

Path integral and Sommerfeld quantization

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(Dated: September 13, 2018)

The path integral formulation can reproduce the right energy spectrum of the harmonic oscillator potential, but it cannot resolve the Coulomb potential problem. This is because the path integral cannot properly take into account the boundary condition, which is due to the presence of the scattering states in the Coulomb potential system. On the other hand, the Sommerfeld quantization can reproduce the right energy spectrum of both harmonic oscillator and Coulomb potential cases since the boundary condition is effectively taken into account in this semiclassical treatment. The basic difference between the two schemes should be that no constraint is imposed on the wave function in the path integral while the Sommerfeld quantization rule is derived by requiring that the state vector should be a single-valued function. The limitation of the semiclassical method is also clarified in terms of the square well and $\delta(x)$ function potential models.

PACS numbers: 25.85.-w,25.85.Ec

I. INTRODUCTION

Quantum field theory is the basis of modern theoretical physics and it is well established by now [1–4]. If the kinematics is non-relativistic, then one obtains the equation of quantum mechanics which is the Schrödinger equation. In this respect, if one solves the Schrödinger equation, then one can properly obtain the energy eigenvalue of the corresponding potential model.

Historically, however, the energy eigenvalue is obtained without solving the Schrödinger equation, and the most interesting method is known as the Sommerfeld quantization rule which is the semiclassical method [5–8]. In this case, the Sommerfeld quantization rule is to first assume

$$\oint p dr = nh \quad (1.1)$$

where n denotes an integer and h is the Planck constant. This method can be applied to the Coulomb potential problem of $V(r) = -\frac{Ze^2}{r}$. In fact, it can be solved exactly by the Sommerfeld quantization. Here, the momentum p is related to the energy E as

$$E = \frac{p^2}{2m} - \frac{Ze^2}{r} \quad (1.2)$$

where m denotes the mass of electron which is bound in the Coulomb potential. In this case, eq. (1.1) can be written as

$$\oint p dr = 2\sqrt{2m|E|} \int_0^{r_0} \sqrt{\frac{r_0 - r}{r}} dr = nh \quad (1.3)$$

where $r_0 = \frac{Ze^2}{|E|}$ is introduced. After the integration of eq.(1.3), we obtain the energy eigenvalue E as

$$E = -\frac{m(Ze^2)^2}{2\hbar^2 n^2} \quad (1.4)$$

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which is a correct expression. The advantage of this method is clear in that it does not require the solution of the differential equation. Instead, one should make an integration of the space coordinates over the limited range of space.

The similar type of advantage is also known in the path integral formulation, and indeed the path integral method is formulated so that the spectrum can be obtained by the infinitely many dimensional integration over the discretized space coordinates. However, the path integral method can be successfully applied only to the harmonic oscillator potential case. The reason of the successful description of the harmonic oscillator potential is clear because there is no scattering state in the harmonic oscillator potential system. On the other hand, the path integral cannot reproduce the energy spectrum of the Coulomb potential case. This is related to the fact that the Coulomb case contains scattering states, and thus the value of $\int_{-\infty}^{\infty} |\psi(x)|^2 dx$ is not necessarily unity. Therefore, the boundary condition cannot be properly taken into account in the path integral method, which should be an intrinsic defect arising from the formulation itself.

In addition, we discuss the Sommerfeld quantization rule [5–7] and clarify why it is successful for obtaining the energy spectrum of both the Coulomb and the harmonic oscillator potential systems. As we see below, the integration of the Sommerfeld quantization rule over coordinate space can be limited to the finite range of space. Therefore, the boundary condition is effectively taken into account in this treatment. However, the scattering problem cannot be treated in this semiclassical method, and the scattering states can be obtained by the WKB method which is the semiclassical approximation for the Schrödinger wave function. This WKB method is, however, not exact and only valid for the limited range of applications. The exact calculation of the scattering problem should be possible only when one solves the Schrödinger equation.

II. BOUNDARY CONDITION IN PATH INTEGRAL FORMULATION

Here, we discuss the problem of the boundary condition how we can consider the physics of the boundary condition into the path integral expression. In fact, there is no way to include the boundary condition in the path integral formulation since the path integral does not make use of any information on the wave function. This is the basic reason why one cannot solve the Coulomb potential problem in the path integral calculation since the Coulomb case contains the scattering states in which the boundary condition in the scattering state is completely different from the bound state problem. In this section, we take the representation of $\hbar = 1$.

