

Global Derivation of the Fluctuation Determinant from Group Property of Time Evolution.

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The Van Vleck-Pauli-Morette fluctuation determinant is derived from the global group property of the time evolution amplitude in a continuous formulation of path integrals.

I. INTRODUCTION

In the semiclassical limit, the quantum mechanical time evolution amplitude consists of an exponential of the classical action $\exp(iA)$, multiplied by a fluctuation factor F containing the inverse square root of the functional fluctuation determinant of harmonic eigenmodes of the system. The standard derivations of F rely on the local group properties of the time evolution amplitude [1]. The initial historic paper of DeWitt-Morette [2] determined F by enforcing these properties for infinitesimal time slices of the amplitude, which are necessarily semiclassical by Dirac's observation [3]. The full fluctuation factor F for finite times was then composed by a limiting procedure from the F 's of the time slices. The result was expressed as a square root of an ordinary matrix determinant, the Van Vleck-Pauli-Morette determinant [2].

Later, Gelfand and Yaglom [4] related the fluctuation determinant to the solution of a second-order differential equation, again via time-slicing techniques. This solution can, of course, be related to the Van Vleck-Pauli-Morette determinant.

In this note, we point out a more compact way of obtaining the fluctuation factor from the global, finite-time group property of the time evolution operator. Only the continuum formulation of path integrals is used. Our derivation involves neither time-sliced actions nor differential equations.

II. SEMICLASSICAL APPROXIMATION

In Schrödinger theory, a point particle in a D -dimensional euclidean space has associated with it a Hamilton operator $\hat{H}(t)$, and a time evolution operator $\hat{U}(t)$, which determines the amplitude to go from a position x_a at time t_a to a position x_b at time t_b by the matrix elements [1]

$$(x_b t_b | x_a t_a) = \theta(t_b - t_a) \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle. \quad (1)$$

The Heaviside function $\theta(t_b - t_a)$ ensures causality by the vanishing of the amplitude for times $t_b < t_a$. As elements of a one-parameter Lie group, the time evolution operators for different times satisfy the group multiplication law

$$\hat{U}(t_b, t_a) = \hat{U}(t_b, t) \hat{U}(t, t_a). \quad (2)$$

For matrix elements, this reads

$$\langle x_b | \hat{U}(t_b, t) \hat{U}(t, t_a) | x_a \rangle = \int_{-\infty}^{\infty} d^D x \langle x_b | \hat{U}(t_b, t) | x \rangle \langle x | \hat{U}(t, t_a) | x_a \rangle \quad (3)$$

so that the time evolution amplitudes satisfy the integral relation

$$(x_b t_b | x_a t_a) = \prod_{i=1}^D \left[\int_{-\infty}^{\infty} dx^i \right] (x_b t_b | x t) (x t | x_a t_a). \quad (4)$$

The matrix elements in (1) have a path integral representation

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$$\langle x_b | \hat{U}(t_b, t_a) | x_a \rangle = \int \mathcal{D}x \exp \left[\frac{i}{\hbar} \mathcal{A}(x) \right] \quad (5)$$

where

$$\mathcal{A}(x) = \int_{t_a}^{t_b} dt L(x, \dot{x}, t) \quad (6)$$

is the action and L the Lagrangian of the system. The semiclassical approximation is defined rewriting the result of the path integration as a product

$$\langle x_b | \hat{U}(t_b, t_a) | x_a \rangle \approx \exp \left[\frac{i}{\hbar} A(x_b, x_a; t_b, t_a) \right] F(x_b, x_a; t_b, t_a) \quad (7)$$

where $A(x_b, x_a; t_b, t_a)$ is the associated classical action, i.e., the action $\mathcal{A}[x]$ evaluated for the solution $x_{\text{cl}}(t)$ of the Euler-Lagrange classical equation of motion which extremizes $\mathcal{A}[x]$ with fixed endpoints at x_a, t_a and x_b, t_b . In the semiclassical approximation, the factor F contains no \hbar and contains the fluctuation determinant arising from the quadratic fluctuations around the classical path. Its logarithm is the quantum-mechanical analog of the entropy of harmonic fluctuations in quantum statistical mechanics. Since the end points of the paths are fixed, $x(t_a) = x_a$, $x(t_b) = x_b$, the boundary conditions for the fluctuations $\delta x(t)$ are of the Dirichlet type: $\delta x(t_a) = 0$, $\delta x(t_b) = 0$.

For a point particle moving in a time-dependent potential $V(x, t)$, the Lagrangian reads

$$L = \frac{M}{2} \dot{x}^2 - V(x, t), \quad (8)$$

and the fluctuation factor is

$$F(x_b, x_a; t_b, t_a) = \frac{1}{\sqrt{2\pi i \hbar (t_b - t_a) / M}^D} \sqrt{\frac{\det_D(\partial^2 / \partial t^2)}{\det_D[\partial^2 / \partial t^2 + \mathbf{V}^{(2)}(t) / M]}} \quad (9)$$

where $\mathbf{V}^{(2)}(t)$ is a $D \times D$ derivative matrix collecting the second derivatives of the potential along the classical path:

$$V_{ij}^{(2)}(t) = \left. \frac{\partial^2}{\partial_i \partial_j} V(x, t) \right|_{x=x_{\text{cl}}(t)}, \quad (10)$$

where the indices i, j denote the vector components. The fluctuation determinants \det_D consist of the product of eigenvalues of the $D \times D$ differential operator for Dirichlet boundary conditions.

The fluctuation determinant is most easily evaluated with the help of the Gelfand-Yaglom method [4], and the result can be reexpressed in terms of the Van Vleck-Pauli-Morette determinant [2]

$$F(x_b, x_a; t_b, t_a) = \frac{1}{(2\pi i \hbar)^{D/2}} \left\{ \det_D[-\partial_{x_a^i} \partial_{x_b^j} A(x_b, x_a; t_b, t_a)] \right\}^{1/2}, \quad (11)$$

The minus sign inside the determinant makes the argument of the square root positive as long as the classical trajectories do not reach a turning point. The continuation to longer intervals can always be done with the help of Maslov indices [1].

