AMERICAN JOURNAL of PHYSICS

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Citation: American Journal of Physics **42**, 304 (1974); doi: 10.1119/1.1987677
View online: http://dx.doi.org/10.1119/1.1987677
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/42/4?ver=pdfcov
Published by the American Association of Physics Teachers

Solution of the Schrödinger Equation for Some Electric Field Problems

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(Received 26 June 1973)

An alternate treatment of the Schrödinger equation for a charged particle in a uniform, constant electric field is given. The time-varying field is then treated. Next, using a Hamiltonian which gives the classical equations of motion for a particle in a viscous medium subject to a uniform constant, or time-varying field, the corresponding Schrödinger equation is solved. This procedure yields the classical electrical conductivity expressions for both dc and ac fields.

I. INTRODUCTION

While the solution of the Schrödinger equation for a particle in a uniform, constant electric field has long been known,[1] the solution for a uniform but time-varying field is less familiar. Further, while the problem of dissipation has normally been approached either *via* time-dependent perturbation theory or the *ad hoc* introduction of relaxation times, the exact solution of the Schrödinger equation for Hamiltonians which classically incorporate friction *ab initio* has only recently been studied.[2]

We first give an alternate treatment of the Schrödinger equation for a charged particle in a uniform, constant electric field; then the time-varying field is treated. Next, starting with a Hamiltonian which gives the classical equations of motion for a particle in a viscous medium subject to a uniform constant or arbitrarily time-varying field, we solve the corresponding Schrödinger equation and show that this procedure yields the classical electrical conductivity expressions for both dc and ac fields.

II. PARTICLE IN A UNIFORM CONSTANT FIELD

The equation of motion for a particle of mass m and charge q in an electromagnetic field is

$$m\dot{\mathbf{v}}=q[\mathbf{E}+(\mathbf{v}/c)\times\mathbf{B}],$$

for which the Hamiltonian is

$$H=\frac{(\mathbf{p}-q\mathbf{A}/c)^2}{2m}+q\Phi,$$

where

$$\mathbf{B}=\nabla\times\mathbf{A}\quad\text{and}\quad\mathbf{E}=-\nabla\Phi-(1/c)\partial\mathbf{A}/\partial t.$$

For the case of a constant electric field E_0 along the x-axis, the usual procedure is to choose

$$\Phi=-E_0x, \tag{1a}$$

$$\mathbf{A}=0. \tag{1b}$$

Then, considering the time-independent Schrödinger equation for the x motion

$$-(\hbar^2/2m)(d^2\psi/dx^2)-qE_0x\psi=\epsilon\psi, \tag{2}$$

the solutions are found to be

$$\psi=z^{1/2}J_{\pm1/3}(\tfrac{2}{3}z^{3/2}),$$

where

$$z=(2m/q^2\hbar^2E_0^2)^{1/3}(\epsilon+qE_0x),$$

and $J_{\pm1/3}$ are the Bessel functions of order $\pm\frac{1}{3}$. As in the case for the free particle, a continuous set of energy levels exists. If, however, there is at $x=0$ a perfectly reflecting plane [so that $\psi(x\leq 0)=0$], then the energy levels form a discrete set of bound states.

Let us now consider an alternate treatment of this problem. The aforementioned electric field may also be generated by setting[3]

$$\Phi=0, \quad (3a)$$

$$A_x=-E_0 ct, \quad (3b)$$

$$A_y=A_z=0, \quad (3c)$$

so that the Hamiltonian (for the x motion) becomes[4]

$$H=(p+qE_0 t)^2/2m. \quad (4)$$

The Schrödinger equation can then be written[5]

$$-(\hbar^2/2m)(\partial^2\psi/\partial x^2)-(i\hbar qE_0 t/m)(\partial\psi/\partial x) = i\hbar(\partial\psi/\partial t). \quad (5)$$

Making the transformation[6]

$$\xi=x-qE_0 t^2/2m, \quad (6a)$$

$$\tau=t, \quad (6b)$$

Eq. (5) becomes

$$-(\hbar^2/2m)(\partial^2\psi/\partial\xi^2)=i\hbar(\partial\psi/\partial\tau), \quad (7)$$

which is just the Schrödinger equation for a free particle. The solution ψ is thus

$$\psi=\exp(-i\hbar k^2\tau/2m)[A\exp(ik\xi)+B\exp(-ik\xi)] \quad (8)$$

or

$$\psi=\exp(-i\hbar k^2 t/2m)\{A\exp[ik(x-qE_0 t^2/2m)] + B\exp[-ik(x-qE_0 t^2/2m)]\}, \quad (9)$$

where k is a constant.