A. Path integral in quantum mechanics

Here, we briefly describe the path integral formulation in quantum mechanics [9–11]. First, we define the transition amplitude $K(x', x : t)$ as

$$K(x', x : t) = \langle x' | e^{-iHt} | x \rangle = \sum_n \psi_n^*(x') \psi_n(x) e^{-iE_n t} \quad (2.1)$$

where Hamiltonian H is defined as

$$H = \frac{\hat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (2.2)$$

and $\psi_n(x)$ is an eigenstate of the Hamiltonian H

$$H\psi_n(x) = E_n\psi_n(x). \quad (2.3)$$

In this case, the path integral formulation is written as

$$K(x', x : t) = \int \mathcal{D}x \exp \left\{ i\Delta t \sum_{i=1}^n \left(\frac{m(x_i - x_{i-1})^2}{2(\Delta t)^2} - V(x_i) \right) \right\} \quad (2.4)$$

where many dimensional integration $\int \mathcal{D}x$ is introduced as

$$\int \mathcal{D}x \equiv \lim_{n \rightarrow \infty} \left(\frac{m}{2i\pi\Delta t} \right)^{\frac{n}{2}} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{n-1} \quad (2.5)$$

which is a symbolic notation in the path integral formulation. Therefore, the transition amplitude can be written in terms of the path integral formulation as

$$K(x', x : t) = \langle x' | e^{-iHt} | x \rangle = \int \mathcal{D}x \exp \left(i \int_0^t L(x, \dot{x}) dt \right) \quad (2.6)$$

where $L(x, \dot{x})$ is defined as

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - V(x) \quad (2.7)$$

which is the Lagrangian of the corresponding classical system.

B. Boundary condition in path integral formulation

Now a question may arise as to whether we may take into account the boundary condition for the wave function $\psi(x)$ in order to solve a bound state problem. That is, we must take into account the condition

$$\psi(\pm\infty) = 0 \quad (2.8)$$

in the path integral expression of eq.(2.1) and eq.(2.6) in some way or the other. However, one sees that the boundary condition cannot be taken into account in the path integral formulation in which any condition on the wave function never appears in this formulation. This will be shown below more in detail.

C. Boundary condition in the harmonic oscillator potential system

There is one example which is solved exactly in terms of the path integral formulation, that is, the harmonic oscillator potential system. Why is it that the harmonic oscillator potential system can be successfully solved? The reason is, of course, simple in that the harmonic oscillator potential system does not contain any scattering states, and in fact, all the states are bound. Therefore, it is clear that

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1 \quad (2.9)$$

is always guaranteed. Thus, we obtain from eq.(2.1)

$$\int K(x, x : t) dx = \int \langle x | e^{-iHt} | x \rangle dx = \int dx \sum_n |\psi_n(x)|^2 e^{-iE_n t} = \sum_n e^{-iE_n t}. \quad (2.10)$$

In fact, we obtain the $K(x', x : t)$ for the harmonic oscillator potential system as

$$K(x', x : t) = \sqrt{\frac{m\omega}{2i\pi \sin \omega t}} \exp \left\{ i \frac{m\omega}{2} \left[(x'^2 + x^2) \cot \omega t - \frac{2x'x}{\sin \omega t} \right] \right\} \quad (2.11)$$

and therefore

$$\int K(x, x : t) dx = \int_{-\infty}^{\infty} dx \sqrt{\frac{m\omega}{2i\pi \sin \omega t}} e^{-im\omega x^2 \tan \frac{\omega t}{2}} = \frac{1}{2i \sin \frac{\omega t}{2}} = \sum_{n=0}^{\infty} e^{-iE_n t}. \quad (2.12)$$

Here, we make use of the following equation

$$\frac{1}{2i \sin \frac{\omega t}{2}} = \frac{e^{-\frac{i}{2}\omega t}}{1 - e^{-i\omega t}} = \sum_{n=0}^{\infty} e^{-i\omega t(n+\frac{1}{2})} \quad (2.13)$$

and thus find

$$E_n = \omega \left(n + \frac{1}{2} \right) \quad (2.14)$$

which is a correct energy for the harmonic oscillator potential system.