There exists various ways of rewriting the right-hand side of Eq. (11). A convenient form is obtained by using the fact that the momentum at the final time is given by the derivative of the classical action:

$$p_b^j = \frac{\partial A(x_b, x_a; t_b, t_a)}{\partial x_b^j}, \quad (12)$$

allowing to rewrite (11) as

$$F(x_b, x_a; t_b, t_a) = \frac{1}{(2\pi i \hbar)^{D/2}} \left[\det_D(-\partial_{x_a^i} p_b^j) \right]^{1/2}. \quad (13)$$

For the decomposition (7) of the matrix elements of the time evolution operator, the group property (3) takes the form

$$e^{\frac{i}{\hbar}A(x_b, x_a; t_b, t_a)} F(x_b, x_a; t_b, t_a) = \left[\prod_{i=1}^D \int_{-\infty}^{\infty} dx^i \right] e^{\frac{i}{\hbar}A^L(x_b, x; t_b, t)} F(x_b, x; t_b, t) \times e^{\frac{i}{\hbar}A^R(x, x_a; t, t_a)} F(x, x_a; t, t_a) \quad (14)$$

Here we have introduced superscripts L and R to emphasize the left and right positions of the action in the product. The configuration of the variables is illustrated in Fig. 1.

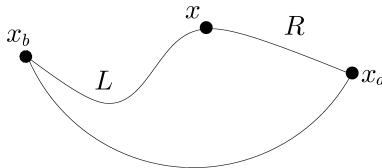


FIG. 1. The upper curve shows two classical paths running from x_a to x and from x to x_b . The intermediate point x has to be determined by the saddle point condition. The lower curve shows the direct classical path.

The fluctuation factor (11) has the property that the semiclassical approximation (7) satisfies this equation providing that the intermediate x -integrals are evaluated in the saddle-point approximation. This operation is done explicitly as follows. We denote the extremum of the intermediate integration over x by \tilde{x} , and expand the integrand around \tilde{x} up to quadratic terms in $\delta x \equiv x - \tilde{x}$. Since the fluctuation factor contains no \hbar , only the action in the exponent has to be expanded, and the semiclassical approximation to (14) reads

$$\begin{aligned} \exp \left[\frac{i}{\hbar} A(x_b, x_a; t_b, t_a) \right] F(x_b, x_a; t_b, t_a) &= \exp \left[\frac{i}{\hbar} A^L(x_b, \tilde{x}; t_b, t) + \frac{i}{\hbar} A^R(\tilde{x}, x_a; t, t_a) \right] \\ &\times F(x_b, \tilde{x}; t_b, t) F(\tilde{x}, x_a; t, t_a) \int_{-\infty}^{\infty} \prod_{i=1}^D d\delta x^i \exp \left[\frac{i}{2! \hbar} \delta x^i \frac{\partial^2}{\partial \tilde{x}^i \partial \tilde{x}^j} (A^R + A^L) \delta x^j \right]. \end{aligned} \quad (15)$$

The saddle point condition for \tilde{x} is

$$\frac{\partial}{\partial \tilde{x}^i} (A^R + A^L) = 0. \quad (16)$$

Just as in Eq. (12), the derivatives are equal to the momenta at the intermediate time t ,

$$\frac{\partial}{\partial \tilde{x}^i} A^R(\tilde{x}, x_a; t, t_a) = p_i^R(t), \quad (17)$$

$$\frac{\partial}{\partial \tilde{x}^i} A^L(x_b, \tilde{x}; t_b, t) = -p_i^L(t), \quad (18)$$

so that the saddle point condition (16) implies the equality of the intermediate momenta:

$$p_i^L(t) = p_i^R(t). \quad (19)$$

Our proof will be straightforward for a general Lagrangian which is at most quadratic in the velocities:

$$L(x, \dot{x}; t) = \frac{1}{2} \dot{x}_i g_{ij}(x, t) \dot{x}_j + \dot{x}_i a_i(x, t) - V(x, t), \quad (g_{ij} = g_{ji}) \quad (20)$$

The kinetic metric $g_{ij}(x, t)$ is also known as the Hessian, whose determinant is assumed to be nonzero to have a nondegenerate quantum system.

The canonical momenta are

$$p_i \equiv \frac{\partial L}{\partial \dot{x}^i} = g_{ij} \dot{x}_j + a_i, \quad (21)$$

and the Hamiltonian is the Legendre transform of $L(x, \dot{x}; t)$:

$$H(t) \equiv p_i \dot{x}^i - L = \frac{1}{2} [p_i(x, t) - a_i(x, t)] g^{ij}(x, t) [p_j(x, t) - a_j(x, t)] + V(x, t), \quad (22)$$

where $g^{ij}(x, t)$ is the inverse matrix of the Hessian $g_{ij}(x, t)$.

The Euler-Lagrange equations of motion following from (20) are

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0. \quad (23)$$

They are second-order differential equations in time. Due to this property, the condition (19) at the junction between the left and right paths ensures that the saddle point \tilde{x} is located on the the classical trajectory $x_{\text{cl}}(t)$ running all the way from x_a to x_b . The upper curve of Fig. 1 coincide then with the lower one. Moreover, the sum of the actions is equal to the total classical action along this combined path:

$$A^L(x_b, \tilde{x}; t_b, t) + A^R(\tilde{x}, x_a; t, t_a) = A(x_b, x_a; t_b, t_a). \quad (24)$$

Performing the Gaussian integral in Eq. (15), we therefore find the semiclassical consequence of the group property (14) for of the fluctuation factor:

$$F(x_b, x_a; t_b, t_a) = F(x_b, x; t_b, t)F(x, x_a; t, t_a)(2\pi i\hbar)^{D/2} \left\{ \det_D \left[\frac{\partial^2 (A^L + A^R)}{\partial x^i \partial x^j} \right] \right\}^{-1/2}, \quad (25)$$

where we have omitted the tilde on top of the intermediate position x on the classical path. This equation is an algebraic version of the eikonal equation in Schrödinger theory.

