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THE STORY OF VAN VLECK's AND MORETTE - VAN HOVE's DETERMINANTS *

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Abstract

The genesis of Pauli's formula dating from late 1949 or early 1950, for the semi-classical approximation to Feynman's propagator (which is identical to Dirac's transformation function of type $(q|Q)$ introduced in 1933) and that of Van Vleck's, in 1928, for the second order approximation to Dirac's transformation function introduced in 1927, and which can be identified as being of type $(q|P)$, are carefully reexamined.

We show that the action integrals and generating functions which enter Pauli's and Van Vleck's formulae are of type commonly called 1 and 2, respectively, the same being of course true for their Jacobians.

Convincing evidence is provided that the determinant which enters Pauli's formula is due to Morette and Van Hove and not to Van Vleck as usually referred to in the literature on this subject.

*In honour of Klaus Hepp und Walter Hunziker at the occasion of their 60th birthday.

1 Introduction and summary

In the last decades, quantum properties of classically non-integrable and piecewise integrable Hamiltonian systems have been extensively investigated by means of the semiclassical approximation to Feynman's propagator [12]. In particular, in the field of "quantum chaos", the semiclassical propagator is the starting point in the derivation of Gutzwiller's celebrated trace formula [12, ch. 17] which is a basic tool to understand quantum spectra of systems whose classical limit is strongly chaotic.

The phase and amplitude of the semiclassical propagator are known to be directly related to solutions of the Hamilton-Jacobi equation and to their Jacobian matrix.

It has become a widespread, though inaccurate custom, to call the determinant which occurs through its square root in this amplitude Van Vleck's determinant, on the basis of Van Vleck's work of 1928 [3] on the second approximation to Dirac's transformation function of 1927 [2]. It happens even that the semiclassical propagator itself is unduly called Van Vleck's formula. On the other hand, and for reasons to become clear later, an improved designation of this determinant is sometimes given as Van Vleck-Pauli-Morette determinant [13, section 4.3].

Indeed we shall recall in this paper and we shall provide additional evidence that Pauli is the author of the semiclassical approximation to Feynman's propagator which, in fact, is Dirac's transformation function of 1933 [4]. Furthermore, we prove that the determinant which occurs in Pauli's formula is, up to a sign factor, due to Morette and Van Hove.

This paper is organized in a way which makes it self-contained, including several quotations from the original papers. The second section reviews briefly Dirac's transformation theory as published in his papers of 1927 [2] and 1933 [4], the last one containing his celebrated Action Principle. The third section deals with Van Vleck's second approximation to Dirac's transformation function of 1927. The genesis of his determinant is fully reproduced and it is shown that the determinant of Van Vleck is not identical to the determinant which appears in the semiclassical Feynman propagator. Furthermore this section contains a piece of work which we imagine that Van Vleck might have done after publication of Dirac's 1933 paper. The next section is of historical nature: it reports on the interactions which occurred in Princeton in the fall of 1949 between Cécile Morette, Wolfgang Pauli and Léon Van Hove when they were together at the Institute for Advanced Study and on some of their works published in 1951. It is here that we unveil where Van Hove published his result on the determinant which enters the semiclassical propagator in the final form as given by Pauli. The fifth section is made of comments of technical and historical nature concerning in particular the network of quotations in the papers reviewed. Lastly, an appendix has been added with the aim of identifying unambiguously the phases and amplitudes of Van Vleck's and Pauli's approximations, respectively, to Dirac's transformation functions of 1927 and 1933, the latter being Fourier transforms of one another. Throughout this paper, we keep the original notation of the authors, unless misleading, and we indicate their modern version whenever needed.

2 About Dirac's theory of transformation functions

This is to review briefly some technical points concerning P. A. M. Dirac's papers [2, 4] published in 1927 and 1933 under the titles "*The Physical Interpretation of the Quantum Dynamics*" and "*The Lagrangian in Quantum Mechanics*".

In the first paper [2] , Dirac exposes the motivations for his q-number picture of Quantum Dynamics and the ensuing theory of transformation functions, later called probability amplitudes by Pauli. One considers a dynamical system of n degrees of freedom, with a Hamiltonian $H(p,q,t)$, possibly time-independent, described by sets of conjugate variables $(p,q),(\eta,\xi)$ and (α,β) which, at the classical level, are connected via canonical transformations. Since Hamilton-Jacobi's equation is the classical analog and the classical limit of Schrödinger's wave equation, it is appropriate to choose solutions of Hamilton-Jacobi's equation as the generating functions of the canonical transformations. This means that the new variables are constants of integration, i.e., coordinates and momenta at a specified time. In his first paper [2], Dirac considers the initial and final sets of conjugate variables (η,ξ) and (α,β) and chooses ξ and α to be the independent variables of a generating function $S(\xi,\alpha,t)$. For the dependent variables, he writes [2, eq.13]

$$\eta = \frac{\partial S}{\partial \xi}, \qquad \beta = \frac{\partial S}{\partial \alpha} \quad . \tag{2.1}$$

In the appendix we show that this generating function is of type 2.

