Accelerating wave packet solution to Schrödinger's equation

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Most textbooks on quantum mechanics discuss a Gaussian wave packet, whose center is either stationary or moving at constant velocity.[1–3] Here, a *uniformly accelerating* wave packet is introduced. This solution to Schrödinger's equation for constant applied force, though not an energy eigenstate, is simpler than the standard non-wave-packet solution expressed in terms of Airy functions.[1] In the limit that the wave packet's initial width vanishes, it becomes a propagator,[1,2] permitting a general solution to be expressed in terms of initial conditions, $\psi(x,t)=\int\psi(x',0)K(x',x,t)dx'$. In contrast to Ehrenfest's theorem,[1–3] no *a priori* understanding of ''operator'' or ''expectation value'' is needed to establish a correspondence between Schrödinger's equation and a familiar kinematic equation of motion for uniform acceleration,

$$x(t)=x_0+v_0t+\tfrac{1}{2}at^2. \tag{1}$$

Start with Schrödinger's equation for a uniform force,

$$\frac{\hbar}{-i}\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-Fx\psi, \tag{2}$$

and with any solution, ψ_0, to Schrödinger's equation for the special case $F=0$. For example, the Gaussian wave packet,[1–3]

$$\psi_0(x,t)=\frac{[8b/\pi]^{1/4}}{\sqrt{4b+2i\hbar t/m}}\exp\left(-\frac{x^2}{4b+2i\hbar t/m}\right), \tag{3}$$

is well known. Without delving into the interpretation of ψ, one easily sees that (3) remains ''centered'' at $x=0$ for all time. One might expect that a uniform applied force, $F\neq0$, would permit a wave packet ''centered'' at a point which accelerates according to (1). Thus we attempt a solution of the form,

$$\psi(x,t)=\psi_0(x-x_0-v_0t-\tfrac{1}{2}at^2,t)e^{iS(x,t)}. \tag{4}$$

It is reasonable to assume that application of a uniform force is equivalent to making a (nonrelativistic) transformation into an accelerated reference frame. As $|\psi|^2$ represents a physical variable (density), which is invariant under this transformation, it follows that both stationary and accelerating observers should perceive the same value for $|\psi|^2$. Therefore, it is reasonable to conclude, without loss of generality, that $S(x,t)$ is a real valued function; this argument, however, does not play a direct role in the particular solution for S we obtain below. The calculation of $S(x,t)$ starts with the chain rule, used to write the partial derivatives in Schrödinger's equation (2) as:

$$\frac{\partial\psi}{\partial t}=\frac{\partial\psi_0}{\partial t}e^{iS}+(-v_0-at)\frac{\partial\psi_0}{\partial x}e^{iS}+i\frac{\partial S}{\partial t}\psi_0e^{iS},$$

$$\frac{\partial\psi}{\partial x}=\frac{\partial\psi_0}{\partial x}e^{iS}+i\frac{\partial S}{\partial x}\psi_0e^{iS}, \tag{5}$$

$$\frac{\partial^2\psi}{\partial x^2}=\frac{\partial^2\psi_0}{\partial x^2}e^{iS}+2i\frac{\partial S}{\partial x}\frac{\partial\psi_0}{\partial x}e^{iS}+i\frac{\partial^2S}{\partial x^2}\psi_0e^{iS}-\psi_0\left(\frac{\partial S}{\partial x}\right)^2e^{iS}.$$

After substituting (5) into (2), two terms cancel due to the fact that ψ_0 obeys the free-particle ($F=0$) Schrödinger equation. The terms that remain can be arranged as:

$$\left\{\frac{\hbar(v_0+at)}{i}+i\frac{\hbar^2}{m}\frac{\partial S}{\partial x}\right\}\frac{\partial\psi_0}{\partial x}+\left\{-\hbar\frac{\partial S}{\partial t}+i\frac{\hbar^2}{2m}\frac{\partial^2S}{\partial x^2}-\frac{\hbar^2}{2m}\left(\frac{\partial S}{\partial x}\right)^2+Fx\right\}\psi_0=0. \tag{6}$$

Equating to zero both the term in (6) proportional to ψ_0, as well as the term proportional to $\partial\psi_0/\partial x$, is a sufficient though not necessary condition for obtaining a particular solution S. Upon imposing these conditions we obtain:

$$\frac{\hbar}{m}\frac{\partial S}{\partial x}=v_0+at, \tag{7a}$$

$$\frac{\hbar}{m}\frac{\partial S}{\partial t}=ax-\frac{1}{2}(v_0+at)^2+\frac{i\hbar^2}{2m^2}\frac{\partial^2S}{\partial x^2}. \tag{7b}$$

