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## SEMICLASSICAL QUANTUM MECHANICS: A PATH-INTEGRAL APPROACH

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It is well known that one can approach problems in electrodynamics at either the macroscopic or microscopic level. However, we have less knowledge about the same approach in the case of semiclassical quantum mechanics. This case will be discussed here.

### 1 Introduction

When dealing with simple optical phenomena such as transmission and reflection, one can proceed in two quite different but totally equivalent ways. One is macroscopic and utilizes the solution of the Maxwell equations subject to appropriate boundary conditions. The second is microscopic. It is based on the multiple scattering series and follows a simple ray through all possible paths to its final destination. This procedure offers a very visual and a much clearer intuitive picture for what is taking place. The equivalence of macroscopic and microscopic techniques in this case is well known. Less familiar to many physicists is that an equivalent microscopic approach can be used in the case of semiclassical quantum mechanics. This will be discussed here. Our results are implicit in the work of other authors [1], so the presentation will be more of a didactic nature.

### 2 Semiclassical Methods

It is possible to treat quantum mechanics via macroscopic and/or microscopic methods, at least in the situation that the action divided by  $\hbar$  is large – the

so-called semiclassical limit. The macroscopic procedure is well known as the WKB technique, the basic idea of which is that for a slowly varying potential  $V(x)$ , a stationary state solution can be written as [2]

$$\psi_{\text{WKB}}(x, t) \sim \sqrt{\frac{m}{k(x)}} \exp \left\{ i \left( \int_{x_0}^x k(x') dx' - Et \right) \right\}, \quad (1)$$

with the local wave number

$$k(x) = \sqrt{2m(E - V(x))}. \quad (2)$$

This approximation is valid when refraction dominates over reflection, or equivalently when the change in potential energy over a distance of the de Broglie wavelength is much smaller than the local kinetic energy, i.e.

$$\lambda \frac{|dV/dx|}{E - V(x)} \ll 1. \quad (3)$$

This approximation clearly breaks down at a classical turning point  $x = a$ , where  $E = V(a)$ . The usual procedure to deal with this breakdown is to use the WKB form of the wave function except in the immediate vicinity of the turning point, wherein a linear approximation to the potential is used in order to match the form of the wave function. This technique is a standard one and a prototypical problem treated via WKB is that of barrier penetration, i.e. the case of a particle of mass  $m$  and energy  $E$  incident on a potential barrier  $V(x)$  with maximum height such that  $V_{\text{max}} > E$ . The results of this procedure are well known and yield reflection and transmission formulae [3]

$$R = 1 - T = \frac{e^{-2\sigma}}{\left(1 + \frac{1}{4}e^{-2\sigma}\right)^2}, \quad (4)$$

with the WKB penetration factor

$$\sigma = \int_a^b dx \sqrt{2m(V(x) - E)}, \quad (5)$$

and  $a, b$  being the classical turning points. The derivation is straightforward, but using the connection formulae, derived from the asymptotic behavior of Airy functions, renders this procedure somewhat in the realm of black magic, so that one does not really develop a “feel” for the physics.

As an alternative approach, we present below a microscopic version of the semiclassical approximation which is based upon the Feynman path integral. The results obtained in this fashion are totally equivalent to those found via

WKB in most cases. However, the path integral viewpoint generates a more intuitive picture of the physics of the process under consideration and offers ways to treat some aspects, such as the superbarrier penetration [4], which lie outside the simple WKB domain of applicability.

### 2.1 Quadratic Approximation to the Propagator

In order to understand the semiclassical procedure, consider the path-integral form of the propagator

$$D_F(x_2, t; x_1, 0) = \int \mathcal{D}[x(t)] \exp \left\{ \frac{i}{\hbar} S[x(t), \dot{x}(t)] \right\}. \quad (6)$$

