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LETTER TO THE EDITOR

The partition function in the Wigner–Kirkwood expansion

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Online at stacks.iop.org/JPhysA/39/L285**Abstract**

We study the semiclassical Wigner–Kirkwood (WK) expansion of the partition function $Z(t)$ for arbitrary even homogeneous potentials, starting from the Bloch equation. As is well known, the phase-space kernel of Z satisfies the so-called Uhlenbeck–Beth equation, which depends on the gradients of the potential. We perform a chain of transformations to obtain novel forms of this equation that invite analogies with various physical phenomena and formalisms, such as diffusion processes, the Fokker–Planck equation and supersymmetric quantum mechanics.

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1. Introduction

The problem of the semiclassical expansion of physical states and their energies in powers of \hbar rather than the expansions involving oscillating functions of \hbar^{-1} has a long history and was studied and used in different fields of science (see [1] for review) beginning from the Thomas–Fermi (TF) approximation [1–3]. Being the lowest order in \hbar , the TF correction to the classical partition function (heat kernel) takes into account the discreteness of the phase space treating the Hamiltonian classically.

We consider here Hamiltonians of the form $H = T + V$ where T is the kinetic and V is the potential energy, respectively. The non-commutativity of the T and V in the quantum Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\nabla^2 + V(\{x_i\}), \quad (1)$$

where ∇^2 denotes the Laplacian and i labels the coordinates, was taken into account by the Wigner–Kirkwood (WK) approach [4, 5]. (Note: We set the mass $m = 1$, and all quantities are given in units of energy E (implying the dimensions: $[H] = 1$, $[t] = -1$, $[\hbar] = 3/4$,

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$[V] = 1, [x] = 1/4$.) We do not specify the form of the, generally non-central, potential $V(\mathbf{x})$ for n degrees of freedom ($\mathbf{x} = (x_1, x_2, \dots, x_n)$). The case of even homogeneous polynomials satisfying $V(\lambda\mathbf{x}) = \lambda^{2N} V(\mathbf{x})$ includes the potentials of the well-known Yang–Mills classical and quantum mechanics [6–8] (see [9] for a review).

2. The partition function in the WK expansion

The partition function

$$Z(t) = \text{Tr}[\exp(-t\hat{H})] = \sum_{n=0}^{\infty} e^{-E_n t}, \quad (2)$$

which is the Laplace transform of the density of states $\mathcal{L}[\rho(E)]$, is calculated taking the Wigner transform of the quantum operator $\exp(-t\hat{H})$ and integrating it over the phase space with measure

$$d\Gamma = (2\pi\hbar)^{-n} d^n x d^n p, \quad (3)$$

where n is the dimension of the system.

For the semiclassical expansion it is convenient to use the plane waves as a complete set:

$$Z(t) = (2\pi\hbar)^{-n} \int d\Gamma e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} e^{-t\hat{H}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}. \quad (4)$$

The WK method takes into account only part of the quantum features, but ignores the quantum fluctuations defined by the concrete form of the potential and dynamics (see [8] for the discussion of the role of the quantum fluctuations in Yang–Mills quantum mechanics). Following [10], we can account the non-commuting terms in WK approach setting

$$e^{-t\hat{H}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} = e^{-tH} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} W(\mathbf{x}, \mathbf{p}; t) = u(\mathbf{x}, \mathbf{p}; t), \quad (5)$$

where H is the classical Hamiltonian and the function $W(\mathbf{x}, \mathbf{p}; t)$ is to be determined. The function $u(\mathbf{x}, \mathbf{p}; t)$ satisfies the Bloch equation, the analogue of the time-dependent Schrödinger equation:

$$\frac{\partial u}{\partial t} + \hat{H}u = 0 \quad (6)$$

with the initial condition

$$\lim_{t \rightarrow 0} u(\mathbf{x}, \mathbf{p}; 0) = e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}, \quad (7)$$

corresponding to the initial condition $W(\mathbf{x}, \mathbf{p}; 0) = 1$.

