Berry Phases of Classical Trajectories in the Presence of Hard-Wall Boundaries

Hsiu-Hau Lin and Tzay-Ming Hong

Department of Physics, National Tsing-Hua University, Hsinchu 300, Taiwan, Republic of China
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We study the quantum propagator in the semiclassical limit with hard-wall potentials. We show that, upon each reflection by the hard wall, a Berry phase \( \pi \) is accumulated and leads to interferences between different classical trajectories. Including the Berry phase caused by the hard walls, the modified Van Vleck’s formula is derived. We also discuss the close relations among quantum statistics, discrete gauge symmetry, and hard-wall constraints. Most of all, we formulate a new quantization rule that applies to both smooth and sharp boundary potentials. It provides an easy way to compute quantized energies in the semiclassical limit and is extremely useful for many physical systems.

I. INTRODUCTION

Path integral provides an alternative approach to formulate quantum mechanics [1-3]. The quantum propagator \( G(x,x';T) \), that is the key quantity in quantum mechanics, is shown to equal the summation over all possible paths with the same end points. In the semiclassical limit, the dominant contribution comes from classical trajectories and fluctuations around them [3-4]. Within the stationary phase approximation including fluctuations up to the quadratic order, the quantum propagator can be approximated by the Van Vleck’s formula [5]. In general, there would be many classical trajectories that satisfy the same boundary conditions, and the Berry phase interferences between them are important [6].

The interference effects among the classical trajectories were not included until Gutzwiller’s work that enables the earlier short-time result of Van Vleck to be extended past the first conjugate point [4]. By Morse’s theorem, the second variation, considered as quadratic fluctuations around a given trajectory from \( x' \) to \( x \) in time \( T \), has as many negative eigenvalues as there are conjugate (turning) points along the trajectory. These conjugate points give rise to a Berry phase \( \nu \pi/2 \) for the trajectory, where \( \nu \) is the total number of conjugate points along the trajectory, or sometimes referred to as the Maslov or Morse index [4].

Not only elucidating the crossover between classical and quantum mechanics, the semiclassical limit also provides a convenient way to calculate the bound state energy. Instead of solving the Schrödinger equation directly, the bound state energies can also be computed by the WKB approximation [11]. However, the method is only applicable when the confinement potential is reasonably “smooth” (compared with the relevant energy gradient we are interested in). In this paper, we study the semiclassical limit in the presence of hard-wall potentials that is beyond the validity of the WKB approximation. We found that upon each reflection by the hard wall, a Berry phase \( \pi \) accumulates and eventually leads to an additional phase \( r\pi \), where \( r \) is the number of reflection points. In order to account for the interference effects among classical trajectories correctly, we rederive Van Vleck’s formula with an extra Berry phase correction due to hard-wall boundaries. An elegant proof by mirror projection explains the Berry phase \( \pi \) and reveals the close connections among quantum statistics, discrete gauge symmetry, and the hard-wall boundary.

Following the standard stationary phase approximation and making a Legendre transformation of the time variable in the quantum propagator to the energy variable, we are able to generalize the Einstein-Brillouin-Keller (EBK) quantization rule [12-14] with a hard-wall correction term

\[
\int \sqrt{2m(E - V(x))} dx = 2\pi(n + \frac{\nu}{4} + \frac{r}{2}),
\]

where \( \nu \) is the number of conjugate points and \( r \) is the number of reflection points. The usual WKB approximation is the special case \( \nu = 2 \) and \( r = 0 \). The modified EBK quantization rule in Eq. (1.1) relaxes the requirement of the potential smoothness in the WKB approximation. If the trajectory bounces from a smooth potential, it is counted as a conjugate (turning) point. If the trajectory gets reflected by a hard-wall like boundary, it is counted as a reflection point. This is of great advantage because many physical systems including quantum dots, quantum wells, Hall bars, electronic wave guides, etc., have both hard-wall-like potentials (from sample edges) as well as smooth potentials (by applying external fields) at the same time.