Now write

$$x(t) = x_{\text{cl}}(t) + \delta x(t), \quad (7)$$

where  $x_{\text{cl}}(t)$  is a solution of Hamilton's equation  $\delta S[x_{\text{cl}}(t)] = 0$ , and expand the action in terms of  $\delta x(t)$ . The terms linear in  $\delta x, \delta \dot{x}$  vanish after an integration by parts and use of the classical equations of motion, yielding

$$\begin{aligned} D_F(x_2, t; x_1, 0) &\simeq \exp \left\{ \frac{i}{\hbar} S[x_{\text{cl}}(t)] \right\} \int \mathcal{D}[\delta x(t)] \\ &\times \exp \left\{ \frac{i}{\hbar} \int_0^t dt' \left( \frac{1}{2} m (\delta \dot{x}(t'))^2 - \frac{1}{2} V''(x_{\text{cl}}(t')) (\delta x(t'))^2 \right) \right\} \end{aligned} \quad (8)$$

as an approximate representation of the propagator. The exponential phase factor is just the classical action, while the additional multiplicative term is the closed path propagator for a particle of mass  $m$  moving under the influence of the time-dependent potential  $x^2 V''(x_{\text{cl}}(t))/2$ .

Eq. (8) is exact for a quadratic potential, but for a general potential the semiclassical approximation involves dropping terms of higher order than quadratic in  $\delta x$ , since one can show that the contribution of the quadratic order terms to the path integral is of lower order in  $\hbar$  than that from cubic or higher order terms. Indeed, only the classical path survives in the limit  $\hbar \rightarrow 0$ , and deviations  $\delta x(t)$  from this path are only important if the change which they induce in  $S/\hbar$  is of order  $\sim \pi$  or less, i.e.  $\delta^2 S[x_{\text{cl}}]/\hbar \leq \pi$ , since larger deviations imply a rapid oscillation of the integrand and result in a nearly complete cancellation. We conclude that  $\delta x \sim \hbar^{1/2}$  so that  $S[x_{\text{cl}}]/\hbar \sim \mathcal{O}(\hbar^{-1})$  and  $\delta^2 S[x_{\text{cl}}]/\hbar \sim \mathcal{O}(1)$ . However,  $\delta^3 S[x_{\text{cl}}]/\hbar \sim \mathcal{O}(\hbar^{1/2})$ , implying

that cubic and higher order terms in  $\delta x$  can be neglected in the semiclassical limit  $\hbar \rightarrow 0$ .

The quadratic path integration over  $\delta x(t)$  may be performed via a clever analyticity argument due to Coleman [5], or by other means, yielding the so-called Van Vleck determinant (hereafter setting  $\hbar = 1$ )

$$\begin{aligned} & \int \mathcal{D}[\delta x(t)] \exp \left\{ i \int_0^t dt' \left( \frac{1}{2} m (\delta \dot{x}(t'))^2 - \frac{1}{2} (\delta x(t'))^2 V''(x_{\text{cl}}(t')) \right) \right\} \\ &= \left( \frac{m}{2\pi i \dot{x}_{\text{cl}}(0) \dot{x}_{\text{cl}}(t)} \int_{x_1}^{x_2} dx \dot{x}_{\text{cl}}^{-3}(x) \right)^{\frac{1}{2}}. \end{aligned} \quad (9)$$

## 2.2 The WKB Propagator

We can now demonstrate that this quadratic approximation to the path integral is, in general, completely equivalent to the WKB approximation [6]. In order to make this connection, consider the propagator written in terms of WKB solutions of Eq. (1):

$$D(x_2, t; x_1, 0) = \frac{m}{2\pi} \int dE e^{-iEt} \psi_{\text{WKB}}(x_2, E) \psi_{\text{WKB}}^*(x_1, E), \quad x_2 > x_1, \quad (10)$$

where

$$\psi_{\text{WKB}}(x, E) = \frac{1}{\sqrt{k(x)}} \exp \left[ i \int_a^x dx' k(x') \right], \quad (11)$$

with the local wave number (2). The energy integration in Eq. (10) can be performed via the stationary phase approximation, wherein one approximates an integral of the form

$$J = \int_{-\infty}^{\infty} dE e^{if(E)} g(E) \simeq \sqrt{\frac{2\pi i}{f''(E_0)}} g(E_0) e^{if(E_0)}, \quad (12)$$

with  $E_0$  defined by the condition  $f'(E_0) = 0$ . In our case

$$f(E) = \int_{x_1}^{x_2} dx' \sqrt{2m(E - V(x'))} - Et, \quad (13)$$

and the stationary phase energy  $E_0$  is found by requiring

$$0 = \frac{\partial f(E)}{\partial E} = \int_{x_1}^{x_2} dx' \sqrt{\frac{m}{2(E_0 - V(x'))}} - t. \quad (14)$$

