Semiclassical and quantum analysis of a free-particle Hermite wave function

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In this Brief Report we discuss a solution of the free-particle Schrödinger equation in which the time and space dependence are not separable. The wave function is written as a product of exponential terms, Hermite polynomials, and a phase. The peaks in the wave function decelerate and then accelerate around $t = 0$. We analyze this behavior within both a quantum and a semiclassical regime. We show that the acceleration does not represent true acceleration of the particle but can be related to the envelope function of the allowed classical paths. Comparison with other "accelerating" wave functions is also made. The analysis provides considerable insight into the meaning of the quantum wave function.

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I. INTRODUCTION

The Schrödinger equation is at the center of nonrelativistic quantum theory. The usual method of solution is to separate the time and space dependence of the wave function and solve the time independent Schrödinger equation [1]. This can be done analytically for a few simple model potentials and otherwise it is straightforwardly amenable to numerical solution. This approach has had huge success in describing a vast array of physical phenomena, in particular the electronic and structural properties of atoms, molecules, and solids. The Schrödinger equation has also been shown to have more exotic solutions such as accelerating Airy wave functions [2,3]. The wave function introduced by Berry and Balazs [2] also has the remarkable property that it does not broaden with time. However, it does not represent a single particle because it is not square integrable and thus is not an element of a Hilbert space; therefore there is no contradiction with Ehrenfest's theorem. Later, Lekner [3] derived a more general form of the Airy wave function which is both well behaved and square integrable. Both the expectation values of position and momentum show no acceleration, except in the Berry-Balazs limit where the wave function is not square integrable. In a subsequent paper Nguyen and Lekner [4] were able to derive wave functions that describe true acceleration via an extended Galilean transformation of a free-particle wave function, where the extended Galilean transformation also introduces a potential into the Hamiltonian which drives the acceleration. In this Brief Report we derive, describe, and try to gain insight into an exotic, apparently accelerating solution of the free-particle Schrödinger equation that is square integrable and which also displays some unusual characteristics. In Sec. II we write down and describe the solution. In Sec. III A we perform a quantum-mechanical analysis of the wave function and show that the probability density accelerates. Accelerating probability densities for free particles is an apparent contradiction. However, they have been found to be explicable on the basis of classical mechanics [2]. Therefore in Sec. III B we have performed a parallel classical analysis to show how the accelerating probability density can be understood and how the semiclassical and quantum descriptions are related. In Sec. IV we compare the properties of our Hermite wave function with those of a Gaussian and the the Airy wave function of Lekner [3]. In conclusion we discuss the considerable insight this calculation yields into the meaning of the quantum-mechanical wave function.

II. THEORY

The time dependent free-particle Schrödinger equation in $1 + 1$ dimensions is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}. \quad (1)$$

Using a symmetry analysis and separation of the variables [5,6] it is possible to find a solution of Eq. (1) as

$$\psi(x,t) = \sqrt{\frac{1}{n!}}\left(\frac{m}{\hbar t_c \pi}\right)^{1/4}\frac{2^{-n/2}}{\left(1+t^2/t_c^2\right)^{1/4}} \times e^{imx^2t/2\hbar(t_c^2+t^2)}e^{-i(n+1/2)\arctan(t/t_c)} \times e^{-mt_cx^2/2\hbar(t_c^2+t^2)}H_n\left(\left(\frac{mt_c}{\hbar(t_c^2+t^2)}\right)^{1/2}x\right). \quad (2)$$

Wave functions similar to this have been obtained previously [7] although not in precisely this form to our knowledge. Here t_c is an arbitrary positive constant with the dimensions of time. $H_n(y)$ are the Hermite polynomials [8]. Square integrability requires that n be an integer. This wave function has been normalized between $\pm\infty$ and the normalization is constant with respect to time, as it must be. Equation (2) reduces to a Gaussian wave packet centered on the origin when $n = 0$. This expression may be checked by direct substitution. Henceforth we will retain constants in equations, but all figures will be calculated in atomic units (a.u.) with $\hbar = 1$ and $m = 1/2$.

