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Approximate solutions of the Schrödinger equation in the semiclassical limit via generalized Fourier integrals

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It is shown in the limit $\hbar \rightarrow 0$ that an approximate solution of the time-dependent Schrödinger equation can be obtained by the use of generalized Fourier integrals. These are constructed by the continuous superposition of eikonals, each generated by solving a problem in classical mechanics. The solution thus generated is valid even in the presence of caustics, provided that they are not too dense. The method applies to localized wave functions and provides a short-time solution. The nature of the solution and its relation to an exact solution is demonstrated in the case of the one-dimensional problem of the surface-state electron. The Wigner distribution f arises in a natural way, leading to the interpretation of the semiclassical limit as classical kinetic theory.

I. INTRODUCTION

Despite 60 years of consideration, the existence and nature of the semiclassical approximation[1,2] to the solution of the Schrödinger equation ($\hbar \rightarrow 0$) is still under active investigation. Current interest stems in part from the observation that the eikonal approximation conventionally employed fails for systems harmonically perturbed by an external force, due to the development of caustics which become more numerous as time goes on. In this paper we shall demonstrate that some of the difficulties can be removed by employing, rather than a single eikonal, a continuous superposition thereof, using the method of the generalized Fourier integral (GFI), introduced by Hazak.[3,4] This technique is particularly well adapted for localized wave functions and leads to an approximate solution of the initial-value problem in terms of a Green's function which can be constructed using classical mechanics and reduced in complexity via stationary phase integration. One consequence of the theory is that the spatically coarse-grained probability density can be calculated by integrating over velocity a distribution function which obeys the Vlasov equation. This provides the connection with the quantum theory, and justification of the classical techniques used for example to calculate the ionization of Rydberg states by microwave electric fields.[5,6] While this work is confined to the Schrödinger equation for one particle in a given space-time-dependent potential, it offers the possibility of ready generalization to many-body systems.

The paper proceeds as follows. Section II is devoted to the development and extension of the conventional single eikonal theory in a form convenient for the GFI, namely the systematic use of Lagrangian coordinates. It is shown that the classical limit thus generated is describable as cold fluid mechanics, with the probability density determinable from a continuity equation for which the velocity obeys the momentum equation of cold irrotational fluid dynamics. Caustics occur when there is crossing of the trajectories associated with the Lagrangian variables. They can be located by integrating along each trajectory a system of ordinary differential equations akin to and including the particle equations of motion. This procedure is feasible even in three dimensions using modern computers. The well-known result that the caustic is an envelope of the trajectories is demonstrated in simple fashion, as well as the behavior of the eikonal approximation as one approaches a caustic surface. This last permits a simple solution of the Schrödinger equation by means of a matched asymptotic expansion in a boundary layer straddling a moving caustic. The well-known expression in terms of Airy functions is the result. It is pointed out that the single eikonal approximation is useful for scattering problems which display a limited number of caustics, but is deficient for driven time-dependent problems, both because of the absence of a unique way to fit an arbitrary localized initial condition, and the problem of coping conveniently with many caustics.

Section III is devoted to the application of the GFI to the general problem. A brief derivation of the method is given, and it is employed to construct a solution of the initial-value problem associated with the one-particle Schrödinger equation. The solution is in terms of a Green's function which is constructed following classical trajectories, and which in the absence of dense caustics can be simplified using the method of stationary phase.

The solution is valid, roughly speaking, as long as the volume of caustic boundary layers is sufficiently small. It is then demonstrated that the probability density $|\psi(\mathbf{r},t)|^2$, suitably coarse grained, can be computed from a distribution function, a Wigner distribution associated with the initial wave function, which satisfies the Vlasov equation, by means of integration over the velocity variable. The Wigner distribution enters naturally and this work serves as a justification of its use. Thus the classical limit can be described as governed by kinetic theory. Finally, it is demonstrated that if one employs in the GFI solution the classical one-particle phase-space variables, the local velocity and position, then the integrand is analytic away from caustics, if the potential in the Schrödinger equation is analytic.

Section IV is devoted to a one-dimensional problem for which the Schrödinger equation can be solved exactly, namely the surface-state electron problem (SSE) (Refs. 5 and 6) in the absence of external fields. In this case the electron is bound to a surface of liquid helium by its image charge. The potential is $-e^2/\epsilon x$, where x is the distance from the surface, and ϵ the dielectric constant of the helium. The surface itself acts as an infinite potential barrier. A Laplace transform in time converts the equation into an inhomogeneous ordinary differential equation in x which can be solved in terms of Whittaker functions by the method of variation of parameters. Inversion of the Laplace transform by deformation into the lower half transform plane yields a representation in terms of the discrete and continuum eigenstates. A different inversion technique employing the Wentzel-Kramers-Brillouin (WKB) asymptotic forms in the upper half transform plane yields a representation useful for short times, and provides an estimate of the time of validity. This latter representation is shown to coincide with the GFI result when both can be reduced by the method of stationary phase.

II. SINGLE EIKONAL THEORY

Consider the one-particle Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi+W\psi\ , \tag{1}$$

where $W(\mathbf{r},t)$ is a given potential. We wish to find solutions in the limit $\hbar\to 0$. The conventional procedure is to seek an eikonal solution[1,2] of the form

$$\psi=a\exp(S/\hbar)\ . \tag{2}$$

Let

$$m\mathbf{v}=\nabla S\ , \tag{3}$$

$$H=-\frac{\partial S}{\partial t}\ . \tag{4}$$

Then (1) implies

$$0=(H-\tfrac{1}{2}mv^2-W)a+i\hbar\left[\frac{\partial a}{\partial t}+\mathbf{v}\cdot\nabla a+\frac{1}{2}a\nabla\cdot\mathbf{v}\right]+\frac{\hbar^2}{2m}\nabla^2 a\ . \tag{5}$$

We wish solutions which in the limit $\hbar\to 0$ have a nonzero amplitude a. This requires that

$$H=\tfrac{1}{2}mv^2+W \tag{6}$$

or on using (3) and (4)

$$\frac{\partial S}{\partial t}+\frac{(\nabla S)^2}{2m}+W=0\ . \tag{7}$$

Equation (7) is a nonlinear first-order partial differential equation for S, the Hamilton-Jacobi equation.[7]

