A Time Dependent Version of the Quantum WKB Approximation

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Abstract
The phenomenon of quantum tunneling is reviewed and an overview of applying approximate methods for studying this effect is given. An approach to a time-dependent formalism is proposed in one dimension and generalized to higher dimensions. Some physical examples involving the resulting wavefunction which is determined are presented.

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There is a great deal of interest in integrable systems at the moment and their quantization. The semiclassical treatment of integrable systems has its roots in Bohr’s atomic model as well as in Einstein’s well known paper on the quantization of regular motion [1]. It is known that semiclassical quantization is exact only for so-called solvable potentials, which would include the harmonic oscillator [2,3]. The nonsolvable case yields approximate results which may be asymptotic in nature [4,5]. Of course there are summation techniques which can be applied to divergent series. Recently [6] a quantum phase was derived which gives exact quantization of nonsolvable potentials and avoids many of these complications. A consistent divergence-free scheme is still an active area of research.

The phenomenon of tunneling has been a characteristic property of many types of quantum mechanical processes, especially those which involve confining potential wells [7]. Their mathematical description has generated many different types of results. Due to the wide variety of applied applications where tunneling plays some role, the study of mathematical methods which would be useful in this context is still very active. Along these lines, the quantum WKB approximation is very important, and not a great deal exists in the literature for the time-dependent case [8]. An important example of a system where this approximation can be useful is the case of the decay of a system from a long-lived metastable state which frequently arises in physics. There has always been considerable interest in understanding the quantum tunneling of a macroscopic coordinate. If the height of a potential barrier is greater than the total energy $E$ of a particle, the kinetic energy of the particle is negative and so the study of the tunneling of a particle appears to have a paradoxical aspect to it. However this approach implies that we can assign values to the coordinate $x$ and the momentum $p$ simultaneously [7]. This however would violate the uncertainty principle. If however for a very short time $\Delta t$, the uncertainty in the energy $\Delta E$ is such that the total energy of the particle is greater than the height of the barrier, then tunneling takes place in time $\Delta t$ if the particle can traverse the barrier in this time interval. The continued interest in the Josephson effect, and the fact that high precision measurements are possible for such systems probably accounts for some of this interest. Another reason is that decay rates can be calculated theoretically based on models for such systems. The purpose here is to begin to introduce the
treatment of time dependence into these applications, and to discuss some of their quantum con-
sequences. A perturbative time-dependent wavefunction will be developed for the time-dependent
Schrödinger equation, and some applications will be considered. In particular, this type of wave
function is applicable to the study of the Berry phase.

The time-dependent Schrödinger equation in three space dimensions has the form

\[
i\hbar \frac{\partial \psi}{\partial t} = H\psi,
\]

where \( H \) is the Hamiltonian for the system. The case in which the Hamiltonian contains a potential
function will be of interest here, in which case (1) can be written

\[
i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V\psi.
\]

Here \( \Delta \) is the Laplacian operator in terms of the position coordinates. To motivate the approach,
consider a function \( \psi \) which is to satisfy (2) which has the particular form

\[
\psi(x, t) = A(x, t)e^{i S(x, t)}.
\]

In (3), both \( A \) and \( S \) depend on both the spatial variables and the time variable. Substituting (3)
into (2), after differentiating with respect to the given variables, (2) takes the form

\[
i\hbar \frac{\partial A}{\partial t} - A \frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m} \left[ \Delta A + 2i \frac{\hbar}{\hbar} \nabla A \cdot \nabla S + i \frac{\hbar^2}{\hbar} A \Delta S - \frac{1}{\hbar^2} A (\nabla S)^2 \right] + VA.
\]

Equating the real and imaginary parts on both sides of (4), two independent, coupled equations
in terms of the variables \( A \) and \( S \) then result and are given by

\[
\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + V - \frac{\hbar^2}{2mA} \Delta A = 0,
\]

\[
\frac{\partial A}{\partial t} + A \frac{\Delta S}{2m} + \frac{1}{m} \nabla S \cdot \nabla A = 0.
\]

Of course, by neglecting the term proportional to \( \hbar^2 \) in (5), the classical Hamilton-Jacobi equation
in terms of the single function \( S \) results. In this approximation, a solution to (5) in (6) gives an
equation for the function \( A \).