From (7a), we see that this condition causes $\partial^2S/\partial x^2$ to vanish. Both partial derivatives in (7) can be integrated, each with arbitrary constants which are functions of the other variable:

$$\frac{\hbar}{m}S(x,t)=v_0x+axt-\frac{1}{2}av_0t^2-\frac{1}{6}a^2t^3-\frac{1}{2}v_0^2t+\text{constant}. \tag{8}$$

Equations (3), (4), and (8) combine to form an accelerating Gaussian wave packet, subject to a uniform force. As the derivation of (7) did not make explicit use of the Gaussian wave packet (3), we actually have a class of solutions to Schrödinger's equation which can be generated from any solution ψ_0 of the free-particle ($F=0$) Schrödinger equation.

A propagator, $K(x,x',t)$, is a solution to Schrödinger's equation, subject to any imposed boundary conditions, where the variables are taken as x and t. Also, at $t=0$, the propagator must collapse to a Dirac delta function centered at x', so that $K(x,x',0)=\delta(x-x')$. In order to construct a propagator for a uniform applied force, multiply the free-particle

stationary Gaussian wave packet (3) by a constant, to obtain a differently normalized stationary Gaussian wave packet, $\phi_0(x,t)=(8\pi b)^{-1/4}\psi_0(x,t)$. At $t=0$, it is easily verified that $\phi_0(x,0)$ is real, and that $\int\phi_0(x,0)dx=1$. Next, allow the initial width, b, to vanish. This establishes $\phi_0(x,0)=\delta(x)$. Use the procedure indicated by (4) and (8), with $x_0=x'$ and $v_0=0$, and let the $\phi(x,t)$ be the solution, generated for $F\neq 0$. From (8), we see that $S=0$ at $t=0$, which implies $\phi(x,0)=\phi_0(x-x',0)=\delta(x-x')$. Thus, $\phi(x,t)=K(x,x',t)$ satisfies the necessary conditions for being a propagator, and a general solution can be written as $\psi(x,t)=\int K(x,x',t)\psi(x,0)dx$.

As another aside, a referee pointed out a connection to Hamilton's principal function.[4] Start with (7), and combine $v=v_0+at$ with $dS/dt=\partial S/\partial t+v\,\partial S/\partial x$, to show that $dS/dt=\hbar L$, where $L=T-U$ (kinetic minus potential energy) is the Lagrangian. Thus, Hamilton's principal function is $\hbar S(x,t)$. Also, one can recover both de Broglie relations, $E=\hbar\omega$ and $p=\hbar k$, by equating ω to $-\partial S/\partial t$ and k to $\partial S/\partial x$, and evaluating these derivatives at $x=x_0+v_0t+\frac{1}{2}at^2$.

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Field pattern of a magnetic dipole

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A calculation is presented which gives the field pattern due to a dipole field. The approach should be within the reach of an undergraduate student.

The magnetic field due to a dipole is well known[1] and given in a coordinate free form as[2]

$$\mathbf{B}=\frac{\mu_0}{4\pi}\frac{1}{r^3}[3(\mathbf{m}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}-\mathbf{m}]+\frac{2}{3}\mu_0\mathbf{m}\delta(\mathbf{r}). \tag{1}$$

Here, $\mathbf{m}$ is the magnetic dipole moment and $\mathbf{r}$ is the vector from the source to the field point.

Often depicted with this result is an accompanying figure, which indicates the pattern of the field. However, it seems never to be explained in any detail how this field pattern is derived.

It is the object of this note to show that it is quite straightforward to derive the lines of force (or characteristic curves or streamlines). This derivation is one that an undergraduate student should be able to follow.

We begin by first dropping the delta function term in (1) since we will be deriving the field lines for nonzero r. We next simplify matters by taking the dipole moment, $\mathbf{m}$, to lie along the y direction, i.e., $\mathbf{m}=m\mathbf{j}$. This involves no loss of generality since if the dipole moment points in some other direction, an adroit change of coordinate system can always be made so that our assumption is valid.

Because of azimuthal symmetry we can also restrict our discussion to the case $z=0$. Once we have determined the field pattern in the xy plane, then rotation about the y axis gives the field everywhere.