It is straightforward to verify that the Van Vleck-Pauli-Morette fluctuation factor (11) satisfies (25). We shall prove this using the equivalent form (13). Inserting this into (25), and using (17) and (18), we have to show that

$$\det_D \left(- \frac{\partial p_b}{\partial x_a} \Big|_{x_b} \right) = \frac{\det_D \left(- \partial p_b^L / \partial x \Big|_{x_b} \right) \det_D \left(- \partial p^R / \partial x_a \Big|_x \right)}{\det_D \left(\partial p^R / \partial x \Big|_{x_a} - \partial p^L / \partial x \Big|_{x_b} \right)}, \quad (26)$$

where we have ignored vector indices, for simplicity, and emphasized the variable kept constant in the partial differentiations. We also used $p_b^L = p_b$. The proof follows from the chain rule for the Jacobians. Taking the left-hand side of Eq. (26) to the right-hand side, we must verify that

$$1 = \frac{\det_D \left(- \partial p^R / \partial x_a \Big|_x \right) \det_D \left(\partial x_a / \partial x \Big|_{x_b} \right)}{\det_D \left(\partial p^R / \partial x \Big|_{x_a} - \partial p^L / \partial x \Big|_{x_b} \right)}. \quad (27)$$

The saddle-point condition (19) is, in a more explicit notation,

$$p^L[x_b, x(x_a, x_b)] = p^R[x_a, x(x_a, x_b)]. \quad (28)$$

This equality allows to derive

$$\frac{\partial p^L}{\partial x} \Big|_{x_b} \equiv \frac{\partial p^R}{\partial x} \Big|_{x_b} \equiv \frac{\partial p^R[x_a, x(x_a, x_b)]}{\partial x} \Big|_{x_b} = \frac{\partial p^R}{\partial x_a} \Big|_x \frac{\partial x_a}{\partial x} \Big|_{x_b} + \frac{\partial p^R}{\partial x} \Big|_{x_a}. \quad (29)$$

Inserting this equation into the denominator of (27) proves that (26) is indeed satisfied.

III. GLOBAL DERIVATION OF FLUCTUATION FACTOR

We are now prepared for the essential part of this paper, in which we *derive* the Van Vleck-Pauli-Morette formula (11) from the semiclassical group property (25) of the fluctuation factor. We proceed in two steps: first we move the intermediate time t infinitesimally close to the initial time t_a . This time is called t_{a+} . The corresponding intermediate position x will then lie at a point x_{a+} near x_a , as illustrated in Fig. 2. For this configuration, the fluctuation factor (25) reads more explicitly



FIG. 2. Classical path from x_a to an intermediate position $x = x_{a+}$ very close to x_a , followed by a classical path from x_{a+} to x_b .

$$F(x_b, x_a; t_b, t_a) = F(x_b, x_{a+}; t_b, t_{a+})F(x_{a+}, x_a; t_{a+}, t_a)(2\pi i\hbar)^{D/2} \\ \times \left\{ \det_D \left[\frac{\partial^2 A^L(x_b, x_{a+}; t_b, t_{a+})}{\partial x^i \partial x^j} + \frac{\partial^2 A^R(x_{a+}, x_a; t_{a+}, t_a)}{\partial x^i \partial x^j} \right] \right\}^{-1/2}. \quad (30)$$

In the limit $t_{a+} \rightarrow t_a$ we now extract the behavior of $F(x_{a+}, x_a; t_{a+}, t_a)$. Intuitively, this should be determined by the kinetic term of the action only, since the potential has no time to become active. Let us see how this comes about. First we use the equations for the momenta (17) and (18), express these in terms of the derivatives of the Lagrangian with respect to the velocities via (21), and derive the relations

$$\frac{\partial^2}{\partial x^i \partial x^j} A^R(x, x_a; t, t_a) = \frac{\partial}{\partial x^i} p_j^R(t) = \frac{\partial^2 L}{\partial x_i \partial \dot{x}_j} + \frac{\partial^2 L}{\partial \dot{x}_k \partial \dot{x}_j} \frac{\partial}{\partial x^i} \dot{x}_k^R(t) \quad (31)$$

$$\frac{\partial^2}{\partial x^i \partial x^j} A^L(x_b, x; t_b, t) = -\frac{\partial}{\partial x^i} p_j^L(t) = -\frac{\partial^2 L}{\partial x_i \partial \dot{x}_j} - \frac{\partial^2 L}{\partial \dot{x}_k \partial \dot{x}_j} \frac{\partial}{\partial x^i} \dot{x}_k^L(t). \quad (32)$$

On the right-hand side we have taken into account that the arguments x and \dot{x} of the Lagrangian are classical trajectories fixed by their end points, i.e., $x(t) = x_{cl}(x, x_a; t)$ in Eq. (31) and $x(t) = x_{cl}(x_b, x; t)$ in Eq. (32). The derivatives with respect to the end points produce therefore an extra term coming from the velocity dependence of $L(x, \dot{x}; t)$. Then we use the Lagrangian (20) once more to express

$$\frac{\partial L}{\partial x_k} = \frac{1}{2} \dot{x}_i [\partial_k g_{ij}(x, t)] \dot{x}_j + \dot{x}_i \partial_k a_i(x, t) - \partial_k V(x, t) \quad (33)$$

$$\frac{\partial^2 L}{\partial \dot{x}_i \partial \dot{x}_j} = [\partial_j g_{ik}(x, t)] \dot{x}_k + \partial_j a_i(x, t) \quad (34)$$

$$\frac{\partial^2 L}{\partial \dot{x}_i \partial \dot{x}_j} = g_{ij}(x, t) \quad (35)$$

such that the brackets in Eq. (30) lead, via (31) and (32), to

$$\frac{\partial^2 A^R(x, x_a; t, t_a)}{\partial x^i \partial x^j} + \frac{\partial^2 A^L(x_b, x; t_b, t)}{\partial x^i \partial x^j} \quad (36) \\ = \{[\partial_j g_{ik}(x, t)] \dot{x}_k(t) + \partial_j a_i(x, t)\}^R - \{[\partial_j g_{ik}(x, t)] \dot{x}_k(t) + \partial_j a_i(x, t)\}^L + g_{ik}(x, t)^R \frac{\partial}{\partial x^j} \dot{x}_k^R(t) - g_{ik}(x, t)^L \frac{\partial}{\partial x^j} \dot{x}_k^L(t).$$