Boundary conditions on $u(\mathbf{x}, \mathbf{p}; t)$ at $|x| = \infty$ are in correspondence with the boundary conditions on $W(\mathbf{x}, \mathbf{p}; t)$. From (5) and (6) we obtain an exact equation for $W(\mathbf{x}, \mathbf{p}; t)$, which we call the Uhlenbeck–Beth (UB) equation):

$$\frac{\partial W}{\partial t} = \frac{\hbar^2}{2} \left[\nabla^2 - t(\nabla^2 V) + t^2(\nabla V)^2 - 2t(\nabla V) \cdot \nabla + \frac{2i}{\hbar} \mathbf{p} \cdot (\nabla - t\nabla V) \right] W. \quad (8)$$

Next we expand W in powers of \hbar [5]:

$$W = \sum_{k=0}^{\infty} \hbar^k W_k \quad (9)$$

and equate the terms with the same power of \hbar on both the sides. The result is

$$\frac{\partial W_k}{\partial t} = \frac{1}{2} [\nabla^2 - t(\nabla^2 V) + t^2(\nabla V)^2 - 2t(\nabla V) \cdot \nabla] W_{k-2} + i\mathbf{p} \cdot (\nabla - t\nabla V) W_{k-1}. \quad (10)$$

with conditions $W_0 = 1, W_k = 0$ for $k < 0$.

3. New forms of the UB equation

The expressions (8) and (10) can be written in more compact form, if we introduce the ‘covariant’ derivative $\mathcal{D} = \nabla - t(\nabla V)$:

$$\frac{\partial W}{\partial t} = \frac{\hbar^2}{2} \left[\mathcal{D}^2 + \frac{2i}{\hbar} \mathbf{p} \cdot \mathcal{D} \right] W = \frac{1}{2} [(\hbar \mathcal{D} + i\mathbf{p})^2 + \mathbf{p}^2] W, \quad (11)$$

or its recursive form

$$\frac{\partial W_k}{\partial t} = \frac{1}{2} [\mathcal{D}^2 W_{k-2} + 2i\mathbf{p} \cdot \mathcal{D} W_{k-1}]. \quad (12)$$

We note that the symbol \mathbf{p} in (11), (12) denotes a classical phase-space variable and not an operator. To our knowledge, the forms (11) and (12) of equations (8) and (10) are novel and have not been given in the literature.

In terms of the operator \mathcal{D} , equation (11) resembles a Fokker–Planck equation (FPE) for $W(\mathbf{x}, \mathbf{p}; t)$ with the diffusion constant \hbar^2 and the constant drift vector $-i\hbar\mathbf{p}$. The relation to the FPE can be further elucidated by noting that the ‘vector potential’ $\mathbf{A} = t\nabla V$ is a complete gradient and thus may be ‘gauged out’ by the transformation $W \rightarrow \exp(tV)W'$, yielding an alternative form of (11):

$$\frac{\partial W'}{\partial t} = \frac{\hbar^2}{2} \left[\nabla^2 + \frac{2i}{\hbar} \mathbf{p} \cdot \nabla \right] W' - V W'. \quad (13)$$

If we interpret $W'(\mathbf{x}, \mathbf{p}; t)$ as an one-time probability density and introduce the probability current (sometimes called the probability flux in the literature [11, 12]):

$$\mathbf{J} = -i\hbar\mathbf{p}W' - \frac{\hbar^2}{2}\nabla W' = W' \left(-i\hbar\mathbf{p} - \frac{\hbar^2}{2}\nabla \ln W' \right), \quad (14)$$

we may write (13) in the form of the continuity equation

$$\frac{\partial W'}{\partial t} + \nabla \cdot \mathbf{J}' = -V(x)W'(\mathbf{x}, \mathbf{p}; t), \quad (15)$$