Let us now consider another version of this process. In other words, let \( \psi \) have the basic
structure given in (3), and then require that \( S \) satisfy the classical Hamilton-Jacobi equation. In
fact, it proves more appropriate to introduce a function which is a superposition of such functions in powers of $\hbar$.

Consider a classical system which is governed by a Hamiltonian $H$, then the associated classical Hamilton-Jacobi equation has the following form in terms of $r$-space variables

$$\frac{\partial S}{\partial t} + H(q_1, \cdots, q_r, \frac{\partial S}{\partial q_1}, \cdots, \frac{\partial S}{\partial q_r}, t) = 0.$$  \(7\)

Although it should be possible to generalize what follows to higher dimensions, let us suppose that there is just one spatial variable in order to simplify the discussion. Then for a Hamiltonian of the form that generates (2), equation (7) takes the form

$$\frac{1}{2m}(S_x)^2 + V + \frac{\partial S}{\partial t} = 0.$$  \(8\)

The Schrödinger equation (2) in one variable reduces to the form

$$\left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V + i\hbar \frac{\partial}{\partial t}\right)\psi = 0.$$  \(9\)

Define the linear operator

$$L = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V + i\hbar \frac{\partial}{\partial t}.$$  \(10\)

Equation (9) then takes the compact form

$$L\psi = 0.$$  \(11\)

Now the wave function $\psi$ in (3) will be generalized to the following series form in ascending powers of $\hbar$ by writing

$$\Psi(x,t) = \sum_{k=0}^{N} (i\hbar)^k a_k(x,t) \exp\left(\frac{i}{\hbar} S(x,t)\right).$$  \(12\)

In expression (12), the functions $S(x,t)$ and the coefficients $a_k(x,t)$ depend on both the space and time variables. Moreover, the $a_k$ are to be real-valued $a_k : \mathbb{R} \to \mathbb{R}$. It will be seen that it is possible to force (12) to satisfy (11) up to a single error term which is proportional to a power of $\hbar$ by imposing a set of differential constraint equations on the coefficients $a_k$ which appear in (12).

The second derivative of $\Psi$ is required in (9) and it is given by

$$\frac{\hbar^2}{2m} \Psi_{xx} = \frac{1}{2m} \left\{-i\hbar \sum_{k=1}^{N} (i\hbar)^k a_{k-1,xx} + 2i\hbar S_x \sum_{k=0}^{N} (i\hbar)^k a_{k,x} - (S_x)^2 \sum_{k=0}^{N} (i\hbar)^k a_k \right\}.$$
\[-(i\hbar)^{N+2}a_{N,xx} + i\hbar S_{xx} \sum_{k=0}^{N} (i\hbar)^{k}a_{k} \exp(i\frac{S}{\hbar}) \]  
(13)

The time derivative is given by

\[ i\hbar \Psi_t = \sum_{k=0}^{N} (i\hbar)^{k+1}a_{k,t} \exp(i\frac{S}{\hbar}) - S_t \Psi. \]  
(14)

Here, the variable subscript indicates differentiation with respect to \(x\) or \(t\). Substituting these derivatives into Schrödinger equation (9), we obtain

\[ \frac{\hbar^2}{2m} \Psi_{xx} - V \Psi + i\hbar \Psi_t = \frac{1}{2m}i\hbar \exp(i\frac{S}{\hbar}) \sum_{k=1}^{N} \{-(i\hbar)^{k}a_{k-1,xx} + 2S_{x}(i\hbar)^{k}a_{k,x} + S_{xx}(i\hbar)^{k}a_{k}\} \]

\[-\frac{1}{2m}(i\hbar)^{N+2}a_{N,xx} \exp(i\frac{S}{\hbar}) + \frac{1}{2m}i\hbar\{2S_{x}a_{0,x} + S_{xx}a_{0}\} \exp(i\frac{S}{\hbar}) \]

\[-\frac{1}{2m}(S_x^2\Psi + V\Psi + S_t \Psi) + \sum_{k=0}^{N} (i\hbar)^{k+1}a_{k,t} \exp(i\frac{S}{\hbar}). \]  
(15)