At the quantum level, Dirac considers and constructs representations of the operators corresponding to ξ and α in which they are diagonal matrices and he introduces transformation functions, (ξ/α) in his notation, which connect the two representations. A result of his transformation theory is that, given any dynamical variable $f(\xi,\eta)$, the matrix elements of f in the α representation are given in his notation by

$$f(\xi,\eta)(\alpha',\alpha'') = \int\int (\alpha'/\xi')d\xi' f(\xi',\frac{\hbar}{i}\frac{\partial}{\partial \xi'})(\xi'/\alpha''), \tag{2.2}$$

where (α/ξ) is the hermitian conjugate of (ξ/α). Next, Dirac shows that, if the Hamiltonian is time-dependent, then (q/α) satisfies Schrödinger's wave equation [2, eq. 12].

In the second paper [4] which contains the celebrated Action Principle that inspired Feynman [5], Dirac considers again two sets of conjugate variables (p,q) and (P,Q) but supposes now that, at the classical level, the independent variables of the generating function are q and Q. Let R be the corresponding generating function. The dependent variables are consequently given by [4, eq. 1]

$$p = \frac{\partial R}{\partial q}, \qquad P = -\frac{\partial R}{\partial Q}, \tag{2.3}$$

where $R = R(q,Q,t)$. Notice here the difference in the sign factors between (2.1) and (2.3). In the appendix we show that this generating function is of type 1.

At this point, let us quote Dirac [4, p. 66]: "*In the quantum theory we may take a representation in which the q's are diagonal, and a second representation in which the Q's are diagonal. There will be a transformation function $(q'|Q')$ connnecting the two representations. We shall now show that this transformation function is the quantum analogue of* $e^{iR/\hbar}$".

Next, after the proof, in relabeling q,p as q_t,p_t ; Q,P as q_T,p_T and designating the corresponding transformation function by $(q_t|q_T)$, Dirac writes [4, p. 68]: "*The work of the preceding section now shows that*

$$(q_t|q_T) \quad \textit{corresponds} \quad \textit{to} \quad e^{\frac{i}{\hbar}\int_T^t L\,dt'}, \tag{2.4}$$

where L is the Lagrangian." Dirac gives also the composition law of $(q_t|q_T)$ in the form

$$(q_t|q_T) = \int (q_t|q_m)dq_m(q_m|q_{m-1})dq_{m-1}\dots(q_2|q_1)dq_1(q_1|q_T), \tag{2.5}$$

where q_k denotes q at the intermediate time t_k, $k = 1,...,m$. Lastly, when discussing the classical limit when $\hbar$ tends to zero, Dirac approximates $(q_t|q_T)$ by $exp(\frac{i}{\hbar}R(q_t,q_T,t,T))$ disregarding the question of the pre-exponential factor. At this point it is appropriate to consider Van Vleck's work.

3 About J. H. Van Vleck's second order approximation

In his paper of 1928 [3], entitled "*The Correspondence Principle in the Statistical Interpretation of Quantum Mechanics,*" Van Vleck acknowledges his difficulty "*in understanding how the quantum formulae for averages and probabilities merge into the analogous classical expressions in the region of large quantum numbers and also, of course, in the limit $\hbar = 0$* ".

His starting point is the diagonal part of Dirac's matrix elements (2.2), i.e.

$$f(p,q)(\alpha,\alpha) = \int (\alpha/q) f\left(i\hbar\frac{\partial}{\partial q}, q\right)(q/\alpha)dq_1\cdots dq_n\,. \tag{3.1}$$

He recalls that (q/α) "*is the probability amplitude or transformation function associated with the passage from the* p,q *to* α,β *system of variables*", that "*the expression*

$$|(q/\alpha)|^2 dq_1\ldots dq_n \tag{3.2}$$

is the probability of a given configuration in the q*'s when the* α*'s are specified*", that "(q/α) *is identical with a Schrödinger wave function* $\psi(q,\alpha,t)$" and that "*it is often convenient to choose the* α*'s and* β*'s to be a set of action and angle variables*" but "*unnecessary*".

Then Van Vleck seeks the classical analog of these statements. For this purpose he evokes Hamilton-Jacobi's equation

$$H(\frac{\partial S}{\partial q}, q, t) + \frac{\partial S}{\partial t} = 0\,. \tag{3.3}$$

He considers a complete integral $S(q,\alpha,t)$ and gives, for the dependent variables, the relations

$$p = \frac{\partial S}{\partial q}\,, \qquad \beta = \frac{\partial S}{\partial \alpha}\,, \tag{3.4}$$

which are identical to Dirac's relations (2.1) and define a canonical transformation of type 2 (see appendix) from the (p,q) system to a set of new variables (α,β).

