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Action-dependent wave functions: Definition

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This paper contains the formalism for a new object: an ''action-dependent wave function.'' The peaks and valleys of this function move through space as the action is varied. For some simple action-dependent wave packets, this motion mimics the trajectories of a classical particle. Unlike time-dependent wave packets, the action-dependent wave packets do not disperse when the classical motion is separable. I will present the results for three simple cases. For one-dimensional systems and separable multidimensional systems, a large number of states can be superposed to give a sharply peaked function, which exactly tracks the classical motion.

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I. INTRODUCTION

Time-dependent wave functions evolve in time so that peaks and valleys of the function move through space. This movement is reminiscent of classical motion for some simple types of time-dependent wave functions. Dispersion of the wave packets is almost always present because a packet is composed of several eigenstates and the energy spacing between successive eigenstates is usually energy dependent. The classical distribution in phase space also disperses because the ''periods'' of motion depend on the energy. Unfortunately, the quantum dispersion can greatly hinder the simple interpretation of the wave packets since the interference between initially separated parts of the packet can be the source of complicated features.

In this paper, I present one possible definition for a theoretical object, which I call an ''*action*-dependent wave function.'' This function has many points of similarity with the more usual *time*-dependent wave functions. The time-dependent wave function is the solution of a linear, partial differential equation (Schrödinger's equation) [1] that governs the dependence of the function of space coordinates on the scalar parameter t (time). The action-dependent wave function is the solution of a linear, partial differential equation that governs the dependence of the function of space coordinates on the scalar parameter $\tilde{S}$ (action). Unlike the time-dependent wave function, the action-dependent wave function does not disperse for the cases examined to date. This is because the action-dependent wave packets evolve in action like a classical distribution of particles-all with *the same energy*.

The action-dependent wave packet appears to be an artificial construct to a large extent. There does not appear to be a simple method to transform an action-dependent to a time-dependent wave function. Despite the artificiality, one aspect of action-dependent wave functions has been observed-the action dependence of an autocorrelation function. Also, the Fourier transform of the action-dependent wave function with respect to action gives the correct quantum eigenstates of the Hamiltonian.

Perhaps, the main usefulness of these functions will arise from the aid in interpreting quantum phenomena. Perhaps, also, the properties of a new wave equation that generates classical-like motion will be interesting in itself. Finally, it is possible that the wave equation will be the source of new approximations for handling complicated quantum systems. It is these possibilities that have led to the initial studies presented in this paper. I have used the action-dependent wave function to study a few simple systems; these results are presented in this paper. Atomic units will be used unless explicitly specified otherwise.

II. TIME-DEPENDENT RECURRENCE

Before describing the action-dependent wave functions, it is instructive to first present some features of time-dependent wave functions. As a specific example, I will focus on the time-dependent recurrence of a wave packet that is defined as $R(t)=\langle\Psi(0)|\Psi(t)\rangle$. The time-dependent recurrence of a wave function can be directly measured in a Ramsey-type procedure [2] or can be obtained from the Fourier transform of the photoabsorption spectrum. For bound states, this can be shown in a few steps.

The dependence of the photon absorption spectrum as a function of the final energy E, can be written as a sum of delta functions

$$\rho(E)=\sum_n |D_n|^2\delta(E-E_n), \tag{1}$$

where E_n is an eigenenergy of the Hamiltonian, $H|\psi_n\rangle=|\psi_n\rangle E_n$, and the strength of each term is given by the squared magnitude of the dipole matrix element $D_n=\langle\psi_n|D|\psi_i\rangle$ between the nth final state and the initial state $|\psi_i\rangle$.

The Fourier transform of the absorption spectrum is interesting if it is multiplied by a window function $W^2(E)$. Generically, the window function is smooth and is sizeable only over a relatively small range of energy. Two possible examples of W are $W(E)=\exp[-(E-E_{\rm av})^2/\Delta E^2]$ or $W(E)=\exp[-(E-E_{\rm av})^4/\Delta E^4]$. The window function is used to pick out a small range of energy so the types of motion and periods of the system do not wildly change over the window. It can be shown that if the time-dependent wave function is given by