Equation (2) has one remarkable property. If we look at its form at $t = 0$ and define the frequency $\omega = 1/t_c$ it becomes

$$\psi(x,t) = \sqrt{\frac{1}{2^n n!}}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}e^{-m\omega x^2/2\hbar}H_n\left(\left(\frac{m\omega}{\hbar}\right)^{1/2}x\right). \quad (3)$$

Surprisingly, this is exactly the form of the eigenfunctions of the harmonic oscillator. Of course this is only true at $t = 0$ because our wave function evolves according to the free-particle Schrödinger equation, not the one describing the harmonic oscillator.

This identification helps us because we already know that for the quantum harmonic oscillator the kinetic-energy and potential-energy operators provide an equal contribution to the total energy of the oscillator. Our Hamiltonian only contains the kinetic-energy operator, so at $t = 0$ and hence at all times

$$E_n = \frac{1}{2}(n + 1/2)\hbar\omega = \frac{1}{2}(n + 1/2)\frac{\hbar}{t_c} = \frac{1}{2m}\langle \hat{p}^2\rangle, \quad (4)$$

where the last equality has been confirmed computationally.

Of course, it would always be possible to use Eq. (3) as an initial state of our system and then to integrate the Schrödinger equation directly, or to expand it in terms of some basis functions such as plane waves with time dependent coefficients and integrate that. However, such a procedure is essentially numerical and would in general require large numbers of basis functions, making it rather opaque and unwieldy.

III. RESULTS

A. Quantum-mechanical results and analysis

In Fig. 1 we show a contour plot of the probability density associated with this wave function as a function of time for $n = 2$ and $t_c = 1$. The principal effect of t_c is to set the time scale. The wave function itself is strongly oscillatory but the oscillatory nature cancels in the probability density to produce three peaks. At all times the probability density is symmetric about $x = 0$. For $t \ll 0$ the probability density consists of a pair of broad peaks on either side of $x = 0$ moving toward $x = 0$ at approximately constant velocity and a central peak which has its maximum at $x = 0$ at all times. As the two outer peaks get close together their contour lines, shown in Fig. 1, describe a curve indicating that the peaks are decelerating and narrowing, and at $t = 0$ they form two well-localized peaks close to the origin. For $t > 0$ this behavior is reversed with the outer peaks accelerating away from each other and broadening, and as t continues to increase the peaks move asymptotically to a constant velocity. The peak at the origin simply broadens as time increases in either the negative or positive direction from zero.

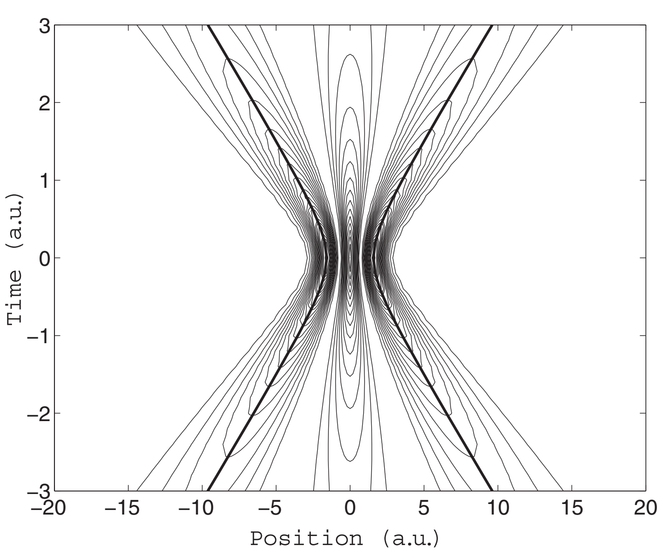

FIG. 1. Contour map of the density associated with the wave function of Eq. (2) as a function of time and space. This was evaluated for $t_c = 1$ a.u. with $n = 2$. Superimposed on this are the hyperbolas given by Eq. (6).

