Wave Functions in the Presence of a Time-Dependent Field: Exact Solutions and Their Application to Tunneling

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Solutions to the time-dependent Schrödinger equation for a particle in a spatially uniform time-dependent field and some potentials of arbitrary form are proved to be like the time-independent eigenfunctions for an identical static potential. The field phase modulates the wave function and translates its envelope. This work applies directly to constant, linear, and parabolic static potentials and is self-consistent. Results for the modulation by a time-dependent field of the current through a rectangular barrier are relevant to the traversal time for tunneling and associated device limitations.

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A novel transformation of the coordinate system of the Schrödinger equation for a charged particle in a time-dependent field is presented which eliminates the field and gives rise to a new exact solution. Significant features are that it may be applied directly to major physical problems and that it is self-consistent in the simultaneous solution of Poisson and Schrödinger equations. It is used here to calculate the modulation by a field of the current tunneling through a rectangular potential barrier.

The wave functions of some systems respond to a time varying, spatially uniform force, $f(t)$, by a superposition of phase modulation and classical motion. This is a consequence of the transformation that yields a time-independent Schrödinger equation for one set of potentials which includes several of physical importance. Constant, linear, and parabolic potentials have exact solutions as do all which can be written as

$$V_A\left[x-m^{-1}\int\int f(t)dt^2\right]+V_B(t)\,.$$

In general, the problem of a uniform field applied to a finite potential, which gives divergent wave functions, transforms to one in which the potential has a localized time dependence and is therefore easier to analyze; for example, iterative methods may allow all quantum systems in time varying spatially uniform fields to be investigated.

The proof that time-dependent fields may be eliminated by a coordinate transformation starts with a Schrödinger equation in which the potential explicitly includes a spatially uniform field that is an arbitrary function of time, $V(x,t)-xf(t)$, and a solution $\Psi(x,t)$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+[V(x,t)-xf(t)]\Psi=i\hbar\frac{\partial\Psi}{\partial t}\,. \tag{1}$$

This is transformed to the coordinate system ξ,t, where $\xi=x-q(t)$, the displacement $q(t)=m^{-1}\int^t p(t')dt'$, and $p(t)=\int^t f(t')dt'$, by substituting the product $\phi(\xi,t)\times\chi(x,t)$ for $\Psi(x,t)$, with

$$\chi(x,t)=\exp\left[-\frac{iET}{\hbar}+\frac{ixp(t)}{\hbar}-\int^t\frac{ip^2(t')dt'}{2\hbar m}\right].$$

After division by $\chi(x,t)$ and subtracting

$$\left[xf(t)+\frac{p^2(t)}{2m}\right]\phi(\xi,t)+\frac{i\hbar p(t)}{m}\frac{\partial\phi(\xi,t)}{\partial\xi}$$

from both sides, Eq. (1) gives

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}+U(\xi,t)-E\right]\phi(\xi,t)=i\hbar\frac{\partial\phi(\xi,t)}{\partial t}\,, \tag{2}$$

where $U([x-q(t)],t)=V(x,t)$ and the partial derivatives are taken at constant t and ξ. Since $\chi(x,t)$ is continuous and nonzero, Eqs. (1) and (2) are equivalent.

This transformation may be used in three ways: First, when $U(\xi,t)$ is independent of t or the sum of two terms, one independent of t and the other of ξ, the solutions to Eq. (2) will be, correspondingly, functions of ξ alone or products of these with a phase factor $\exp[i\Theta(t)]$. When found, either analytically or numerically, they lead to exact solutions in the presence of a uniform time-dependent field. Second, the time-dependent Schrödinger equation (1) applies at each point x and time t; Eq. (2) shows that correct local solutions may be found wherever the potential $U(\xi,t)$ is either independent of t or the sum of separate functions of ξ and t. This is used in the calculation in this Letter. Third, for all other potentials the variables in the function $\phi(\xi,t)$ will not be separable; however, when $U(\xi,t)$ is a series of terms, each having a simple time dependence, an iterative approach solves Eq. (2) approximately, allowing the transformation to be used on problems in which the potential is not a function of ξ alone. For a fixed potential $V(x)$, a Taylor series may be used to express $U(\xi,t)$; its time-dependent part will equal $\sum q(t)^n[\partial^n V(\xi)/\partial\xi^n]/n!$. This will be zero where $V(x)$ is constant, e.g., far from the system under investigation in many experiments. In general, potentials with a global time dependence are transformed to ones with a localized time dependence.