The paper is organized in the following way. In Sec. II, we introduce the Van Vleck’s formula and apply it to two simple systems without and with hard-wall boundaries. We explicitly show that the Van Vleck’s approximation is incorrect in the presence of hard walls. In Sec III, We show that the Berry phase due to the reflection by a simple hard-wall boundary is \( \pi \) and derive the modified Van Vleck’s formula. In Sec. IV, a more elegant proof by mirror projection is presented. Finally, in Sec V, we derive the key result of this paper – the modified EBK quantization rule. We apply it to physical systems with both smooth and hard confinement potentials and show that the modified term is necessary to obtain the correct energy levels. Then a brief conclusion follows.
II. QUANTUM PROPAGATOR AND CLASSICAL TRAJECTORIES

In the path integral formalism, the quantum propagator equals the sum over all possible paths with the same end points,

\[ G(x, x'; T) = \langle x | e^{-iHT} | x' \rangle = \int_{x'}^{x} D[x] \exp \left( i \int_{0}^{T} L(x, \dot{x}, t) dt \right) , \quad (2.1) \]

where the measure \( D[x] \) denotes all possible paths with end points \( x(0) = x' \) and \( x(T) = x \). In the semiclassical limit, the phase inside the path integral oscillates rapidly except in the neighborhood of the classical trajectories. Within the stationary phase approximation including fluctuations up to quadratic order, the propagator is approximated by the Van Vleck’s formula,

\[ G(x, x'; T) \simeq \frac{1}{\sqrt{2\pi i}} \sum_{p} \sqrt{C_{p}} \exp \left[ i A_p - i \nu \frac{\pi}{2} \right] , \quad (2.2) \]

where \( A_p(x, x'; T) \) is the action of the classical trajectory starting from \( x(0) = x' \) and ending at \( x(T) = x \), and the subscript \( p \) denotes all classical paths with the desired end points. The strength of the quadratic fluctuations around the classical trajectory is

\[ C_p = \left| \frac{\partial^2 A}{\partial x \partial x'} \right| . \quad (2.3) \]

Finally, the total number of conjugate (or turning) points along the classical trajectory is denoted by \( \nu \). Notice that, for each conjugate point, there is a \( \pi/2 \) Berry phase associated with it. Van Vleck’s formula provides a completely classical approximation of the quantum propagator, in the sense that all relevant elements can be computed from the classical trajectories.

A straightforward example of the Van Vleck’s formula is a free particle moving on a finite ring with length \( L \). There are infinite classical paths which satisfy the conditions \( x(0) = x' \) and \( x(T) = x \). The total (route) distance of each classical trajectory is \( d_n = x - x' + nL \), where \( n \) is an integer. The action for each trajectory is

\[ A_n(x, x'; T) = \frac{m}{2T} (x - x' + nL)^2 . \quad (2.4) \]

Taking the derivative of the action, the strength of fluctuations around each trajectory \( C_n = m/T \) is independent of the end points and the choice of trajectories. Since the particle moves at constant velocity, it is obvious that there is no conjugate point along any classical trajectory and thus \( \nu_n = 0 \). Besides, because the fluctuations of the classical trajectory of a free particle are exactly quadratic, we expect the Van Vleck’s formula to be exact for this system,

\[ G(x, x'; T) = \sqrt{\frac{m}{2\pi i T}} \sum_{n} \exp \left[ \frac{im}{2T} (x - x' + nL)^2 \right] . \quad (2.5) \]

This infinite sum can be re-written in terms of its Fourier function with the use of Poisson summation formula in Appendix A. Notice that

\[ f(y) = e^{i\alpha(y^2)} \leftrightarrow F(p) = \sqrt{\frac{i\alpha}{2\pi}} e^{-ik^2/4\alpha + ik\beta} \quad (2.6) \]

Choosing \( a = L \), the summation over coordinate \( y = na \) can be turned into the summation over momentum \( k_n = 2n\pi/L \). The propagator is then

\[ G(x, x'; T) = \frac{1}{L} \sum_{n} \exp[ik_n(x - x') - iE_nT] , \quad (2.7) \]

where \( k_n = 2n\pi/L \) is the quantized momentum and \( E_n = k_n^2/2m \) is the quantized energy. It is obvious that the propagator \( G(x, x'; T) \) calculated by the Van Vleck’s formula is exact in this case.

Let us now apply the Van Vleck’s formula to another physical system – a free particle bouncing back and forth between two hard walls. We would calculate the propagator explicitly and show that the Van Vleck’s formula leads to incorrect results.