To avoid the difficulty of an infinite norm as well as to insure conservation of probability, the particle is enclosed in a box of edge-length L centered at the origin. Periodic boundary conditions are assumed, so that $k=2\pi n/L$, $n=0, 1, 2, \ldots$. By the usual procedure, the probability current density can be shown to be

$$Q=\mathrm{Re}\{\psi^*[(\hbar/im)\partial/\partial x+qE_0 t/m]\psi\}, \quad (10)$$

where

$$v=(\hbar/im)(\partial/\partial x)+(qE_0 t/m) \quad (11)$$

is identified as the velocity operator.

It is instructive to determine the development in time of the minimum wave packet[7]

$$\phi(x)=[2\pi(\Delta x)^2]^{-1/4}\exp\left[\frac{-x^2}{4(\Delta x)^2}+\frac{imv_0 x}{\hbar}\right], \quad (12)$$

where we have chosen $\langle x\rangle=0$ and $\langle p\rangle=mv_0$ at time $t=0$. Using the general form of the wave functions

$$\psi_k(x,t)=(1/L)^{1/2}\exp[\pm ik(x-qE_0 t^2/2m) - (i\hbar k^2 t/2m)]$$

and expanding Eq. (12) in terms of the $\psi_k(x,0)$, as they form a complete orthonormal set,

$$\phi(x,0)=\sum_k A_k\psi_k(x,0),$$

we can obtain the constant coefficients A_k. Then, in the usual way, we follow the development of Eq. (12) in time, writing

$$\phi(x,t)=\sum_k A_k\psi_k(x,t),$$

obtaining for the position probability density

$$|\phi(x,t)|^2=\left\{2\pi\left[(\Delta x)^2+\frac{\hbar^2t^2}{4m^2(\Delta x)^2}\right]\right\}^{-1/2} \times\exp\left\{\frac{-[x-(qE_0t^2/2m)-v_0t]^2}{2[(\Delta x)^2+\hbar^2t^2/4m^2(\Delta x)^2]}\right\}. \quad (13)$$

It is thus seen that the center of the packet moves like a classical charged particle in a uniform electrical field, with initial position $x=0$ and initial velocity v_0. The breadth of the packet spreads out just as in the free-particle case, a result of the free-particle form of the wave function.

III. PARTICLE IN A VISCOUS MEDIUM SUBJECT TO AN EXTERNAL FIELD

As was shown in the previous section, for a charged particle in a uniform electric field, the method employing the static scalar potential yields stationary states, while the method employing the vector potential leads to a nonstationary quantum dynamical treatment. Related to the latter result is the fact that fixed boundary conditions can be found which conserve probability flux, but not which make the wave function vanish at the boundaries.

Let us now apply this method to study the flow of electric current through a conductor under an applied electric field. We approximate the energy loss (resistance) experienced by the charges with linear damping and investigate the one-dimensional case. For the nth charge, the classical equation of motion is

$$m\ddot{x}+a\dot{x}=qE(t), \qquad (14)$$

where $E(t)$ is the applied electric field. It can easily be verified that a suitable single-particle Hamiltonian is

$$H=e^{-\gamma t}p^2/2m-e^{\gamma t}qE(t)x, \qquad (15)$$

or, of the form (4),

$$H=e^{-\gamma t}[p+q\int e^{\gamma t}E(t)dt]^2/2m, \qquad (16)$$

where $\gamma\equiv a/m$. Using the latter, the Schrödinger equation becomes[5]

$$-e^{-\gamma t}\left(\frac{\hbar^2}{2m}\right)\frac{\partial^2\psi}{\partial x^2}-\left(\frac{iq\hbar e^{-\gamma t}}{m}\right)\left[\int e^{\gamma t}E(t)dt\right]\frac{\partial\psi}{\partial x}=i\hbar\frac{\partial\psi}{\partial t}. \qquad (17)$$