In order to deal with (7) it is convenient to take its gradient. On using the property $\mathbf{v}\cdot\nabla\nabla S=(\nabla\nabla S)\cdot\mathbf{v}$ the result can be expressed in the form

$$m\left[\frac{\partial v}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right]=-\nabla W\ . \tag{8}$$

Note that the curl of (8) is

$$\frac{\partial}{\partial t}(\nabla\times\mathbf{v})=\nabla\times[\mathbf{v}\times(\nabla\times\mathbf{v})]\ . \tag{9}$$

Thus if $\nabla\times\mathbf{v}$ vanishes initially, Eq. (8) maintains its zero, whence if $\mathbf{v}$ has been found one can construct $S=S_0(\mathbf{r})_0+m\int_{\mathbf{r}_0}^{\mathbf{r}}d\mathbf{r}\cdot\mathbf{v}$, where the result is independent of path in any region in which $\mathbf{v}$ is a single-valued function of $\mathbf{r}$. Note that thus far no approximations have been made. One has only introduced new dependent variables a and $\mathbf{v}$ which hopefully do not change much in a local wave length h/mv or local period h/H.

Equation (5) in the limit $\hbar\to 0$ next implies

$$0=\frac{\partial a}{\partial t}+\mathbf{v}\cdot\nabla a+\tfrac{1}{2}a\nabla\cdot\mathbf{v}\ . \tag{10}$$

Note that the mass density is given exactly by

$$\rho=m|\psi|^2=m|a|^2 \tag{11}$$

and it is readily seen that (10) implies

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{v})=0\ , \tag{12}$$

the continuity equation. Equations (8) and (12) multiplied by ρ, with the constraint that initially $\nabla\times\mathbf{v}=0$, are those governing the potential flow of a cold ideal fluid acted on by a body force derivable from a potential. This suggests that the semiclassical limit $\hbar\to 0$ be described as fluid dynamics. For example, the scattering of an initially plane wave by a repulsive center can be interpreted in this limit as flow around an obstacle.

In order to present the problem in a form amenable to solution by the method of characteristics it is convenient to denote by a dot the convective derivative

$$\dot{a}=\frac{\partial a}{\partial t}+\mathbf{v}\cdot\nabla a\ . \tag{13}$$

Then (8) and (10) can be expressed as

$$m\dot{\mathbf{v}}=-\nabla W\ , \tag{14}$$

$$\dot{a}=-\tfrac{1}{2}a\nabla\cdot\mathbf{v}\ , \tag{15}$$

while

$$\dot{S}=\frac{\partial S}{\partial t}+\mathbf{v}\cdot\nabla S=-H+mv^2=\tfrac{1}{2}mv^2-W\ . \quad (16)$$

If one introduces characteristics (rays, trajectories) via[8]

$$\dot{\mathbf{r}}=\mathbf{v} \quad (17)$$

and requires at $t=t_0$ that $\mathbf{r}=\mathbf{r}_0$, $a=a_0(\mathbf{r}_0)$, $S=S(\mathbf{r}_0)$, and $m\mathbf{v}_0=\nabla_0 S_0(\mathbf{r}_0)$, then integration of the system of ordinary differential equations (14)—(17) yields the desired solution. Note that since (15) involves $\nabla\cdot\mathbf{v}$, the computation of which requires a knowledge of $\mathbf{v}$ on adjacent characteristics, one must deal with a bundle of characteristics.

The problem can be reduced to consideration of one characteristic at a time by introducing an enlarged system of ordinary differential equations. Advantage is taken of the feature that if the Jacobian

$$J=\frac{\partial(\mathbf{r})}{\partial(\mathbf{r}_0)}=|\det\nabla_0\mathbf{r}(\mathbf{r}_0,t)| \quad (18)$$

is known, then (15) can be immediately integrated, viz.,

$$a=a_0J^{-1/2}\ . \quad (19)$$

To derive (18) note that if $U(t)$ is an arbitrary volume enclosed by a surface $\Sigma(t)$ such that all the points interior to and on Σ move with the velocity $\mathbf{v}$, then

$$U=\int d^3r=\int d^3r_0\,J\ . \quad (20)$$

But

$$\dot{U}=\frac{d}{dt}\int d^3r=\int_\Sigma d^2\mathbf{r}\cdot\mathbf{v}=\int d^3r\,\nabla\cdot\mathbf{v}=\int d^3r_0\,J\nabla\cdot\mathbf{v} \quad (21)$$

and alternatively

$$\dot{U}=\frac{d}{dt}\int d^3r_0\,J=\int d^3r_0\,\dot{J}\ . \quad (22)$$

If we equate the two rightmost expressions in (21) and (22) it follows, since the domain is arbitrary, that

$$\dot{J}=J\nabla\cdot\mathbf{v}\ . \quad (23)$$

When (23) is used in (15) to eliminate $\nabla\cdot\mathbf{v}$ there results

$$0=\dot{a}+\tfrac{1}{2}a\dot{J}\ , \quad (24)$$

which can be directly integrated to obtain (19). In order to compute J it is convenient to define

$$\underline{A}=\nabla_0\mathbf{r}\ . \quad (25)$$

Then $J=|\det\underline{A}|$. Let

$$\underline{B}=\nabla_0\mathbf{v}\ . \quad (26)$$

Then the gradient of (17) with respect to $\mathbf{r}_0$ yields

$$\dot{\underline{A}}=\underline{B}\ , \quad (27)$$

while the gradient of (14) with respect to $\mathbf{r}_0$ yields on, using the chain rule,

$$m\underline{B}=-\nabla_0\nabla W=-(\nabla_0\mathbf{r})\cdot\nabla\nabla W=-\underline{A}\cdot\nabla\nabla W\ . \quad (28)$$

At $t=t_0$ we require that $\underline{A}=\underline{I}$ and $m\underline{B}=\nabla_0\nabla_0 S_0(\mathbf{r}_0)$. Note that the closed set of equations (14), (16), (17), (27), and (28) do not involve the gradient with respect to $\mathbf{r}$ of any of the unknowns, and that $\nabla\nabla W$ is given. Thus the system can be integrated along one characteristic at a time. If W is an analytic function of $\mathbf{r}$, then $\mathbf{r}(\mathbf{r}_0,t)$ will be an analytic function of $\mathbf{r}_0$.