Then we use the fact that $x(t)$ and $\dot{x}(t)$ are continuous at the junction between the left and right paths, such that we can collect the terms on the right-hand side to

$$\frac{\partial^2 A^R(x, x_a; t, t_a)}{\partial x^i \partial x^j} + \frac{\partial^2 A^L(x_b, x; t_b, t)}{\partial x^i \partial x^j} = g_{ik}(x, t) \left[\frac{\partial}{\partial x^j} \dot{x}_k^R(t) - \frac{\partial}{\partial x^j} \dot{x}_k^L(t) \right]. \quad (37)$$

If we now take the limit $t \rightarrow t_{a+}$, the contribution from the path R to the derivatives inside the brackets becomes much larger than that of the path L . Indeed, the associated short classical path is

$$\dot{x}_k^R(t_{a+}) \approx \frac{x_k(t_{a+}) - x_k(t_a)}{t_{a+} - t_a}, \quad (38)$$

implying a very large derivative

$$\frac{\partial}{\partial x^j} \dot{x}_k^R(t_{a+}) \approx \frac{\delta_{kj}}{t_{a+} - t_a}. \quad (39)$$

Inserting this dominant contribution into Eq. (37), this further into (30), and factorizing out the approximately equal unknown fluctuation factors $F(x_b, x_a; t_b, t_a) \approx F(x_b, x_{a+}; t_b, t_{a+})$, we obtain the fluctuation factor for the infinitesimal time interval:

$$F(x_{a+}, x_a; t_{a+}, t_a) \approx \frac{1}{(2\pi i\hbar)^{D/2}} \left\{ \det_D \left[\frac{g_{ij}(x_a, t_a)}{t_{a+} - t_a} \right] \right\}^{1/2}. \quad (40)$$

This is the well-known free-particle result, as anticipated. It will be used twice: first to obtain Eq. (41), and later to fix the sign of the solution in Eq. (53).

We turn now to the second step in the derivation. It is based on the observation that the group property (25) is not only valid for causal time configurations $t_b > t > t_a$, but also for acausal time configurations $t > t_b > t_a$. The causality is only a property of the time evolution amplitude (1), not of the matrix elements (7), such that also (14) and (25) are valid for $t_b > t > t_a$ and $t > t_b > t_a$. This means that we can also bring the time t_b close to t_a , leaving t much larger than these two adjacent times, as indicated in Fig. 3.

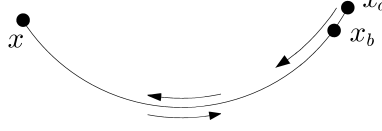


FIG. 3. Classical path from x_a to x , followed by a classical path backward in time from x to x_b along the same path.

In this limit $t_b \rightarrow t_{a+}$, Eq. (25) reads

$$F(x_{a+}, x_a; t_{a+}, t_a) = F(x_{a+}, x; t_{a+}, t)F(x, x_a; t, t_a)(2\pi i\hbar)^{D/2} \left\{ \det_D \left[\frac{\partial^2 (A^L + A^R)}{\partial x^i \partial x^j} \right] \right\}^{-1/2} \quad (41)$$

where A^L and A^R are now abbreviations for $A^L \equiv A(x_{a+}, x; t_{a+}, t)$, $A^R \equiv A(x, x_a; t, t_a)$. Using (40), this can be rewritten as

$$F(x_{a+}, x; t_{a+}, t)F(x, x_a; t, t_a) = \frac{1}{(2\pi i\hbar)^D} \left\{ \det_D \left[\frac{g_{ij}(x_a, t_a)}{t_{a+} - t_a} \right] \right\}^{1/2} \left\{ \det_D \left[\frac{\partial^2 (A^R + A^L)}{\partial x^i \partial x^j} \right] \right\}^{1/2}. \quad (42)$$

Let us study the behavior of the brackets in the last determinant for t_{a+} close to t_a . It reads more explicitly

$$\left. \frac{\partial^2 A^R(x, x_a; t, t_a)}{\partial x^i \partial x^j} + \frac{\partial^2 A^L(x_{a+}, x; t_{a+}, t)}{\partial x^i \partial x^j} \right|_{t_{a+} \approx t_a}, \quad (43)$$

where x_{a+} is very close to x_a . As the limit $t_{a+} \rightarrow t$ is reached, the two paths coincide, and have the same classical action, except for a negative relative sign, since the corresponding paths have the opposite direction in time. Thus for $t_{a+} = t_a$, the sum in (43) vanishes. For small $t_{a+} - t$, we perform a Taylor expansion of the second term around the first and have, omitting the now superfluous distinction between L and R , and using double primes to abbreviate the second derivatives $\partial^2 / \partial x_i \partial x_j$,

$$A''(x_{a+}, x; t_{a+}, t) \approx A''(x_a, x; t_a, t) + \left[\frac{\partial}{\partial t_a} A''(x_a, x; t_a, t) \right] (t_{a+} - t_a) + \left[\frac{\partial}{\partial x_a^k} A''(x_a, x; t_a, t) \right] (x_{a+}^k - x_a^k). \quad (44)$$

Inserting here $x_{a+}^k - x_a^k \approx (t_{a+} - t_a) \dot{x}^k(t_a)$, we may replace (43) by

$$\left\{ \left[\frac{\partial}{\partial t_a} \frac{\partial^2 A(x_a, x; t_a, t)}{\partial x^i \partial x^j} \right] + \left[\frac{\partial}{\partial x_a^k} \frac{\partial^2 A(x_a, x; t_a, t)}{\partial x^i \partial x^j} \right] \dot{x}^k(t_a) \right\} (t_{a+} - t_a), \quad (45)$$

and (42) becomes

$$F(x, x_a; t, t_a)F(x_a, x; t_a, t) = \frac{1}{(2\pi i\hbar)^D} \{ \det_D [g_{ij}(x_a, t_a)] \}^{1/2} \times \left(\det_D \left\{ \left[\frac{\partial^2}{\partial x^i \partial x^j} \frac{\partial A(x_a, x; t_a, t)}{\partial t_a} \right] + \left[\frac{\partial^2}{\partial x^i \partial x^j} \frac{\partial A(x_a, x; t_a, t)}{\partial x_a^k} \right] \dot{x}^k(t_a) \right\} \right)^{1/2}. \quad (46)$$