Clearly the path of the outer peaks is hyperbolic, and we can find the equation for this path. We can find the maximum of the probability density by differentiating it with respect to x. This leads to

$$2nH_{n-1}\left(\left(\frac{mt_c}{\hbar(t_c^2+t^2)}\right)^{1/2}x\right) = \left(\frac{mt_c}{\hbar(t_c^2+t^2)}\right)^{1/2} xH_n\left(\left(\frac{mt_c}{\hbar(t_c^2+t^2)}\right)^{1/2}x\right) \quad (5)$$

as the condition for a wave-function peak. We can insert the explicit expressions for the Hermite polynomials here to find the condition for any given n. For $n = 2$ we find

$$x = \pm\sqrt{\frac{5\hbar}{2mt_c}}\left(t_c^2+t^2\right)^{1/2}. \quad (6)$$

These two hyperbolas are shown superimposed on the density in Fig. 1. Clearly they represent the motion of the wave-function peaks as a function of time.

B. Semiclassical analysis

Accelerating wave functions have been observed previously [2]. In that case the acceleration of the wave function was shown to have a classical origin. In this Brief Report we simply perform a similar analysis on the wave function Eq. (2) and obtain an analogous result. The key insight found originally and here is that the wave function should really be regarded as representing families of particle paths rather than an individual classical particle. The present wave function can be regarded as the simplest possible case of this because the initial phase-space orbits are simply circular. We will show what we mean by this explicitly as we proceed.

We will analyze the classical motion using Hamilton's equations. To do this we need an initial position and momentum for the particle. This can be provided by the analogy with the harmonic oscillator at $t = 0$. The harmonic oscillator has a Hamiltonian:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 = E. \quad (7)$$

At $t = 0$ we can write the energy of our system in the same way. Writing this down with zero subscripts to indicate that the quantity is valid at $t = 0$ only and dividing through by E gives

$$\frac{p_0^2}{\sqrt{2mE_n}} + \frac{m\omega^2}{2E_n}x_0^2 = 1. \quad (8)$$

This allows a simple parametrization of the position and momentum at $t = 0$:

$$p_0(\theta) = \sqrt{2mE}\sin\theta, \quad x_0(\theta) = \sqrt{\frac{2E_n}{m\omega^2}}\cos\theta. \quad (9)$$

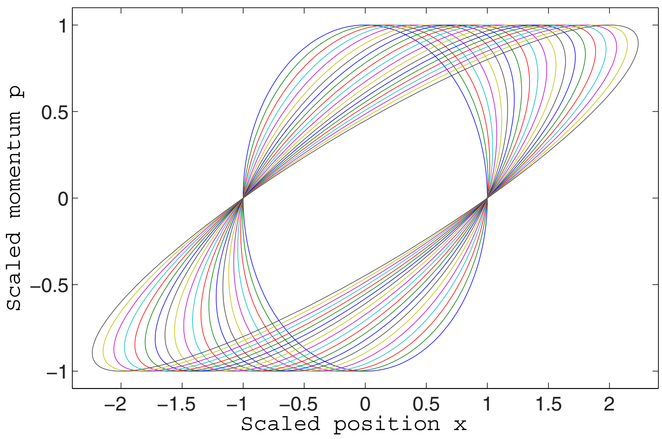

FIG. 2. (Color online) Phase-space curves (p vs x for the family of paths described by Eqs. (9) and (10). At $t = 0$ this is a circle in phase space which shears into an ellipse as time proceeds.