Since  $\sqrt{2(E - V(x))/m} = \dot{x}_{\text{cl}}$  is the classical velocity, we find  $t = \int_{x_1}^{x_2} dx' / \dot{x}_{\text{cl}}(x')$  as the defining equation for  $E_0$ , i.e.  $E_0 = E_{\text{cl}}$ , where  $E_{\text{cl}}$  is the classical energy for the trajectory  $x_{\text{cl}}(t)$  connecting  $(x_1, 0)$  and  $(x_2, t)$ . Also, since

$$f''(E_{\text{cl}}) = -\frac{1}{2} \int_{x_1}^{x_2} dx' \left( \frac{m}{2(E_{\text{cl}} - V(x'))^3} \right)^{\frac{1}{2}} = -\frac{1}{m} \int_{x_1}^{x_2} dx \dot{x}_{\text{cl}}^{-3}(x) \quad , \quad (15)$$

the WKB propagator becomes

$$D(x_2, t; x_1, 0) = \left( \frac{m}{2\pi i \dot{x}_{\text{cl}}(t) \dot{x}_{\text{cl}}(0) \int_{x_1}^{x_2} dx \dot{x}_{\text{cl}}^{-3}(x)} \right)^{1/2} \times \exp \left( i \int_{x_1}^{x_2} dx k(x) - i E_{\text{cl}} t \right) \quad , \quad (16)$$

which is identical in form to the quadratic approximation to the path integral, since the prefactor is obviously the same, while the classical action can be written as

$$\begin{aligned} S[x_{\text{cl}}(t)] &= \int_0^t dt' \left( \frac{1}{2} m \dot{x}_{\text{cl}}^2(t') - V(x_{\text{cl}}(t')) \right) = \int_0^t dt' (m \dot{x}_{\text{cl}}^2(t') - E_{\text{cl}}) \\ &= \int_{x_1}^{x_2} dx m \dot{x}_{\text{cl}}(x) - E_{\text{cl}} t = \int_{x_1}^{x_2} dx \sqrt{2m(E_{\text{cl}} - V(x))} - E_{\text{cl}} t. \end{aligned} \quad (17)$$

We conclude that any problem which can be treated via WKB methods can equally well be handled using path-integral techniques in the quadratic approximation.

### 2.3 Barrier Penetration: Semiclassical Approach

An example of such a problem is that of barrier penetration. We shall demonstrate here how the same results found via WKB can be derived via semiclassical path-integral methods. In order to do so, it is necessary to generalize the idea of a classical path. In the case of barrier penetration a conventional classical trajectory connecting points  $x_1, x_2$  far to the left or right of the barrier, respectively, and with classical energy *less* than the height of the barrier, does not exist since the particle must be completely reflected. Nevertheless, there *do* exist trajectories connecting the two space-time points  $(x_1, 0)$  and

$(x_2, t)$  which satisfy

$$m\ddot{x}_{\text{cl}} = -\left.\frac{dV}{dx}\right|_{x_{\text{cl}}}, \quad (18)$$

provided we allow the time  $t$  to become complex, and such paths can be chosen to have a real classical energy  $E < V_{\text{max}}$ . In fact, for given  $x_1, x_2, E$ , there exists a denumerably *infinite* set of such paths which can be labeled by their propagation “times” with  $t^{(n)}$ ,  $n = 0, 1, 2, \dots$ :

$$t^{(n)} = \int_{x_1}^a + \int_b^{x_2} dx \sqrt{\frac{m}{2(E - V(x))}} - i(2n + 1) \int_a^b dx \sqrt{\frac{m}{2(V(x) - E)}}. \quad (19)$$