Making the transformation

$$\xi=x-(q/m)\int^t e^{-\gamma\nu}\int^\nu e^{\gamma\lambda}E(\lambda)d\lambda d\nu, \quad \tau=t, \qquad (18)$$

Eq. (17) becomes

$$-e^{-\gamma\tau}(\hbar^2/2m)(\partial^2\psi/\partial\xi^2)=i\hbar(\partial\psi/\partial\tau), \qquad (19)$$

which is the Schrödinger equation for a particle in a viscous medium with the Hamiltonian

$$H=e^{-\gamma t}p^2/2m, \qquad (20)$$

and whose classical equation of motion is

$$m\ddot{\xi}+m\gamma\dot{\xi}=0.$$

In discussing the "quantization" of the above dissipative system, we must emphasize that it is really a semi-classical treatment, in that the particle is quantized but the system (conductor) with which the particle interacts is not. It is expected that Eq. (19) should be a good approximation for a charged particle of high energy moving in the "large system" (conductor) of much lower average (thermal) energy. Under these conditions, the charged particle slowly and almost continuously loses energy to the conductor, while other effects of the conductor on the particle can be ignored.

Proceeding to solve Eq. (19), the variables ξ and τ can be separated, and the wave function is found to be of the form

$$\psi_k(\xi,\tau)=\exp[\pm ik\xi+(i\hbar k^2e^{-\gamma\tau}/2m\gamma)], \qquad (21)$$

and in terms of variables x and t,

$$\psi_k(x,t)=A_\pm\exp\{\pm ik[x-(q/m)\int^t e^{-\gamma\nu}\int^\nu e^{\gamma\lambda}E(\lambda)d\lambda d\nu]+(i\hbar k^2e^{-\gamma t}/2m\gamma)\}. \qquad (22)$$

Again to conserve probability flux,[8] we employ box normalization with periodic boundary conditions, so that $k=2\pi n/L$, $n=0, 1, 2, \ldots$, insuring normalization of the wave function

$$\int_{-L/2}^{L/2}\psi^*\psi dx=1.$$

To determine the temporal development of the minimum wave packet (12), we use the general form of the wave function

$$\psi_k(\xi, t) = (1/L)^{1/2} \exp[ik\xi + (i\hbar k^2 e^{-\gamma t}/2m\gamma] \quad (23)$$

and follow the same procedure as was done previously. The resulting position probability density at time t is

$$| \phi(\xi, t) |^2 = \left\{ 2\pi \left[(\Delta\xi)^2 + \frac{\hbar^2(1-e^{-\gamma t})^2}{4m^2\gamma^2(\Delta\xi)^2} \right] \right\}^{-1/2}$$

$$\times \exp\left\{ \frac{-[\xi - v_0(1-e^{-\gamma t})/\gamma]^2}{2[(\Delta\xi)^2 + \hbar^2(1-e^{-\gamma t})^2/4m^2\gamma^2(\Delta\xi)^2]} \right\}. \quad (24)$$

Thus, the center of the packet moves like a classical particle in a viscous medium with initial position $\xi = 0$ and initial velocity v_0. The breadth of the packet also spreads out with the same time dependence as the classical particle. For $t \to \infty$, the center approaches v_0/γ (classical range), and the packet ceases to spread out, the width approaching

$$[(\Delta\xi)^2 + \hbar^2/4m^2\gamma^2(\Delta\xi)^2]^{1/2}. \quad (25)$$

As a specific example, let us assume that the applied electric field is an alternating one, so that

$$E(t) = E_0 \exp(i\omega t), \quad (26)$$

and proceed to calculate the dynamic value of electrical conductivity. From Eq. (26) and the Hamiltonian (16), the velocity operator is

$$\dot{x} = (e^{-\gamma t}p/m) + [e^{i\omega t}qE_0/m(\gamma + i\omega)], \quad (27)$$