where the potential term acts as a source term leading to a ‘probability loss’ and violates the local conservation law associated with FPE. Integrating over volume and using the Gauss’ theorem in (15) we obtain

$$\frac{\partial}{\partial t} \int W' d^n x + \int_S d\sigma \cdot \mathbf{J}' = - \int V W' d^n x, \quad (16)$$

where S is the surface confining the volume. If the flux vanishes at infinity we have

$$\frac{\partial}{\partial t} \int W' d^n x = - \int V W' d^n x. \quad (17)$$

Note that in the right-hand side of (13) and (15) we may substitute the total energy H instead of the potential V by making the transformation $W' = W'' \exp(-p^2 t/2)$, since p commutes with gradients on the right-hand side of (13) and (14).

The presence of the potential term $V W'$ (or $U W'$) in (13) and (15) invalidates the standard result for the FPE (see, e.g. [11, 12]) that under rather loose conditions on the drift and diffusion kernels (which are satisfied in our case) all solutions of the FPE must coincide for sufficiently large times. If drift and diffusion functions do not depend on time, a stationary solution may exist, and this solution is unique in the sense that all other solutions agree with it after sufficiently long time. Having the stationary solution of the FPE, one is able to find the general solution with given initial and boundary conditions (see, e.g. [13, 14]).

In our case it is clear that stationary solutions to the Bloch equation (6) exist only for the trivial case of vanishing V . This is evident from (1), (5) and (6): using the second expression for the probability flux in (14), setting $\dot{W}_{\text{st}} = 0$ and using U instead of V in (15), we obtain the equation

$$(\nabla \ln u_{\text{st}})^2 = \frac{2}{\hbar^2} V(\mathbf{x}). \quad (18)$$

Since $u_{\text{st}} = \exp(i\mathbf{p} \cdot \mathbf{x}/\hbar)$ is the solution of the Bloch equation (6) with $\partial u/\partial t = 0$, we arrive at the stated conclusion that there are no stationary solutions to the Bloch equation for non-vanishing potential. Similarly, for the FPE (13) resulting from the substitution $W = \exp(tV)W'$, it is clear from (5) that the only stationary solution is $W' = 1$ for $V(\mathbf{x}) = 0$.

Keeping this in mind, let us divide the solution to (13) into a stationary and a time-dependent part:

$$W'(\mathbf{x}, \mathbf{p}; t) = W'_{\text{st}}(\mathbf{x}, \mathbf{p}) + w'(\mathbf{x}, \mathbf{p}; t). \quad (19)$$

For $V = 0$ there exists the stationary solution

$$L_{\text{FP}}(\mathbf{x}, \mathbf{p})W'_{\text{st}} \equiv \frac{\hbar^2}{2} \left[\nabla^2 + \frac{2i}{\hbar} \mathbf{p} \cdot \nabla \right] W'_{\text{st}} = 0. \quad (20)$$

Inserting (19) into (13) we obtain

$$\frac{\partial w'}{\partial t} = (L_{\text{FP}} - V)w' - V W'_{\text{st}}. \quad (21)$$

Following the standard approach to the solution of inhomogeneous first-order differential equations, we can obtain a formal solution of (21) in the form

$$w'(\mathbf{x}, \mathbf{p}; t) = - \int_{-\infty}^t dt' e^{[L_{\text{FP}} - V](t-t')} V(\mathbf{x}) W'_{\text{st}}(\mathbf{x}, \mathbf{p}). \quad (22)$$

To this we need to add the general solution of the homogeneous equation

$$\frac{\partial \tilde{w}}{\partial t} = (L_{\text{FP}} - V)\tilde{w}. \quad (23)$$