Next comes the famous Van Vleck determinant. We quote [3, p. 180-181]:

"*By this transformation a function* $f(p;q)$ *of the original variables is converted into a function* $F(\alpha;\beta)$ *of the new ones. Let us suppose that for given* α*'s all values of the* β*'s are equally probable so that probability is proportional to the volume in the* β *-space. Like the usual assumptions concerning "weight" in statistical mechanics, this is a statistical hypothesis not included in the classical analytical dynamics by itself. The average value of* $f(p;q) = F(\alpha;\beta)$ *for given* α*'s is then*

$$A\int\ldots\int F(\alpha;\beta)d\beta_1\ldots d\beta_n \quad . \tag{3.5}$$

Let us change the variables of integration from the β*'s to the* q*'s. The integrand then is expressed in terms of the* q*'s and* α*'s and by (3.4) the expression (3.5) thus becomes*

$$A\int\ldots\int f\left(\frac{\partial S}{\partial q};q\right)\Delta dq_1\ldots dq_n \tag{3.6}$$

where Δ is the functional determinant

$$\Delta = \frac{\partial(\beta_1, \dots \beta_n)}{\partial(q_1, \dots q_n)} = det\left(\frac{\partial^2 S}{\partial q_k \partial \alpha_j}\right) \tag{3.7}$$

of the transformation from the β's to the q's with the α's kept fast. With our statistical assumption the probability that the system will be in a given configuration $dq_1 \dots dq_n$ is clearly

$$Ad\beta_1 \dots d\beta_n = A\Delta dq_1 \dots dq_n\,. \tag{3.8}$$

The constant A is determined by the requirement that the total probability be unity so that

$$A^{-1} = \int \dots \int \Delta dq_1 \dots dq_n\,. \tag{3.9}$$

For the correspondence principle to be valid, equation (3.1) must pass into (3.6) and (3.2) into (3.8) in the limiting case of very large quantum numbers (or, more generally, large values of the variables α_k). This is equivalent to letting $\hbar$ approach zero, as in either case the ratios $\hbar/\alpha_k$ vanish in the limit. It is well known that for small values of the $\hbar/\alpha_k$, a first approximation to the wave or transformation function (q/α) is $Ce^{S/i\hbar}$, where C is a constant and S is the classical action function satisfying (3.3). This approximation is, however, not adequate to yield the correspondence principle, for it is easily shown that with only this approximation equation (3.1) and (3.2) approach expressions analogous to (3.6) and (3.8) except for the important difference that the functional determinant Δ is wanting. It is, however, proved below that a second approximation is

$$(q/\alpha) = A^{1/2}\Delta^{1/2}e^{S/i\hbar} \tag{3.10}$$

where the constant A has the value (3.9). From this it follows immediately that (3.1) and (3.2) do indeed merge asymptotically into (3.6) and (3.8) for it is readily seen that

$$f\left(i\hbar\frac{\partial}{\partial q}; q\right)\left(\Delta^{1/2}e^{S/i\hbar}\right) = \Delta^{1/2}e^{S/i\hbar} f\left(\frac{\partial S}{\partial q}; q\right) + \dots \tag{3.11}$$

where the dots denote terms which vanish in the limit $\hbar = 0$, and where $f\left(\frac{\partial S}{\partial q}; q\right)$ means the function obtained by replacing the operators $i\hbar\frac{\partial}{\partial q_k}$ by the expressions $\frac{\partial S}{\partial q_k}$.

The essential contribution of the present paper is the proposition that (q/α) when calculated to the second approximation, always contains the factor $\Delta^{1/2}$ involving the functional determinant (3.7)".

Lastly, Van Vleck shows that his formula applies also to the case where the Hamiltonian is time-dependent.

At this point it is instructive to imagine the following scenario:
Suppose that, after Dirac's paper of 1933, Van Vleck would have liked to derive

the second approximation to Dirac's probability amplitude $(q_t|q_T) \equiv (q|Q) \equiv (q/\beta)$. He would have assumed that, for given $Q, i.e., \beta$ the values of $P, i.e., \alpha$ are equally probable and then, that the average value of $F(P;Q)$ for fixed Q would have been

$$B \int \ldots \int F(P;Q) dP_1 \ldots dP_n \tag{3.12}$$

which becomes

$$B \int \ldots \int f\left(\frac{\partial R}{\partial Q}, Q\right) D dq_1 \ldots dq_n \,, \tag{3.13}$$

where according to the relations (2.3)

$$D = \frac{\partial (P_1, \ldots, P_n)}{\partial (q_1, \ldots, q_n)} = det\left(-\frac{\partial^2 R}{\partial q_k \partial Q_\ell}\right) \tag{3.14}$$

and

$$B^{-1} = \int \ldots \int D dq_1 \ldots dq_n \,. \tag{3.15}$$

The result would have been that the second approximation to $(q_t|q_T)$ is

$$B^{1/2} D^{1/2} e^{\frac{i}{\hbar} R} \,. \tag{3.16}$$

But this is precisely Pauli's semiclassical approximation to Dirac's probability amplitude, re-christened Feynman's propagator $K(q, t; q_0, t_0)$, where q_0 has replaced Q. The determinant D will turn out to be nothing but Morette - Van Hove's determinant, up to a sign factor. Why this gap of so many years? We have no explanation.