so that if we set $A_+ = A_-$, the expectation value of $\dot{x}$ becomes

$$\langle \dot{x} \rangle = e^{i\omega t}qE_0/m(\gamma + i\omega) \quad (28)$$

as $\langle p \rangle$ vanishes. If there are N charges per unit volume, then the expectation value of the current density j is

$$\langle j \rangle = Nq\langle \dot{x} \rangle = e^{i\omega t}Nq^2E_0/m(\gamma + i\omega), \quad (29)$$

so that writing $\langle j \rangle = \sigma\langle E \rangle$ gives for the dynamic value of the conductivity

$$\sigma = Nq^2/m(\gamma + i\omega), \quad (30)$$

in agreement with the classical result (setting $\omega = 0$ yields the value for the dc field).

IV. CONCLUSIONS

For a charged particle in a uniform constant electric field, note the completely different structure between the stationary solution for the scalar potential $\Phi = -E_0 x$ and the conventional form of Schrödinger's equation, and the nonstationary solution (9) for the time-dependent vector potential (3) in the Hamiltonian (4). Further, the appropriate boundary conditions in the two cases are quite different; so that, although a gauge transformation in theory affects the solution only by a phase factor, in practice the two approaches are quite distinct.

We also note that the inclusion of linear damping in Schrödinger's equation *via* the Hamiltonians (15) and (16), although not well understood quantum-mechanically, leads without approximation to values of the conductivity which are correct in the classical regime.

APPENDIX A

In this Appendix, we show the connection between the two treatments of the uniform field problems given in Sec. II. For the Hamiltonian

$$H = \frac{(\mathbf{p} - q\mathbf{A}/c)^2}{2m} + q\Phi, \quad (A1)$$

let us perform the gauge transformations

$$\mathbf{A}' = \mathbf{A} + \nabla f,$$
$$\Phi' = \Phi - (1/c)(\partial f/\partial t) \quad (A2)$$

and consider the (primed) Hamiltonian

$$H' = \frac{(\mathbf{p} - q\mathbf{A}'/c)^2}{2m} + q\Phi'. \quad (A3)$$

It is known that if ψ is a solution to the Schrödinger equation

$$H\psi = i\hbar(\partial\psi/\partial t), \qquad \text{(A4)}$$

then

$$\psi' = \exp(iqf/\hbar c)\psi, \qquad \text{(A5)}$$

is a solution to the Schrödinger equation

$$H'\psi' = i\hbar(\partial\psi'/\partial). \qquad \text{(A6)}$$

Let us use this procedure to obtain an alternate solution of Eq. (2).

In this case, H is as given by Eq. (4), where

$$\Phi = 0,$$
$$A_x = -E_0 ct,$$
$$A_y = A_z = 0. \qquad \text{(A7)}$$

In order to obtain the Hamiltonian

$$H' = (p^2/2m) - qE_0 x, \qquad \text{(A8)}$$

where

$$\mathbf{A}' = 0, \qquad \Phi' = -E_0 x, \qquad \text{(A9)}$$

we must choose

$$f = E_0 ctx, \qquad \text{(A10)}$$

apart from an arbitrary constant. Thus, an alternate solution of Eq. (2) is

$$\psi' = \exp(iqE_0 tx/\hbar)\psi, \qquad \text{(A11)}$$

where

$$\psi = \exp\left[-\frac{i(\hbar^2 k^2 t + q^2 E_0{}^2 t^3/3)}{2m\hbar}\right] \times (A \exp ik\xi + B \exp - ik\xi), \qquad \text{(A12)}$$

and

$$\xi = x - qE_0 t^2/2m. \qquad \text{(A13)}$$

APPENDIX B

Let us present an alternate method of solving the Schrödinger equation for particles acted upon by a uniform (time-dependent) field, with and without linear damping.[9] As will be seen, the resulting solutions have an elegant form.