Now suppose that the function \(S(x,t)\) satisfies the Hamilton-Jacobi equation (8), then (15) takes the form

\[ L\Psi = \frac{1}{2m} \exp(i\frac{S}{\hbar})\{\sum_{k=1}^{N} (i\hbar)^{k+1}(-a_{k-1,xx} + 2S_{x}a_{k,x} + S_{xx}a_{k} + 2ma_{k,t})\} \]

\[ + \frac{1}{2m}i\hbar \exp(i\frac{S}{\hbar})\{2S_{x}a_{0,x} + S_{xx}a_{0} + 2ma_{0,t}\} - \frac{1}{2m}(i\hbar)^{N+2}a_{N,xx} \exp(i\frac{S}{\hbar}). \]  
(16)

It is now required that for a given function \(S\), the coefficient functions \(a_{k}\) must satisfy the following system of first-order partial differential equations with the definition \(a_{-1} = 0\),

\[ 2S_{x}a_{0,n} + S_{xx}a_{0} + 2ma_{0,t} = 0, \]  
(17)

\[ 2S_{x}a_{k,n} + S_{xx}a_{k} + 2ma_{k,t} - a_{k-1,xx} = 0, \quad k = 1, \ldots, N. \]  
(18)

Equation (18) is non-homogeneous since the coefficient \(a_{k-1}\) and hence \(a_{k-1,xx}\) has been determined from (17)-(18) at the previous order \(k-1\). In the event that (17) and (18) hold, all the terms in the brackets on the right-hand side of (16) vanish, and the Schrödinger equation reduces to simply

\[ L\Psi = -\frac{1}{2m}(i\hbar)^{N+2}a_{N,xx} \exp(i\frac{S}{\hbar}). \]  
(19)
If wavefunction (12) had been an exact solution of (9), the right-hand side of (19) would have reduced to zero. Thus this procedure in which $\Psi$ is taken in the form (12) provides a solution of (9) up to an error term proportional to $\hbar^{N+2}$, provided that $S$ is a solution of the classical Hamilton-Jacobi equation (8), and the $a_k$ satisfy the set of partial differential equations (17)-(18). Upon letting $N \to \infty$, an asymptotic solution to equation (11) results which has the form

$$\Psi \sim \left( \sum_{k=0}^{\infty} a_k(x, t) \hbar^k \right) \exp\left(\frac{i}{\hbar} S\right).$$

(20)

Once $S$ has been determined, the coefficients $a_k$ are obtained recursively as solutions of equations (17)-(18) which generate a time dependent solution. Convergence of (20) will not be discussed here.

This procedure can be generalized to higher spatial dimensions by using the linearity of the Schrödinger equation (2). The Hamilton-Jacobi equation has the form

$$\partial_t S + \frac{1}{2m} (\nabla S)^2 + V = 0.$$  

(21)

Thus, if the wavefunction $\Psi$ depends on three spacial coordinates $x$, the analogue of (12) will be written

$$\Psi(x, t) = \sum_{k=0}^{N} (i\hbar)^k a_k(x, t) \exp\left(\frac{i}{\hbar} S(x, t)\right).$$

(22)

The $\Delta \Psi$ term in (2) will include three expressions of the form (13) for each of the variables. Therefore, we can write

$$L \Psi = \frac{\hbar^2}{2m} \Delta \Psi - V \Psi + i\hbar \partial_t \Psi$$

$$= \frac{1}{2m} i\hbar \exp\left(\frac{i}{\hbar} S\right) \sum_{k=1}^{N} \left[ -(i\hbar)^k \Delta a_{k-1} + 2(i\hbar)^k (\nabla S) \cdot \nabla a_k + (i\hbar)^k a_k \Delta S \right]$$

$$- (i\hbar)^{N+2} \Delta a_n \exp\left(\frac{i}{\hbar} S\right) + \frac{i}{2m} \hbar [2(\nabla S) \cdot (\nabla a_0) + \Delta S a_0] \exp\left(\frac{i}{\hbar} S\right)$$

$$- \left( \frac{1}{2m} (\nabla S)^2 + V + \partial_t S \right) \Psi + \sum_{k=0}^{N} (i\hbar)^{k+1} a_{k+1} \exp\left(\frac{i}{\hbar} S\right).$$

(23)