4 At the Institute for Advanced Study in 1949/50

Cécile Morette, Wolfgang Pauli and Léon Van Hove happened to be simultaneously in Princeton during the fall of 1949 and the following winter. Morette was interested in developing Feynman's functional integral formalism [5], Pauli was working, among other subjects in Quantum Field Theory, on Feyman's Lagrangian approach to Quantum Mechanics [5], while Van Hove was concentrating on his "*Thèse d'agrégation*" to be submitted to the Université Libre de Bruxelles (ULB).

The work of Morette, submitted in July 1950 to Physical Review, appeared in 1951 under the title "*On the Definition and Approximation of Feynman's Path Integrals*" [7]. Pauli presented his results in a series of lectures given at ETH Zürich during the winter term 1950-51 and entitled "*Ausgewählte Kapitel aus der Feldquantisierung*" with an appendix on "*Der Feynman'sche Zugang zur Quantenelektrodynamik*" [6]†.

†The lectures notes, written by U. Hochstrasser and M.R. Schafroth were mimeographed in 1951 in Zürich and reprinted by Boringheri, in Turin in 1952. Later, C.P. Enz edited an English version of these notes as Volume 6 of Pauli Lectures in Physics and published by the MIT Press in 1973 [6].

It is also in 1951 that Van Hove published his "*Thése d'agrégation*" [8] to which we shall return later.

Morette's paper contains an original derivation, based in part on the use of a unitarity condition, of Feyman's propagator for infinitesimal (proper) time intervals [7.2] which reads

$$K\left(x^{k+1}, x^k\right) = \left(\frac{1}{2i\pi\hbar}\right)^{n/2} \left(det \frac{\partial^2 \bar{S}}{\partial x_\mu^{k+1}\, \partial x_\nu^k}\right)^{1/2} e^{\frac{i}{\hbar}\bar{S}(x^{k+1}, x^k)} \tag{4.1}$$

where $\bar{S}$ is the classical action‡ and $n = 4$§.

The paper contains also an infinite product representation of Feynman's propagator for finite (proper) time intervals and, more importantly, an original construction, by means of a saddle point expansion of the action integral, of a functional approximation, called K_a [7.31], to Feynman's propagator. This approximation is shown to be equivalent to the WKB approximation.

Concerning the derivation of (4.1), Morette acknowledges the help received from Van Hove in a, for our purpose historically important footnote, namely: "*We are greatly indebted to Dr. Van Hove for giving us formula 12 (the relation between Feynman's normalisation factors and the absolute value of* $det(\partial^2\bar{S}/\partial x_\mu^{k+1}\partial x_\nu^k)$ *times* h^{-2}*) before publication and for very many helpful discussions in the course of this work. For a more general study of Eq.2 (4.1) we refer the reader to a work of Dr. Van Hove (unpublished as yet).*"

We have recently clarified the mystery of Van Hove's unidentified paper on this subject. It happens that Van Hove's "*Thèse d'agrégation*" published in 1951 [8] appeared in two versions, the front pages of which are reproduced below (facsimile 1 and 2). The second facsimile bears the mention "*Exemplaire hors commerce*". Here is the explanation: according to the regulation at ULB at that time, a candidate to the "*agrégation*" had to submit three "*thèses ou questions accessoires*" also called "*propositions annexes*" in addition to the "*dissertation*" or main thesis, but it is the main thesis only which had to be published in the "*Mémoires de la Classe des Sciences de l'Académie royale de Belgique*" after approval by two academicians. As to the "*propositions annexes*", reproduced below (facsimile 3 and 4), the second of which containing Van Hove's determinant without derivation, they where incorporated

‡Notice here, that since the momentum at the initial position is minus times the derivative of the action integral with respect to that position (generating function of type 1), Eq. [7] contains an error of sign which consequently affects the elements of the Jacobian matrix of $\bar{S}$ (A.9).

§In fact, Morette considers a relativistic framework and introduces the proper time τ. A generalisation of Hamilton-Jacobi's equation is indeed possible provided that one eliminates ultimately the auxiliary proper time variable through $\partial\bar{S}(x^{k+1}, x^k; \tau^{k+1} - \tau^k = \epsilon)/\partial\epsilon = 0$ [9, p. 134].

in the "*Exemplaires hors commerce*" given by the Academy, free of charge, to the candidate.

So far, we have reported about Morette's and Van Hove's contributions to the subject of this paper, and we have proved that the determinant which enters the amplitude of Feynman's propagator for infinitesimal time interval is, up to a sign factor, due to Morette and Van Hove and not to Van Vleck.

What about Pauli's contribution? This can be answered, thanks to a personal recollection of Morette which is that, at the occasion of an appointment of herself and Van Hove with Pauli, she asked Van Hove to present her work as well as his, i.e., their definition of the infinitesimal propagator and her formula for a functional WKB type approximation. As a result of the discussion with Morette and Van Hove, Pauli wrote a couple of research notes, one, entitled *Van Hove* (PN 8/150 ¶ of the Pauli archives at CERN) where he considers Feynman's propagator for infinitesimal time intervals, argues about and corrects the sign factor in Van Hove's formula and, the other one, entitled "*Diskutiere Van Hove's Formel*" (PN 8/154-159) where he considers small but finite time intervals‖ and shows, with the help of other notes on the subject (PN 8/113-116, 121-123, 130-133) that the Ansatz