Note that the derivative $\partial^2 / \partial x^i \partial x^j$ does *not* act on $\dot{x}^k(t_a)$, so that the total argument in the last determinant of (46) is not the double prime of the total derivative of the action with respect to time t_a , in which case it could have been simplified to $(\partial^2 / \partial x^i \partial x^j) dA(x_a, x; t_a, t) / dt_a = (\partial^2 / \partial x^i \partial x^j) L(x_a, \dot{x}(t_a), t_a)$. Since this is not the case, we can only do a partial simplification using the Hamilton-Jacobi equation

$$\frac{\partial}{\partial t_a} A(x_a, x; t_a, t) + E(x_a, x; t_a, t) = 0, \quad (47)$$

where $E(x_a, x; t_a, t)$ is the energy at the time t_a for the classical trajectory $x(t_a) = x_{\text{cl}}(x_a, x; t_a, t)$ running backwards from x at t to x_a at t_a . It is the value of the Hamiltonian $H(t_a)$ of Eq. (22) evaluated for this trajectory. If $p(t_a) = p_{\text{cl}}(x_a, x; t_a, t)$ denotes the associated trajectory in momentum space, the energy is given by

$$\begin{aligned} E(x_a, x; t_a, t) &= H(t)|_{x(t)=x_{\text{cl}}(x_a, x; t_a, t), p(t)=p_{\text{cl}}(x_a, x; t_a, t)}, \\ &= \frac{1}{2} [p_i(x_a, t_a) - a_i(x_a, t_a)] g^{ij}(x_a, t_a) [p_j(x_a, t_a) - a_j(x_a, t_a)] + V(x_a, t_a). \end{aligned} \quad (48)$$

With this, Eq. (47) allows to rewrite (46) as

$$\begin{aligned} F(x, x_a; t, t_a) F(x_a, x; t_a, t) &= \frac{\{\det_D [g_{ij}(x_a, t_a)]\}^{1/2}}{(2\pi i \hbar)^D} \\ &\times \left(\det_D \left\{ -\frac{\partial^2}{\partial x^i \partial x^j} E(x_a, x; t_a, t) + \left[\frac{\partial^2}{\partial x^i \partial x^j} \frac{\partial A(x_a, x; t_a, t)}{\partial x_a^k} \right] \dot{x}^k(t_a) \right\} \right)^{1/2}. \end{aligned} \quad (49)$$

At this point we observe that for a purely harmonic Lagrangian, which is at most quadratic in the velocities and positions, the functions $g_{ij}(x, t)$ in the general expression (20) are position-independent, the vector potential $a_i(x, t)$ is at most linear in x , and the scalar potential $V(x, t)$ has the general form $V = x_i \Omega_{ij}(t) x_j / 2$. Then the classical action is at most quadratic in the end points. This implies a vanishing second term in the brackets of the second determinant in (49). Then, we have

$$F(x, x_a; t, t_a)^2 \underset{\text{for quadratic actions}}{=} \frac{\{\det_D [g_{ij}(t_a)]\}^{1/2}}{(2\pi i \hbar)^D} \left\{ \det_D \left[\frac{\partial^2}{\partial x^i \partial x^j} E(x_a, x; t_a, t) \right] \right\}^{1/2}. \quad (50)$$

Note the sign change of the second derivative of $E(x_a, x; t_a, t)$. This is caused by the replacement

$$F(x, x_a; t, t_a) F(x_a, x; t_a, t) \rightarrow i^D F(x, x_a; t, t_a)^2. \quad (51)$$

The reason for the factor i^D lies in the Fresnel nature of the path integral over the fluctuations. The exponent is the second functional derivative of the action with a factor i . Assuming stable orbits, the factor of i is positive or negative, depending on the time direction of the path. This sign change implies that the Fresnel integrals are related by

$$F(x, x_a; t, t_a) \sqrt{i^D} = F(x_a, x; t_a, t) / \sqrt{i^D}. \quad (52)$$

We can now take the square root of (50) and obtain

$$F(x_b, x_a; t_b, t_a) \underset{\text{for quadratic actions}}{=} \frac{\{\det_D [g_{ij}(t_a)]\}^{1/4}}{(2\pi i \hbar)^{D/2}} \left\{ \det_D \left[\frac{\partial^2}{\partial x_b^i \partial x_b^j} E(x_a, x_b; t_a, t_b) \right] \right\}^{1/4}, \quad (53)$$

The sign of this square root is fixed by the fact that in the limit of short intervals $t_b - t_a$, the fluctuation factor has to reduce to the free-particle result (40).

Note that in the semiclassical limit the fluctuations are always harmonic. For a vanishing vector potential $a_i(x, t)$ in Eq. (20), these would be driven by a time-dependent frequency matrix

$$\Omega_{ij}(t) = g^{ik}(x_{\text{cl}}(t), t) \partial_k \partial_j V(x_{\text{cl}}(t), t). \quad (54)$$

This harmonic property does not, however, allow us to use formula (53) for the fluctuation factor, since the frequency matrix depends on the end points via the classical solution $x_{\text{cl}}(t)$ of the equations of motion, so that the full formula (49) must be used, which we now investigate in detail.

We must evaluate

$$-\frac{\partial^2}{\partial x^i \partial x^j} E(x_a, x; t_a, t) + \left[\frac{\partial^2}{\partial x^i \partial x^j} \frac{\partial A(x_a, x; t_a, t)}{\partial x_a^k} \right] \dot{x}^k(t_a) \quad (55)$$

with $\partial A(x_a, x; t_a, t) / \partial x_a^k = p_k(t_a)$. Since $\partial x_a^k / \partial x^j = 0$, expression (55) can be rewritten as

$$-\frac{1}{2} g_{kl}(x_a, t_a) \frac{\partial^2}{\partial x^i \partial x^j} \dot{x}^k(t_a) \dot{x}^l(t_a) + \dot{x}^k(t_a) g_{kl}(x_a, t_a) \frac{\partial^2}{\partial x^i \partial x^j} \dot{x}^l(t_a). \quad (56)$$

Using the symmetry $g_{kl}(x_a, t_a) = g_{lk}(x_a, t_a)$, this becomes

$$-g_{kl}(x_a, t_a) \frac{\partial}{\partial x^i} \dot{x}_k(t_a) \frac{\partial}{\partial x^i} \dot{x}_l(t_a). \quad (57)$$