$$\Psi(\mathbf{r},t)=\sum_n \psi_n(\mathbf{r})D_nW(E_n)\exp(-iE_nt) \tag{2}$$

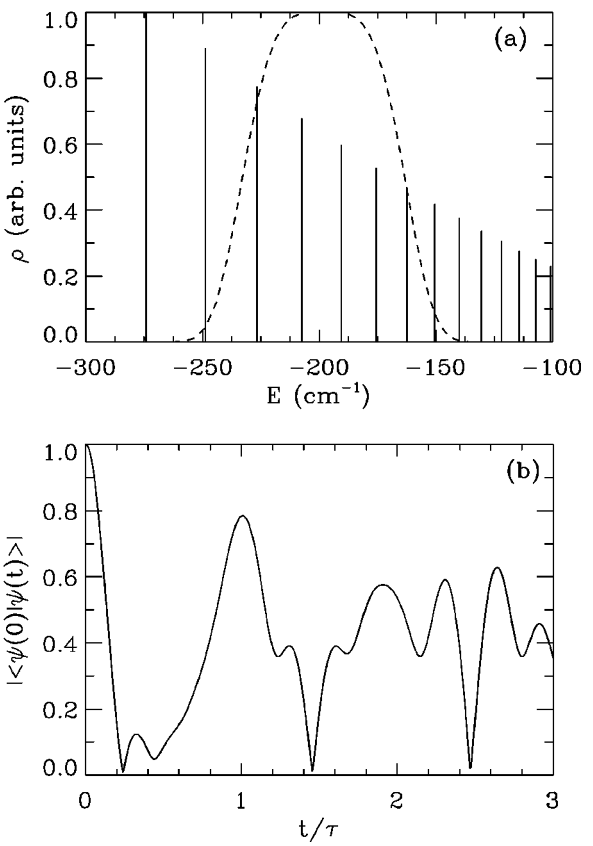

FIG. 1. (a) Solid line—the absorption of light by an H atom in its ground state as a function of the final energy. Dashed line—weight function used to emphasize a small energy region of energy. (b) The absolute value of the recurrence function using the absorption and window function of (a). The time is given in units of the classical period τ, at the central energy of the window function.

then the time-dependent recurrence is given by

$$R(t)=\langle\Psi(0)|\Psi(t)\rangle=\int dE W^2(E)\rho(E)e^{-iEt}. \tag{3}$$

To show this result, the orthonormality properties of the energy eigenstates $\langle\psi_{n'}|\psi_n\rangle=\delta_{n'n}$ have been used. From the properties of the eigenstates, one can also show that $\Psi(\mathbf{r},t)$ is a solution of the time-dependent Schrödinger equation.

In Fig. 1, I show a typical and moderately simple case for a one-dimensional system. The solid line in Fig. 1(a) gives the absorption spectrum for H excited from the 1s ground state using 1 photon; the states shown are $n=20-32$. The dashed line in Fig. 1(a) is a window function that was used to make a time-dependent recurrence. The absolute value of the recurrence is shown in Fig. 1(b), where the time is plotted in units of the classical period at the central energy. In Fig. 2, I have plotted the radial density at a few specific times. There are some features that can be interpreted easily. For example, the rapid drop of the recurrence at short time is due to the electron moving away from small r to the outer turning point. The wave packet first reaches the outer turning point at time equal to 1/2 the classical period. The electron returns to small r after one classical period at which point there is a peak in the recurrence. The longer time behavior of this packet is hard to interpret due to the large amount of dispersion for the parameters that were chosen. As an example, after three periods the radial distribution is mostly at the outer turning point instead of at small r.

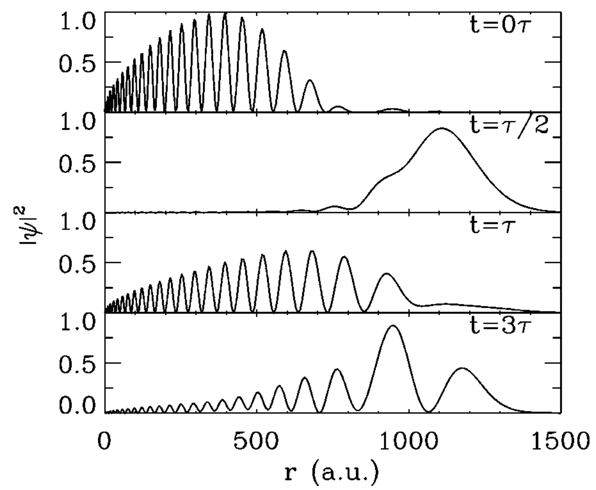

FIG. 2. The time-dependent radial probability corresponding to the conditions of Fig. 1. τ is the classical period of an electron at the central energy of Fig. 1. Note that over the first period the probability moves like a classical electron but that dispersion gives most of the probability at $t=3\tau$ at the outer turning point instead of the inner turning point.

There is an interesting point of physics to which I will return in a later section. Notice that the wave packet at $t=0$ extends over a much larger range of r than that for the initial 1s state. The 1s state covers a range of only ~1 a.u. whereas the wave packet at $t=0$ covers several hundred atomic units. This difference can be directly traced to the presence of the window function $W(E)$. As the energy range covered by $W(E)$ increases, the radial width of the $t=0$ packet decreases; in the limit of infinite range, the $t=0$ packet has exactly the same radial form as $r\psi_i(\mathbf{r})$. The $W(E)$ plays exactly the same role as a bandpass filter: a pulsed optical signal is stretched in time when the range of frequency components is reduced.

The case that was shown in Figs. 1 and 2 was deliberately chosen to have a large amount of dispersion. By reducing the number of states in the packet or keeping the number of states fixed and going to higher n, the dispersion can be reduced. However, it must be remembered that dispersion is always present unless the packet only consists of two states or the system has equally spaced energy levels.