$$K_c = \left(\frac{1}{2i\pi\hbar}\right)^{n/2} \left[det\left(-\frac{\partial^2 R}{\partial q_k \partial q_{0\ell}}\right)\right]^{1/2} e^{\frac{i}{\hbar}R(q,t\,;\,q_0,t_0)} \tag{4.2}$$

satisfies Schrödinger's equation up to terms of order $\hbar^2$, called "*wrong terms*", proportional to $D^{-1/2}\,\nabla^2\,D^{1/2}$, the coefficient of $\hbar^0$ being Hamilton-Jacobi's equation and that of $\hbar^1$ the continuity equation satisfied by the probability density D, the square of the amplitude of K_c. Like the exact propagator K, the semiclassical one, K_c, reduces to Dirac's $\delta(q - q_0)$ distribution when $t \to t_0$.

¶The meaning of PN 8/150 is "Pauli Nachlass" Box 8 p.150.

‖Here, one should qualify the meaning of small but finite time intervals. One condition is that $t - t_o$ has to be smaller than $\tau_1(t_0) - t_0$ which is the time interval corresponding to the first conjugate point (in the sense of Jacobi) which follows q_0 on the trajectory of the system, a point at which the inverse determinant $D^{-1}(q, \tau_1, q_0, t_0) = 0$ [11, p.86]. To the best of our knowledge the singularities of D have been investigated for the first time in [9, p. 114-119] for conservative systems with non-singular, confining potentials. This is a class of systems which allows an infinity of trajectories passing through q_0 at time t_0 (which can be set $= 0$ by translational invariance) and q at time t. It was shown in [9, p.114] that the manifold of conjugate points is given by $(\partial q/\partial E)_{q_0,t} = 0$ with $E = -\frac{\partial R}{\partial t}$. Quantitative results were given for a one-dimensional anharmonic x^{2n} model. Near a conjugate point Q, D is proportional to $\pm|q - Q|^{-1/2}$. Going beyond the conjugate points for conservative systems with singular, attractive potentials, a class of systems which allows for a finite number of trajectories going from q_0 to q in the time t, has first been achieved by Gutzwiller in 1967 [12, p. 184-187]. Another condition is that the effect of the "*wrong terms*", interpreted as a quantum potential, be smaller in magnitude, than that of the classical potential [9, p. 110]. For the model discussed above, the absolute value of this quantum potential behaves as $|q - Q|^{-2}$ close to the singularity.

Next, concerning Morette's functional WKB approximation, there is no evidence that Pauli has reacted in one way or another. The only indirect allusion can be found in a letter of April 1951, congratulating Bryce Seligman-DeWitt and Cécile Morette on their marriage [15, #1230, p.294]. At the end of this letter, Pauli writes, in parentheses "*By the way, Cécile may be interested in the way I treated the Feynman-action principle in my mimeographed lectures. It is a kind of generalization of the WKB method to time-dependent solutions.*"

It seems to us that one reason why Pauli did not react to Morette's functional WKB formula is that at that time is was not known that the saddle point approximation to Feynman's path integral yields exactly the same result as the time-dependent WKB approximation; in other words, that $K_a = K_c$ [11, ch. 12; 13, sect. 2.5, 4.2 and 4.3].

It should lastly be pointed out that it is in the fall of 1951 that one of us (Ph.Ch.) started his Ph.D. thesis under the direction of Pauli who mentioned to him Van Hove's formula but did not give him the reference [9, p. 91] nor that of Morette. Why van Hove did not give a separatum of these "propositions annexes" to Morette and Pauli and why Morette did not give a reprint to Pauli and Van Hove, is not clear.

5 Comments on quotations

This is to provide the reader with a few additional informations of technical and historical nature.

i) We have not mentioned P. Jordan's work of 1926 on canonical transformation in Quantum Mechanics [1]. It is true that Dirac, Van Vleck and Morette quote this paper since the Jacobian of a particular canonical transformation of type 2 occurs in order to make the old momenta hermitian. The reason is that Jordan's work of 1926 and later concerns time-independent canonical transformations which have nothing to do with solutions of Hamilton-Jacobi's equation.

ii) It is interesting to observe that Van Vleck's paper of 1928 is:

- quoted by Van Hove and Morette
- not quoted by Dirac until the third edition (1947) of his book "The Principles of Quantum Mechanics" (p. 128 in section 3.2 : the Action Principle)

- not quoted by Pauli (is it not intriguing?) who, in his lecture notes quotes the Action Principle in Dirac's second edition (1935, sec. 33, p. 123), but does not quote Van Hove nor Morette
- not quoted by Feynman who, in ref. [5], quotes the Action Principle in Dirac's second edition.

iii) Van Hove's quotation of Van Vleck is erroneous since, as we prove in the appendix, Van Vleck's generating function is of type 2 not of type 1. However, Morette - Van Hove's determinant is also valid in non cartesian coordinates.

iv) An up to date derivation of the semiclassical propagator can be found in Sect. IV. 1 of an article by P. Cartier and C. DeWitt-Morette entitled "*A new perspective on functional integration*" and published in Ref. 14. See, in particular, p. 2254, the remark concerning the infinitesimal propagator and the WKB approximation.