The complete solution (19) thus has three contributions:

$$W'(\mathbf{x}, \mathbf{p}; t) = W'_{\text{st}}(\mathbf{x}, \mathbf{p}) + w'(\mathbf{x}, \mathbf{p}; t) + \sum_n C_n \tilde{w}_n(\mathbf{x}, \mathbf{p}; t), \quad (24)$$

where the C_n are derived from the initial condition $W'(\mathbf{x}, \mathbf{p}; 0) = 1$. The solutions \tilde{w}_n of the homogeneous equation are obtained by separation of variables, $\tilde{w}_n(\mathbf{x}, \mathbf{p}; t) = T_n(t)X_n(\mathbf{x}, \mathbf{p})$, in the form

$$T_n(t) = e^{-\lambda_n t}, \quad (25)$$

$$(L - V)X_n(\mathbf{x}, \mathbf{p}) = -\lambda_n^2 X_n(\mathbf{x}, \mathbf{p}), \quad (26)$$

where $-\lambda_n^2$ are the eigenvalues of the operator $L - V$. Finally, the solution of (20) is the plane wave:

$$W'_{\text{st}}(\mathbf{x}, \mathbf{p}) = \frac{c}{\hbar^2} e^{-2i\mathbf{p} \cdot \mathbf{x}/\hbar}. \quad (27)$$

4. Chain of transformations of the UB equation

By the transformation $W = \exp(tV)W'$ (or $W = \exp(tU)W'$) we obtained the equation (13) which is intermediate between the Bloch and UB equations. Going one step further by setting $W' = \exp(-i\mathbf{p} \cdot \mathbf{x}/\hbar)\tilde{W}$ we arrive, of course, at the Bloch equation (6) as is evident from the chain of transformations

$$W \rightarrow e^{tU}W'' \rightarrow e^{tU-i\mathbf{p}\cdot\mathbf{x}/\hbar}\tilde{W}, \quad (28)$$

with the identification $\tilde{W} = u$. Each link of this chain opens up new analogies with the important physical processes and equations which govern them. We elaborate this issue below in more detail. Before we address this subject, however, we note that the expansion in \hbar proposed by Kirkwood [5] is also an expansion in powers of the gradient operator as emphasized in [10]: the gradient operator occurs k times for each W_k in equation (10). In the general case, one needs to expand in powers of \hbar or, equivalently, in powers of the gradient operator using (10) and (12), as done in [7, 8].

In some special cases the compact form of (11) or (13) and the Bloch equation itself may be the starting point of another approximation scheme, which can bring to bear the knowledge of approximation techniques developed for the Fokker–Planck and Schrödinger equations. With this in mind, we explore here several modified forms of the diffusion equation (13), before we consider some aspects of the Bloch equation. Going back to our original function $W(\mathbf{x}, \mathbf{p}; t) = \exp(tU)W'(\mathbf{x}, \mathbf{p}; t)$ we may write (13) in the form

$$\frac{\partial W}{\partial t} = e^{tH}(\hat{L}_{\text{FP}}W)e^{-tH}, \quad (29)$$

where

$$\hat{L}_{\text{FP}} = \frac{\hbar^2}{2} \left[\nabla^2 + \frac{2i}{\hbar} \mathbf{p} \cdot \nabla \right]. \quad (30)$$

For (15) we then obtain

$$\frac{\partial W}{\partial t} = e^{tH}(\nabla \cdot \mathbf{J})e^{-tH}, \quad (31)$$

with

$$\mathbf{J} = \frac{\hbar^2}{2} \left[\nabla + \frac{2i}{\hbar} \mathbf{p} \right] W. \quad (32)$$

Equations (29) and (31) are of form of a FPE, just like equation (8).

Another, equivalent form of the same equation (13) is easily derived:

$$\frac{\partial W}{\partial t} = \frac{1}{2} e^{tH}(\hat{\mathcal{P}}^2 - \mathbf{p}^2)e^{-tH}, \quad (33)$$

with the quantum operator

$$\hat{\mathcal{P}} = \mathbf{p} - i\hbar\nabla. \quad (34)$$

This is the Bloch–Schrödinger form of equation (8).