In many studies the time dependence of the field is harmonic with a potential: $U(\xi,t)-xF\cos(\omega t)$; ξ will equal $x+F\cos(\omega t)/m\omega^2$ and $\chi(x,t)$ will be

$$\exp\left\{-\frac{iEt}{\hbar}+\frac{iFx\sin(\omega t)}{\hbar\omega}-\frac{iF^2[2\omega t-\sin(2\omega t)]}{8\hbar m\omega^3}\right\}.$$

Three simple potentials are sums of separate functions of ξ and t. The constant potential, $V(x)=V_0$, can be written as $V(\xi)=V_0$. A linear potential, V_0-xV_1, may be written as $V_0-V_1q(t)-\xi V_1$. To express a quadratic potential, $V(x)=\frac{1}{2}x^2V_2$, in the presence of a field as separate functions of ξ and t, it is necessary to scale the field, giving, for a harmonic force, a total potential

$$\tfrac{1}{2}\xi_g^2V_2-xG\cos(\omega t)-(V_2G^2/2m^2\omega^4)\cos^2(\omega t),$$

where the scaled amplitude of the force, G, equals $F/(1-V_2/m\omega^2)$ and $\xi_g=x+G\cos(\omega t)/m\omega^2$. The exact wave functions for the linear and quadratic cases are

$$\phi(\xi)\chi(x,t)\exp\left[i(V_1/\hbar)\int^t q(t')dt'\right],$$

$$\phi(\xi_g)\chi(x,t)\exp\left\{\frac{iG^2V_2[2\omega t+\sin(2\omega t)]}{8\hbar m^2\omega^5}\right\},$$

respectively, where $\phi(\xi)$ and $\phi(\xi_g)$ are solutions to the time-independent form of Eq. (2). With a quadratic potential the equation of motion for $q(t)$ is identical to the classical equation for the same potential. T. Tanuiti [1] noted that in this case such a transform eliminates the term due to an arbitrarily varying uniform force; his analysis exploited the parabolic potential and would not extend to the general result presented here.

When a set of exact solutions $\{\Psi_I(x,t)\}$ exists, two important properties may be demonstrated. The orthonormality of the wave functions $\{\Psi_I(x,t)\}$ over the space $\{\xi\}$ is proved from that of the set $\{\phi_I(\xi)\}$ by evaluating $\int\Psi_A^*(x,t)\Psi_B(x,t)dx$ to give

$$\int\phi_A^*(\xi)\phi_B(\xi)\exp[i(E_A-E_B)t/\hbar]d\xi=\delta_{AB}.$$

The completeness of the set $\{\Psi_i(x,t)\}$ at a time $t=\tau$ follows from the argument that, if a function $F(x)$ orthogonal to the elements of the set $\{\Psi_I(x,\tau)\}$ were to exist, then there would be a function $F(x)\exp[-ixp(\tau)/\hbar]$ outside $\{\phi_I(x-q(\tau))\}$ which is complete [2].

The transformation applies to N particles of mass m interacting through potentials $V_{ij}(\mathbf{r}_i-\mathbf{r}_j)=V_{ij}(\mathbf{r}_{ij})$ and subject to the external potential

$$V(\{\mathbf{r}_i\},t)=\sum_i V_i(\mathbf{r}_i,t)-x_if(t),$$

where $\{\mathbf{r}_i\}$ represents the space coordinates of all the particles and x_i is the x component of $\mathbf{r}_i$. Write the wave function $\Psi(\{\mathbf{r}_i\},t)$ as the product $\phi(\{\boldsymbol{\rho}_i\},t)\chi(\{\mathbf{r}_i\},t)$ with $\boldsymbol{\rho}_i=\mathbf{r}_i-\hat{\mathbf{x}}q(t)$ and $\chi(\{\mathbf{r}_i\},t)$ given by

$$\exp\left\{-\frac{iEt}{\hbar}-\sum_i\frac{ix_ip(t)}{\hbar}-\int^t\frac{iNp^2(t')dt'}{2\hbar m}\right\}.$$

