) in using the Ornstein-Zernicke relation between the pair and direct correlation function and

(iii) in calculating $\text{grad } c(|x_1 - x_4|)$ from the second equation of the hierarchy for the homogenous system, namely

$$\begin{aligned} \text{grad } \rho_2(|x_1 - x_2|, \rho) = \beta F(|x_1 - x_2|) \rho_2(|x_1 - x_2|, \rho) \\ + \int dx_3 \beta F(|x_1 - x_3|) \rho_3(x_1, x_2, x_3, \rho) \end{aligned}$$

then, the first B.B.G.K.Y. equation, correctly linearized, becomes

$$\begin{aligned} \text{grad } f(x_1) = \int dx_2 dx_4 \beta F(|x_1 - x_2|) \rho_2(|x_1 - x_2|, \rho) \chi(|x_2 - x_4|) f(x_4) \\ + \int dx_2 dx_3 dx_4 \beta F(|x_1 - x_2|) \rho_3(x_1, x_2, x_3, \rho) \chi(|x_3 - x_4|) f(x_4) \end{aligned}$$

while

$$\begin{aligned} \rho \text{ grad } c(|x_1 - x_4|) = \int dx_2 \beta F(|x_1 - x_2|) \rho_2(|x_1 - x_2|, \rho) \chi(|x_2 - x_4|) \\ + \int dx_2 dx_3 \beta F(|x_1 - x_3|) \rho_3(x_1, x_2, x_3, \rho) \chi(|x_2 - x_4|) \end{aligned}$$

Thus

$$\text{grad } f(x_1) = \rho \int dx_4 \text{ grad } c(|x_1 - x_4|) f(x_4)$$

provided the three particle correlation function of the homogenous system is symmetric in its three arguments. Violation of this condition explains why the above relation is not satisfied in some truncation scheme used to determine $\rho_2(|x_1 - x_2|, \rho)$ e.g. in the H.N.C. scheme. Furthermore, it can be shown that the above relation applies also to systems with long range forces.

It follows that the Kirkwood liquid-'solid' instability criterion is equivalent to the Ornstein-Zernicke phase instability criterion for non-zero wave vectors.

This observation suggests that the onset of the long range ordering considered here results from a singular (discontinuous) bifurcation mechanism governing $\rho_1(x) - \rho$ rather than from a continuous bifurcation as frequently searched for by approximative linearizations of the first B.B.G.K.Y. equation. With $\tilde{c}(|k|)$ designating the Fourier transform of $c(|x|)$, the case of a continuous bifurcation would indeed imply the occurrence of zeros for real $|k| \neq 0$ of the function $1 - \rho \tilde{c}(|k|)$. And there is no such evidence from available data on one-component systems, whether models (hard sphere gas, one-component plasma) or real (noble gas liquids). On the other hand it is clear that singular bifurcation of an order parameter is consistent with a first-order phase transition.

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