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HELVETICA PHYSICA ACTA
Zusammenfassungen der letzten eingegangenen Arbeiten
Résumés des derniers articles reçus

Coupled State Calculation of Proton Hydrogen Collisions in a Gaussian Basis

by V. Dose and C. Semini
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(10. VII. 74)

Abstract. Proton hydrogen scattering has been used to investigate the usefulness of Gaussian functions as a basis set for the description of atomic collisions. An impact-parameter close-coupling calculation is carried out and cross-sections for ground-state electron capture, total electron capture and free electron production are obtained. Generally, promising agreement of the results of this work with other theoretical and experimental investigations is observed.

Molecular Multipole Moments Derived from Collisional Quenching of H(2s)

by V. Dose and C. Semini
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(10. VII. 74)

Abstract. In this paper we try to improve on existing Born approximation treatments [1] of collisional quenching of metastable hydrogen atoms by molecules in thermal energy collisions. A four-state coupled-channel impact parameter calculation is carried out. The molecule is treated as a static charge distribution whose rotational motion is neglected. Cross-section results from the present calculation are used to calculate new values of multipole moments for CH_3I, N_2, CO_2, and CCl_4 from available experimental data.

On a Generalized Moment Problem

by V. A. Yatsun
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(16. VII. 74)

Abstract. The generalized moment problem, (1.1) which arises from analysis of the Froissart–Gribov formula for partial amplitudes is considered. The necessary and sufficient conditions of solvability of problem (1.1) by reducing it to the power problem (3.1) are obtained.

On the Approach to Equilibrium in Fluid Mechanics

by Miroslav Grmela
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(20. VIII. 74)

Abstract. The method which has been developed for the study of solutions of the family of the kinetic equations of the Enskog–Vlasov type [J. Math. Phys. *15*, 35 (1974)] is formulated generally and applied in fluid dynamics. The theory of solving the equations of fluid dynamics is in this way put into the relationship with the theory of solving other dynamical equations of non-equilibrium statistical mechanics. Some basic results in fluid dynamics are reproduced and a new contribution to the problem of finding a natural (both from the physical and mathematical point of view) structure for the space on which the equations of fluid mechanics are defined is made.

On the Approach to Equilibrium in Kinetic Theory. II. Fluid Mechanics

by Miroslav Grmela
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(20. VIII. 74)

Abstract. The long time behaviour of solutions to the Enskog–Vlasov type kinetic equations is studied in detail. It is found that for this purpose the Enskog–Vlasov dynamics can be reduced to fluid dynamics. The quantities that are phenomenological in fluid dynamics appear as functions of the quantities that are phenomenological in the Enskog–Vlasov dynamics and of the properties of the fixed point of the Enskog–Vlasov dynamics approached as time goes to infinity. The interesting case where the fixed point corresponds to a near critical state is also discussed.

Effet Jahn–Teller quadratique sur un ion de configuration d^9 dans une structure fluorine

par R. Lacroix
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(26. VIII. 74)

Résumé. Le cas général d'un système dans un état triplet orbital T_{2g} soumis à l'effet Jahn–Teller dû au mode vibrationnel T_{1u} a été examiné. On montre que la déformation résultante, due à un effet quadratique, correspond à un déplacement dans l'espace de configuration dans l'une des trois directions (100, (111) ou (110), selon la valeur numérique des constantes. Dans le problème particulier traité, ces constantes sont évaluées par l'approximation de Wolfsberg et Helmholz. Les valeurs numériques obtenues pour le cas de Ag^{2+} dans $SrCl_2$ montrent un déplacement de l'ion Ag^{2+} dans la direction (111).

Abstract. The general case of an orbital triplet T_{2g} undergoing a Jahn–Teller effect due to a T_{1u} vibrational mode has been studied. The occurring deformation, produced by a quadratic effect, is shown to result in a configurational space displacement along one of the (1000), (111) or (110) directions, depending on the numerical value of the constants. In the particular case in consideration, the constants were estimated by the Wolfsberg–Helmholz method. Numerical application to the Ag^{2+} ion in $SrCl_2$ crystal shows a displacement of this ion in the (111) direction.

Grüneisen Gamma of Some Cubic Crystals from Third-Order Elastic Constants Data

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(30. VIII. 74)

Abstract. A simple procedure is described to calculate the generalized Grüneisen parameters for longwave acoustic modes in cubic crystals from third-order elastic constants data. This procedure is used to calculate the limits $\bar{\gamma}_L$ and $\bar{\gamma}_H$ of the Grüneisen gamma of sixteen cubic crystals for which the measured third-order elastic constants are available. The agreement between the calculated limits and the experimental values from thermal expansion data is, in general, good. It is found that the alkali halides NaCl and NaF confirm Barron's predictions and the unusual behaviour of KCl and LiF is discussed within the framework of negative mode gammas. In the alkaline-earth fluorides CaF_2 and BaF_2 the elastic $\bar{\gamma}_H$ is found to be smaller than the thermal $\bar{\gamma}_H$ indicating a large contribution to $\bar{\gamma}_H$ from optical modes at high temperatures for these fluorides. In silver, gold and aluminium, farther neighbour interactions appear to be predominant. In indium antimonide, the calculated $\bar{\gamma}_L$ is negative which is, perhaps, suggestive of the experimental fact of the existence of a negative thermal expansion region at low temperatures for this insulator.