Every different value of θ in these equations represents the initial conditions for one member of the family of paths. With these initial conditions we can solve Hamilton's equations for a free particle to give

$$\begin{aligned} p &= p_0(\theta) = \text{const}, \\ x &= x_0(\theta) + pt/m = x_0(\theta) + p_0(\theta)t/m. \end{aligned} \tag{10}$$

These equations all represent paths that are straight lines representing uniform motion. As time passes, x increases linearly and p remains constant. The phase-space curve associated with $p_0(\theta)$ and $x_0(\theta)$ is a circle [9], but as time passes it shears into an ellipse. This is shown in Fig. 2 for times $0 \leqslant t < 2$ a.u. Next we plot the possible particle paths described by Eq. (10) with initial conditions Eq. (9). This is shown in Fig. 3. These paths form a characteristic shape as shown. The edges of this shape form a hyperbolic caustic or envelope function in space-time. An equation for the caustic can be found using standard methods [10]; i.e., we have to

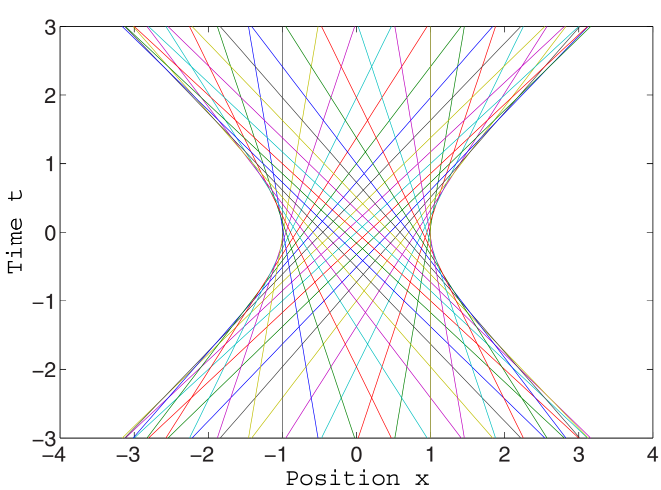

FIG. 3. (Color online) The family of allowed classical paths for the system described by Eq. (10). All quantities are in atomic units.

satisfy

$$x(t) = x(t,\theta), \quad \frac{\partial x(t,\theta)}{\partial \theta} = 0. \tag{11}$$

This is easily done using Eqs. (9) and (10) and results in

$$x(t) = \pm\sqrt{\frac{2E_n}{m}}\left(t_c^2 + t^2\right)^{1/2}. \tag{12}$$

For $n = 2$ this comes out as

$$x(t) = \pm\sqrt{\frac{5\hbar}{2mt_c}}\left(t_c^2 + t^2\right)^{1/2}, \tag{13}$$

which is identical to Eq. (6). Clearly the peak in the space-time representation of the wave function in Fig. 1 corresponds exactly to the caustic enveloping the classically allowed paths.

IV. EXPECTATION AND UNCERTAINTY

Lekner has derived the normalizable Airy wave function [3]:

$$\begin{aligned} \psi(x,t) = {} & \mathrm{Ai}\left[q\left(x - ut + ivt - \tfrac{1}{2}at^2\right)\right]e^{ima(x-ut-at^2/3)t/\hbar} \\ & \times e^{mv(x-ut+ivt/2-at^2)/\hbar}e^{imu(x-ut/2)/\hbar}. \end{aligned} \tag{14}$$

Here u and v are velocities that are real, v is positive, and a is an acceleration. We will consider this wave function in its rest frame ($u = 0$) and compare it with the one derived in this Brief Report. Although checked by us, all results for this wave function quoted here were originally published by Lekner and are reproduced here for comparative purposes only. It is instructive to compare the expectation values of position and momentum for the various wave functions. This is done in Table I. To make the comparison with the Airy wave function as meaningful as possible we have identified $t_c = v/a$. The uncertainties have the usual definitions:

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2, \quad (\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2. \tag{15}$$

For the Airy wave function,

$$(\Delta x)^2 = \frac{1}{8}\left(\frac{\hbar}{mv}\right)^2 + \frac{\hbar}{2m}(t_c + t^2/t_c). \tag{16}$$

TABLE I. Comparison of the expectation values of the Airy, Gaussian, and Hermite ($n = 1$ and 2) wave functions and evaluation of the uncertainty principle. $\langle x^2\rangle$ has not been included for the Airy wave function because the expression is too long. However, it can easily be found from $\langle x\rangle$ and the uncertainty in Eq. (16).