As a check, from $Z(t) = \int d\Gamma W e^{-tH}$ we have, using (33):

$$\frac{\partial Z}{\partial t} = - \int d\Gamma \left(\frac{1}{2} \hat{\mathcal{P}}^2 + V(\mathbf{x}) \right) W e^{-tH}. \quad (35)$$

Integrating over t we have

$$Z(t) = \int d\Gamma \left(\frac{1}{2} \hat{\mathcal{P}}^2 + V(\mathbf{x}) \right) \int_t^\infty dt' e^{-t'H} W(\mathbf{x}, \mathbf{p}; t'). \quad (36)$$

In the limit $\hbar = 0$, $\hat{P} = \mathbf{p}$, (and thus $W = 1$) equation (36) reduces to the Thomas–Fermi term

$$Z(t) = \int d\Gamma e^{-tH}. \quad (37)$$

Finally, we mention another form of the basic equation (8), or its equivalent, equation (11). If one introduces instead of W the new function $\tilde{W} = \exp(-tV)W$, then (11) can be written in the form

$$\frac{\partial \tilde{W}}{\partial t} = \left[\frac{\hbar^2}{2} \tilde{\mathcal{D}}^2 + i\hbar \mathbf{p} \cdot \tilde{\mathcal{D}} \right] \tilde{W} - \frac{1}{2} V \tilde{W}, \quad (38)$$

where the operator $\tilde{\mathcal{D}}$ is given by

$$\tilde{\mathcal{D}} = e^{-tV/2} \nabla e^{-tV/2}. \quad (39)$$

Equation (38) corresponds to the FPE used in supersymmetric quantum mechanics in one dimension in association with the Darboux transformation (see, e.g. [12]).

5. More on the Bloch equation

We see that WK semiclassical expansion leads to several equations with interesting connections to fundamental branches of physics. The basis of this expansion is the Bloch equation (6). Having obtained the solution of (6) we find the partition function

$$Z(t) = \int d\Gamma e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} u(\mathbf{x}, \mathbf{p}; t). \quad (40)$$

The initial condition

$$u(\mathbf{x}, \mathbf{p}; 0) = e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \quad (41)$$

may appear somewhat unusual taking into account that the potentials $V(\mathbf{x})$ considered here are generally associated with the bound states of the corresponding Schrödinger equation. Nevertheless, starting from (6), we may represent $u(\mathbf{x}, \mathbf{p}; t)$ as an expansion in terms of plane waves satisfying the initial condition (41):

$$u(\mathbf{x}, \mathbf{p}; t) = \int d^n p' a(\mathbf{p}, \mathbf{p}'; t) e^{i\mathbf{p}'\cdot\mathbf{x}/\hbar - p'^2 t/2}. \quad (42)$$

Equation (41) translates into the following initial condition for the amplitude $a(\mathbf{p}, \mathbf{p}'; t)$:

$$a(\mathbf{p}, \mathbf{p}'; 0) = \delta(\mathbf{p} - \mathbf{p}'), \quad (43)$$

and equation (6) gives, after multiplying the resulting equation by $\exp(-i\mathbf{p}\cdot\mathbf{x}/\hbar)$ and integrating both sides over x :

$$\frac{\partial}{\partial t} [a(\mathbf{p}, \mathbf{p}'; t) e^{-p'^2 t/2}] = - \int \frac{d^n p'}{(2\pi\hbar)^n} a(\mathbf{p}, \mathbf{p}'; t) e^{-p'^2 t/2} \int d^n x V(\mathbf{x}) e^{i(\mathbf{p}' - \mathbf{p})\cdot\mathbf{x}/\hbar}. \quad (44)$$