Now the determinant of a product of matrices factorizes into a product of determinants, and Eq. (49) becomes

$$F(x, x_a; t, t_a)^2 = \frac{\det_D [g_{ij}(x_a, t_a)]}{(2\pi i \hbar)^D} \det_D \left[\frac{\partial}{\partial x^i} \dot{x}_j(t_a) \right], \quad (58)$$

where the phase factor (51) has been taken into account. Using the relation

$$\frac{\partial^2}{\partial x_a^i \partial x^j} A(x, x_a; t, t_a) = -\frac{\partial}{\partial x^j} p_i(t_a) = -g_{ik}(x_a, t_a) \frac{\partial}{\partial x^j} \dot{x}_k(t_a) \quad (59)$$

we can finally rewrite (58) as

$$F(x, x_a; t, t_a)^2 = \frac{1}{(2\pi i \hbar)^D} \det_D \left[-\frac{\partial^2}{\partial x_a^i \partial x^j} A(x, x_a; t, t_a) \right] \quad (60)$$

from which it is straightforward to obtain

$$F(x_b, x_a; t_b, t_a) = \frac{1}{(2\pi i \hbar)^{D/2}} \left\{ \det_D \left[-\frac{\partial^2}{\partial x_a^i \partial x_b^j} A(x_b, x_a, t_b, t_a) \right] \right\}^{1/2}. \quad (61)$$

This is the Van Vleck-Pauli-Morette formula (11).

Our derivation has ignored zero modes in the intermediate integration, which may be treated in the standard way [1].

IV. APPLICATIONS

Here we shall apply our formula to three systems of point particles:

A. the free point particle with a mass matrix, with a Lagrangian

$$L = \frac{1}{2} \dot{x}_i M_{ij} \dot{x}_j, \quad (62)$$

B. the harmonic oscillator space with a time-dependent frequency matrix $\omega_{ij}(t)$, a mass matrix and a Lagrangian

$$L = \frac{1}{2} \{ \dot{x}_i M_{ij} \dot{x}_j - x_i [M\omega^2(t)]_{ij} x_j \}, \quad (63)$$

C. an ordinary particle in a constant magnetic field perpendicular to the plan spanned by x_1 and x_2 , with a Lagrangian

$$L = L = \frac{1}{2} M \sum_{i=1}^D \dot{x}_i^2 - \frac{e}{c} B \dot{x}_2 x_1. \quad (64)$$

In each cases, the boundary conditions are $x(t_a) = x_a, x(t_b) = x_b$.

A. Free Particle

The free particle case is particularly simple. The Lagrangian (62) implies the equations of motion

$$M_{ij} \frac{d^2}{dt^2} x_j = 0. \quad (65)$$

Since the matrix \mathbf{M} is symmetric, it can be diagonalized by a similarity transformation with an orthogonal matrix $\mathbf{S} = \mathbf{S}^{-T}$. Let $\mathbf{M}^d = \mathbf{S}^{-1}\mathbf{M}\mathbf{S}$ be the resulting diagonal mass matrix. The normal modes of the motion are $y(t) = \mathbf{S}^{-1}x(t)$. The latter satisfy

$$\frac{d^2}{dt^2}y_j = 0 \quad (66)$$

and have the time dependence

$$y_i(t) = \frac{1}{t_b - t_a} [y_a^i(t_b - t) + y_b^i(t - t_a)]. \quad (67)$$

The associated classical Hamiltonian is

$$H = \frac{1}{2}\dot{x}_i M_{ij} \dot{x}_j = \frac{1}{2}\dot{y}_i M_{ij}^d \dot{y}_j, \quad (68)$$

and the trajectories have the energy

$$E(x_a, x_b; t_a, t_b) = \frac{1}{2} \sum_{k=1}^D \frac{(y_b^k - y_a^k) M_{kk}^d (y_b^k - y_a^k)}{(t_b - t_a)^2}, \quad (69)$$

Using the relation

$$\frac{\partial}{\partial x_b^i} = \frac{\partial y_b^k}{\partial x_b^i} \frac{\partial}{\partial y_b^k} = S_{ki}^{-1} \frac{\partial}{\partial y_b^k}, \quad (70)$$

we deduce

$$\frac{\partial^2}{\partial x_b^i \partial x_b^j} E(x_a, x_b; t_a, t_b) = \frac{M_{ij}}{(t_b - t_a)^2}. \quad (71)$$

Inserting this into Eq. (53), we obtain the well-known fluctuation factor

$$F(x_b, x_a; t_b, t_a) = \frac{(\det_D \mathbf{M})^{1/2}}{[2\pi i \hbar (t_b - t_a)]^{D/2}}. \quad (72)$$

B. Harmonic Oscillator with Time-Dependent Frequency

The case of the harmonic oscillator with a time-dependent frequency is slightly more involved. One cannot solve the equations of motion to get the solution in a closed form. We will however give a formal solution, showing how the well-known result can be recovered when the frequency is time independent. The equations of motion associated with (63) are

$$\frac{d^2}{dt^2}x_i + \omega_{ij}^2(t)x_j = 0. \quad (73)$$

With the help of two matrices \mathbf{A} and \mathbf{B} , the solution can be decomposed as $x = \mathbf{A}x_a + \mathbf{B}x_b$. Since x_a and x_b are independent, each of the matrices satisfies a same equation as (73):

$$\frac{d^2}{dt^2}\mathbf{A} + \omega^2(t)\mathbf{A} = 0, \quad (74)$$

$$\frac{d^2}{dt^2}\mathbf{B} + \omega^2(t)\mathbf{B} = 0. \quad (75)$$

The boundary conditions are

$$A_{ij}(t_a) = \delta_{ij}, A_{ij}(t_b) = 0, \quad (76)$$

$$B_{ij}(t_a) = 0, B_{ij}(t_b) = \delta_{ij}. \quad (77)$$

Formula (53) contains a double derivative with respect to the end point x_b . For this reason, it will depend only on the part of the solution with the matrix \mathbf{B} . This simplifies the evaluation of the Hamiltonian and, taking derivatives with respect to the end point x_b , we have