III. ACTION-DEPENDENT RECURRENCE

The study of atomic Rydberg states in static fields has been greatly aided by ideas arising from scaled energy spectroscopy [3,4]. One of the more important ideas is that the absorption spectrum is obtained by simultaneously varying the energy and the field strength so the classical scaled energy remains fixed. As two examples, consider the classical Hamiltonian for an H atom in a static electric field or the diamagnetic H atom. If the classical variables are scaled as

$$\mathbf{r}=\tilde{\mathbf{r}}\left(\frac{\omega}{2\pi}\right)^{2},\quad t=\tilde{t}\left(\frac{\omega}{2\pi}\right)^{3},$$

$$E=\varepsilon\left(\frac{2\pi}{\omega}\right)^{2},\quad S=\tilde{S}\left(\frac{\omega}{2\pi}\right), \tag{4}$$

with $F=(2\pi/\omega)^4$ for the H atom in static electric field and $B=(2\pi/\omega)^6$ for the diamagnetic H atom, then the motion is only determined by the scaled energy ε, and the initial position and momenta of the classical particle. In all that follows, scaled variables (except the scaled energy ε) and functions of scaled variables will have a tilde. The reason that the classical scaled dynamics is interesting is that the absorption can be represented by the imaginary part of the expectation value of a Green's function and a semiclassical approximation to the Green's function is simply $\exp(i2\pi S)$; to be consistent with the conventions used in scaled energy spectroscopy, the action is defined as $S=(2\pi)^{-1}\int \mathbf{p}\mathbf{v}\,dt$. Thus the Fourier transform of the absorption spectrum with respect to the scaling parameter ω is expected to have peaks at the classical values of the scaled action $\tilde{S}$.

The scaled energy absorption spectrum can be obtained from the imaginary part of the expectation value of the Green's function as

$$\rho(\omega)=\mathrm{Im}\{\langle\psi_i|D[E(\omega)-H(\omega)-i\delta]^{-1}D|\psi_i\rangle\}, \tag{5}$$

where $\delta\rightarrow 0^{+}$. In the bound-state region, the eigenstates and ''eigenscalings'' can be used to obtain an expression for the absorption:

$$\rho(\omega)=\sum_{n}|D_n|^2\delta(\omega-\omega_n), \tag{6}$$

where ω_n is an ''eigenscaling'' that determines the eigenstate $H(\omega_n)\psi_n=E(\omega_n)\psi_n$; compare this equation with Eq. (1). The orthonormality properties of the eigenstates will be discussed below. The strength of the nth delta function is a generalization of the dipole matrix element:

$$D_n=\langle\psi_n|D|\psi_i\rangle/\sqrt{|\langle\psi_n|N(\omega_n)|\psi_n\rangle|}, \tag{7}$$

where the ''normalization'' operator $N(\omega)=\partial[E(\omega)-H(\omega)]/\partial\omega$ accounts for the rate of change of the $E-H$ denominator in the Green's function. As an example, $N(\omega)=-2[E(\omega)+2F(\omega)z]/\omega$ for the hydrogen atom in a static electric field.

The action-dependent recurrence function is defined to be the Fourier transform with respect to the scaling ω of the windowed absorption spectrum:

$$R(\tilde{S})\equiv\int d\omega W^2(\omega)\rho(\omega)e^{-i\omega\tilde{S}}, \tag{8}$$

which should be compared to the $E\rightarrow t$ transform in Eq. (3). The action-dependent recurrence function tends to have peaks whenever $\tilde{S}$ equals a classical scaled action for a closed trajectory that starts near the nucleus and returns to the nucleus. This can be understood because $D\psi_i$ is substantial only for a small region near the nucleus and a semiclassical approximation of the Green's function is simply $\Sigma_j\exp(i2\pi S_j^{\mathrm{cl}})=\Sigma_j\exp(i\tilde{S}_j^{\mathrm{cl}}\omega)$, where j is an index that numbers the classical orbits that begin and end at the nucleus [3,5]. A very interesting feature is that dispersion is greatly suppressed because all trajectories are at the same scaled energy; thus peaks in the action-dependent recurrence function do not get broader as the action increases. This should be contrasted with the situation of the previous section.

The comparison between the time-dependent and the action dependent recurrence functions, Eqs. (3) and (8), suggests that the action-dependent recurrence can be written as an autocorrelation for an action-dependent wave function. The straightforward translation, $R(\tilde{S})=\langle\Psi(0)|\Psi(\tilde{S})\rangle$ with the action-dependent function defined as $\Psi(\mathbf{r},\tilde{S})=\Sigma_n\psi_n(\mathbf{r})D_nW(\omega_n)\exp(-i\omega_n\tilde{S})$ will not work because the ψ_n are solutions of *different* Hamiltonians and thus they do not have simple orthonormality properties when using the spatial coordinate $\mathbf{r}$. Fortunately, this difficulty can be overcome if one extra idea from classical scaling is incorporated.