Note that H as given by (6) is just the Hamiltonian, and $L=\frac{1}{2}mv^2-W$ is the Lagrangian, whence if $\mathbf{p}=m\mathbf{v}$ Eqs. (17) and (14) can be written in the Hamiltonian form

$$\dot{\mathbf{r}}=\frac{\partial H}{\partial p},\quad \dot{\mathbf{p}}=-\frac{\partial H}{\partial r}\ , \quad (29)$$

while consequent to (16) S is clearly the action.

It is evident from (18) that the neglect of the term in $\nabla^2 a$ in (5) becomes invalid as one approaches a surface $J=0$, conventionally termed a caustic. One can, however, solve (1) locally in a neighborhood straddling the caustic and display how that solution matches onto the eikonal approximation. For this we require the normal to the caustic and the behavior of J as one approaches the caustic. Now if $W(\mathbf{r},t)$ is at least thrice differentiable with respect to $\mathbf{r}$ it follows from differentiation of (27) and (28) that $\nabla_0\nabla_0\mathbf{r}$ exists, and hence on viewing J as a function of $\mathbf{r}_0,t$ that $\nabla_0 J$ exists, since J is cubic in terms of the form $\partial x_i/\partial x_{0j}$, where x_i and x_{0j} are Cartesian components. But on using the chain rule

$$\nabla_0 J=(\nabla_0\mathbf{r})\cdot\nabla J=\underline{A}\cdot\nabla J\ . \quad (30)$$

Let $\underline{A}^a$ be the adjoint of $\underline{A}$, that is, that matrix the elements of which are the cofactors of their counterparts in $\underline{A}$. Then

$$\underline{A}^{-1}=J^{-1}\underline{A}^a\,\mathrm{sgn}\det\underline{A}$$

and

$$\nabla J=J^{-1}\underline{A}^a\cdot(\nabla_0 J)\,\mathrm{sgn}\det\underline{A}\ . \quad (31)$$

Now the elements of $\underline{A}^a$ are also products of terms of the form $\partial x_i/\partial x_{0j}$, whence it follows from (31) that ∇J diverges as one approaches the caustic $J=0$. But returning to (30), since $\nabla_0 J$ is bounded as one approaches the caustic and ∇J diverges, it follows that ∇J must tend towards parallelism with the unit vector $\mathbf{n}$ satisfying

$$\underline{A}\cdot\mathbf{n}=\mathbf{0} \quad (32)$$

which exists since $J=\det\underline{A}=\det\underline{A}=0$. Moreover, if we multiply (30) by J there results

$$\nabla(\tfrac{1}{2}J^2)=\underline{A}^a\cdot(\nabla_0 J)\,\mathrm{sgn}\det\underline{A} \quad (33)$$

which is well behaved as $J\to 0$. Let $\mathbf{R}(t)$ be a point on the caustic. Then if we introduce a local Cartesian coordinate system ξ,η,ζ, with the ζ axis parallel to $\mathbf{n}(\mathbf{R})$ and its origin at $\mathbf{R}$, Eq. (33) implies

$$\left.\frac{\partial J^2}{\partial\zeta}\right|_{\mathbf{r}=\mathbf{R}}=2\mathbf{n}\cdot\underline{A}^a\cdot\nabla_0 J\,|_{\mathbf{r}=\mathbf{R}}=G(\xi,\eta,t) \quad (34)$$

whence near $\mathbf{r}=\mathbf{R}$

$$J^2=\zeta G(\xi,\eta,t)+O(\zeta^2)\ . \quad (35)$$

The square root of (35) employed in (18) yields

$$a \approx a_0 G^{-1/4}\zeta^{-1/4} = a_0 G^{-1/4} \,|\, \mathbf{n}\cdot(\mathbf{r}-\mathbf{R}) \,|^{-1/4} , \quad (36)$$

giving the local behavior near a caustic, provided that $G \neq 0$ as we shall assume. When G vanishes one must work to higher order in ζ.

The velocity relative to the, in general, moving caustic is tangent to the caustic. To demonstrate this note that on any surface $J = $const,

$$\dot{J} = \frac{\partial J}{\partial t} + \mathbf{v}\cdot\nabla J . \quad (37)$$

Moreover, since $\mathbf{R}$ is a position vector which moves with this surface

$$0 = \frac{\partial J}{\partial t} + \dot{\mathbf{R}}\cdot\nabla J . \quad (38)$$

Thus (37) can be written

$$\dot{J} = (\mathbf{v}-\dot{\mathbf{R}})\cdot\nabla J . \quad (39)$$

But $\dot{J}$ is bounded, even on the caustic where ∇J is not. Thus on the caustic

$$\mathbf{n}\cdot(\mathbf{v}-\dot{\mathbf{R}}) = 0 . \quad (40)$$

That is, the caustic is an envelope of the characteristic curves.

One can solve (1) approximately in a boundary layer straddling the caustic and match asymptotically to the eikonal solution. To this end we require an approximate expression for S in the neighborhood of the caustic. This may be determined via a local integration of

$$\nabla\mathbf{v} = (\nabla\mathbf{r}_0)\cdot\nabla_0\mathbf{v} = J^{-1}(\nabla_0\mathbf{r})^a\cdot\nabla_0\mathbf{v} \,\mathrm{sgn}\det\nabla_0\mathbf{r} , \quad (41)$$

which near the caustic, on using (35), behaves like

$$\nabla\mathbf{v} = \zeta^{-1/2}\mathbf{n}\mathbf{b} , \quad (42)$$

where $\mathbf{b} = G^{-1/2}\mathbf{n}(\nabla_0\mathbf{r})^a\cdot\nabla_0\mathbf{v}$. The form of the dyadic in (42) is determined by the requirement that $\nabla\times(\nabla\mathbf{v}) = 0$, since $\nabla\zeta = \mathbf{n}$. Integration of (43) locally yields

$$\mathbf{v}(\mathbf{r},t) = \mathbf{v}(\mathbf{R},t) + 2\zeta^{1/2}\mathbf{b} + \cdots . \quad (43)$$