$$\frac{\partial^2}{\partial x_b^i \partial x_b^j} E(x_a, x_b; t_a, t_b) = \left\{ \left[\frac{d}{dt} \mathbf{B}(t) \right]_{t=t_a} \mathbf{M} \left[\frac{d}{dt} \mathbf{B}(t) \right]_{t=t_a} \right\}_{ij} = \left[\dot{\mathbf{B}}(t_a) \mathbf{M} \dot{\mathbf{B}}(t_a) \right]_{ij} \quad (78)$$

where the last equality defines $\dot{\mathbf{B}}$ as the time derivative of the matrix \mathbf{B} . Using this relation in Eq. (53), the fluctuation factor is given by

$$F(x_b, x_a; t_b, t_a) = \frac{(\det_D \mathbf{M})^{1/2}}{[2\pi i \hbar (t_b - t_a)]^{D/2}} \left[\det_D \dot{\mathbf{B}}(t_a) \right]^{1/2}, \quad (79)$$

which requires to solve Eq. (75) with the associated boundary conditions (77). A formal solution can be obtained in the following way. Integrating twice (75), using (77), leads to

$$\mathbf{B}(t) = \int_{t_a}^t ds \dot{\mathbf{B}}(t_a) - \int_{t_a}^t ds \int_{t_a}^s \omega^2(y) \mathbf{B}(y) dy \quad (80)$$

which can be iterated to lead to a Neumann series

$$\mathbf{B}(t) = \int_{t_a}^t ds \left\{ \mathbb{1} - \int_{t_a}^s \omega^2(y) dy \int_{t_a}^y ds' + \int_{t_a}^s \omega^2(y) dy \int_{t_a}^y ds' \int_{t_a}^{s'} \omega^2(y') dy' \int_{t_a}^{y'} ds'' - \dots \right\} \dot{\mathbf{B}}(t_a). \quad (81)$$

Using a first order differential formalism, this expansion can be given a compact notation. This comes from the fact that the solution of (75) can be written as

$$\begin{pmatrix} \mathbf{B}(t) & \mathbf{0} \\ \mathbf{0} & \dot{\mathbf{B}}(t) \end{pmatrix} = T \left\{ \cosh \left[\int_{t_a}^t \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\omega^2(s) & \mathbf{0} \end{pmatrix} ds \right] \right\} \begin{pmatrix} \mathbf{B}(t_a) & \mathbf{0} \\ \mathbf{0} & \dot{\mathbf{B}}(t_a) \end{pmatrix} + T \left\{ \sinh \left[\int_{t_a}^t \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\omega^2(s) & \mathbf{0} \end{pmatrix} ds \right] \right\} \begin{pmatrix} \mathbf{0} & \mathbf{B}(t_a) \\ \dot{\mathbf{B}}(t_a) & \mathbf{0} \end{pmatrix}, \quad (82)$$

where the hyperbolic functions are defined through their Taylor expansion and where the symbol T implies a time ordering operation. Using the boundary conditions, we end up with

$$\begin{pmatrix} \mathbf{B}(t) & \mathbf{0} \\ \mathbf{0} & \dot{\mathbf{B}}(t) \end{pmatrix} = T \left\{ \sinh \left[\int_{t_a}^t \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\omega^2(s) & \mathbf{0} \end{pmatrix} ds \right] \right\} \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \dot{\mathbf{B}}(t_a) & \mathbf{0} \end{pmatrix}, \quad (83)$$

where we have multiplied from the right by an appropriate matrix in order to single out the upper left component. We can extract $\dot{\mathbf{B}}(t_a)$ from this relation using the boundary condition $\mathbf{B}(t_b) = \mathbb{1}$. This gives

$$\dot{\mathbf{B}}(t_a) = \left(T \left\{ \sinh \left[\int_{t_a}^{t_b} \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\omega^2(s) & \mathbf{0} \end{pmatrix} ds \right] \right\}_{12} \right)^{-1}, \quad (84)$$

which is indeed equivalent to iterative solution (81). Using this in (79) provides then us with a formal solution for the fluctuation factor.

The case of a time independent frequency matrix is obtained directly from the formal series (84): the time ordering operator disappears, the time integration is trivial and the series easily evaluated:

$$T \left\{ \sinh \left[\int_{t_a}^{t_b} \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\omega^2(s) & \mathbf{0} \end{pmatrix} ds \right] \right\}_{\omega=\text{const.}} = \sin[\omega(t_b - t_a)] \begin{pmatrix} \mathbf{0} & \omega^{-1} \\ -\omega & \mathbf{0} \end{pmatrix}. \quad (85)$$

As stipulated in (84), we need only the upper-right component. We then end up with

$$F(x_b, x_a; t_b, t_a)_{\omega=\text{const.}} = \frac{(\det_D \mathbf{M})^{1/2}}{[2\pi i \hbar (t_b - t_a)]^{D/2}} \left\{ \frac{\det_D \omega}{\det_D \sin[\omega(t_b - t_a)]} \right\}^{1/2}. \quad (86)$$

Denoting by ω_i^2 (no summation over i) the normal modes, this equation can also be written as

$$F(x_b, x_a; t_b, t_a)_{\omega=\text{const.}} = \frac{(\det_D \mathbf{M})^{1/2}}{[2\pi i \hbar (t_b - t_a)]^{D/2}} \prod_{i=1}^D \left\{ \frac{\omega_i}{\sin[\omega_i(t_b - t_a)]} \right\}^{1/2}. \quad (87)$$

