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Curious Features of Semiclassical Formulas for the Sum over Histories

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Abstract

The semiclassical formula for Feynman's path integral and the semiclassical formula for the energy-dependent Green function are revisited. Curious features of these semiclassical formulas are pointed out, which are examined in relation with supersymmetric quantum mechanics. The supersymmetric counterparts of the semiclassical formulas are also proposed.

1. Introduction

Feynman's path integral formula [1] and the semiclassical formula of Van Vleck, Pauli and Morette [2, 3] are equally useful for providing the propagator for a quadratic system. However, the power of either Feynman's formula or the VPM formula is substantially reduced for handling non-quadratic systems. The semiclassical formula of Gutzwiller [4], which calculates the energy-dependent Green function by reckoning the contributions from the classical orbits, can deal with those problems which are not well handled by the formulas for the propagator. Why is the formula for the Green function more flexible than the formulas for the propagator? Is it a myth that the sum over all classical paths for the Green function is exact? Is there anyway to improve the semiclassical approximation? We examine these questions and point out some well-known or not-so-well-known curious facts about the semiclassical formulas. Then we propose the quasiclassical approach to derive the quasiclassical counterparts of the semiclassical formulas. We show that the quasiclassical version of Gutzwiller's formula gives rise to the quantization rules in supersymmetric quantum mechanics.

2. Semiclassical Formula for the Propagator

Feynman [1] provided the path integral formula for calculating the propagator for a point mass m ,

$$K(x'', t'', x', t') = \lim_{N \rightarrow \infty} \int_{x' = x(t')}^{x'' = x(t'')} \prod_{j=1}^N \left[\frac{m}{2\pi i \hbar \Delta t_j} \right]^{1/2} \prod_{j=1}^{N-1} \exp\{ (i/\hbar) S_j \} \prod_{j=1}^{N-1} dx_j, \tag{1}$$

where

$$S_j = \int_{t_{j-1}}^{t_j} L(\dot{x}, x) dt \tag{2}$$

and $x_j = x(t_j)$, $\Delta t_j = t_j - t_{j-1} > 0$, $t'' - t' = \sum_{j=1}^N \Delta t_j$. For a system whose Lagrangian $L(\dot{x}, x)$ has a quadratic form in its variables, this path integration can be explicitly carried out to yield an exact expression for the propagator in question. The polar coordinate treatment helps only slightly to extend the list of exactly path integrable examples by including in it the rigid rotator, the inverse-square potential [5, 6], and the spherical top [7, 8]. Otherwise, even if the system is soluble by standard methods, Feynman's prescription does not work. If the Lagrangian is of the form,

$$L = \frac{1}{2} m \dot{x}^2 - V(x), \tag{3}$$

the propagator may as well be found by the semiclassical formula of Van Vleck, Pauli and Morette (VPM) [3],

$$K(x'', t'', x', t') = \sqrt{\frac{i}{2\pi\hbar} \frac{\partial^2 S_c}{\partial x' \partial x''}} \exp \left[\frac{i}{\hbar} S_c(x'', t'', x', t') \right], \tag{4}$$

where S_c is the action calculated along the classical path. In fact, the VPM formula can be derived from Feynman's path integral. For convenience of our later discussions, let us review the essence of the derivation. The semiclassical calculation is based on the expansion of the action functional $S[x]$ about the classical path,

$$S \cong S_c + \delta S + \frac{1}{2} \delta^2 S. \tag{5}$$

The classical path $x_c(t)$ is determined by Hamilton's principle,

$$\delta S = \delta \int_{t'}^{t''} \left[\frac{1}{2} m \dot{x}^2 - V(x) \right] dt = 0, \tag{6}$$

or as the solution $x(t) = x_c(t)$ of the classical equation of motion,

$$m \ddot{x} + V'(x) = 0, \tag{7}$$

where $V'(x) = dV(x)/dx$. The first term of (5) is the classical action,

$$S_c \equiv S[x_c] = \int_{t'}^{t''} \left[\frac{1}{2} m \dot{x}_c^2 - V(x_c) \right] dt \tag{8}$$

evaluated along the classical path $x_c(t)$. If $\xi(t) = x(t) - x_c(t)$ denotes the quantum deviation from the classical path, satisfying the end point conditions $\xi(t') = \xi(t'') = 0$, the third term of (5), which is the quantum correction to the action, is given by,

$$\frac{1}{2} \delta^2 S = \int_{t'}^{t''} \left[\frac{1}{2} m \dot{\xi}^2 - \frac{1}{2} V''(x_c) \xi^2 \right] dt, \tag{9}$$

where $V''(x) = d^2V(x)/dx^2$. Consequently, the propagator must be found in the form,

$$K(x'', t'', x', t') = K_c(0, t'', 0, t') \exp \left[\frac{i}{\hbar} S_c(x'', t'', x', t') \right]. \tag{10}$$

The first factor of (10) is the path integral for the propagator associated with the deviation variable ξ , which can be exactly calculated. Expressing it in terms of the classical action S_c , one obtains the VPM formula (4).