With these simplifying assumptions we find that the x and y values of the magnetic field $\mathbf{B}$ are given, respectively, by

$$B_x=\frac{\mu_0}{4\pi}\frac{1}{r^3}\left(3m\frac{xy}{r^2}\right) \tag{2}$$

and

$$B_y=\frac{\mu_0}{4\pi}\frac{1}{r^3}\left(3m\frac{y^2}{r^2}-m\right), \tag{3}$$

where $r=\sqrt{x^2+y^2}$.

According to Davis and Snider,[3] the field lines are determined from the equation

$$\frac{dx}{B_x}=\frac{dy}{B_y}. \tag{4}$$

Substituting from (2) and (3) into (4), cancelling out like terms on each side leads to

$$\frac{dx}{3xy}=\frac{dy}{3y^2-r^2}=\frac{dy}{2y^2-x^2}. \tag{5}$$

From (5) we obtain the equation of the field lines as

$$\frac{dy}{dx}=\frac{2y^2-x^2}{3xy}. \tag{6}$$

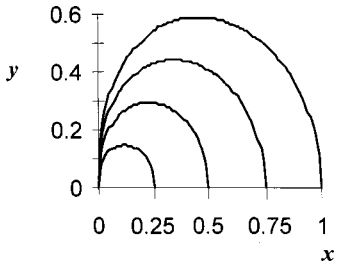

Fig. 1. The field lines for the magnetic dipole.

To solve this we introduce the variables $Y=y^2$ and $X=\ln x$, so that we can rewrite (6) as

$$\frac{dY}{dX}=\frac{4}{3}Y-\frac{2}{3}e^{2X}. \tag{7}$$

This first-order differential equation is straightforward to solve if we introduce the integrating factor[4] $e^{-4X/3}$ and write (7) as

$$\frac{d}{dX}(Ye^{-4X/3})=-\frac{2}{3}e^{2X}e^{-4X/3}=-\frac{2}{3}e^{2X/3}. \tag{8}$$

From this we easily obtain

$$Y=Ce^{4X/3}-e^{2X}, \tag{9}$$

where C is an arbitrary constant. Finally, we can write the solution in terms of the original variables x and y,

$$x^2+y^2=Cx^{4/3}. \tag{10}$$

Equation (10) is the desired result, i.e., the form of field pattern for the dipole field.

We now give a brief discussion of the significance of the constant C. If we write C in the form $C=D^{2/3}$ then D has the dimensions of length and (10) can be written as

$$\left(\frac{x}{D}\right)^2+\left(\frac{y}{D}\right)^2=\left(\frac{x}{D}\right)^{4/3}. \tag{11}$$

We note that the field line describes a curve from the origin which extends as far as the distance D, so that D clearly sets the length scale.

Shown in Fig. 1 is the result of plotting Eq. (11) for the cases $D=0.25$, 0.5, 0.75 and 1.0, with $0<x\leqslant D$ and $y>0$.

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[1]The references on this subject are extensive, see for example, D. J. Griffiths, *Introduction to Electrodynamics* (Prentice–Hall, New York, 1989), 2nd ed., pp. 235–239; J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975), 2nd ed., pp. 180–184; P. Lorrain, D. R. Corson, and F. Lorrain, *Electromagnetic Fields and Waves* (Freeman, New York, 1988), 3rd ed., pp. 337–340; J. Vanderlinde, *Classical Electromagnetic Theory* (Wiley, New York, 1993), Sec. 2.1, p. 37.

[2]D. J. Griffiths, *Introduction to Electrodynamics* (Prentice–Hall, New York, 1989), 2nd ed., pp. 248–249.

[3]H. F. Davis and A. D. Snider, *Introduction to Vector Analysis* (Allyn and Bacon, Boston, 1987), 5th ed., pp. 110–113.

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Erratum: "Ideal capacitor circuits and energy conservation" [Am. J. Phys. 67 (8), 737–739 (1999)]

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The expression below Eq. (11) for the electric current should be $\omega CV_0\sqrt{q_0(2-q_0/CV_0)/CV_0}$. Equation (12) should be replaced by $E_L=L_Ci_0^2/2=q_0V_0-q_0^2/2C$. The energy conservation, however, holds valid. The sum of the energies stored in the capacitor and the inductor is equal to q_0V_0, which is the energy supplied by the battery.

CHEMISTS AND MOLECULES

It is not chemists who make molecules react. That is done by the molecules. The chemists only set the conditions, and then watch.

George Wald, in the Introduction to Lawrence J. Henderson, *The Fitness of the Environment* (Macmillan, New York, 1913, reprinted 1958), p. xxiv.