D. Boundary condition with scattering states

The harmonic oscillator potential is a very special and exceptional case in quantum mechanics, and it is, of course, unrealistic and cannot be applied to the description of nature. The reason why we often find the harmonic oscillator potential is simple. If we treat many body systems and make some approximations to obtain an effective one body potential, then we always obtain the harmonic oscillator potential near the minimum point. Namely, if we treat it in terms of the small vibration around the minimum point $x = x_0$ of the complicated potential, then we find

$$V(x) = V(x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \dots \quad (2.15)$$

and here the first term is a constant and the second term is just the harmonic oscillator potential. However, it is clear that this is only valid for the small vibrations.

The complicated realistic potential should contain the scattering states since the potential $V(x)$ should vanish at the large value of x . For any systems with scattering states $\psi_s(x)$, the condition

$$\int |\psi_s(x)|^2 dx < \infty \quad (2.16)$$

is not necessarily satisfied. Therefore, eq.(2.10) cannot be used, and thus there is no way to obtain the energy eigenvalues of the corresponding system from the path integral method. This indicates that eq.(2.1) should normally contain some infinity in the integrations of the left hand side.

III. SOMMERFELD QUANTIZATION AND BOUNDARY CONDITION

As we see in the Introduction, the Sommerfeld quantization scheme is quite successful for obtaining the energy eigenvalue in some of the potential problems. Here, we briefly review the derivation of the Sommerfeld quantization rule from the Schrödinger equation in terms of the semiclassical approximation.

A. Sommerfeld quantization rule

We start from the Schrödinger equation in one dimension

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E\psi(x). \quad (3.1)$$

Now we assume the wave function in the following shape

$$\psi(x) = Ae^{i\frac{\Sigma}{\hbar}} \quad (3.2)$$

and expand the S in terms of \hbar as $S = S_0 + \hbar S_1 + \dots$. By inserting the S into the Schrödinger equation, we obtain the S_0 to the lowest order of \hbar

$$\frac{dS_0(x)}{dx} = \pm \sqrt{2m(E - V(x))}. \quad (3.3)$$

Therefore, the wave function $\psi(x)$ becomes

$$\psi(x) = Ae^{\pm \frac{i}{\hbar} \int \sqrt{2m(E - V(x))} dx}. \quad (3.4)$$

At this point, we require that the wave function should be a single-valued function, and therefore obtain the following constraint equation

$$\oint p dx \equiv \oint \sqrt{2m(E - V(x))} dx = 2\pi\hbar n, \quad (n : \text{integer or half integer}) \quad (3.5)$$

which is just the Sommerfeld quantization rule.

B. Boundary condition in the Sommerfeld quantization

The constraint equation of eq.(3.5) is obtained from the requirement that the wave function should be a single-valued function. This should not necessarily correspond to a boundary condition at infinity, but should be an important physical imposition on the state vector, and therefore we can obtain the energy spectrum from this condition. However, it should be noted that the Sommerfeld quantization scheme can reproduce the right description of the energy eigenvalue only if the system has some semiclassical nature like the Coulomb potential system.

The boundary condition at large x should reflect the quantum effect in the wave function of the corresponding particle. This can be viewed from the uncertainty law that the large x corresponds normally to the small momentum regions in which the quantum effect becomes most important.

• **Coulomb potential** ($V(r) = -\frac{Ze^2}{r}$) : In the Coulomb potential, the strong part should be found in the small r region, and therefore the large momentum region is most important, and thus it can be considered to be almost semiclassical. Indeed, the Sommerfeld quantization scheme can give the right answer for the energy spectrum of the Coulomb potential system. We show the calculated result which is given in Introduction

$$\oint p dr = 2\sqrt{2m|E|} \int_0^{\frac{Ze^2}{|E|}} \sqrt{\frac{Ze^2}{|E|} - r} dr = nh \quad \implies \quad E = -\frac{m(Ze^2)^2}{2\hbar^2 n^2}. \quad (3.6)$$

The boundary condition of eq.(2.8) is effectively included in the above equation. This can be seen since the integration is limited to the finite region of space coordinate which is physically acceptable area of space.