Since $\nabla\times\mathbf{v} = 0$ it follows that $\mathbf{b} = c\mathbf{n}$, with $c = G^{-1/2}\mathbf{n}\cdot(\nabla_0\mathbf{r})^a\cdot(\nabla_0\mathbf{v})\cdot\mathbf{n}$ evaluated at $\mathbf{r} = \mathbf{R}$. Since $m\mathbf{v} = \nabla S$ a further integration yields

$$S(\mathbf{r},t) = S(\mathbf{R},t) + m\mathbf{v}(\mathbf{R},t)\cdot(\mathbf{r}-\mathbf{R}) + \tfrac{4}{3}\zeta^{3/2}cm + \cdots . \quad (44)$$

Note that (43) implies on using (40)

$$[\mathbf{v}(\mathbf{r},t) - \dot{\mathbf{R}}]^2 = [\mathbf{v}(\mathbf{R},t) - \dot{\mathbf{R}}]^2 + 4c^2\zeta . \quad (45)$$

In order to solve (1) in the boundary layer straddling the caustic we factor out the dominant variation tangent to the caustic by writing

$$\psi = \phi e^{i\sigma/\hbar} , \quad (46)$$

where

$$\sigma(\mathbf{r},t) = S(\mathbf{R},t) + m\mathbf{v}(\mathbf{R},t)\cdot(\mathbf{r}-\mathbf{R}) . \quad (47)$$

Then (1) implies, on using (8) to eliminate $\partial\mathbf{v}/\partial t$,

$$0 = -\left[\frac{\partial S(\mathbf{R},t)}{\partial t} + \frac{1}{2}m\mathbf{v}(\mathbf{R},t)^2 + W(\mathbf{r},t) - m[\mathbf{v}(\mathbf{R},t) - \dot{\mathbf{R}}]\cdot[\nabla_R\mathbf{v}(\mathbf{R},t)]\cdot(\mathbf{r}-\mathbf{R}) - (\mathbf{r}-\mathbf{R})\cdot\nabla_R W(\mathbf{R},t)\right]\phi$$
$$+ i\hbar\left[\frac{\partial\phi}{\partial t} + \mathbf{v}(\mathbf{R},t)\cdot\nabla\phi\right] + \frac{\hbar^2}{2m}\nabla^2\phi . \quad (48)$$

But if we use (7) evaluated at $\mathbf{r} = \mathbf{R}$, Eq. (48) can be rewritten as

$$0 = \left((\mathbf{r}-\mathbf{R})\cdot\nabla_R\{\tfrac{1}{2}m[\mathbf{v}(\mathbf{R},t) - \dot{\mathbf{R}}]^2\} - \tfrac{1}{2}(\mathbf{r}-\mathbf{R})(\mathbf{r}-\mathbf{R}):\nabla_R\nabla_R W(\mathbf{R},t) + \cdots\right)\phi$$
$$+ i\hbar\left[\frac{\partial\phi}{\partial t} + \dot{\mathbf{R}}\cdot\nabla\phi + [\mathbf{v}(\mathbf{R},t) - \dot{\mathbf{R}}]\cdot\nabla\phi\right] + \frac{\hbar^2}{2m}\nabla^2\phi , \quad (49)$$

where we have made a Taylor-series expansion of $W(\mathbf{r},t)$, and used the property that $\nabla\mathbf{v} = \nabla\nabla S$ is symmetric. Now in the boundary layer we expect that $\mathbf{n}\cdot\nabla\phi$ is much larger than $\mathbf{n}\times\nabla\phi$, and that $\partial\phi/\partial t + \dot{\mathbf{R}}\cdot\nabla\phi$, the time derivative of ϕ as seen by an observer moving with the caustic, is small. Thus (49) may be approximated near $\zeta = 0$ by

$$0 = 2mc^2\zeta\phi + \frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial\zeta^2} \quad (50)$$

provided that c is not so small as to require retention of higher terms in the Taylor series, which we shall assume.

Let

$$\frac{1}{l^3} = \frac{4m^2c^2}{\hbar^2} . \quad (51)$$

Then with l positive that solution of (50) which vanishes for $\zeta \to -\infty$ is[9]

$$\phi = D\,\mathrm{Ai}(-\zeta/l) , \quad (52)$$

where $\mathrm{Ai}(z)$ is the Airy function, whence ϕ has the asymptotic forms in ζ

$$\phi \sim \begin{cases} D\pi^{-1/2}\zeta^{-1/4}\sin\left[\dfrac{2}{3}\left[\dfrac{\zeta}{l}\right]^{3/2} + \dfrac{\pi}{4}\right] & \text{as } \zeta \to \infty , \quad (53) \\[2ex] \dfrac{D}{2\pi^{1/2}}(-\zeta)^{-1/4}\exp\left[-\dfrac{2}{3}\left[-\dfrac{\zeta}{l}\right]^{3/2}\right] & \text{as } \zeta \to -\infty . \end{cases}$$
$$(54)$$

Now, as $\zeta=\mathbf{n}\cdot(\mathbf{r}-\mathbf{R})\to 0+$, that characteristic incident on the caustic has $\mathbf{n}\cdot[\mathbf{v}(\mathbf{r},t)-\dot{\mathbf{R}}]<0$. Equation (42) with $\mathbf{b}=c\mathbf{n}$ then implies $c<0$. Thus following (44) the associated eikonal behaves near $\zeta\approx 0$ like

$$\psi_{\rm in}=a_{\rm in}\zeta^{-1/4}\exp\left\{i\left[\frac{\sigma}{\hbar}-\frac{2}{3}\left[\frac{\zeta}{l}\right]^{3/2}\right]\right\}, \tag{55}$$

where $a_{\rm in}$ is independent of ζ. But (53) implies that near $\zeta=0$

$$\psi=F(\xi,\eta,t)\zeta^{-1/4}\exp\left[i\frac{\sigma}{\hbar}\right]\times\left\{\exp\left[-i\frac{2}{3}\left[\frac{\zeta}{l}\right]^{3/2}\right]-i\exp\left[-i\frac{2}{3}\left[\frac{\zeta}{l}\right]^{3/2}\right]\right\}. \tag{56}$$

Let $\psi_{\rm out}$ be a second eikonal which near $\zeta=0$ behaves likes

$$\psi_{\rm out}=-ia_{\rm in}\zeta^{-1/4}\exp\left\{i\left[\frac{\sigma}{\hbar}+\frac{2}{3}\left[\frac{\zeta}{l}\right]^{3/2}\right]\right\}. \tag{57}$$

In order to have a matched asymptotic expansion with (56) we must write ψ as the sum of (55) and (57). Note that the local wavelength associated with an eikonal is $\lambda=h/mv$, while l measures the width of the boundary layer straddling the caustic. Clearly, in order that the boundary-layer analysis be valid it is necessary that l be much less than the smaller principal radius of curvature of the caustic at the point $\mathbf{R}$ in the neighborhood of which one makes the local analysis. Moreover, if there is more than one caustic, they must be separated by distances much greater than l, or else the boundary-layer analysis must be modified to allow for barrier penetration. Evidently as the number of caustics goes up the bookkeeping associated with the asymptotic matching becomes complicated. If c is small or zero the boundary-layer analysis must be modified, which calculation we will not present here.