The propagation from  $x_1$  to  $x_2$  can be considered as occurring in three successive steps. First the particle travels from the initial point  $x_1$  to the left-hand classical turning point  $a$  in the real time interval

$$\Delta t_a = \int_{x_1}^a dx \sqrt{\frac{m}{2(E - V(x))}}, \quad (20)$$

and then makes  $2n + 1$  traversals of the interval between  $a$  and  $b$  in pure *imaginary* time

$$\Delta t_i^{(n)} = -i(2n + 1) \int_a^b dx \sqrt{\frac{m}{2(V(x) - E)}}. \quad (21)$$

Finally, the particle propagates from the right-hand turning point  $b$  to  $x_2$  in the real time interval

$$\Delta t_b = \int_b^{x_2} dx \sqrt{\frac{m}{2(E - V(x))}}. \quad (22)$$

The total temporal interval is then  $t^{(n)} = \Delta t_a + \Delta t_i^{(n)} + \Delta t_b$ , as given in Eq. (19).

Physically, the different values  $t^{(n)}$  ( $n = 0, 1, 2, \dots$ ) correspond to the possibility of internal reflections from the walls inside the barrier. This interpretation follows from writing Newton’s equations in terms of imaginary time  $\tau = it$

$$m \frac{d^2 x}{d\tau^2} = -m \frac{d^2 x}{dt^2} = \left.\frac{dV(x)}{dx}\right|_{x=x(\tau)}. \quad (23)$$

Equation (23) describes the motion of a classical particle of mass  $m$  moving inside a potential well  $-V(x)$ . The particle can travel from turning point  $a$  to turning point  $b$  in an infinite number of ways, corresponding to the direct path plus an *arbitrary* number ( $n = 1, 2, \dots$ ) of complete loops from  $a$  to  $b$  and back again to  $a$ . Thus the “trajectory” labeled by  $t^{(0)}$  represents a path which enters the forbidden region at point  $a$ , “propagates” directly to turning point  $b$  and exits. The path labeled by  $t^{(1)}$  passes into the barrier at point  $a$ , “propagates” to  $b$  where it is reflected, returns to  $a$  where it is reflected again, and finally “propagates” to point  $b$  where it exits the barrier. Similarly, paths labeled by  $t^{(n)}$  correspond to “trajectories” with  $2n + 1$  traversals of the forbidden region before final exit at point  $b$ .

Obviously these “classical” paths cannot be directly utilized to produce a semiclassical propagator. They become relevant, however, if the propagator is analytically continued through the introduction of its Fourier transform<sup>a</sup>

$$D(x_2, x_1; E) = \int_0^\infty dt e^{iEt} D(x_2, t; x_1, 0) . \quad (24)$$

In fact, it is this energy-space form of the propagator which is relevant for calculating the barrier reflection/transmission properties, since wavepackets are constructed to have fixed energy.

The form of  $D(x_2, t; x_1, 0)$  to be used here is given by

$$D(x_2, t; x_1, 0) \cong \left( \frac{1}{2\pi i k(x_2) k(x_1) \int_{x_1}^{x_2} dx k^{-3}(x)} \right)^{1/2} \times \exp \left( i \int_{x_1}^{x_2} k(x) dx - i\tilde{E}t \right) . \quad (25)$$

The integral  $\int_{x_1}^{x_2} k(x) dx$  is to be understood as a line integral that can loop around the edges of the barrier  $2n$  times ( $n = 0, 1, 2, \dots$ ). In the immediate vicinity of a turning point, the quadratic approximation to the propagator is no longer valid, and an additional factor  $\lambda = i/2$  is produced each time one passes through such a point, as shown by careful study of the turning point region [7]. Thus for the “classical” path labeled by integer  $n$ , we interpret

$$\int_{x_1}^{x_2} dx k(x) = \int_{x_1}^a + \int_b^{x_2} dx k(x) + i(2n + 1) \int_a^b \kappa(x) dx - i2n \ln \lambda, \quad (26)$$

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<sup>a</sup>The lower limit of integration is set by the feature that the Feynman propagator  $D(x_2, t; x_1, 0)$  is defined to vanish for  $t < 0$  by the  $i\epsilon$  prescription.

where  $\kappa(x) = \sqrt{2m(V(x) - E)}$  and where the energy  $\tilde{E}(t^{(n)})$  is defined implicitly in terms of the time  $t^{(n)}$  via

$$t^{(n)} = \int_{x_1}^a + \int_b^{x_2} dx \sqrt{\frac{m}{2(\tilde{E} - V(x))}} + i(2n+1) \int_a^b dx \sqrt{\frac{m}{2(V(x) - \tilde{E})}} . \quad (27)$$

Here the turning points  $a$  and  $b$  are functions of  $\tilde{E}(x_2, x_1, t^{(n)})$ , but  $\lambda$  is independent of energy (and time).