6 Appendix

The aim of this appendix is to identify unambiguously the phases and amplitudes of Van Vleck's and Pauli's approximations to Dirac's transformation functions of 1927 and 1933, respectively, and also their initial conditions at $t = t_0$. In these approximations the phases are specific solutions of Hamilton-Jacobi's equation divided by $\hbar$ and the amplitudes are proportional to the square root of their Jacobians.

Let $H(p, q, t)$ be the Hamiltonian, possibly time-independent, of a dynamical system of n degrees of freedom with canonically conjugate variables $p, q \in R^n$ and phase space $\Gamma \subset R^n \times R^n$. Let $L(q, \dot{q}, t)$ be its Lagrangian with $\dot{q} = \partial H/\partial p$ and let Y be a solution of Hamilton-Jacobi's equation

$$\frac{\partial Y}{\partial t} + H\left(\frac{\partial Y}{\partial q}, q, t\right) = 0\,. \tag{A.1}$$

A complete solution of (A.1), say $Y(q, C, t) + C_0$ depends, apart from the disposable constant C_0, upon n constants of integration C_k and, since Y is the generating function of a canonical transformation from the variables (p, q) to new variables (P, Q) which are constants, $Y(q, C, t)$ has to depend upon n of these new variables. There are 2^n possibilities since each one of the C_k can be a Q_k or a P_k . Only two of them have to be considered in the present context, namely $Y = R$, i.e., $C_k = Q_k$ and $Y = S$, i.e., $C_k = P_k$, $k = 1, \ldots, n$. At this point there is no loss of generality in saying that the Q_k's are constants of integration of the motion at a specific time t_0, so we set

$$Q_k = q_{0k} \tag{A.2}$$

and the same with P_k which we set

$$P_k = p_{0k}\,. \tag{A.3}$$

Notice here that, in addition to being constants of integration at a specified time t_0, some of the p_{0k}'s might be constants of the motion depending upon the structure, symmetries and invariant properties of the Hamiltonian.

Following the traditional labelling of time-independent generating functions of canonical transformations which convert $H(p,q)$ into a $H(P,Q)$, namely $F_1 = F_1(q,Q)$, $F_2 = F_2(q,P), F_3 = F_3(p,Q)$ and $F_4 = F_4(p,P)$ we call

$$R(q,Q,t) = S_1(q,t\,;\,q_0,t_0) \tag{A.4}$$

and

$$S(q,P,t) = S_2(q,t;p_0,t_0)\,. \tag{A.5}$$

Clearly S_1 and S_2 are Legendre transforms of one another with respect to q_0 and p_0. Notice furthermore that one might also consider $S_3 = S_3(p,t;q_0,t_0)$ and $S_4 = S_4(p,t\,;\,p_0,t_0)$. They would satisfy the equation

$$\frac{\partial S_{3,4}}{\partial t} + H\left(p, \frac{\partial S_{3,4}}{\partial p}, t\right) = 0\,, \tag{A.6}$$

a kind of dual of (A.1). Although we shall ignore S_3 and S_4 in the sequel of this appendix, one should nevertheless realize that, in permuting the role of (p,q) and (P,Q), i.e., in saying that p and q are constants of integration at time t, and t_0 is the running time variable, we see that S_1 and S_2 satisfy the following equations

$$-\frac{\partial S_1}{\partial t_0} + H\left(-\frac{\partial S_1}{\partial q_0}, q_0, t_0\right) = 0 \tag{A.7}$$

and

$$-\frac{\partial S_2}{\partial t_0} + H\left(p_0, \frac{\partial S_2}{\partial p_0}, t_0\right) = 0\,. \tag{A.8}$$

For the dependent variables, p and p_0 for S_1 and p and q_0 for S_2 we have the relations

$$p = \frac{\partial S_1}{\partial q} = p\,(q,t\,;\,q_0,t_0)\,, \qquad p_0 = -\frac{\partial S_1}{\partial q_0} = p_0\,(q,t\,;\,q_0,t_0) \tag{A.9}$$

and

$$p = \frac{\partial S_2}{\partial q} = p\,(q,t;p_0,t_0)\,, \qquad q_0 = \frac{\partial S_2}{\partial p_0} = q_0\,(q,t;p_0,t_0)\,. \tag{A.10}$$

Let us give lastly the formal solutions of (A.1) for S_1 and S_2. Consider S_1 first and let $x(q,t\,;\,q_0,t_0,t')$ be a solution of Hamilton's or Lagrange's equations of motion satisfying the boundary conditions $x(t_0) = q_0$ and $x(t) = q$; keeping in mind that, since we have to deal with a boundary value problem and not with an initial value one, the solutions are generally not unique [9, p. 93]. The formal solution of (A.1) is now given by the action integral known to be Hamilton's principal function

$$S_1(q,t\,;\,q_0,t_0) = \int_{t_0}^{t} L\left(\dot{x}(q,t\,;\,q_0,t_0,t'), x(q,t\,;\,q_0,t_0,t'), t'\right) dt' . \tag{A.11}$$