There is also the problem of fitting a single eikonal to a given initial condition $\psi(\mathbf{r},0)$. For a steady-state scattering problem the task is easy since one has only to stipulate the incident monochromatic plane wave. For a bound-state problem the association of the eikonal with $\psi(\mathbf{r},0)$ is not unique. Indeed, when one notes that for any square-integrable initial condition with $W=0$ the natural tool would be a Fourier integral in $\mathbf{r}$, an integral over eikonals would seem to be the natural extension for a slowly varying W. This latter notion is developed in detail in Sec. III.

III. THE GENERALIZED FOURIER INTEGRAL AND THE LIMIT $h\to 0$

We now develop a method for solving the Schrödinger equation appropriate to localized wave functions of short local wavelength in the limit $h\to 0$. This involves so-called generalized Fourier integrals introduced by Hazak[3,4] for similar problems in the geometric optics of plasmas. The technique involves the approximate construction of the Green's function for the initial-value problem associated with (1) and leads to a representation involving integrals over eikonals. That is, we wish to write

$$\psi(\mathbf{r},t)=\int d^3r_0\,K(\mathbf{r},\mathbf{r}_0,t)\psi(\mathbf{r}_0,0)\ . \tag{58}$$

For this purpose we define a transformation from independent variables $\mathbf{r}_0,\mathbf{v}_0$ to $\mathbf{r},\mathbf{v}$ via the system of ordinary differential equations

$$\dot{\mathbf{r}}=\mathbf{v},\quad \mathbf{r}(0)=\mathbf{r}_0\ , \tag{59}$$

$$m\dot{\mathbf{v}}=-\nabla V,\quad \mathbf{v}(0)=\mathbf{v}_0\ , \tag{60}$$

with the associated action generated via

$$\dot{S}=\tfrac{1}{2}mv^2-V,\quad S(0)=m\mathbf{v}_0\cdot\mathbf{r}_0\ . \tag{61}$$

Clearly one can use any of the sets $\mathbf{k},\mathbf{v}$; $\mathbf{k}_0,\mathbf{v}_0$; $\mathbf{k}_0,\mathbf{v}$; or $\mathbf{k},\mathbf{v}_0$ as variables to locate a point in the six-dimensional phase space. Since $\mathbf{v}_0$ is now an independent variable it follows from the theory of ordinary differential equations that the transformation from $\mathbf{r}_0,\mathbf{v}_0$, to $\mathbf{r},\mathbf{v}$ is one-to-one.

Parallel to (18) we define

$$J(\mathbf{v}_0,\mathbf{r},t)=\frac{\partial(\mathbf{v}_0,\mathbf{r})}{\partial(\mathbf{v}_0,\mathbf{r}_0)}=|\det\nabla_0\mathbf{r}(\mathbf{v}_0,\mathbf{r}_0,t)|\ . \tag{62}$$

Since (59) and (60) are Hamiltonian the Jacobian

$$\frac{\partial(\mathbf{v}_0,\mathbf{r}_0)}{\partial(\mathbf{v},\mathbf{r})}=1\ . \tag{63}$$

But one can write[10]

$$\frac{\partial(\mathbf{v}_0,\mathbf{r}_0)}{\partial(\mathbf{v},\mathbf{r})}=\frac{\partial(\mathbf{v}_0,\mathbf{r})}{\partial(\mathbf{v},\mathbf{r})}\frac{\partial(\mathbf{v}_0,\mathbf{r}_0)}{\partial(\mathbf{v}_0,\mathbf{r})}=\frac{\partial(\mathbf{v}_0,\mathbf{r})}{\partial(\mathbf{v},\mathbf{r})}\left[\frac{\partial(\mathbf{v}_0,\mathbf{r})}{\partial(\mathbf{v}_0,\mathbf{r}_0)}\right]^{-1} \tag{64}$$

whence on using (62) and (63)

$$J=\frac{\partial(\mathbf{v}_0,\mathbf{r})}{\partial(\mathbf{v},\mathbf{r})}\ . \tag{65}$$

Note that initially $J=1$, and that by the same arguments used in Sec. II it is bounded. Moreover, J is independent of $\hbar$.

The GFI are defined in terms of objects akin to $e^{i\mathbf{k}\cdot\mathbf{r}}$, viz.,

$$g(\mathbf{v}_0,\mathbf{r},t)=[J(\mathbf{v}_0,\mathbf{r},t)]^{-1/2}\exp[iS(\mathbf{v}_0,\mathbf{r},t)/\hbar] \tag{66}$$

which in the limit $\hbar\to 0$ enjoy the property

$$\int d^3v_0\,g^*(\mathbf{v}_0,\mathbf{r},t)g(\mathbf{v}_0,\mathbf{r}',t)=\int d^3v_0[J(\mathbf{v}_0,\mathbf{r},t)J(\mathbf{v}_0,\mathbf{r}',t)]^{-1/2}\times\exp\{i[S(\mathbf{v}_0,\mathbf{r},t)-S(\mathbf{v}_0,\mathbf{r}',t)]/\hbar\}\sim(2\pi\hbar/m)^3\delta(\mathbf{r}-\mathbf{r})\ . \tag{67}$$