Introducing the function

$$A(\mathbf{p}, \mathbf{p}'; t) = a(\mathbf{p}, \mathbf{p}'; t) e^{-p'^2 t/2} \quad (45)$$

we obtain

$$\frac{\partial}{\partial t} A(\mathbf{p}, \mathbf{p}'; t) + \frac{p'^2}{2} A(\mathbf{p}, \mathbf{p}'; t) = - \int d^n p' A(\mathbf{p}, \mathbf{p}'; t) \tilde{V}(\mathbf{p} - \mathbf{p}'), \quad (46)$$

where

$$\tilde{V}(\mathbf{p}) = \int \frac{d^n x}{(2\pi\hbar)^n} V(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}. \quad (47)$$

Inserting (42) into equation (40) we find that

$$Z(t) = \int d^n p A(\mathbf{p}, \mathbf{p}; t). \quad (48)$$

This form is analogous to the expression for $Z(t)$ in terms of the Bloch density matrix (see, e.g. [1]):

$$C(\mathbf{x}, \mathbf{x}'; t) = \sum_n \psi_n^*(\mathbf{x}) \psi_n(\mathbf{x}') e^{-tE_n} = \langle \mathbf{x} | e^{-t\hat{H}} | \mathbf{x}' \rangle, \quad (49)$$

from which it is obvious that the quantity

$$A(\mathbf{p}, \mathbf{p}'; t) = \langle \mathbf{p} | e^{-t\hat{H}} | \mathbf{p}' \rangle, \quad (50)$$

whose trace is the partition function, is the counterpart of $C(\mathbf{x}, \mathbf{x}'; t)$ in the momentum representation.

As an example, we consider the case of $n = 2$, i.e. the Yang–Mills quantum mechanics (YMQM) with the potential

$$V(x, y) = \frac{g^2}{2} x^2 y^2, \quad (51)$$

which was the subject of numerous studies (see [9] for a review). This potential leads to a non-separable and non-integrable Schrödinger equation. Its Fourier transform is given by

$$\tilde{V}(\mathbf{p}' - \mathbf{p}) = \frac{g^2 \hbar^4}{2} \frac{\partial^2}{\partial p_x'^2} \frac{\partial^2}{\partial p_y'^2} \delta(\mathbf{p}' - \mathbf{p}), \quad (52)$$

which lets (46) take the form

$$\frac{\partial}{\partial t} A(\mathbf{p}, \mathbf{p}; t) + \frac{p^2}{2} A(\mathbf{p}, \mathbf{p}; t) = - \frac{g^2 \hbar^4}{2} \frac{\partial^2}{\partial p_x'^2} \frac{\partial^2}{\partial p_y'^2} A(\mathbf{p}, \mathbf{p}'; t) \Big|_{\mathbf{p}'=\mathbf{p}}. \quad (53)$$

From (53) one finds that the quantum corrections to the classical result for $Z(t)$ generally begin at the order \hbar^4 for the YMQM model [7]. In the same way, one may show that the quantum corrections to $Z(t)$ for the harmonic oscillator begin at the order \hbar^2 , in agreement with the result found by the expansion of the well-known exact expression for $Z(t)$. The generalization of (53) to higher dimensions ($n > 2$) is straightforward.

6. Conclusions

In the present paper we have presented several different forms of the differential equation for the quantum corrections to the partition function $Z(t)$. Some of these forms appear to be novel. Any one of these equivalent equations can be used to generate the gradient expansion of $Z(t)$ for a wide class of potentials or could serve as the starting point for a numerical evaluation. The analogy between some forms of the equation and other well-studied equations of theoretical physics, such as the Fokker–Planck equation, suggests the possibility of novel approaches or approximation schemes for the calculation of $Z(t)$. As an example, we have used the integral representation of the Bloch equation in momentum space to give a simple proof of the fact that the quantum corrections to $Z(t)$ for the anharmonic Yang–Mills quantum mechanics begins at the order \hbar^4 [7]. We have also found a hitherto unknown correspondence with the Fokker–Planck equation occurring in supersymmetric quantum mechanics.

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