$\psi(x,t)$	$\langle x\rangle$	$\langle x^2\rangle$	$\langle p\rangle$	$\langle p^2\rangle$	$(\Delta x\Delta p)^2$
Airy	$\frac{v^2}{2a} - \frac{\hbar}{4mv}$		0	$\frac{\hbar m}{2t_c}$	$\frac{\hbar^2}{4}(1 + \frac{\hbar}{mv^2t_c} + t^2/t_c^2)$
Gaussian ($n = 0$)	0	$\frac{\hbar}{2m}(t_c + t^2/t_c)$	0	$\frac{\hbar m}{2t_c}$	$\frac{\hbar^2}{4}(1 + t^2/t_c^2)$
Hermite ($n = 1$)	0	$\frac{3\hbar}{2m}(t_c + t^2/t_c)$	0	$\frac{3\hbar m}{2t_c}$	$\frac{9\hbar^2}{4}(1 + t^2/t_c^2)$
Hermite ($n = 2$)	0	$\frac{5\hbar}{2m}(t_c + t^2/t_c)$	0	$\frac{5\hbar m}{2t_c}$	$\frac{25\hbar^2}{4}(1 + t^2/t_c^2)$

It is easy to show from the table that the uncertainty in position for all the wave functions is in accord with the general result [11]

$$(\Delta x)^2 = (\Delta x)^2_{t=0} + \left(\frac{\Delta p}{m}\right)^2 t^2. \quad (17)$$

Surprisingly the Airy wave function has an identical uncertainty in momentum as the Gaussian wave function. The uncertainties in position look very different partially because the Airy wave function is not centered on $x = 0$, and whether the Airy wave function is broader or narrower than the Gaussian wave function depends on the size of v when $t_0 = v/a$ is kept constant.

V. CONCLUSIONS

As an exact solution of one of the fundamental equations of physics, the free-particle Schrödinger equation, the wave function of Eq. (2) is of great interest from a mathematical perspective. Furthermore the fact that it exhibits some unusual properties such as the apparent acceleration of the probability densities while remaining normalizable means that it provides profound insight into the meaning of the single-particle wave function. However, practical applications of this work are not immediately clear. We note however that the Schrödinger equation has an identical mathematical form to the paraxial wave equation, and so such solutions have been employed as the basis of solutions of Maxwell's equations to describe electromagnetic radiation that can change direction as it propagates through interference effects [12–14]. We hope this work will provoke similar experiments. In fact, if light is set up with the profile shown at negative times in Fig. 1 it will focus down to the profile shown at $t = 0$ in that figure, a property that may well have significant applications.

The wave function described here illustrates a number of quantum phenomena very clearly. At the undergraduate level wave functions are normally interpreted in terms of time independent probability densities. Along with the Airy wave packets derived by Berry and Balazs [2] and Lekner [3] the present wave function provides a very different perspective where the wave function is a description of the family of allowed paths of the particle it describes. The Berry-Balazs wave function has a second remarkable property that it does not spread out with time. However, it has the drawbacks that it is not square integrable, is infinite in extent, and as a result of this has undefined energy. Along with the Lekner wave function the current wave function does broaden with increasing (and decreasing) time, but is square integrable and has a well-defined energy, thus making it easier to think about and more straightforward for interpretation purposes. This analysis also illustrates the fact that accelerating wave functions do not necessarily correspond to accelerating particles as many might think. Indeed, the expectation values of momentum and energy are constant with respect to time. This wave function does have the unusual property that it consists of more than one peak that separate as time proceeds, despite the fact that it represents a single particle. However, this can be understood if we think about the wave function in the semiclassical way discussed here. Moreover, the analysis introduces caustics into quantum theory in an interesting and mathematically simple way.

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