• **Harmonic oscillator potential** ($V(x) = \frac{1}{2}m\omega^2 x^2$) :

$$\oint p dx \equiv \oint \sqrt{2m(E - V(x))} dx = 2m\omega \oint_{-\sqrt{\frac{2E}{m\omega^2}}}^{\sqrt{\frac{2E}{m\omega^2}}} \sqrt{\frac{2E}{m\omega^2} - x^2} dx = 2m\omega \frac{2E}{m\omega^2} \frac{n}{2} = 2\pi\hbar n. \quad (3.7)$$

Thus, by considering the fact that the value of n in eq.(3.5) can be an integer as well as a half integer, we obtain the energy E

$$E = \hbar\omega \left(n + \frac{1}{2} \right), \quad (n = 0, 1, 2, \dots). \quad (3.8)$$

• **Square well potential** ($V(x) = -V_0$ for $|x| < a$, otherwise $V(x) = 0$) :

$$\oint p dx \equiv \oint \sqrt{2m(E - V(x))} dx = 2\sqrt{2m(E + V_0)} 2a = 2\pi\hbar n. \quad (3.9)$$

Thus, we obtain

$$E = -V_0 + \frac{\hbar^2 \left(\frac{\pi n}{2}\right)^2}{2ma^2}. \quad (3.10)$$

This can be compared with the result obtained from the quantum mechanics calculation for the square well potential model. This energy cannot be given in terms of the analytical expression. Instead, one should solve the following equation for E

$$\alpha = \sqrt{\frac{2m(E + V_0)a^2}{\hbar^2}}, \quad \beta = \sqrt{-\frac{2mEa^2}{\hbar^2}} \quad (3.11)$$

$$\beta = \alpha \tan \alpha. \quad (3.12)$$

Approximate solutions can be found when $\alpha \simeq \frac{\pi}{2}n$ which should be expected from $\tan \alpha \simeq 0$. In this case, we can immediately obtain the energy E as

$$E \simeq -V_0 + \frac{\hbar^2 \left(\frac{\pi n}{2}\right)^2}{2ma^2} \quad (3.13)$$

which is just the same as the semiclassical result of eq.(3.10). In this case, however, eq.(3.12) is not necessarily satisfied, and thus the result of the bound state energy should be far from reliable.

• **δ function potential** ($V(x) = -V_\delta \delta(x)$) : The limitation of the Sommerfeld quantization rule can be well exhibited if one solves the energy spectrum of the δ function potential with the semiclassical method. The answer is that there is no way to express the energy E in terms of V_δ . This is partly because of the mathematical difficulty due to the generalized function of $\delta(x)$ in the square root, but mainly because of the limitation of the Sommerfeld quantization rule itself. This difficulty is better understood if we calculate the energy spectrum of the δ function potential from the square well potential result. In this case, we start from eq.(3.12)

$$\sqrt{-\frac{2mEa^2}{\hbar^2}} = \sqrt{\frac{2m(E + V_0)a^2}{\hbar^2}} \tan \sqrt{\frac{2m(E + V_0)a^2}{\hbar^2}}. \quad (3.14)$$

Here, we make $a \rightarrow 0$, $V_0 \rightarrow \infty$, but keep $V_\delta = 2aV_0$ finite. Therefore, eq.(3.14) can be written to a good approximation as

$$\sqrt{\frac{-2mE}{\hbar^2}} \simeq \sqrt{\frac{mV_\delta}{\hbar^2}} \sqrt{\frac{mV_\delta}{\hbar^2}} \quad (3.15)$$

which leads to the energy E

$$E = -\frac{mV_\delta^2}{2\hbar^2} \quad (3.16)$$

and this is indeed a correct energy eigenvalue of the δ function potential in quantum mechanics problem.

As we note above, the energy of the square well potential from the Sommerfeld quantization rule is obtained without making use of eq.(3.12) while the energy of the δ function potential is obtained only if we make use of eq.(3.12). From this discussion, we see that the Sommerfeld quantization rule cannot be applied to the δ function potential.

IV. SUMMARY

We have clarified the similarity and difference between the path integral formulation and the Sommerfeld quantization rule. The similarity of the two methods is concerned with the classical mechanics since both approaches start from the equations of classical mechanics.

On the other hand, there is a significant difference between them. The Sommerfeld quantization rule can properly take into account the boundary condition which is crucial for solving the bound state problem. On the other hand, the path integral method cannot include any of the wave function information, and therefore it cannot consider the boundary condition at infinity. Therefore, the path integral method can only solve the harmonic oscillator potential problem in which there is no need of the boundary condition.

The investigation of the present paper may not contain any new physics except that the limitation of the path integral method is made clear for the first time. In this respect, it should present an important step for readers to realize that any numerical calculations based on the path integral formulation cannot give the right energy spectrum of physically interesting potential models.

In addition, it is shown that the Sommerfeld quantization rule can be quite useful for calculating the spectrum of some quantum mechanics models, but at the same time, we explicitly present the limitation of the semiclassical picture in terms of the square well potential calculation.

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