![Fig. 1. Classical trajectories in the presence of two hard walls. On the left is a trajectory with even reflection points \( r = 2 \), while the right with odd reflection points \( r = 3 \).](image)

The trajectories in this problem can be classified by the number of collisions with the hard walls, as seen in Fig. 1. For those trajectories that collide with the hard walls even times, the route distance is \( d_{m} = x - x' + 2nL \), while the distance is \( d_{m} = x + x' + 2nL \) for trajectories that collide with the walls odd times. The action for each trajectory can be computed straightforwardly

\[ A_0^+(x, x'; T) = \frac{m}{2T} (x - x' + 2nL)^2 , \quad (2.8) \]

\[ A_0^-(x, x'; T) = \frac{m}{2T} (x + x' + 2nL)^2 . \quad (2.9) \]

Here \( A_0^+(x, x'; T) \) denotes the action for trajectories with even/odd reflection points. The fluctuations along all trajectories contribute the same \( C_n = m/T \) as in the previous example. For an one-dimensional motion, a conjugate point is identified as the position where the velocity vanishes. However, for a free particle bouncing back and forth between two hard walls, the velocity is constant up to a minus sign and does not vanish at any point along...
the classical trajectory. Thus, the number of conjugate points is zero, $\nu = 0$.

The propagator without any Berry phase interference is

$$G_{VV}(x, x'; T) = \sqrt{\frac{m}{2\pi i T}} \sum_{n} \left\{ \exp\left[ \frac{im}{2T} (x - x' + 2nL)^2 \right] + \exp\left[ \frac{im}{2T} (x + x' + 2nL)^2 \right] \right\}. \quad (2.10)$$

Both infinite sums can be turned into summations over discrete momentum again by mean of the Poisson summation formula. The prefactors cancel as in the previous example and we are left with the simple result,

$$G_{VV}(x, x'; T) = \frac{1}{L} \sum_{n=0}^{\infty} \exp[-iE_n t] \times$$

$$\times \left\{ \cos[k_n(x - x')] + \cos[k_n(x + x')] \right\}, \quad (2.11)$$

where $k_n = n\pi/L$ is the quantized momentum and $E_n = k_n^2/2m$ is the quantized energy. Combining two cosines would lead to $\cos(k_n x) \cos(k_n x')$, while the correct form should be $\sin(k_n x) \sin(k_n x')$. Indeed one can recover the exact answer (with all prefactors right!) if we change the sign of the second term in Eq. (2.11). That is, only if we assign an extra Berry phase $\pi$ to trajectories with odd reflection points, will the modified Van Vleck’s formula become correct!

In the following section, we study the path integral formalism in the presence of a single hard-wall boundary and show that there is an additional Berry phase.

III. BERRY PHASES DUE TO HARD WALLS

Consider a particle moving under the influence of a regular potential $V(x)$ and a hard-wall potential $V_c(x)$. The Hamiltonian is

$$H = \frac{p^2}{2m} + V(x) + V_c(x), \quad (3.1)$$

where $V_c(x)$ is the hard-wall potential at $x = 0$,

$$V_c(x) = \begin{cases} 0, & x > 0; \\ \infty, & x < 0. \end{cases} \quad (3.2)$$

The regular potential is treated in the ordinary way while the hard-wall one is viewed as the depletion of Hilbert space. The complete set of the Hilbert space is now reduced,

$$\int_{0}^{\infty} dr |r| = 1, \quad (3.3)$$

$$\sum_{\phi \in [0, \pi]} \int \frac{dp}{2\pi} e^{i\phi} |p\rangle \langle p| = 1. \quad (3.4)$$

It would become clear later that the phase $\phi$ is associated with the Berry phase in the path integral. Slicing the time interval $T$ into infinitesimal pieces and inserting complete sets of the coordinate space, the propagator is

$$G(r, r'; T) = \langle r'| e^{-iHT} |r \rangle$$

$$= \int_{0}^{\infty} dr_N \prod_{n=0}^{N-1} \langle r_{n+1} | e^{-iE_n} | r_n \rangle, \quad (3.5)$$

where $r_N = r$ and $r_0 = r'$ are all positive. Each matrix element in the product is computed by inserting the complete set in momentum space into Eq. (3.4).