The Fourier transform is performed via the stationary phase approximation. Writing  $D(x_2, t; x_1, 0) = \rho(t) e^{i\phi(t)}$  (where we have suppressed the dependence upon  $x_2, x_1$ ) we have

$$D(x_2, x_1; E) = \int_0^\infty dt e^{i(Et + \phi(t))} \rho(t), \quad (28)$$

and the stationary phase point  $\bar{t}$  is determined via

$$\begin{aligned} 0 &= \frac{\partial}{\partial t} (Et + \phi(t)) = \frac{\partial}{\partial t} \left( Et + \int_{x_1}^{x_2} k(x) dx - \tilde{E}t \right) \\ &= E - \tilde{E}(t) - t \frac{\partial \tilde{E}}{\partial t} + \int_{x_1}^{x_2} dx \frac{\partial k}{\partial \tilde{E}} \frac{\partial \tilde{E}}{\partial t} . \end{aligned} \quad (29)$$

However,  $t - \int_{x_1}^{x_2} dx \partial k / \partial \tilde{E} = 0$ , since this is the equation which defined  $\tilde{E}(t)$  in the first place. Thus the stationary phase point  $\bar{t}$  is defined via  $E = \tilde{E}(\bar{t})$ . Finally, using

$$\frac{\partial^2}{\partial t^2} (Et + \phi(t)) \Big|_{t=\bar{t}} = - \frac{\partial \tilde{E}}{\partial t} \Big|_{t=\bar{t}} = - \frac{1}{\int_{x_1}^{x_2} dx \frac{\partial^2 k}{\partial \tilde{E}^2}} = \left( m^2 \int_{x_1}^{x_2} dx k^{-3}(x) \right)^{-1}, \quad (30)$$

the stationary phase approximation yields

$$D(x_2, x_1; E) = \left( \frac{m^2}{k(x_2)k(x_1)} \right)^{1/2} \exp \left\{ i \int_{x_1}^{x_2} k(x) dx \right\}, \quad (31)$$

where the integration is understood in the sense of Eq. (26).

As the  $\bar{t}^{(n)}$  are complex, the stationary phase procedure requires that the path from  $t = 0$  to  $t = +\infty$  is deformed into the complex plane in such a way that it passes through *each*  $\bar{t}^{(n)}$  with  $n = 0, 1, 2, \dots$ . We then find

$$D(x_2, x_1; E) = \sum_{n=0}^{\infty} D^{(n)}(x_2, x_1; E)$$



$$\begin{aligned}
 &= \left( \frac{m^2}{k(x_2)k(x_1)} \right)^{1/2} \exp \left( i \int_{x_1}^a + i \int_b^{x_2} k(x) dx \right) \\
 &\quad \times \sum_{n=0}^{\infty} \lambda^{2n} \exp \left( -(2n+1) \int_a^b \kappa(x) dx \right) . \quad (32)
 \end{aligned}$$

The contribution from paths involving  $n \geq 1$  are exponentially suppressed and of questionable accuracy, as the corrections to the semiclassical approximation to the path integral could well be larger. Nevertheless, it is important to include the effects of these “interior bounce” solutions since only then we have a unitary and fully consistent picture of the transmission and reflection process which conserves probability. Thus calculating the propagator for transmission, as given above, we can perform the summation over  $n$ , yielding

$$D(x_2, x_1; E) = \left( \frac{m^2}{k(x_2)k(x_1)} \right)^{1/2} \exp \left( i \int_{x_1}^a + i \int_b^{x_2} k(x) dx \right) \frac{e^{-\sigma}}{1 - \lambda^2 e^{-2\sigma}}, \quad (33)$$

where  $\sigma \equiv \int_a^b \kappa(x) dx$ .