The time-dependent Schrodinger equation

$$-\frac{\hbar^2}{2m}\sum_i\nabla_i^2\Psi+V(\{\mathbf{r}_i\},t)\Psi+\sum_i\sum_j V_{ij}(\mathbf{r}_{ij})\Psi=i\hbar\frac{\partial\Psi}{\partial t},$$

where the double summation is over all pairs counted once, simplifies after division by $\chi(\{\mathbf{r}_i\},t)$ to

$$\sum\left[-\frac{\hbar^2}{2m}\nabla_i^2+U_i(\boldsymbol{\rho}_i,t)+\sum V_{ij}(\boldsymbol{\rho}_{ij})\right]\phi=E\phi+i\hbar\frac{\partial\phi}{\partial t},$$

where the Laplacian is with respect to $\boldsymbol{\rho}_i$ and the summations remain over all particles and pairs. The transformation eliminates the field without affecting the interparticle potential; the response of identical particles to a field is therefore independent of those interactions. For example, if electrons are confined within a parabolic potential such as may be produced by compositional grading of an alloy semiconductor [3], their dispersion properties will not be affected by the flattening of the potential by electron-electron repulsion but will be identical to that of N independent electrons each with a resonant frequency $(V_2/4\pi^2m)^{1/2}$. This argument also applies to certain molecular vibrational modes.

To investigate the traversal time for particle tunneling Büttiker and Landauer [4] calculated the modulation of the tunneling current produced by a spatially uniform time variation of a thick rectangular barrier. This will be repeated here for the physically realizable case of modulation by a uniform field using the transformation and time-dependent wave functions. The two sets of results show significant differences relevant to the concept of a traversal time. The calculation, using the notation of the earlier study, starts with noninteracting charge carriers and barrier of width d, and height V_0 between two conducting regions whose relative potential varies at a frequency $\omega/2\pi$, subjecting the barrier to a time-varying uniform field. The potential is zero for $x\leq-\frac{1}{2}d$; $V_0-(x+\frac{1}{2}d)F\cos(\omega t)$ for x between $-\frac{1}{2}d$ and $\frac{1}{2}d$; and $-Fd\cos(\omega t)$ for $x\geq\frac{1}{2}d$. This is an unbounded problem with a continuous set of wave functions for all positive values of energy E. In the first region the general form of the wave function for a particle of energy E will be $\Psi=A\exp[\pm ikx-iEt/\hbar]$ where $\hbar^2k^2=2mE$, while in the third it will be the product of this with $\exp[i(Fd/\hbar\omega)\sin(\omega t)]$. In the barrier a wave function is required that is a solution of the Schrödinger equation in the presence of the oscillating field. This work has shown that the general form will be

$$\Psi=A\exp[\mp\kappa\xi]\chi(x,t)\exp\left[\frac{iFd\sin(\omega t)}{2\hbar\omega}\right],$$

where $\hbar^2\kappa^2=2m(V_0-E)$. Substitution confirms that this satisfies Eq. (1) at all points in the barrier.

When a wave of unit amplitude and energy $E_i < V_0$ is incident at $x = -\frac{1}{2}d$, part will be reflected and part will penetrate into the barrier where its amplitude will decay with distance. At $x = -\frac{1}{2}d$ the amplitude of the component in the barrier at energy E_i will be

$$C\left\{1 - \frac{\kappa F[\exp(i\omega t) + \exp(-i\omega t)]}{2m\omega^2}\right\}\exp\left(\frac{\kappa d}{2} - \frac{iE_i t}{\hbar}\right).$$

The time dependences of this expression and that for $\partial\Psi/\partial x$ are such that the continuity equations at $x = \pm\frac{1}{2}d$ can only be satisfied to first order always if the waves that are reflected, within the barrier, and transmitted have components with energies E_i and $E_i \pm \hbar\omega$. The separate continuity equations for terms with time dependence $\exp[-iE_i t/\hbar]$, $\exp[-iE_i t/\hbar - i\omega t]$, and $\exp[-i \times E_i t/\hbar + i\omega t]$ at both ends of the barrier give each of the transmitted amplitudes: D, which equals $[-4ik\kappa/(\kappa - ik)^2]\exp(-\kappa d)$, identical to the solution of the static problem, and D_+ and D_- given by

$$D_\pm = \frac{D\kappa F}{2m\omega^2}[\exp(\kappa d - \kappa_\pm d) - 1]\exp[i(k - k_\pm)d/2],$$

where terms of the order of $1/\hbar\omega$ have been neglected in comparison with $\kappa^2/m\omega^2$ and as have changes in k and κ that are small in comparison with the exponential term, consistent with a barrier thick compared with κ^{-1} and a modulation frequency small compared to $(V_0 - E_i)/\hbar$. It is also consistent to write the first bracketed term in this expression as $[\exp(\pm m\omega d/\hbar\kappa) - 1]$.