C. Particle in Constant Magnetic Field

Here the calculation looks somewhat more complicated, although it is still trivial. The equations of motion associated with the Lagrangian (64) are

$$\frac{d^2}{dt^2}x_1 - \omega \frac{d}{dt}x_2 = 0, \quad (88)$$

$$\frac{d^2}{dt^2}x_2 + \omega \frac{d}{dt}x_1 = 0, \quad (89)$$

$$\frac{d^2}{dt^2}x_j = 0, \quad j = 3, \dots, D. \quad (90)$$

The index j will be limited to $j = 3, \dots, D$ throughout in this section. The frequency ω is the Larmor frequency $\omega = eB/(cM)$, where e is the electron charge and c the speed of light. The classical trajectories are

$$x_1 = \frac{1}{\sin \omega(t_b - t_a)} [(x_b^1 - x_0^1) \sin \omega(t - t_a) + (x_a^1 - x_0^1) \sin \omega(t_b - t)] + x_0^1, \quad (91)$$

$$x_2 = \frac{1}{\sin \omega(t_b - t_a)} [(x_b^2 - x_0^2) \sin \omega(t - t_a) + (x_a^2 - x_0^2) \sin \omega(t_b - t)] + x_0^2, \quad (92)$$

$$x_j = \frac{1}{t_b - t_a} [x_a^j(t_b - t) + x_b^j(t - t_a)], \quad (93)$$

where x_0^1 and x_0^2 are determined from (88) and (89) as [1]:

$$x_0^1 = \frac{1}{2} \left[(x_b^1 + x_a^1) + (x_b^2 - x_a^2) \cot \frac{\omega(t_b - t_a)}{2} \right], \quad (94)$$

$$x_0^2 = \frac{1}{2} \left[(x_b^2 + x_a^2) - (x_b^1 - x_a^1) \cot \frac{\omega(t_b - t_a)}{2} \right]. \quad (95)$$

For the classical Hamiltonian we obtain the only non-vanishing contributions (no summation over j)

$$\frac{\partial^2}{\partial x_b^1 \partial x_b^1} E(x_a, x_b; t_a, t_b) = \frac{\partial^2}{\partial x_b^2 \partial x_b^2} E(x_a, x_b; t_a, t_b) = \frac{M\omega^2}{4 \sin^2 [\omega(t_b - t_a)/2]}, \quad (96)$$

$$\frac{\partial^2}{\partial x_b^j \partial x_b^j} E(x_a, x_b; t_a, t_b) = \frac{M}{(t_b - t_a)^2}, \quad (97)$$

from which it is trivial to find

$$\det_D \frac{\partial^2}{\partial x_b^i \partial x_b^k} E(x_a, x_b; t_a, t_b) = \left[\frac{M}{(t_b - t_a)^2} \right]^{D-2} \left\{ \frac{M\omega^2}{4 \sin^2 [\omega(t_b - t_a)/2]} \right\}^2, \quad (98)$$

such that Eq. (53) yields [1]

$$F(x_b, x_a; t_b, t_a) = \sqrt{\frac{M}{2\pi i \hbar (t_b - t_a)}}^D \frac{\omega(t_b - t_a)/2}{\sin [\omega(t_b - t_a)/2]}. \quad (99)$$

D. Particle in Arbitrary One-Dimensional Potential

For a particle moving in an arbitrary time-dependent potential in one dimension, it is possible to construct an explicit solution to the general relation (25). The matrix in the determinant on the right-hand side is

$$\frac{\partial}{\partial x} \dot{x}^R(t) - \frac{\partial}{\partial x} \dot{x}^L(t). \quad (100)$$

Using the equation of motion

$$\frac{d^2}{dt^2}x + \partial_x V(x, t) = 0 \quad (101)$$

and taking the derivative with respect to time we obtain

$$\frac{d^2}{dt^2}\dot{x} + V''(x, t)\dot{x} = 0, \quad (102)$$

and a similar equation for a derivative with respect to any other parameter λ :

$$\frac{d^2}{dt^2}\partial_\lambda x + V''(x, t)\partial_\lambda x = 0. \quad (103)$$

Hence $\partial_\lambda x$ can be expressed as a linear combination of two fundamental solutions of (102). One of them is the time derivative of the classical trajectory, $\partial_\lambda x^{(1)} = \dot{x}$. The other can be obtained from the D'Alembert construction [1] and is $\partial_\lambda x^{(2)} = \dot{x} \int^t dt/\dot{x}^2$. Combining these into solutions satisfying the boundary conditions $\partial_x x(t_a) = 0$, $\partial_x x(t_b) = 0$ and $\partial_x x(t) = 1$, we then obtain

$$\partial_x x^R = \frac{\dot{x}^R}{\dot{x}(t)} \frac{\int_{t_a}^t dt/\dot{x}^2}{\int_{t_a}^t dt/\dot{x}^2}, \quad (104)$$

$$\partial_x x^L = \frac{\dot{x}^L}{\dot{x}(t)} \frac{\int_t^{t_b} dt/\dot{x}^2}{\int_t^{t_b} dt/\dot{x}^2}, \quad (105)$$

from which we deduce

$$\partial_x \dot{x}^R(t) - \partial_x \dot{x}^L(t) = \frac{1}{\dot{x}^2(t)} \frac{\int_{t_a}^{t_b} dt/\dot{x}^2}{\left(\int_{t_a}^t dt/\dot{x}^2\right) \left(\int_t^{t_b} dt/\dot{x}^2\right)}. \quad (106)$$

Inserting this result in (25), we have in the limit $t \rightarrow t_{a+}$

$$\left(\dot{x}^2(t_a) \int_{t_a}^{t_{a+}} \frac{dt}{\dot{x}^2}\right)^{-1/2} = \sqrt{2\pi i \hbar} F(x_{a+}, x_a; t_{a+}, t_a). \quad (107)$$

Taking the limit $t_b \rightarrow t_a$ at an arbitrary t in (25), and inserting (107), we obtain

$$\left[\dot{x}^2(t_a) \dot{x}^2(t) \left(\int_{t_a}^t \frac{dt}{\dot{x}^2}\right) \left(\int_t^{t_a} \frac{dt}{\dot{x}^2}\right)\right]^{-1/2} = (2\pi i \hbar) F(x_a, x; t_a, t) F(x, x_a; t, t_a). \quad (108)$$

and thus a fluctuation factor

$$F(x_b, x_a; t_b, t_a) = \frac{1}{\sqrt{2\pi i \hbar}} \left[\dot{x}(t_a) \dot{x}(t_b) \int_{t_a}^{t_b} \frac{dt}{\dot{x}^2}\right]^{-1/2}. \quad (109)$$

which agrees, of course, with formula (11).

V. CONCLUSION

We have shown that the Van Vleck-Pauli-Morette determinant in the fluctuation factor (11) can be obtained directly from the group property of the time evolution operator (1) and the semiclassical expansion (7). In addition, we have derived a formula which allows us to find the fluctuation factor from the classical Hamiltonian function if the Lagrangian is at harmonic velocities and positions.

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