IV. ACTION-DEPENDENT WAVE FUNCTION

The difficulty in defining an action-dependent wave function lies in the lack of orthonormality properties of the eigenstates at scaled energy. This can be overcome if the functions are defined using the scaled distance. Thus, the eigenfunctions in scaled coordinates and the eigenscalings are determined by

$$\left(\frac{\omega_n}{2\pi}\right)^{2}[\varepsilon-\tilde{V}(\tilde{\mathbf{r}})]\tilde{\psi}_n(\tilde{\mathbf{r}})=-\frac{1}{2}\tilde{\nabla}^2\tilde{\psi}_n(\tilde{\mathbf{r}}),$$

$$\int d^3\tilde{\mathbf{r}}\tilde{\psi}^{*}_{n'}(\tilde{\mathbf{r}})[\varepsilon-\tilde{V}(\tilde{\mathbf{r}})]\tilde{\psi}_n(\tilde{\mathbf{r}})=\delta_{n'n}, \tag{9}$$

where ε is the scaled energy from Eq. (4) and $\tilde{V}(\tilde{\mathbf{r}})$ equals $-1/\tilde{r}+\tilde{z}$ for the H atom in static electric field and $-1/\tilde{r}+(\tilde{x}^2+\tilde{y}^2)/8$ for the diamagnetic H atom. (In Ref. [6], the techniques of scaled energy spectroscopy are extended to systems without classical scaling in order to interpret complicated spectra.) The definition can be extended to continuum states by replacing the Kronecker delta function by a Dirac delta function.

The simple orthonormality properties of Eq. (9) removes the only difficulty in defining an action-dependent wave function. If the action-dependent wave function is defined as

$$\Psi(\tilde{\mathbf{r}},\tilde{S})=\sum_{n}\tilde{\psi}_n(\tilde{\mathbf{r}})D_nW(\omega_n)\exp(-i\omega_n\tilde{S}), \tag{10}$$

then the action-dependent recurrence is exactly equal to a generalized autocorrelation function:

$$R(\tilde{S})=\int d^3\tilde{\mathbf{r}}\Psi^{*}(\tilde{\mathbf{r}},0)[\varepsilon-\tilde{V}(\tilde{\mathbf{r}})]\Psi(\tilde{\mathbf{r}},\tilde{S}). \tag{11}$$

These two equations should be compared to Eqs. (2) and (3) for the time-dependent situation. The reasons why I think the definition of an action-dependent wave function, given in Eq. (10), should be preferred, will be given in the next section.

The action-dependent wave function has been defined through a superposition of eigenstates, but it is natural to require it to also be the solution of a wave equation. Using the eigenstate and orthonormality properties of Eq. (9) and the definition of Eq. (10), it is possible to show that

$$\frac{1}{4\pi^2}[\varepsilon-\tilde{V}(\tilde{\mathbf{r}})]\frac{\partial^2}{\partial\tilde{S}^2}\Psi(\tilde{\mathbf{r}},\tilde{S})=-\frac{1}{2}\tilde{\nabla}^2\Psi(\tilde{\mathbf{r}},\tilde{S}) \tag{12}$$

is the simplest wave equation for the present definition of an action-dependent wave function [7]. The definition of the action-dependent wave function, Eq. (10), and its corresponding wave equation, Eq. (12), are the most important results of this paper.

While the action-dependent wave equation is perfectly well defined, it does not seem likely that it can be used to numerically solve for the action-dependent wave function. The problem is that the operator $[\varepsilon-\tilde{V}(\tilde{\mathbf{r}})]$, which multiplies the second derivative with respect to action, is not positive definite for most problems of interest. The partial differential equation is of a mixed, elliptic-hyperbolic character. A famous equation of this type is the Tricomi equation, $xy_{tt}+y_{xx}=0$. This means that while there are oscillating solutions like Eq. (10) there are also solutions that exponentially diverge with increasing action. The exponentially diverging solutions are never part of the initial conditions; unfortunately, numerical round off and other inaccuracies will mix the diverging solutions into the numerical propagation (even small admixture of a diverging term will quickly dominate the solution). It may be possible to prevent admixture of diverging solutions by using special numerical techniques [8].

There still may be use for the wave equation even if its direct numerical solution is impossible. It is possible that new semiclassical approximations can be derived from the wave equation instead of through the indirect procedure of Fourier transforming the Green's function. It is also possible that the action-dependent wave functions will themselves be the source of insight into the origins and problems with semiclassical approximations.

V. APPLICATION

In this section, I will give results for the action-dependent wave function for three different cases. The section on the H atom in a static electric field addresses the recent mystery about peaks in the recurrence spectrum without corresponding closed orbits [9].

A. One-dimensional semiclassical

It is relatively easy to define objects like action-dependent wave functions; however, it is not necessary that the resulting construct behaves in the desired manner. The purpose of this section is to show that the action-dependent wave function behaves in a very simple and intuitive manner for one-dimensional problems. In fact, it is possible to show that the action-dependent wave function has very little dispersion, has peaks that move like a classical particle, and has a semiclassical approximation that gives extremely narrow peaks in space.