$$\langle r_{n+1} | e^{-iE_n} | r_n \rangle = \int \frac{dp_n}{2\pi} \exp[-iE_n] \times$$

$$\times \sum_{x_n = \pm r_n} e^{i\phi_n(r_{n+1} - x_n) - i\phi_n}, \quad (3.6)$$

where the phase $\phi = 0$ for $x_n = r_n$, and $\phi = \pi$ when $x_n = -r_n$. Since $x_n = \pm r_n$, the two terms can be combined and lead to the unconstraint integral over $x_n$. After changing the constrained variable $r_n$ to $x_n$, it is convenient to write the Berry phase $\phi_n$ in the following way

$$\phi_n = \pi[\Theta(x_{n+1}) - \Theta(x_n)]. \quad (3.7)$$

Notice that the Berry phase is zero if the path does not pass through $x = 0$ in the infinitesimal time interval $dt_n$ and $\pi$ if the path passes through. The integral over momentum can be carried out easily and the propagator is

$$G(r, r'; T) \approx \sum_{x' = \pm r'} \sum_{n=0}^{\infty} e^{i\phi_B} \int_{x'}^{r} D[x] \exp[iA(r, x'; T)]. \quad (3.8)$$

The total Berry phase $\phi_B = \pi[\Theta(r) - \Theta(x')]$ is a boundary term and can be pulled out of the path integral [2]. The paths are divided into two topologically distinct classes. For all possible paths starting from $r$ to $r'$, the Berry phase is zero, while for those starting from $r$ to $-r'$, the Berry phase is $\pi$ that causes a minus sign. The classical trajectories among the paths can be then classified in the same way. Furthermore, trajectories with end points $r$ and $r'$ can be identified as trajectories (in the physical half plane) with even reflection points and those with end points $r$ and $-r'$ are trajectories with odd reflection points.

Therefore, in the semiclassical limit, the Van Vleck’s formula is modified with an extra Berry phase term,

$$G(r, r'; T) \approx \sum_{n=0}^{\infty} \sqrt{\nu_p} \exp[iA_p - i\nu_p \pi - i\nu_p \pi], \quad (3.9)$$

where $\nu_p$ is the number of reflection points. The proof for more than one hard wall is straightforward but tedious. A more general and elegant proof would be given by mirror projection in the next section. However, I would like to emphasize that the proof given in this section explains clearly the origin of the minus sign – an extra Berry phase due to hard-wall boundaries.
IV. MIRROR PROJECTION

In the previous section, we treat the hard-wall boundary as depletion of the Hilbert space. An alternative way is to view it as a discrete $Z_2$ gauge symmetry of the wave function

$$\psi(x) = -\psi(-x). \quad (4.1)$$

The minus sign is chosen here to make the wave function vanishes at $x = 0$ so that the boundary condition $\psi(0) = 0$ is always satisfied. Since the propagator can be written down as the summation of eigenfunctions, $G(x, x'; T) = \sum_n \psi_n(x)\psi_n(x')\exp[-iE_n T]$, where $\psi_n(x)$ is the eigenfunction with eigenenergy $E_n$. The discrete gauge symmetry of the wave function implies that the quantum propagator has the symmetry

$$G(x, x'; T) = -G(x, -x'; T). \quad (4.2)$$

Now choose both $x = r$ and $x' = r'$ to be positive, the propagator can also be viewed as the wave function $G(r, r'; T) = \psi_\nu(r, t)$ that satisfies the Schrödinger equation with a delta function source at $(x, t) = (r', 0)$. The propagator $G_0(r, r'; T)$ without the hard-wall boundary satisfies exactly the same differential equation except that the boundary condition at $x = 0$ is not met. Notice that the mirrored propagator $\overline{G}_0(r, r'; T) = G_0(r, -r'; T)$ satisfies the Schrödinger equation without the source term since the delta function $\delta(r + r') = 0$ for positive coordinates. Therefore, the propagator that satisfies the correct boundary condition is constructed as