To prove (67) note that the condition that the phase $[S(\mathbf{v}_0,\mathbf{r},t)-S(\mathbf{v}_0,\mathbf{r}',t)]/\hbar$ be stationary is

$$\mathbf{R}(\mathbf{v}_0,\mathbf{r},t)=\mathbf{R}(\mathbf{v}_0,\mathbf{r}',t)\ , \tag{68}$$

where

$$m\,\mathbf{R}(\mathbf{v}_0,\mathbf{r},t)=\partial S(\mathbf{v}_0,\mathbf{r},t)/\partial \mathbf{v}_0 \,. \tag{69}$$

[Note that this use of the symbol $\mathbf{R}$ is distinct from that after Eq. (33).] But since $m\mathbf{v}=\nabla S(\mathbf{v}_0,\mathbf{r},t)$

$$\begin{aligned} m\dot{\mathbf{R}} &= m\left[\frac{\partial \mathbf{R}}{\partial t}+\dot{\mathbf{r}}\cdot\nabla\mathbf{R}\right] \\ &= m\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right]\frac{\partial S}{\partial \mathbf{v}_0} \\ &= m\frac{\partial}{\partial \mathbf{v}_0}\left[\frac{\partial S}{\partial t}+\mathbf{v}\cdot\nabla S\right]-m\left[\frac{\partial}{\partial \mathbf{v}_0}\mathbf{v}\right]\cdot\nabla S \\ &= m\frac{\partial}{\partial \mathbf{v}_0}\left[\frac{1}{2}mv^2-V\right]-m\left[\frac{\partial}{\partial \mathbf{v}_0}\mathbf{v}\right]\cdot m\mathbf{v} \\ &= 0\,, \end{aligned} \tag{70}$$

where we have employed (61). Thus

$$\mathbf{R}(\mathbf{v}_0,\mathbf{r},t)=\mathbf{R}(\mathbf{v}_0,\mathbf{r}_0,0)=\frac{\partial}{\partial \mathbf{v}_0}\frac{1}{m}S(\mathbf{v}_0,\mathbf{r}_0,0)=\frac{\partial}{\partial \mathbf{v}_0}\mathbf{v}_0\cdot\mathbf{r}_0 = \mathbf{r}_0 \tag{71}$$

whence (68) requires that $\mathbf{r}_0=\mathbf{r}_0'$ which implies $\mathbf{r}=\mathbf{r}'$ since the transformation $\mathbf{v}_0,\mathbf{r}_0$ to $\mathbf{v}_0,\mathbf{r}$ is one-to-one. Thus if $\mathbf{r}\neq\mathbf{r}'$, in the limit $\hbar\rightarrow 0$, the integral in (67) must vanish because of the rapidly oscillating phase and smooth $\hbar$ independent behavior of J. When $\mathbf{r}'\sim\mathbf{r}$ one can make a Taylor-series expansion about $\mathbf{r}'=\mathbf{r}$, whence on keeping lowest-significant-order terms (67) becomes, on using (65) and transforming to $\mathbf{v}$ as the variable of integration,

$$\begin{aligned} &\int d^3v_0[J(\mathbf{v}_0,\mathbf{r},t)]^{-1}\exp[i(\mathbf{r}-\mathbf{r}')\cdot\nabla S(\mathbf{v}_0,\mathbf{r},t)/\hbar] \\ &\quad= \int d^3v\frac{\partial(\mathbf{v}_0,\mathbf{r})}{\partial(\mathbf{v},\mathbf{r})}[J(\mathbf{v}_0,\mathbf{r},t)]^{-1}\exp[i(\mathbf{r}-\mathbf{r}')\cdot m\mathbf{v}/\hbar] \\ &\quad= \int d^3v\,\exp[i(\mathbf{r}-\mathbf{r}')\cdot m\mathbf{v}/\hbar] \\ &\quad=(2\pi\hbar/m)^3\delta(\mathbf{r}-\mathbf{r}'),\quad \text{Q.E.D.} \end{aligned} \tag{72}$$

It can be argued in parallel fashion that

$$\int d^3r\,g^*(\mathbf{v}_0,\mathbf{r},t)g(\mathbf{v}_0',\mathbf{r},t)=(2\pi\hbar/m)^3\delta(\mathbf{v}_0-\mathbf{v}_0')\,. \tag{73}$$

These properties can be used to solve (1) in the limit $\hbar\rightarrow 0$. Multiply (1) by $g^*(\mathbf{v}_0,\mathbf{r},t)$ and integrate with respect to $\mathbf{r}$:

$$\begin{aligned} 0 &= \int d^3r\,g^*\left[i\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m}\nabla^2\psi-V\psi\right] \\ &= \int d^3r\left[i\hbar\frac{\partial}{\partial t}(g^*\psi)+\frac{\hbar^2}{2m}\nabla\cdot(g^*\nabla\psi-\psi\nabla g^*)\right. \\ &\qquad\left.+\psi\left[-i\hbar\frac{\partial g^*}{\partial t}+\frac{\hbar^2}{2m}\nabla^2 g^*-Vg^*\right]\right]. \end{aligned} \tag{74}$$

The divergence in the integrand, on using Gauss' theorem, integrates to zero for the localized wave functions considered here. Moreover, g is just the eikonal discussed in Sec. I with $\mathbf{v}_0$ the same for all $\mathbf{r}_0$, whence

$$-i\hbar\frac{\partial g^*}{\partial t}+\frac{\hbar^2}{2m}\nabla^2 g^*-Vg^*=\frac{\hbar^2}{2m}[\exp(-iS/\hbar)]\nabla^2 J^{-1/2}\,. \tag{75}$$

Clearly, away from caustics one can neglect the right-hand side in the limit $\hbar\rightarrow 0$.