The basic idea of this section is to use a WKB type of approximation in order to obtain approximations to the eigenscaling, ω_n and eigenstates, $\tilde{\psi}_n$. To get repeating motion, I assume that the classical motion is bounded within a finite region with an inner turning point at $\tilde{x}_0$ and an outer turning point at $\tilde{x}_f$. The eigenvalue equation in Eq. (9) reduces to

$$\left(\frac{\omega_n}{2\pi}\right)^2\tilde{p}^2(\tilde{x})\tilde{\psi}_n(\tilde{x})+\frac{\partial^2}{\partial\tilde{x}^2}\tilde{\psi}_n(\tilde{x})=0, \tag{13}$$

where the square of the scaled momentum as a function of scaled distance is $\tilde{p}^2(\tilde{x})=2[\varepsilon-\tilde{V}(\tilde{x})]$. From the assumptions about repeating motion, the scaled kinetic energy is only positive over the range $\tilde{x}_0<\tilde{x}<\tilde{x}_f$. The WKB approximation [1] to this equation is

$$\tilde{\psi}_n(\tilde{x})\simeq\frac{1}{\sqrt{\tilde{p}(\tilde{x})}}\sin[\omega_n\tilde{S}_{\rm cl}(\tilde{x})+\delta],$$

$$\omega_n\tilde{S}_{\rm cl}(\tilde{x}_f)\simeq\left(n+\frac{1}{2}\right)\pi, \tag{14}$$

where the classical, position dependent scaled action

$$\tilde{S}_{\rm cl}(\tilde{x})=\frac{1}{2\pi}\int_{\tilde{x}_0}^{\tilde{x}}\tilde{p}(\tilde{x}')d\tilde{x}' \tag{15}$$

is defined so that it is zero at the inner turning point $\tilde{x}_0$.

The WKB approximation can be thought of as a power series in $\hbar$; in the eigenscaling equations $2\pi/\omega_n$ plays the role of $\hbar$. Thus, the approximate solutions should give a good qualitative approximation to the exact solutions. The first point to notice about the approximation is that the ω_n are *exactly* equally spaced. This equal spacing means there will be *no* dispersion of the action-dependent wave functions at this level of approximation. This property is independent of the type of potential! Thus, the action-dependent wave function should never show a large amount of dispersion when it is constructed from states with large *n*. Unlike the time-dependent wave packets, the action-dependent wave packets can be constructed from a very large number of states without dispersion causing any problems. The physical reason for this is that every eigenstate is at the same scaled energy, thus the main cause of dispersion in the time-dependent wave functions (variation of periods with energy) is removed.

The WKB approximation can also be used to show that a peak in the action-dependent wave function will move in space so that it accurately follows the classical result. To see this, the WKB wave functions can be used to obtain the approximate action-dependent wave function:

$$\Psi(\tilde{x},\tilde{S}) \simeq \frac{1}{\sqrt{\tilde{p}(\tilde{x})}} \sum_n A_n e^{-i\omega_n \tilde{S}} \sin[\omega_n \tilde{S}_{\mathrm{cl}}(\tilde{x})+\delta], \quad (16)$$

where A_n are coefficients. At this level of approximation, $\Psi(\tilde{x},\tilde{S})=\Psi(\tilde{x},\tilde{S}+2\tilde{S}_{\mathrm{cl}}[\tilde{x}_f])$, which shows the lack of dispersion after one cycle. If the A_n is a real, smooth function of n that is nonzero for a large number of n, then the action-dependent wave function is a single peak centered at $\tilde{S}=\tilde{S}_{\mathrm{cl}}(\tilde{x})$ for $0 \leqslant \tilde{S} \leqslant \tilde{S}_{\mathrm{cl}}(\tilde{x}_f)$ and $\tilde{S}=2\tilde{S}_{\mathrm{cl}}(\tilde{x}_f)-\tilde{S}_{\mathrm{cl}}(\tilde{x})$ for $\tilde{S}_{\mathrm{cl}}(\tilde{x}_f) \leqslant \tilde{S} \leqslant 2\tilde{S}_{\mathrm{cl}}(\tilde{x}_f)$. This is exactly the classical result.

The exact return of the wave function to its original form after one cycle with the behavior of the wave function during the first cycle (exactly tracking the classical result) shows that the action-dependent wave function at this level of approximation will exactly follow the classical result to any size of action. This shows that the action-dependent wave function behaves in many respects like a classical particle. Thus, the definition of action-dependent wave function in Eq. (10) gives a reasonable behavior for a one-dimensional system.

B. Hydrogen atom—no field

To my knowledge, this is the first study of an action-dependent wave function so it makes sense to apply it to an effective one-dimensional case. In this section, I will present results for the case of an H atom in zero field. This is a good trial system since the eigenscalings and wave functions may be obtained analytically.

The wave function can be obtained using a separation of variables in spherical coordinates: $\tilde{\psi}_{nlm}=R_{nl}(\tilde{r})Y_{lm}(\theta,\phi)$. The eigenscaling can be obtained from Eq. (9) directly when $\tilde{V}(\tilde{\mathbf{r}})=-1/\tilde{r}$: $\omega_n=2\pi n\sqrt{-2\varepsilon}$. Note that the eigenscaling is proportional to n; this means that the action-dependent wave function will exactly repeat after an action increment of $1/\sqrt{-2\varepsilon}$. Unlike the result from the previous section the repetition $\Psi(\tilde{\mathbf{r}},\tilde{S})=\Psi(\tilde{\mathbf{r}},\tilde{S}+1/\sqrt{-2\varepsilon})$ is an exact result. Most standard quantum textbooks give the eigenstates for the H atom. These eigenstates simply need to be multiplied by a constant and the distances rescaled; if $\psi_{nlm}(\mathbf{r})$ is an eigenstate of the unscaled Hamiltonian and is space normalized to 1, then the eigenstate in Eq. (9) is $\tilde{\psi}_{nlm}(\tilde{\mathbf{r}})=-2\varepsilon\sqrt{2}n^3\psi_{nlm}(-\tilde{\mathbf{r}}2\varepsilon n^2)$. Finally, the normalization operator is $-2E(\omega)/\omega$, which gives the dipole matrix elements as $D_n \propto \langle\psi_n|D|\psi_i\rangle n^{3/2}$, which is proportional to a constant as $n\rightarrow\infty$.