Again, for a quadratic system, the propagator obtained from the VPM formula is identical with the result from Feynman's formula and hence exact. It is an interesting fact that the semiclassical approximation gives an exact result. Historically, this fact was not only noted with interest by Feynman [9] but also stressed by others [10] with the expectation that the sum over all classical paths could be exact in a broader extent.

The harmonic oscillator in three dimensions, if based on cartesian coordinates, is decomposable into three linear harmonic oscillators. Naturally, its propagator is given as a product of three one-dimensional propagators. Therefore, as long as cartesian coordinates are employed, the exact three-dimensional propagator follows from the VPM formula (4) as well as Feynman's formula (1). Strange though it may be, the same is not true in polar coordinates.

The propagator for an isotropic harmonic oscillator in three dimensions can be separated in polar coordinates as

$$K(\mathbf{r}'', t'', \mathbf{r}', t') = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\cos(\mathbf{r}' \cdot \mathbf{r}'' / r' r'')) K_l(r'', t'', r', t'), \tag{11}$$

where $P_l(\cos \theta)$ is the Legendre polynomial and $K_l(r'', t'', r', t')$ is the radial propagator ($\mathbf{r} = |\mathbf{r}|$). It is a curious fact that the VPM formula cannot produce exactly the radial propagator for the harmonic oscillator. The presence of the centrifugal potential makes the semiclassical calculation difficult. In contrast, Feynman's prescription enables us to carry out radial path integration explicitly, resulting in the exact radial propagator for the harmonic oscillator [5, 6]. What the exact polar coordinate analysis has revealed is that the radial path integral is not a Gaussian path integral but a Besselian path integral. The radial path integral is calculated not by the Gaussian integral formula but by Weber's integral formula for the Bessel functions. This would be the reason why the semiclassical approach based on the Gaussian approximation is good for the calculation on cartesian basis but

unsuited for evaluation of the radial propagator.

3. Semiclassical Formula for the Green Function

Instead of the propagator, Gutzwiller [4] paid attention to the energy-dependent Green function which is a Fourier transform of the propagator,

$$G(x'', x'; E) = \frac{1}{i\hbar} \int_0^\infty K(x'', \tau; x', 0) \exp\{(i/\hbar)E\tau\} d\tau, \quad (12)$$

where $\text{Im } E > 0$. Substituting the VPM formula (4) into (12), making the stationary phase approximation for the time integration of (12), and counting the contributions from all classical paths, one can derive the semiclassical expression for the Green function. According to Schulman's derivation [11], Gutzwiller's formula can be given in the form,¹

$$G(x'', x'; E) = \frac{1}{i\hbar} \left[\frac{m}{2\sqrt{(E - V(x''))}(E - V(x'))} \right]^{1/2} \times \frac{1}{1 - \exp\{(i/\hbar)(J - \pi\hbar)\}} \sum_{k=1}^4 \exp \left[\frac{i}{\hbar} \left(W_k - \frac{1}{2} n_k \pi \hbar \right) \right], \quad (13)$$

where

$$W_k = w(x'', E) + (-1)^k w(x', E) \quad \text{for } k = 1, 2 \quad (14)$$

$$W_k = -w(x'', E) + (-1)^k w(x', E) + J \quad \text{for } k = 3, 4 \quad (15)$$

with

$$w(x, E) = \int_{x_L}^x \sqrt{2m(E - V(x))} dx \quad (16)$$

and

$$J = 2w(x_R, E) \quad (17)$$

where x_L and x_R are, respectively, the left and right turning points where $V(x_L) = V(x_R) = E$. This is a consequence of collecting only the contributions from classical paths. Schulman pointed out that the poles of the semiclassical formula (13) give rise to the well-known WKB quantization rule,

$$\int_{x_L}^{x_R} \sqrt{2m(E - V(x))} dx = \left(n + \frac{1}{2} \right) \pi \hbar, \quad n \in \mathbb{N}_0. \quad (18)$$

As is also well-known, the WKB quantization formula can reproduce exact energy spectra for the radial harmonic oscillator and the hydrogen atom provided that the Langer replacement $l(l+1) \rightarrow (l+1/2)^2$ is made. For other soluble systems, other Langer-type

¹Note that the multiple constant here differs from the one in Schulman's book, Equation (18.20).

modifications are needed. Usually, such a modification is applied in an *ad hoc* manner to meet the end and generally without grounds. Nevertheless, it is a remarkable fact that Gutzwiller's formula can provide at least an approximate result for a class of systems which cannot be handled by the VPM formula.