Let us for the time being assume that there are no caustics. Then to lowest significant order in the small parameter h

$$0=\frac{\partial}{\partial t}\int d^3r\,g^*\psi \tag{76}$$

whence

$$\int d^3r'\,g^*(\mathbf{v}_0,\mathbf{r}',t)\psi(\mathbf{r}',t) = \int d^3r_0\,g^*(\mathbf{v}_0,\mathbf{r}_0,0)\psi(\mathbf{r}_0,0)\,. \tag{77}$$

Multiply (77) by $g(\mathbf{v}_0,\mathbf{r},t)$ and integrate with respect to $\mathbf{v}_0$. There results, on using (67),

$$\psi(\mathbf{r},t)=(m/2\pi\hbar)^3\int d^3v_0\,g(\mathbf{v}_0,\mathbf{r},t) \times\int d^3r_0\,g^*(\mathbf{v}_0,\mathbf{r}_0,0)\psi(\mathbf{r}_0,0) \tag{78}$$

whence

$$K(\mathbf{r},\mathbf{r}_0,t)=(m/2\pi\hbar)^3\int d^3v_0\,g(\mathbf{v}_0,\mathbf{r},t)g^*(\mathbf{v}_0,\mathbf{r}_0,0)\,. \tag{79}$$

Note that by virtue of the initial condition in (61), $J(\mathbf{v}_0,\mathbf{r}_0,t_0)=1$, and

$$g^*(\mathbf{v}_0,\mathbf{r}_0,0)=\exp(i\mathbf{v}_0\cdot\mathbf{r}_0/\hbar)\,. \tag{80}$$

Thus if

$$a_0(\mathbf{v}_0)=(m/2\pi\hbar)^3\int d^3r_0\,\psi(\mathbf{r}_0,0)\exp(-im\mathbf{v}_0\cdot\mathbf{r}_0/\hbar) \tag{81}$$

then

$$a(\mathbf{v}_0,\mathbf{r},t)=[J(\mathbf{v}_0,\mathbf{r},t)]^{-1/2}a_0(\mathbf{v}_0) \tag{82}$$

and (77) can be written

$$\psi(\mathbf{r},t)=\int d^3v_0\,a(\mathbf{v}_0,\mathbf{r},t)\exp[iS(\mathbf{v}_0,\mathbf{r},t)/\hbar]\,, \tag{83}$$

an integral over eikonals. If we use $\mathbf{v}$ in place of $\mathbf{v}_0$ as the variable of integration (83) yields

$$\psi(\mathbf{r},t)=\int d^3v\,Ja_0g=\int d^3v\,J^{1/2}a_0\exp(iS/\hbar)\,. \tag{84}$$

Alternatively one can write

$$\psi(\mathbf{r},t)=\int d^3v_0\,a_0(\mathbf{v}_0)g(\mathbf{v}_0,\mathbf{r},t)\,. \tag{85}$$

Consider (85) and let there now be caustics. Note that for those points $\mathbf{v}_0,\mathbf{r}$ away from caustics the generalized Fourier amplitude g has been constructed to satisfy the Schrödinger equation (1) with a fractional error proportional to $\hbar$. This property fails in a boundary layer straddling a caustic $J(\mathbf{v}_0,\mathbf{r},t)=0$, which is now a surface in $\mathbf{v}_0$ space, with $\mathbf{r}$ and t fixed. This defect can be remedied by using (56) or its counterpart matched asymptotically to $g(\mathbf{v}_0,r,t)$ in such a boundary layer. But the effective width Δ of the boundary layer is determined by the condition that $\zeta/l=-\mathbf{n}\cdot(\mathbf{r}-\mathbf{R})/l=-\mathbf{n}\cdot(\mathbf{r}-\mathbf{R})\times(4mc^2c^2/h^2)^{3/2}\approx 1$. Let $\mathbf{r}$ be a point on the caustic. Then if $\boldsymbol{\Delta}$ is the change in $\mathbf{r}$ required to change ζ from zero to l, it follows that $\boldsymbol{\Delta}\cdot\partial\zeta/\partial\mathbf{v}\approx l$ whence $\Delta=O(h^{4/3})$. Clearly, as long as the volume in $\mathbf{v}_0$ space associated with boundary layers around caustics is small compared with the volume external to boundary layers which contributes dominantly to the integral in (85), then (85) will be a good approximation. The details of the development of caustics in two and three dimensions when $\partial W/\partial t\neq 0$ is still an open question, but clearly there are difficulties when the caustics become so dense that the effective volume of their associated boundary layers is dominant, and the generalized Fourier integral method may be expected to fail. Note, however, that formally, for a fixed distribution of caustics, the thickness of the boundary layers and hence their volume go to zero so $\hbar\to 0$. Note too that if one uses (84) where the Jacobian occurs as $J^{1/2}$, the contribution of caustic boundary layers would seem reduced.

Under certain circumstances the integral over $\mathbf{v}_0$ in (85) can be carried out approximately. To this end we write (85) in the form

$$\psi(\mathbf{r},t)=(m/h)^3\int d^3r_0'\int d^3v_0\,\psi(\mathbf{r}_0',0)[J(\mathbf{v}_0,\mathbf{r},t)]^{-1/2}\times\exp\{(i/\hbar)[S(\mathbf{v}_0,\mathbf{r},t)-m\mathbf{v}_0\cdot\mathbf{r}_0']\}\ . \quad (86)$$

Consider the $\mathbf{v}_0$ dependence of the integrand in (86). Note that $J_0(\mathbf{v}_0,\mathbf{r},t)$ is independent of $\hbar$, while the phase $(i/\hbar)[S(\mathbf{v}_0,\mathbf{r},t)-m\mathbf{v}_0\cdot\mathbf{r}_0']$ is large in the limit $\hbar\to 0$ and gives rise to very rapid oscillations when exponentiated. The phase is stationary[12] when

$$0=\frac{\partial S(\mathbf{v}_0,\mathbf{r},t)}{\partial\mathbf{v}_0}-m\mathbf{r}_0'=m[\mathbf{r}_0(\mathbf{v}_0,\mathbf{r},t)-\mathbf{r}_0']\ , \quad (87)$$

where we have used (69) and (71). Equation (87) has but one solution since the transformation from $\mathbf{r}_0,\mathbf{v}_0,t_0$ to $\mathbf{r},\mathbf{v},t$ is one-to-one. Let $\mathbf{u}(\mathbf{r}_0',\mathbf{r},t)$ be such that $\mathbf{r}_0(\mathbf{u},\mathbf{r},t)=\mathbf{r}_0'$. Then if

$$\underline{Q}(\mathbf{r}_0',\mathbf{r},t)=\left.\frac{\partial^2 S(\mathbf{v}_0,\mathbf{r},t)}{\partial\mathbf{v}_0\,\partial\mathbf{v}_0}\right|_{\mathbf{v}_0=\mathbf{u}} \quad (88)$$

one can on Taylor-series expansion write (86) as

$$\psi(\mathbf{r},t)=(m/h)^3\int d^3r_0'\int d^3v_0\,\psi(\mathbf{r}_0',0)[J^2(\mathbf{u},\mathbf{r},t)+\cdots]^{-1/4}\times\exp\{(i/\hbar)[S(\mathbf{u},\mathbf{r},t)+\tfrac{1}{2}(\mathbf{v}_0-\mathbf{u})(\mathbf{v}_0-\mathbf{u}){:}\underline{Q}+\cdots-m\mathbf{u}\cdot\mathbf{r}_0']\}\ . \quad (89)$$