The squared absolute value of the radial part of the action-dependent wave function is shown at 5 values of the scaled action in Fig. 3: $\tilde{S}=0$, and 1/4, 2/4, 3/4, and 4/4 of the classical action for an electron to reach the outer turning point at $\tilde{r}=-1/\varepsilon$ (the function for the smallest action cannot be distinguished from the vertical axis at $\tilde{r}=0$). The scaled energy was chosen to be -4. For this figure, states from $n=1-200$ were superposed with coefficients given by $W \propto \exp[-16(n-100)^2/100^2]$. The squared absolute value has been multiplied by the function $\sqrt{|\varepsilon+1/\tilde{r}|}$ as suggested by the semiclassical derivation of the previous section in order to keep the height roughly constant.

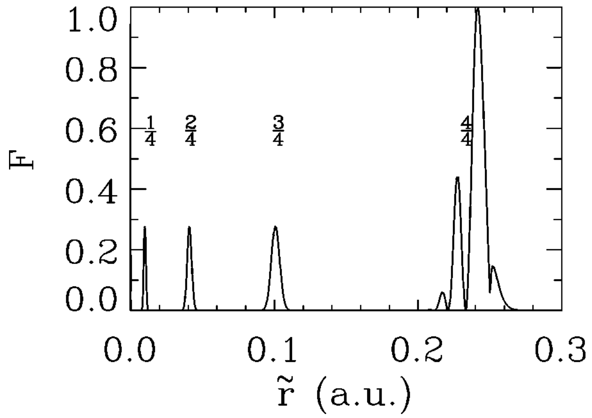

FIG. 3. For an H atom in zero field, the radial part of the renormalized scaled density $F=|\varepsilon+1/\tilde{r}|^{1/2}|\tilde{\Psi}(\tilde{r},\tilde{S})|^2$ at 5 values of the scaled action: 0, 1/4, 2/4, 3/4, and 4/4 of the classical action to reach the outer turning point. Note that F for $\tilde{S}=0$ is indistinguishable from the vertical axis at $\tilde{r}=0$. The scaled energy is -4, which gives the outer turning point at $\tilde{r}=1/4$. States from $n=1-200$ are part of the packet. The function F at action of 5/4, 6/4, 7/4, and 8/4 of the classical action to reach the outer turning point is identical to the function at 3/4, 2/4, 1/4, and 0, respectively. For an H atom in zero field $F(\tilde{r},\tilde{S})=F(\tilde{r},\tilde{S}+2\tilde{S}_{\mathrm{cl}}[\tilde{r}_f])$.

There are a number of features of Fig. 3 that can be understood at a qualitative level. First, the height of the function does not change because the $1/\sqrt{\varepsilon-\tilde{V}}$ behavior has been removed. Second, the spatial width of the packet increases as the packet moves to larger $\tilde{r}$; this arises because $1/d\tilde{S}_{\mathrm{cl}}/dr$, which plays the role of speed of the packet, increases as the outer turning point is approached (the $\tilde{S}=0$ function is not distinguishable from the vertical axis at $\tilde{r}=0$). Third, the interference pattern at the outer turning point arises from the interference between the part of the packet that has already reached the outer turning point and the part that has not reached it; the form of this interference pattern could probably be analytically calculated by using a uniform WKB approximation at the outer turning point. Fourth, the peak position of the packet is at the position of a corresponding classical particle to a very good approximation.

C. Hydrogen atom—electric field

I have used the action-dependent wave function to study the recurrence for an H atom in a static electric field. For this case, the scaled potential is $\tilde{V}=-1/\tilde{r}+\tilde{z}$. There is a cylindrical symmetry for this problem, which means it can be reduced to an effective two-dimensional system. There is another symmetry in the problem, which allows the separation of the Hamiltonian in parabolic coordinates; this separability affects the dynamics but has not been used in the calculation that was performed in spherical coordinates. The classical motion for this system is regular.