In particular, for the Coulomb problem, Gutzwiller [4] obtained the exact wave functions from the semiclassical analysis in phase space. This is indeed surprising. While the semiclassical calculation in configuration space leads to the standard WKB approximation, the semiclassical calculation in phase space has given rise to an exact result. With regard to this finding, Schulman [12] wrote, "It is not clear whether this result is related to the exactness of the sum over classical paths for Lie groups ... inasmuch as the Coulomb problem (with given energy) can be recast as a trivial dynamics on the group manifold of $O(4)$." Dowker [13] found that the sum over classical paths for Lie groups is not always exact. Yet, Schulman's observation concerning the Coulomb problem is nearly right on target.

Let us look at the semiclassical formula (13) again from the exact path integration point of view. The energy-dependent Green function cannot be expressed in a path integral form. However, it can be given by

$$G(x'', x'; E) = \frac{1}{i\hbar} \int_0^\infty P(x'', x'; \tau) d\tau \quad (19)$$

where

$$P(x'', x'; \tau) = \langle x'' | \exp \left[\frac{i}{\hbar} \tau (E - H) \right] | x' \rangle, \quad (20)$$

which is sometime called the promotor. The promotor (20) is reducible to the propagator when E tends to zero. Even in the presence of nonzero E , it is expressible in the form of a path integral. For convenience, we further define a modified promotor by

$$\bar{P}(x'', x'; \tau; f'g'') = \langle x'' | \exp \left[\frac{i}{\hbar} (\tau/f'g'') f(x)(E - H) g(x) \right] | x' \rangle, \quad (21)$$

where $f(x)$ and $g(x)$ are positive-definite q -numbers, and $f' = f(x')$ and $g'' = g(x'')$ are c -numbers. It is easy to show that

$$G(x'', x'; E) = \frac{1}{i\hbar} \int_0^\infty \bar{P}(x'', x'; \sigma) (d\tau/d\sigma) d\sigma. \quad (22)$$

This means that the Green function can be calculated by integrating either the promotor (20) or the modified promotor (21). Thus, we can calculate the Green function by using a promotor in the simplest form. For instance, the promotor for the hydrogen atom in \mathbb{R}^3 may be transformed into the promotor for a harmonic oscillator in \mathbb{R}^4 by the Kustaanheimo-Stiefel space-time transformation [14]. The time-integration of the promotor for the Coulomb problem is difficult to perform, but the integration can be completed for the harmonic oscillator without difficulty. In this way, the hydrogen-atom problem has been solved by path integration [15, 16]. This does not immediately prove Schulman's observation that Gutzwiller's exact result may be related to a trivial dynamics on the group manifold of $O(4)$, but suggests that there is a strong link between the exactness of the path integral solution for the Coulomb problem and its dynamical symmetry. The dynamical symmetry $O(4)$ is now realized as the rotational symmetry in \mathbb{R}^4 .

Of course, the Coulomb problem can be solved without use of the Kustaanheimo-Stiefel coordinate mapping $\mathbf{R}^3 \rightarrow \mathbf{R}^4$, thereby being independent of the $O(4)$ dynamical symmetry [6, 17]. The radial Coulomb promotor,

$$P(r'', r'; \tau) = (r'' | \exp \left[-\frac{i}{\hbar} \tau \left(\frac{1}{2m} p_r^2 + \frac{l(l+1)}{2mr^2} - \frac{e^2}{r} - E \right) \right] | r'), \quad (23)$$

with $p_r = -i\hbar r^{-1}(\partial/\partial r)r$, may be transformed by letting $\tau = \rho^2$ and $\tau = 4\rho'\rho''\sigma$ into the promotor of the radial harmonic oscillator [18],

$$\tilde{P}(\rho'', \rho'; \sigma) = \langle \rho'' | \exp \left[-\frac{i}{\hbar} \sigma \left(\frac{1}{2m} p_\rho^2 + \frac{\lambda(\lambda+1)}{2m\rho^2} - \frac{1}{2} m\omega^2 \rho^2 - E' \right) \right] | \rho' \rangle, \quad (24)$$

where

$$\omega^2 = -8E/m, \quad E' = 4e^2, \quad \lambda = 2l + 1/2. \quad (25)$$

It has been shown that the path integral of this radial promotor is more closely related to the spectrum generating Lie algebra $so(2,1)$ [19, 20].