Combining the transmitted wave at energy E_i and the sidebands at $\pm\hbar\omega$ gives, at $x = \frac{1}{2}d$, a single wave of amplitude D multiplied by

$$1 + \alpha(\cosh\theta - 1)\cos(\omega t) - i\alpha\sinh\theta\sin(\omega t), \qquad (3)$$

where $\alpha = \kappa F/m\omega^2$ and $\theta = m\omega d/\hbar\kappa$, which is proportional to frequency and determines the degree of modulation of the transmitted wave. Series expansion of the hyperbolic functions shows the behavior at low frequencies. To first order the amplitude is $D[1 - i(Fd/\hbar\omega)\sin(\omega t)]$, a phase modulation exactly canceling that implicit in this region. The transmitted wave has a phase, relative to the incident wave, unaffected by the modulation of the barrier to this order. The second-order term, $\frac{1}{2}\alpha\theta^2\cos(\omega t)$, describes amplitude modulation in phase with the applied field; it equals $(Fmd^2/2\hbar^2\kappa)\cos(\omega t)$, identical to the quasistatic result. The third-order term is a frequency-dependent phase modulation of the transmitted wave relative to that incident of $-i(Fm^2\omega d^3/6\hbar^3\kappa^2)\sin(\omega t)$. Only a dynamic theory can give such higher-order terms. It is surprising that an approach in which the nominally small parameter, $F/m\omega^2$, diverges so strongly at low frequencies should give the quasistatic result in any calculation. The fact that it can implies that this transform is an effective way of solving all problems at frequencies at which the particle inertia is significant.

These results may be compared with those for a spatially uniform modulation of the barrier potential. The identical simplifications give similar expressions for D_+ and D_- but with $\mp V_1/2\hbar\omega$ replacing $\kappa F/2m\omega^2$, where V_1 is the amplitude of modulation of V_0. Because the polarities of the sidebands are opposite, the terms $(\cosh\theta - 1)$ and $\sinh\theta$ in Eq. (3) are interchanged. The first-order term in θ in the expansion of the hyperbolic functions, $D[1 + (V_1 md/\hbar^2\omega)\cos(\omega t)]$, represents an amplitude modulation identical to the quasistatic result; while the second-order term, $-i(V_1 m^2\omega d^2/2\hbar^3\kappa^2) \times\sin(\omega t)$, gives phase modulation relative to the incident wave.

Hauge and Støvneng [5] have reviewed the status of tunneling times, including that proposed by Büttiker and Landauer. The consensus is that $\hbar^2\kappa/md$ gives the energy scale characterizing the transmission of a rectangular barrier. For $\hbar\omega \ll \hbar^2\kappa/md$, the transmission varies nearly linearly with energy, while its exponential nature appears when $\hbar\omega \gtrsim \hbar^2\kappa/md$. The association of a traversal time with $md/\hbar\kappa$ is disputed; Büttiker and Landauer argued that, if a barrier is modulated at an angular frequency ω, low compared with the inverse of the traversal time for tunneling τ_T, the quasistatic behavior is observed, while if $\omega\tau_T \gtrsim 1$, particles tunnel through a time-averaged barrier with the absorption or emission of quanta causing the degree of modulation to be frequency dependent. For both types of barrier modulation the transmitted sidebands vary as $\exp(\pm m\omega d/\hbar\kappa) - 1$. With a uniform potential variation, the linear term in expanding $\exp(\pm m\omega d/\hbar\kappa)$ accounts for the quasistatic modulation of the tunneling current; hence they argued that the higher-order terms correspond to $\omega\tau_T \gtrsim 1$, i.e., $\tau_T \gtrsim md/\hbar\kappa$. However, with field modulation it is the second-order term in $m\omega d/\hbar\kappa$ which gives the quasistatic result; it follows that quasistatic behavior is not identified with a particular term and therefore the onset of frequency dependence is not a general property of the barrier. This argument cannot therefore identify $md/\hbar\kappa$ as the transit time for tunneling, since this is a parameter which should be independent of the type of modulation. This rejection accords with criticisms made by Hauge and Støvneng and others [6].

Quasiclassically, a barrier modulated by a uniform potential would not exhibit the time averaging expected by Büttiker and Landauer since the (negative) kinetic energy of the particle in the barrier is determined by the instantaneous height on entry. Changes in the barrier height during transit alter the particle's potential energy by external work, but not its kinetic energy or the barrier transmission. Phase modulation would be the only effect of such work. In contrast, a barrier with a varying field would exhibit time averaging of this modulating field, if it existed, since the kinetic energy of the particle changes as it works against the potential gradient of the field.