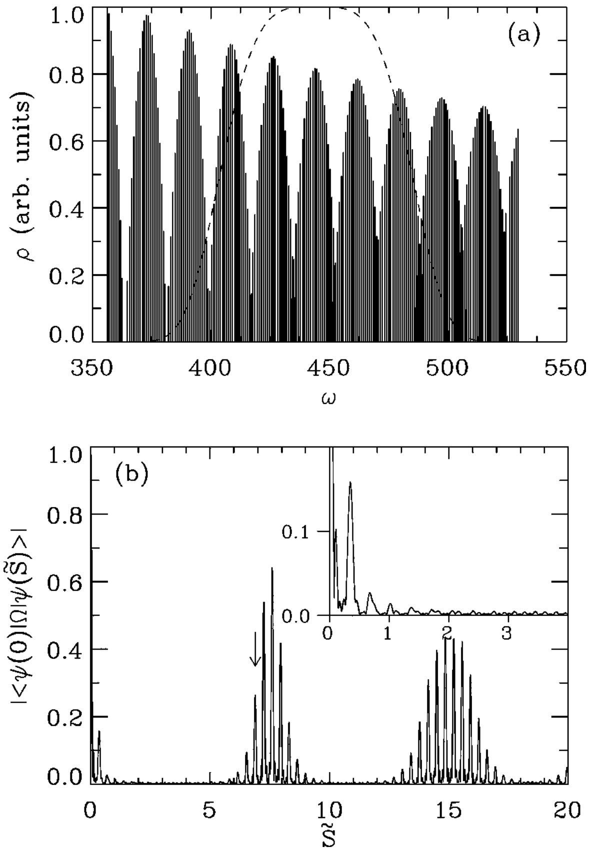

FIG. 4. (a) The scaled energy absorption spectrum from the $1s$ state of an H atom in a static electric field for $\varepsilon = -4$ and a laser polarized perpendicular to the field direction. The dashed line is the window function, $W(\omega)$, used to obtain the action-dependent recurrence of (b). The states shown are from $n = 20-30$. (b) The action-dependent recurrence for the system in (a). The metric $\Omega = \varepsilon - \tilde{V}(\tilde{\mathbf{r}})$ is needed for orthonormality properties of the eigenstates. The inset shows a magnified view of the small action region. The smallest action peak that corresponds to a classical trajectory that returns to the nucleus is marked with an arrow. All peaks (except at $\tilde{S} = 0$) before the arrow are not present in the usual implementation of closed orbit theory.

In Fig. 4, I show the absorption spectrum and the action-dependent recurrence from a recent paper [9]. In this paper, $\varepsilon = -4$ and the H atom is excited from the $1s$ ground state with one photon that is polarized perpendicular to the field direction. The action-dependent recurrence has the usual sequence of peaks at the classical actions of orbits that return to the nucleus.

However, there is one interesting feature of this system that was noted in Ref. [9]. There are peaks in the action-dependent recurrence before the smallest classical action for a trajectory that returns to the nucleus; this smallest action is marked with an arrow in Fig. 4(b). Especially note that there is a substantial recurrence peak at the action of the radial motion in zero field, $\tilde{S} = 1/\sqrt{-2\varepsilon} \simeq 0.35$. These peaks are not present in the usual implementation of semiclassical methods. The classical reason why there should not be peaks before the arrow is that the electron has nonzero $\langle L_z \rangle$, which means that trajectories are not allowed on the z axis and it is only trajectories exactly on the z axis that can return to the region near the nucleus after one radial oscillation; the electric field gives a nonzero torque to any trajectory not on the z axis. In Ref. [9], it was found that performing the calculation as if $L_z = 0$ and thus allowing trajectories on the z axis gave qualitative agreement with the quantum calculation; however, the justification of this procedure was not given. It was suggested in Ref. [10] that the peaks at the small action $\tilde{S} \simeq 0.35$ arise from ghostlike orbits; the difficulty with this suggestion as discussed in Ref. [11] is that these orbits do not reach the region of the ground state. Thus, the origin of the peaks without closed orbits appears to still be an open question.

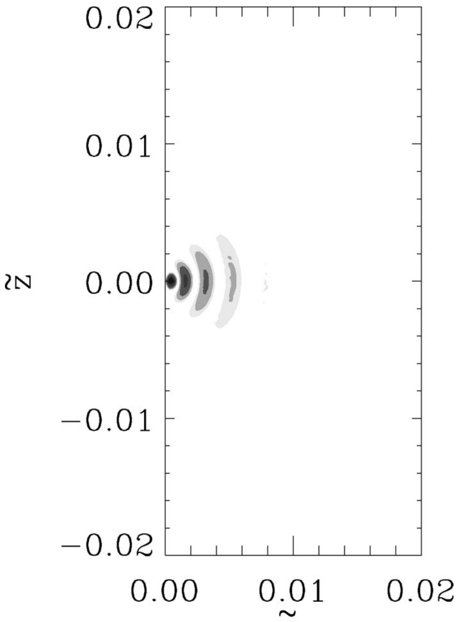

FIG. 5. A contour plot of the squared magnitude of the action-dependent wave function (times $\tilde{\rho}$) at $\tilde{S} = 0$ for the system of Fig. 4. Note this wave function extends to much larger distances than the initial $1s$ state (1 a.u. in real space corresponds to $\sim 2 \times 10^{-4}$ a.u. in scaled distance). Each contour is a factor of 2.

The results from a calculation of the action-dependent wave function suggests a different explanation for the early peaks in the action-dependent recurrence. In Figs. 5, 6, and 7, I show the squared magnitude of the action-dependent wave function at $\tilde{S} = 0$, 0.35, and 0.70, respectively. The $\tilde{S} = 0$ shows the packet localized to small distances but with most of the probability along the plane $\tilde{z} = 0$ because the polarization is perpendicular to the z axis. The $\tilde{S} = 0.35$ shows the first return of the packet to the region near the nucleus; the torque on the electron causes it to approach the nucleus from below the $z = 0$ plane and leave above this plane. The $\tilde{S} = 0.70$ shows the effect of the torque more strongly; the electron packet clearly misses the nucleus.