$$G(x, x'; T) = G_0(x, x'; T) - \overline{G}_0(x, x'; T). \quad (4.3)$$

The above result is equivalent to Eq. (4.2). It is obvious that the discrete gauge symmetry in Eq. (4.2) is satisfied. This method is just the familiar mirror charge trick in the classical electromagnetism. The generalization now becomes clear. In the presence of more than one hard walls, the propagator is just the sum of all path integrals from all mirror points of $x'$ to the final $x$, and the Berry phase correction is either 0 or $\pi$ depending on how many mirror projections are needed to reach the particular mirror point of $x'$. In the example of two hard walls, there are infinite mirror points. Each mirror projection corresponds to a reflection of the classical trajectory. Thus, for those trajectories that are reflected even times, the Berry phase is simply zero, while for those with odd reflection points, the Berry phase is $\pi$ and results in a relative minus sign.

Since we can solve the hard-wall boundary by discrete gauge symmetry, we might as well go the other way around. It is possible to replace the quantum statistics between particles by the hard-wall boundaries. Let us consider the simplest case – two interacting particles with either bosonic or fermionic statistics. The discrete gauge redundancy is

$$\psi(x) = e^{i\phi} \psi(-x), \quad (4.4)$$

where $\phi = 0$ for bosons and $\pi$ for fermions. The discrete gauge symmetry is removed by imposing a hard wall $x_1 = x_2$ in the configuration space, and a Berry phase $\phi$ accumulates upon each reflection due to the hard wall.

![FIG. 2. Classical trajectories of two particles whose quantum statistics is replaced by the equivalent hard wall at $x_1 = x_2$ in the configuration space. In part (a), a direct trajectory is shown and, in part (b), the shown reflected trajectory is equivalent to exchanging two particles which results in an extra Berry phase.](image)
the modified EBK quantization rule can be applied to physical systems with both smooth (soft) and hard confinement potentials. To illustrate this point, let us consider a particle in a harmonic trap, but with a hard wall boundary caused by the sample edge as shown in Fig. 3.

\[ V(x) = \begin{cases} \frac{1}{2}kx^2, & x > 0 \\ \infty, & x < 0 \end{cases} \]  

(5.2)

The classical periodic orbit, shown in Fig. 3, has one conjugate point \( \nu = 1 \) and one reflection point \( r = 1 \) which differs from the assumption of the WKB approximation that there are always two conjugate points. In the semiclassical limit, the quantized energy is given by the new quantization rule,

\[ 2 \int_0^{x_1} \sqrt{2m(E - \frac{1}{2}kx^2)}dx = 2\pi(n + \frac{1}{4} + \frac{1}{2}), \]  

(5.3)

where \( x_1 = \sqrt{2E/k} \) is the conjugate (turning) point. The integral is elementary and leads to the correct energy levels

\[ E_n = (2n + \frac{3}{2})\omega, \]  

(5.4)

where \( n = 0, 1, 2, \ldots \) and \( \omega = \sqrt{k/m} \) is the natural frequency. The result can of course be verified by the parity argument. We emphasize that neither Bohr-Sommerfeld quantization (\( \nu = 0, r = 0 \)) nor WKB approximation (\( \nu = 2, r = 0 \)) leads to the desired result.

In many practical systems, e.g., quantum dots, quantum wells, electronic wave guides, etc., the presence of both soft and hard potentials is inevitable. The modified EBK quantization rule provides us with a convenient tool to estimate the energy level without solving the Schrödinger equation directly. For example, in the quantum well biased by a voltage \( V \) (that needs not to be small) across the well, if the energy is below the bias voltage \( V \), the periodic orbit has one reflection point and one conjugate point. If the energy is above the bias voltage, we have two reflection points. One should not be puzzled that the infinitely sharp hard-wall does not exist in any practical systems and the correction due to hard-wall boundary is only an artifact. As long as the potential profile is sharp in comparison to the relevant energy gradient of the interested system, the Berry phase \( \pi \) correction is reasonably good. On the other hand, if the potential profile is smooth in the same sense, the Berry phase should be \( \pi/2 \) as in the usual WKB approximation.