The reason why Gutzwiller's formula is more generally applicable than the VPM formula may be ascribed to the time-scaling invariance of the integral for the energy-dependent Green function, that is, the equivalence between (19) and (22).

4. Quasiclassical Formulas for the Green Function

Next we look into the semiclassical analysis from a new angle, that is, an angle related to supersymmetric quantum mechanics [21].

In standard semiclassical calculations, as has been shown in Section 2, the action is expanded about the classical path. What we wish to propose is the quasiclassical analysis which differs from the standard semiclassical analysis in the choice of stationary paths. We assume that the potential $V(x)$ may be expressed in the form,

$$V(x) = \phi^2(x) - \frac{\hbar}{\sqrt{2m}} \phi'(x) + \varepsilon, \quad (26)$$

where $\phi(x)$ is a well-behaved scalar function, $\phi'(x) = d\phi/dx$ and ε is a constant. Then we define the quasiclassical path $x_q(t)$ by the following extremum of an action,

$$\delta \int_{t'}^{t''} \left[\frac{1}{2} m \dot{x}^2 - \phi^2(x) \right] dt = 0, \quad (27)$$

or by the solution $x(t) = x_q(t)$ of

$$m\ddot{x} + 2\phi(x)\phi'(x) = 0, \quad (28)$$

with the end-point conditions, $x_q(t') = x_c(t')$ and $x_q(t'') = x_c(t'') = x''$. Now we let $x(t) = x_q(t) + \eta(t)$ where $\eta(t') = \eta(t'') = 0$, and expand the action S around the quasiclassical path $x_q(t)$ as

$$S \simeq S_q + \hbar\varphi + \frac{1}{2} \delta^2 S - \varepsilon(t'' - t'), \quad (29)$$

where $S_q = S[x_q]$ is the action evaluated along the quasiclassical path,

$$\varphi = \frac{1}{\sqrt{2m}} \int_{t'}^{t''} \phi'(x_q) dt, \quad (30)$$

and

$$\frac{1}{2} \delta^2 S = \int_{t'}^{t''} \left[\frac{1}{2} m \dot{\eta}^2 - \phi(x_q) \phi'(x_q) \eta^2 \right] dt. \quad (31)$$

In much the same way that the semiclassical formula (4) was derived, the corresponding propagator can be obtained in the form,

$$K(x'', t''; x', t') = \sqrt{\frac{i}{2\pi\hbar} \frac{\partial^2 S_q}{\partial x' \partial x''}} \exp \left[\frac{i}{\hbar} S_q(x'', t''; x', t') + i\varphi - \frac{i}{\hbar} \varepsilon(t'' - t') \right]. \quad (32)$$

The formula thus obtained is the quasiclassical counterpart of the VPM formula in the semiclassical approach. For the harmonic oscillator potential $V(x) = (m\omega^2/2)x^2$, we choose the scalar function $\phi(x)$ and the constant ε as follows,

$$\phi(x) = \sqrt{\frac{m\omega^2}{2}} x, \quad \varepsilon = \frac{1}{2} \hbar\omega. \quad (33)$$

Obviously, $V(x) = \phi^2(x)$. Therefore, both the semiclassical formula (4) and the quasiclassical formula (32) yield the same exact result for the linear harmonic oscillator. However, thus far, there is no particular merit of introducing the quasiclassical formula (32) because it cannot easily be evaluated for a non-quadratic potential. The merit of the quasiclassical approach becomes apparent when it is applied for the calculation of the Green function.

If we proceed the quasiclassical calculation as Schulman did semiclassically, we can arrive at the quasiclassical counterpart of Gutzwiller's formula,

$$G(x'', x'; E) = \frac{1}{i\hbar} \left[\frac{m}{2\sqrt{\tilde{E} - \phi^2(x'')(\tilde{E} - \phi^2(x'))}} \right]^{1/2} \times \frac{1}{1 - \exp[i(J/\hbar - \pi - a(x_L) + a(x_R))]} \sum_{k=1}^4 \exp \left[\frac{i}{\hbar} \left(W_k - \frac{1}{2} n_k \pi \hbar \right) \right], \quad (34)$$

where $\tilde{E} = E - \varepsilon$ is the shifted energy value. Here the extra phase,

$$a(x) = \arcsin \frac{\phi(x)}{\sqrt{\tilde{E}}}, \quad (35)$$

stems from the integral φ of (31), which takes the following values at the new turning points x_L and x_R defined by $\phi^2(x_L) = \phi^2(x_R) = \tilde{E}$:

$$a(x_R) = -a(x_L) = \pi/2 \quad \text{if} \quad \phi(x_R) = -\phi(x_L) = \pm\sqrt{\tilde{E}} \quad (36)$$

$$a(x_R) = a(x_L) = \pi/2 \quad \text{if} \quad \phi(x_R) = \phi(x_L) = \pm\sqrt{\tilde{E}}. \quad (37)$$