Next, and with $x(q,t\,;\,p_0,t_0,t')$ being a solution of the equations of motion with the boundary conditions $x(t) = q, p(t_0) = p_0$ we have similarly

$$S_2(q,t\,;\,p_0,t_0) = p_0 q_0(q,t\,;\,p_0,t_0) + \int_{t_0}^{t} L\left(\dot{x}(q,t\,;\,p_0,t_0,t'), x(q,t\,;\,p_0,t_0,t'), t'\right) dt'. \tag{A.12}$$

We conclude the above analysis with the assertion that $S_1/\hbar$ and $S_2/\hbar$ are the phases of Pauli's and Van Vleck's formulae respectively and that

$$D = det\left(-\frac{\partial^2 S_1}{\partial q_j \partial q_{0k}}\right) \tag{A.13}$$

and

$$\Delta = det\left(\frac{\partial^2 S_2}{\partial q_j \partial p_{0k}}\right) \tag{A.14}$$

are their respective determinants.

The last points of this appendix concern the initial conditions satisfied by Dirac's transformation functions and their relations. The first transformation function, namely $(\xi/\alpha) \equiv (q,t|p_0,t_0)$ is that solution of the Schrödinger equation which reduces to $exp(\frac{i}{\hbar}p_0 q)$ as $t \longrightarrow t_0$ whereas Dirac's second transformation function $(q|Q) \equiv (q,t|q_0,t_0)$ reduces to $\delta(q-q_0)$ when $t \longrightarrow t_0$. It follows that these transformation functions are related by Fourier transforms, namely

$$(q,t|q_0,t_0) = \int \frac{dp'}{2\pi\hbar} e^{-\frac{i}{\hbar}p'q_0} (q,t|p',t_0) \tag{A.15}$$

and conversely

$$(q,t|p_0,t_0) = \int dq' e^{\frac{i}{\hbar}p_0 q'} (q,t|q',t_0) \ . \tag{A.16}$$

Lastly, if one inserts Van Vleck's formula on the r.h.s. of (A.15) and Pauli's formula on the r.h.s. of (A.16) and if one approximates the integrals by means of the stationary phase method, then, as shown in particular by W. H. Miller [10, p. 80-85], one obtains Pauli's, respectively Van Vleck's formula on the l.h.s.

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References

1. P. Jordan, Z. f. Phys. **38,** 513-517 (1926)

2. P. A. M. Dirac, Proc. Roy. Soc. London **113A,** 621-645 (1927)

3. J. H. Van Vleck, Proc. Nat. Acad. Sci. **14,** 178-188 (1928)

4. P. A. M. Dirac, Phys. Zeits. Sowjetunion **3,** 64-72 (1933)

5. R. P. Feynman, Rev. Mod. Phys. **20,** 367-387 (1948)

6. W. Pauli, *Selected Topics in Field Quantization,* Pauli Lectures, Volume 6, 161-166, MIT Press, (1973)

7. C. Morette, Phys. Rev. **81,** 848-852 (1951)

8. L. Van Hove, Academie Royale de Belgique, classe des sciences, No. 1618, Tome XXVI, Fascicule 6, (1951)

9. Ph. Choquard, Helv. Phys. Acta, **28,** 89-157 (1955)

10. W. H. Miller, Adv. Chem. Phys. **25,** 69-177 (1974)

11. L. S. Schulman, *Techniques and Applications of Path Integrals,* J. Wiley (1981)

12. M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics,* Interdisciplinary Applied Mathematics 1, Springer Verlag (1990)

13. H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, World Scientific, Singapore (1990)

14. P. Cartier and C. DeWitt-Morette, J. Math. Phys. **36**, 2237-2312 (1995), a special issue on Functional Integration, edited by C. DeWitt-Morette.

15. Wolfgang Pauli, Scientific Correspondance, Vol. IV/1, 1950-1952, edited by K. von Meyenn, Springer, 1996.

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FACSIMILE 2

PROPOSITIONS ANNEXES

1. — Soit un système d'un grand nombre de particules identiques se déplaçant sur un segment de droite. Supposons que ces particules soient deux à deux en interaction, le potentiel d'interaction étant une fonction continue de la distance, avec une portée finie et un rayon d'incompressibilité non nul pour les particules. En se basant sur un théorème de Jentzsch concernant les équations intégrales à noyau positif [1], on peut montrer dans le cadre de la Mécanique statistique classique que l'énergie libre par particules du système est une fonction analytique de la température et de la longueur spécifique. Un tel système ne peut donc présenter de phénomènes de condensation [2].

2. — Soit un système dynamique à un nombre fini l de degrés de liberté, traité en Mécanique quantique non relativiste. Feynman a montré que, si l'énergie potentielle est indépendante des vitesses ou les contient linéairement, la solution générale de l'équation de Schrödinger peut s'exprimer en fonction de l'action classique à l'aide d'une expression fonctionnelle, limite d'intégrales multiples

$$K(q^{(0)}, q^{(T)}) =$$

$$\lim_{n\to\infty} \int \exp\left\{\frac{i}{\hbar}\left[S_0(q^{(0)}, q^{(1)}) + \sum_1^{n-1} S_j(q^{(j)}, q^{(j+1)}) + S_n(q^{(n)}, q^{(T)})\right]\right\} \prod_1^n A_j dq_j$$

$q^{(0)}$ et $q^{(T)}$ sont les coordonnées de position aux instants 0, T.