The lowest-order relative phase modulation of the transmitted wave, calculated previously, is consistent with the external work done on a particle traveling at a velocity $\hbar\kappa/m$ for both types of barrier modulation. A point particle traveling in a variable potential $V(x,t)$ is subject to a time rate of change of potential: $\partial V(x,t)/\partial t$; integrating this along the trajectory yields the change in potential energy $V_x(t)$ due to external work. The equation $V_x(t)\phi = i\hbar\partial\phi/\partial t$ gives an additional phase factor equaling $\exp[-(i/\hbar)\int V_x(t)dt]$ that depends on v, the velocity in the barrier. For the two forms of modulation $\partial V(x,t)/\partial t$ will be $V_1\omega\sin(\omega t)$ and $Fx\sin(\omega t)$ giving phase factors $1-(iV_1\tau_T^2\omega/2\hbar)\sin(\omega t)$ and $1-(iFx\tau_T^3\omega/6\hbar)\sin(\omega t)$, respectively, to lowest order in ω. These equal the previous expressions for the phase modulation proportional to ω if the velocity is $\hbar\kappa/m$ and the traversal time τ_T is $md/\hbar\kappa$.

This equality may result from such a velocity of propagation or from an accidental mathematical identity dependent on the energy sensitivity of the barrier. The former interpretation requires, for consistency, that there should be a barrier averaging effect in the amplitude modulation given by Eq. (3). The expressions for the real part of the amplitude proportional to $\cos(\omega t)$ expand to $\frac{1}{2}\alpha\theta^2(1+\theta^2/12)$ and $(V_1\theta/\hbar\omega)(1+\theta^2/6)$ where $\theta = \omega\tau_T$ if $\tau_T = md/\hbar\kappa$. The average gain in kinetic energy of a particle traversing a barrier subject to the varying potential $-Fx\cos(\omega t)$ reaches its maximum value of $Fd(c-c^2+s^2+\omega\tau_T s)/\omega^2\tau_T^2$, where $c=\cos(\omega\tau_T/3)$ and $s=\sin(\omega\tau/3)$, when a particle enters at a time $2n\pi/\omega - \tau_T/3$ and leaves at $2n\pi/\omega + 2\tau_T/3$. This expands to $\frac{1}{2}Fd(1-\omega^2\tau_T^2/36)$ to order ω^2. The amplitude modulation is found by dividing this by the energy scale of the barrier, $\hbar^2\kappa/md$. There is nothing in the comparison of the terms of order ω^2 for the two types of barrier modulation which indicates that a barrier averaging effect of this magnitude exists. This strongly suggests that the tunneling process cannot be described by the picture proposed by Büttiker and Landauer and that the equality of the phase modulations found by the two methods must be attributed to an accidental mathematical relationship. Both expressions for the modulated amplitude of the transmitted wave show that the degree of modulation is a superlinear function of ω. It is clear therefore that, if there is a traversal time for tunneling, it does not necessarily impose a limit to the operating frequency of electronic tunneling devices.

Major differences exist between the calculated tunneling behavior for a modulating field and for the simpler potential modulation. Although both give the quasistatic result to lowest order, the characteristics are significantly different at higher frequencies. Hence conclusions based on analyses using the simpler modulation, popular in studies of tunneling, are probably all incorrect in detail. The wave functions presented here allow the frequency-dependent modulation to be analyzed even for structures which are complex and have parabolic variations of potential in the depletion regions caused by static fields.

The transformation is a key to improved understanding of the dynamics of many physical phenomena. It provides a direct, simple, and intuitive approach to the study of systems in time-dependent fields without the limitations of perturbation theory. Multiquanta effects and scattering by realistic time-dependent potentials are two of the many areas where the basic concepts of this Letter are likely to be used in the solution of important problems.

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[1] Reported by K. Husimi, Prog. Theor. Phys. **9**, 381 (1953).

[2] P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford Univ. Press, Oxford, 1958), 4th ed.

[3] E. G. Gwinn, P. F. Hopkins, A. J. Rimberg, R. M. Westervelt, M. Sundaram, and A. C. Gossard, Phys. Rev. B **41**, 10700 (1990).

[4] M. Büttiker and R. Landauer, Phys. Rev. Lett. **49**, 1740 (1982).

[5] E. H. Hauge and J. A. Støvneng, Rev. Mod. Phys. **61**, 917 (1989).

[6] D. Sokolovski and J. N. L. Connor, Phys. Rev. A **42**, 6512 (1990).