An examination of the action-dependent wave functions at $\tilde{S} = 0.0$ and 0.35 suggests an origin for the short action peaks that is different from that in previous papers [9,10]. The key idea is that the $\tilde{S} = 0.0$ wave function extends out to distances much larger than for the initial state; one a.u. of

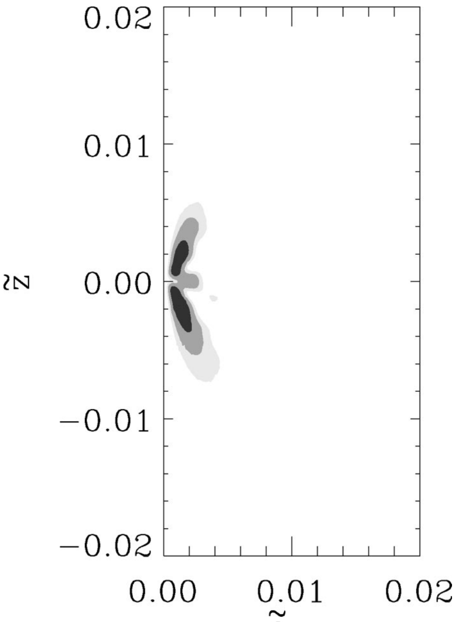

FIG. 6. Same as Fig. 5 but at $\tilde{S}=0.35$ for the system of Fig. 4.

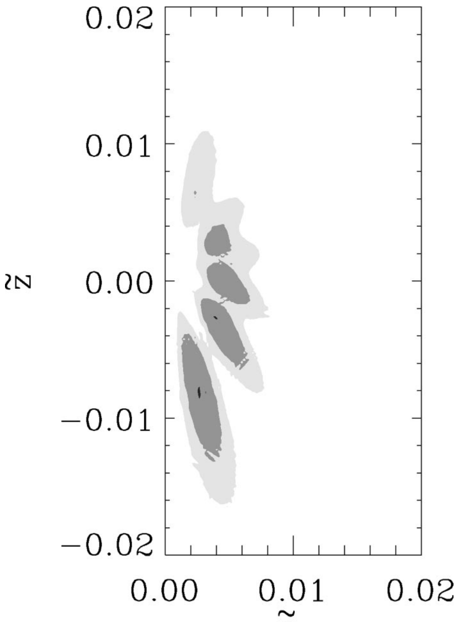

FIG. 7. Same as Fig. 5 but at $\tilde{S}=0.70$ for the system of Fig. 4.

real distance corresponds to 2×10^{-4} a.u. in scaled distance, which is roughly the thickness of a line in Fig. 5. The reason the $\tilde{S}=0.0$ wave function extends out to larger distances is the same as discussed in Sec. II; the weight function W acts as a filter in scaling, which causes the wave function to be spread in space. Since the $\tilde{S}=0.0$ function extends to much larger distances, even trajectories that do not return to within the distance of the ground state can overlap the $\tilde{S}=0.0$ function.

If this idea is correct, then it implies that there may be an idea missing in the usual implementation of closed orbit theory. The action-dependent recurrence is constructed by using a window function that effectively spreads the initial state. However, the recurrence spectrum is calculated by taking orbits all of the way to the nucleus. Perhaps for most situations the corrections that arise are a small fraction of the peaks of the recurrence spectrum. It is only in cases where the orbit cannot reach the nucleus that the effect from the window function becomes clear.

I have calculated the wave function for several values of $\tilde{S}$ and the peak of the wave function follows the classical trajectory without dispersing up to the largest action attempted ($\tilde{S}=20$). Note, that this is an action corresponding to roughly 55 radial oscillations in zero field.

VI. FUTURE DIRECTIONS

The results from this paper show that it is possible to define an action-dependent wave function in a reasonable way. The action-dependent wave function was shown to have a very interesting correspondence to classical motion in a semiclassical approximation of a one-dimensional system; the most interesting aspect is the lack of dispersion shown by the function. The action-dependent wave function does not disperse at all for an H atom in zero field and does not appear to disperse for an H atom in a static electric field (this has not been proven).

There are a number of possibly useful directions to extend this paper. One possibility is to use the action-dependent wave function to interpret quantum-mechanical calculations. Several joint studies comparing action-dependent wave functions and semiclassical approximations could aid in understanding the limitations of semiclassical methods. In particular, the inclusion of scattering by a non-Coulombic potential is only a partially solved problem; the current formulation of scattering appears to work well only for very high n and very few scatterings. Also, the recurrence to states strongly localized in angle does not appear to be correctly handled. Last, the direct solution of the action-dependent wave equation does not appear to be possible for most systems because $(\varepsilon-\tilde{V})$ is not positive everywhere. But the action-dependent wave equation may not have exponential divergence for two outward moving electrons for $\varepsilon\geqslant0$ if they are started on opposite sides of the nucleus. If the direct solution is stable, it may be possible to calculate fully quantum motion out to very large distances and obtain further insight into this very difficult problem.

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