The poles of this Green function lead to the following quantization rules:

Case I: If $\phi(x_R) = -\phi(x_L) = \pm\sqrt{E}$, then

$$\int_{x_L}^{x_R} \sqrt{2m(\tilde{E} - \phi^2(x))} dx = n\pi\hbar, \quad n \in \mathbb{N}_0. \quad (38)$$

Case II: If $\phi(x_R) = \phi(x_L) = \pm\sqrt{E}$, then

$$\int_{x_L}^{x_R} \sqrt{2m(\tilde{E} - \phi^2(x))} dx = \left(n + \frac{1}{2}\right)\pi\hbar, \quad n \in \mathbb{N}_0. \quad (39)$$

Evidently, these quantization formulas differ from the WKB formula (18). In fact, the first quantization formula (38) is identical with the formula of Comtet, Bandrauk and Campbell (CBC) in supersymmetric quantum mechanics [22], and the second formula (39) coincides with the one we have proposed for broken supersymmetry [23, 24]. In supersymmetric quantum mechanics, the scalar function $\phi(x)$ plays the role of the superpotential, and satisfies the antisymmetric boundary conditions of case I when supersymmetry is good and the symmetric boundary conditions of case II when supersymmetry is broken. In this regard, the quasiclassical formula (34) is a supersymmetric version of Gutzwiller's formula.

It is an astonishing fact that the CBC formula provides an exact energy spectrum for a shape-invariant potential [25] without any Langer-type modification [22, 26]. Many systems exactly soluble by Schrödinger's equation belong to the class of shape-invariant potentials. Even for those systems which are not exactly soluble, the CBC formula or the formula for broken supersymmetry give estimates as good as or even better than the WKB results [24, 27, 28]. In this connection, it may be said that the quasiclassical formula (34), which can supply exact energy spectra for shape-invariant potentials with no *ad hoc* Langer-like modification, is an improved version of Gutzwiller's formula.

5. Concluding Remarks

The fact that Gutzwiller's formula for the Green function is more flexible than the VPM formula for the propagator has been related to the property that the Green function remains invariant under a time-scaling of the promotor. For many exactly soluble systems, the promotor is reducible to that of the radial harmonic oscillator or that of a symmetric top, and the corresponding Green function can be obtained exactly. In semiclassical analysis, this is reflected in the fact that Gutzwiller's formula provides exact results for a class of systems with or without the Langer-type modification.

As for the exactness of Gutzwiller's result for the Coulomb problem, it would be interesting to examine if the semiclassical analysis in phase space may be directly linked to the rotational symmetry $O(4)$ in \mathbb{R}^4 , or if the Langer modification or its equivalent may be implicitly implied by a certain computational process.

We have proposed the supersymmetric counterparts of the VPM formula and Gutzwiller's formula. The supersymmetric version of Gutzwiller's formula has been shown to comprise the quantization formula of Comtet, Bandrauk and Campbell which is known as being able to reproduce the exact energy spectra for the shape-invariant potentials without the Langer-

like modification. In addition, it leads to another quantization formula which we have earlier proposed for the broken supersymmetry case [23].

It is unfair to conclude this section without mentioning the shortcoming of the quasiclassical approach. For a shape-invariant potential, the scalar function $\phi(x)$ can be found in a rather simple form. However, it is not easy to find the function $\phi(x)$ for an arbitrary potential $V(x)$. Even if we can get the function in an analytical form, the integration of the CBC formula (38) or the second formula (39) may not be easy. For instance, if $V(x) = \alpha x^n$, we have the Riccati equation,

$$\phi'(x) + a\phi^2(x) = bx^n, \quad (40)$$

with $a = -\sqrt{2m}/\hbar$ and $b = -\alpha\sqrt{2m}/\hbar$, whose solution is given by $\phi(x) = a^{-1}u'(x)/u(x)$ with

$$u(x) = \sqrt{x} Z_{\frac{n+2}{4n+2}} \left(\frac{2i\sqrt{ab}}{n+2} x^{(n+2)/2} \right) \quad (41)$$

where $Z_\nu(z)$ is a solution of Bessel's differential equation; for example, the Bessel function $J_\nu(z)$. Therefore, quantization cannot be done analytically by either the CBC formula or the second formula (39). The WKB formula (18), however, leads to analytical results in this particular case.

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