If we suppose that $S$ is a function which satisfies the classical Hamilton-Jacobi equation (21), then the coefficient functions $a_k$ are required to satisfy the following system analogous to the pair (17)
and (18)
\[2\nabla S \cdot \nabla a_0 + \Delta S a_0 + 2ma_{0,t} = 0,\]  
(24)
\[2\nabla S \cdot \nabla a_k + \Delta S a_k + 2ma_{k,t} - \Delta a_{k-1} = 0, \quad k = 1, \ldots, N\]
Under the constraints (21) and (24), (23) reduces to
\[L\Psi = -\frac{1}{2m}(i\hbar)^{N+2} \Delta a_N \exp \left(\frac{i}{\hbar} S\right).\]  
(25)
Consider as an example the realistic case of the one-dimensional harmonic oscillator Hamiltonian given by
\[H = \frac{1}{2m}p^2 + x^2.\]  
(26) Then it is easy to check that the function
\[S = \int \sqrt{2m(\beta - x^2)} \, dx - \beta t\]  
(27)
is a solution to (8) under the harmonic potential function. In (27), \(\beta\) is a separation constant obtained upon integrating (8). Substituting (27) into (17), \(a_0\) will be given by the first order equation
\[2\sqrt{2m} \sqrt{\beta - x^2} \frac{\partial a_0}{\partial x} - \sqrt{2m} \frac{x}{\sqrt{\beta - x^2}} a_0 + 2m \frac{\partial a_0}{\partial t} = 0.\]  
(28)
This can be solved by the method of characteristics and the general solution is given by
\[a_0(x,t) = (\beta - x^2)^{1/4} \varphi(t - \sqrt{2m/\beta} \arctan(\frac{x}{\sqrt{\beta - x^2}))).\]  
(29)
Using (27), \(a_0\) in (28) can be written in terms of the derivative of \(S\) as
\[a_0(x,t) = \left(\frac{S_x}{\sqrt{2m}}\right)^{1/2} \varphi(t - \sqrt{2m/\beta} \arctan(\frac{\sqrt{2mx}}{S_x})).\]  
In (29), \(\varphi\) is selected to be an arbitrary twice differentiable function of a single variable. The method of characteristics does not specify how \(\varphi\) is to be chosen, however, this can be done on physical grounds. Higher order coefficients for the expansion (12) can be obtained from (18) using (29), however they are rather more complicated and will not be presented here.

As a final application of wavefunction (22), let us consider a curve \(C\) on a manifold of external parameters \(M\), and the adiabatic evolution of the quantum system described by the parameter
dependent Hamiltonian $H = H(v)$ along the curve $C$, and $v$ represents the set of parameters in vector form. A one-form may be defined on $M$ as follows

$$A^{(n)} = -Im(n | d_M n).$$

The integral of the one-form $A^{(n)}$ along a curve $C$ between $v_0$ and $v_1$ in parameter space produces the following geometric quantity

$$\gamma_n(C) = \oint_C A^{(n)} = \int_\Sigma F^{(n)}.$$ 

(30)

This is the Berry phase, where $\Sigma$ is an arbitrary two-dimensional submanifold of $M$ such that $\partial \Sigma = C$ and $F^{(n)} = dA^{(n)}$. In terms of the wave function $\psi_n(x; v)$, the two-form is calculated from $A^{(n)}$ to be

$$F^{(n)} = -Im[d_M \int d^N x \psi^*(x; v) d_M \psi_n(x; v)].$$

There is much interest in the study of the connection between the quantal Berry phase $\gamma_n(C)$ and the classical Hannay angle. An important question in this regard asks if a classical system has a Hannay angle, will it also possess a Berry phase when it is quantized. Wavefunctions of the type discussed here can be useful for discussing questions regarding the relationship between these quantities.

References.

[1] A. Einstein, Verh. Dtsch. Phys. Ges. 19, 82 (1917), A. Stone, Phys. Tod. 8, 57 (2005).
[2] J. B. Keller, Ann. Phys. 4, 180 (1958).
[3] J. B. Keller, Siam Rev. 27, 485 (1985).
[4] T. Hyouguchi, R. Seto, M. Ueda and S. Adachi, Ann. Phys. 312, 177 (2004).
[5] C. M. Bender, K. Olaussen and P. S. Wang, Phys. Rev. D 16, 1740 (1977).
[6] M. Matzkin, Phys. Rev. A72, 054102 (2005).
[7] Quantum Theory of Tunneling, M. Razavy, World Scientific (2003).
[8] M. P. A. Fisher, Phys. Rev. B 37, 75 (1988).