The modified EBK quantization rule can also be applied to physical systems in higher dimensions. Let us consider a spherical or hemispherical quantum dot. We can either apply the modified EBK formula directly to the true three-dimensional trajectories [13] or apply the formula after reducing the system to one dimension. Here we adapt the second approach. After separation of variables, the radial effective Hamiltonian of the three-dimensional spherical (hemispherical) quantum dot becomes one-dimensional with the effective potential

\[ V = \begin{cases} \frac{(l(l+1)}{2m^2a^2}, & r < a \\ \infty, & r > a \end{cases}, \]  

(5.5)

where \( l \) is the quantized angular momentum. For the spherical quantum dot, \( l \) takes on all integer values, while for the hemispherical dot, only odd integers are allowed due to the flat boundary.

The classical trajectory of the electron is confined between the hard-wall boundary at the surface and the centrifugal potential near the origin. Thus, there are one reflection point \( r = 1 \) and one conjugate point \( \nu = 1 \). Applying the modified EBK quantization rule, the approximate energy satisfies the algebraic equation,

\[ \sqrt{(a/r_E)^2 - 1} - \sec^{-1}(a/r_E) = \frac{2\pi(n + \frac{1}{4})}{\sqrt{l(l+1)}}, \]  

(5.6)

where \( r_E = \sqrt{l(l+1)/(2mE)} \) is the conjugate point and \( a \) is the radius of the dot. Instead of solving the Schrödinger equation directly, the energy levels can be determined easily by the algebraic equation. In the semiclassical limit, the conjugate point is close to the origin, i.e., \( a/r_E \gg 1 \). The approximate expression can be further simplified,

\[ E_{n,l} \approx \frac{\pi^2}{2ma^2} \left( n + \frac{3}{4} + \frac{l'}{2} \right)^2, \]  

(5.7)

where \( l' = \sqrt{l(l+1)} \).

Notice that this problem can be solved exactly by the spherical Bessel functions. The hard-wall boundary requires the wave function vanishes at the surface of the sphere, \( j_l(\sqrt{2mE}a) = 0 \), that leads to quantized energy levels. In the same limit \( a/r_E \gg 1 \), the spherical Bessel function is approximated by the asymptotic expansion that leads to
The above exact result does not seem to agree with Eq. (5.7) at first glance. However, if the angular momentum is also semiclassical \((l \gg 1)\), the last term in Eq. (5.7) is \(l'/2 \approx l/2 + 1/4\) up to \(O(1/l)\) corrections. It is then clear that both give the same result. We emphasize again that the agreement is only possible when the modified term due to the hard-wall boundary is included.

VI. CONCLUSIONS

In this paper, we study the Berry phase of classical trajectories due to the hard wall boundaries. It is shown that, upon each reflection by the hard wall, a Berry phase \(\pi\) accumulates. We also relate the hard wall boundary approach to the quantum statistics and the discrete gauge symmetry. A new quantization rule is derived from the modified Van Vleck’s formula and applied to simple examples. Unlike the WKB approximation that is only applicable to smooth potential profiles, the new quantization rule provides us with an easy way to estimate the energy levels in the presence of both smooth and sharp confinement potentials.

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APPENDIX A: POISSON SUMMATION FORMULA

Poisson summation formula provides a convenient way to relate two infinite summations together. Let us consider a physical system on a finite ring with length \(L\) and lattice constant \(a\). The total number of sites is \(N = L/a\). The discrete version of the usual delta function is

\[
\sum_{x=na} e^{ikx} = \left( \frac{L}{a} \right) \sum_{G=2n\pi/a} \delta_{k,G}, \tag{A1}
\]

where \(G\) is the reciprocal lattice vector. Consider the following summation,

\[
\sum_n f(na) = \int \frac{dk}{2\pi} F(k) \sum_{x=na} e^{ikx}, \tag{A2}
\]

where \(x_n = na\) and \(F(k)\) is the Fourier transformation of \(f(x)\). With the help of the identity in Eq. (A1), the summation over coordinates is turned into another summation over reciprocal momenta. Taking the thermodynamical limit \(L \to \infty\), the discrete delta functions are related to the continuous ones by \(L\delta_{k,G} = 2\pi\delta(k-G)\). Finally, we arrive at the useful Poisson summation formula,

\[
\sum_n f(na) = \frac{1}{a} \sum_n F\left(\frac{2n\pi}{a}\right). \tag{A3}
\]