$S_j(q^{(j)}, q^{(j+1)})$ est l'action classique $\int L dt$ pour l'intervalle de temps

$$\big(jT/(n+1),\ (j+1)T/(n+1)\big)$$

prise le long de la trajectoire classique joignant le point $q^{(j)}$ au point $q^{(j+1)}$. A_j est un facteur numérique de normalisation que Feynman détermine de façon que K soit la fonction de Green de l'équation de Schrödinger. Cette formule suppose que l'énergie cinétique soit une forme quadratique à coefficients constants en les vitesses. Elle ne reste donc pas valable en coordonnées q curvilignes [3]. Cela étant, le

(1) R. Jentzsch, *Crelles Journ.*, vol. 141 (1912), p. 235.
(2) L. Van Hove, *Physica*, vol. XVI (1950), p. 137.
(3) R. P. Feynman, *Rev. of Mod. Phys.*, vol. 20 (1948), p. 367.

— 2 —

facteur de normalisation A_j peut être remplacé dans la formule de Feynman par

$$B_j(q^{(j)}, q^{(j+1)}) = (2\pi i \hbar)^{-1/2}\left[\left| \text{dét}\ \frac{\partial^2 S_j(q^{(j)}, q^{(j+1)})}{\partial q^{(j)}\ \partial q^{(j+1)}} \right|\right]^{\frac{1}{2}}.$$

La formule obtenue reste valable en coordonnées curvilignes. Comme l'a montré Van Vleck (¹),

$$B_j(q^{(j)}, q^{(j+1)}) \exp\left\{\frac{i}{\hbar} S_j(q^{(j)}, q^{(j+1)})\right\}$$

est la seconde approximation de la fonction d'onde dans la méthode d'approximation de Wentzel-Kramers-Brillouin.

3. — Soient

$$A_{j\alpha k\beta}(x) = A_{k\beta j\alpha}(x), \quad (j, k = 1, \dots n\ ; \ \alpha, \beta = 1, \dots \mu)$$

des fonctions continues dans un domaine régulier fermé $\mathcal{D}$ de l'espace $(x_1, \dots x_\mu)$. Soit $\mathcal{H}$ l'espace de Hilbert formé par complétion à partir de l'espace vectoriel des systèmes $\zeta = (\zeta_1, \dots \zeta_n)$ de fonctions réelles $\zeta_j(x)$ de classe C^1 dans le domaine $\mathcal{D}$, nulles sur sa frontière, avec le produit scalaire

$$(\zeta, \zeta') = \int_{\mathcal{D}} (\sum_j \zeta_j \zeta'_j + \sum_{j,\alpha} \zeta_{j\alpha} \zeta'_{j\alpha})\, dx_1 \dots dx_\mu, \quad \zeta_{j\alpha} = \partial\zeta_j / \partial x_\alpha, \quad \zeta'_{j\alpha} = \partial\zeta'_j / \partial x_\alpha.$$

Dans $\mathcal{H}$ la relation

$$\int_{\mathcal{D}} A_{j\alpha k\beta}(x)\, \zeta_{j\alpha}\, \zeta'_{k\beta}\, dx_1 \dots dx_\mu = (A\zeta, \zeta')$$

définit un opérateur A, linéaire, autoadjoint et borné (²). Nous faisons la conjecture suivante : si la forme biquadratique

$$A_{j\alpha k\beta}(x)\, \xi_j \xi_k \eta_\alpha \eta_\beta$$

est définie positive en tous les points (x) du domaine $\mathcal{D}$, le spectre de A contient au plus un nombre fini de points dans l'intervalle $-\infty < \lambda < 0$. Cette conjecture se trouve vérifiée dans les cas suivants (²) :

1) $n = 1$ ou $\mu = 1$, d'une manière à peu près triviale ;

2) $n = 2$ ou $\mu = 2$, en vertu d'un théorème de Terpstra (³) et d'un théorème de Rellich (⁴) ;

3) pour des valeurs quelconques de n et μ, si les $A_{j\alpha k\beta}(x)$ sont des constantes, en vertu d'un théorème de Van Hove (⁵).

(¹) J. H. VAN VLECK, *Proc. Nat. Acad. Sci.*, U. S. A., vol. 14 (1928), p. 178.
(²) L. VAN HOVE, *Acad. R. Belg.*, *Mém. Cl. Sc.*, Coll. in-8°, t. XXIV (1949), fasc. 5.
(³) F. J. TERPSTRA, *Math. Ann.*, vol. 116 (1938), p. 166.
(⁴) F. RELLICH, *Gött. Nachr.*, *Math. Phys. Klasse*, (1930), p. 30.
(⁵) L. VAN HOVE, *Proc. Kon. Nederl. Akad. Wet.*, vol. L (1947), p. 18.