We see that this path-integral approach to the semiclassical approximation allows a very appealing and graphical picture of the transmission process. Instead of the sum over *all possible* paths required in calculating the complete path integral, the semiclassical approximation utilizes a sum over *all “classical”* paths connecting the initial and final points. (Here “classical” is used in the sense defined above, wherein analytic continuation into the complex time plane is permitted.) The form of the propagator can be found by using the simple rules:<sup>b</sup>

- i) Propagation from  $x_1$  to  $x_2$  in a classically allowed, forbidden region produces a factor

$$\exp \left\{ i \int_{x_1}^{x_2} k(x) dx \right\} , \quad \exp \left\{ - \int_{x_1}^{x_2} \kappa(x) dx \right\} , \quad (34)$$

respectively;

- ii) Reflection from a classical turning point within a classically forbidden region yields a factor  $\lambda = i/2$ , as discussed in Ref. [7].

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<sup>b</sup>For completeness, it should be noted that there exist corresponding phases  $\exp(\pm i\pi/4)$  which arise upon *transmission* through a barrier. However, these do not play a role when the transmission or reflection probabilities are determined and therefore, for simplicity, will be omitted here.

In order to deal with the corresponding reflection coefficient, we require one additional rule

- iii) Reflection from a classical turning point within a classically allowed region yields a factor  $\eta = -i$ , according to Ref. [7].

The propagator for the reflection process may then be constructed by taking  $x_1, x_2$  both to the left of the barrier and including all possible ‘‘classical’’ trajectories:

- i) Propagation from  $x_1$  to the left-hand wall at  $x = a$  followed by a reflection and propagation back to  $x_2$ ;
- ii) Propagation from  $x_1$  to the left-hand wall at  $x = a$  followed by transmission into the barrier, reflection from the right-hand wall, transmission back to  $x = a$  and then propagation from  $x = a$  to  $x_2$ , etc.

The total contribution to the propagator is then

$$D(x_2, x_1; E) = \left( \frac{m^2}{k(x_2) k(x_1)} \right)^{1/2} \exp \left( i \int_{x_1}^a + i \int_a^{x_2} k(x) dx \right) f \quad (35)$$

with

$$f = \eta + \sum_{n=0}^{\infty} \lambda^{2n+1} e^{-(2n+2)\sigma} = \eta + \frac{\lambda e^{-2\sigma}}{1 - \lambda^2 e^{-2\sigma}}, \quad (36)$$

where  $\sigma$  is defined in Eq. (5). The connection with the transmission and reflection coefficients

$$R = |r(E)|^2 \quad \text{and} \quad T = |t(E)|^2 \quad (37)$$

can now be made via the identifications

$$\begin{aligned} D(x_2, x_1; E) &= \left( \frac{m^2}{k(x_2) k(x_1)} \right)^{1/2} t(E), & x_1 \ll a, \quad b \ll x_2, \\ D(x_2, x_1; E) &= \left( \frac{m^2}{k(x_2) k(x_1)} \right)^{1/2} r(E), & x_1, x_2 \ll a, \end{aligned} \quad (38)$$

and we find, using Eqs. (32) and (35),

$$T = |t(E)|^2 = \frac{e^{-2\sigma}}{|1 - \lambda^2 e^{-2\sigma}|^2} = \frac{e^{-2\sigma}}{(1 + \frac{1}{4}e^{-2\sigma})^2},$$

$$R = |r(E)|^2 = \left| \eta + \frac{\lambda e^{-2\sigma}}{1 - \lambda^2 e^{-2\sigma}} \right|^2 = \left( \frac{1 - \frac{1}{4}e^{-2\sigma}}{1 + \frac{1}{4}e^{-2\sigma}} \right)^2 \quad (39)$$

in complete agreement with the corresponding WKB expressions, Eq. (5).

### 3 Conclusions

We have seen how the problem of barrier penetration can be handled equally well via macroscopic (WKB) or microscopic (semiclassical path integral) techniques. Similarly, it is straightforward to understand how other classic problems usually treated via WKB, such as  $\alpha$  decay [8], can be derived microscopically. The combination of macroscopic and microscopic approaches can provide an improved understanding of the problem and its solution.

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