Consider the Schrödinger equation

$$-(\hbar^2/2m)(\partial^2\psi/\partial x^2) - f(t)x\psi = i\hbar(\partial\psi/\partial t). \qquad \text{(B1)}$$

The substitution

$$z = x - \xi(t) \qquad \text{(B2)}$$

yields

$$-(\hbar^2/2m)(\partial^2\psi/\partial z^2) - f(t)[z + \xi(t)]\psi + i\hbar\dot{\xi}(t)(\partial\psi/\partial z) = i\hbar(\partial\psi/\partial t). \qquad \text{(B3)}$$

Now, setting

$$\psi = \exp\{i[m\dot{\xi}z + \textstyle\int^t L(\tau)d\tau]/\hbar\}\phi \qquad \text{(B4)}$$

gives the result

$$-(\hbar^2/2m)(\partial^2\phi/\partial z^2) - [m\dot{\xi}^2/2 + f(t)\xi - L(t)]\phi + [m\ddot{\xi} - f(t)]z\phi = i\hbar(\partial\phi/\partial t), \qquad \text{(B5)}$$

so that if L is taken to be the Lagrangian that yields the equation of motion for the classical particle, i.e.,

$$L = (m\dot{\xi}^2/2) + f(t)\xi, \qquad \text{(B6)}$$

Eq. (B5) becomes

$$-(\hbar^2/2m)(\partial^2\phi/\partial z^2) = i\hbar(\partial\phi/\partial t). \qquad \text{(B7)}$$

If $f(t) = qE_0$ and only the particular solution for $m\ddot{\xi} = f(t)$ is adopted for ξ, it can be shown that the solution for ψ obtained from (B4) and (B7) is equivalent to that of (A12).

When there is linear damping, Eq. (B1) is modified to

$$-e^{-\gamma t}(\hbar^2/2m)(\partial^2\psi/\partial x^2) - e^{\gamma t}f(t)x\psi = i\hbar(\partial\psi/\partial t). \qquad \text{(B8)}$$

Making the substitutions

$$z = x - \xi(t),$$

$$\psi = \exp\{i[m\dot{\xi}ze^{\gamma t} + \int^t L(\tau)d\tau]/\hbar\}\phi \quad \text{(B9)}$$

yields

$$-e^{-\gamma t}(\hbar^2/2m)(\partial^2\phi/\partial z^2) = i\hbar(\partial\phi/\partial t), \quad \text{(B10)}$$

where

$$L = e^{\gamma t}[m\dot{\xi}^2/2 + f(t)\xi] \quad \text{(B11)}$$

and

$$m\ddot{\xi} + m\gamma\dot{\xi} = f(t), \quad \text{(B12)}$$

only the particular solution of (B12) being taken. It can be shown that the solution ψ obtained from Eqs. (B9)–(B12) is, within a time-dependent phase factor, just the solution (22). They are not identical because the purely time-dependent term of the Hamiltonian (16) was left out of the Schrödinger Eq. (17).

[1] L. Landau and E. Lifshitz, *Quantum Mechanics* (Addison–Wesley, Reading, MA, 1965), 2nd ed., p. 73.

[2] E. Kanai, Progr. Theor. Phys. **3,** 440 (1948); E. H. Kerner, Can. J. Phys. **36,** 371 (1958). L. H. Buch and H. H. Denman, to be published.

[3] That the potentials given by Eqs. (1) and (3) are related by a gauge transformation is shown in Appendix A.

[4] The y and z motions are separable and are trivially free-particle motions, not affected by the applied field.

[5] If the Hamiltonian H for a system is replaced by $H-f(t)$, the classical equations of motion are not affected. See Appendix B for a solution of the Schrödinger equation when the Hamiltonian (15) is used.

[6] Note that classically $\xi = x - qE_0t^2/2m$ is a solution to the free-particle equation of motion.

[7] L. I. Schiff, *Quantum Mechanics* (McGraw–Hill, NY, 1968), 3rd ed., pp. 63–64.

[8] We are treating a problem where energy is dissipated but probability is conserved. This situation differs from that for an optical potential, in which probability is lost.

[9] I. I. Goldman, *et al.*, *Problems in Quantum Mechanics* (Infosearch Ltd., London, 1960), p. 136. See also Ref. 2, E. H. Kerner.