The symmetric dyadic $\underline{Q}$ can be written in its principal axis representation as

$$\underline{Q}=Q_1\mathbf{e}_1\mathbf{e}_1+Q_2\mathbf{e}_2\mathbf{e}_2+Q_3\mathbf{e}_3\mathbf{e}_3\ , \quad (90)$$

where the Q_j are the eigenvalues of $\underline{Q}$, and in parallel fashion one can let

$$\mathbf{v}_0-\mathbf{u}=v_1\mathbf{e}_1+v_2\mathbf{e}_2+v_3\mathbf{e}_3\ . \quad (91)$$

Suppose that $J(\mathbf{v}_0,\mathbf{r},t)$ and $\underline{Q}(\mathbf{v}_0,\mathbf{r},t)$ do not change much when $\mathbf{v}_0-\mathbf{u}$ changes by an amount of the order of $(\min\{|Q_j|\}/\hbar)^{-1/2}$. Then it is adequate to retain only the terms shown explicitly in (89), and since for real β

$$\int_{-\infty}^{\infty}dx\,\exp(\tfrac{1}{2}i\beta x^2)=(2\pi/|\beta|)^{1/2}\exp(\tfrac{1}{4}i\pi\,\mathrm{sgn}\beta)\ , \quad (92)$$

(89) reduces to

$$\psi(\mathbf{r},t)=(m/h)^{3/2}\int d^3r_0'\,\psi(\mathbf{r}_0',0)[J(\mathbf{u},\mathbf{r},t)]^{-1/2}|Q_1Q_2Q_3|^{-1/2}\times\exp\{\tfrac{1}{4}i\pi(\mathrm{sgn}Q_1+\mathrm{sgn}Q_2+\mathrm{sgn}Q_3)+i[s(\mathbf{u},\mathbf{r},t)-m\mathbf{u}\cdot\mathbf{r}_0']/\hbar\}\ . \quad (93)$$

In principle one must verify that the terms neglected in the Taylor series in (89) indeed make a negligible contribution. This is likely to fail when the caustics are dense or stochasticity sets in, since then derivatives are large. When $W(\mathbf{r},t)=0$ Eq. (93) reduces to the exact result

$$\psi(\mathbf{r},t)=(m/ht)^{3/2}\exp(-\tfrac{1}{4}\pi i)\times\int d^3r_0\,\psi(\mathbf{r}_0,0)\exp[im(\mathbf{r}-\mathbf{r}_0)^2/2\hbar t]\ . \quad (94)$$

When J is small in the neighborhood of the stationary point a local expansion can be employed and the integral redone, though the significance of the result is in question.

The probability per unit volume of finding the particle described by $\psi(\mathbf{r},t)$ is $P(\mathbf{r},t)=|\psi(\mathbf{r},t)|^2$. Note that P varies on a scale length L of the order of that characterizing $\psi(\mathbf{r},0)$ or smaller. Moreover, considered as a function the integrand of

$$P(\mathbf{r},t)=\int d^3\mathbf{v}_0\int d^3\mathbf{v}_0'\,a(\mathbf{v}_0,\mathbf{r},t)a^*(\mathbf{v}_0',\mathbf{r},t)\times\exp\{(i/\hbar)[S(\mathbf{v}_0,\mathbf{r},t)-S(\mathbf{v}_0',\mathbf{r},t)]\} \quad (95)$$

has no stationary points of the phase $(i/\hbar)[S(\mathbf{v}_0,\mathbf{r},t)-S(\mathbf{v}_0',\mathbf{r},t)]$ since the condition that there be such

$$0=\nabla S(\mathbf{v}_0,\mathbf{r},t)-\nabla S(\mathbf{v}_0',\mathbf{r},t)=\mathbf{v}(\mathbf{v}_0,\mathbf{r},t)-\mathbf{v}(\mathbf{v}_0',\mathbf{r},t) \quad (96)$$

has no solutions for $\mathbf{v}_0\neq\mathbf{v}_0'$, since the transformation from $\mathbf{v}_0,\mathbf{r}_0,t_0$ to $\mathbf{v},\mathbf{r},t$ is one-to-one. Clearly, as $\hbar\to 0$ with $\mathbf{v}_0\neq\mathbf{v}_0'$ the integrand is a rapidly oscillating function of $\mathbf{r}$ and for calculating an integral of P over a domain of size greater than L^3 we may set $\mathbf{v}_0=\mathbf{v}_0'$. This notion can be made more precise by introducing the new variables

$$\boldsymbol{\nu}=\tfrac{1}{2}(\mathbf{v}_0+\mathbf{v}_0'),\quad \mathbf{u}=\mathbf{v}_0-\mathbf{v}_0' , \tag{97}$$

with the inverse

$$\mathbf{v}_0=\boldsymbol{\nu}+\tfrac{1}{2}\mathbf{u},\quad \mathbf{v}_0'=\boldsymbol{\nu}-\tfrac{1}{2}\mathbf{u} . \tag{98}$$

Then (95) can be written

$$P(\mathbf{r},t)=(m/h)^6\int d^3r_0\int d^3r_0'\int d^3\nu\int d^3u\,\psi(\mathbf{r}_0,0)\psi^*(\mathbf{r}_0',0)[J(\boldsymbol{\nu}+\tfrac{1}{2}\mathbf{u},\mathbf{r},t)J(\boldsymbol{\nu}-\tfrac{1}{2}\mathbf{u},\mathbf{r},t)]^{-1/2}$$
$$\times\exp\{(i/\hbar)[S(\boldsymbol{\nu}+\tfrac{1}{2}\mathbf{u},\mathbf{r},t)-m\mathbf{r}_0\cdot(\boldsymbol{\nu}+\tfrac{1}{2}\mathbf{u})$$
$$-S(\boldsymbol{\nu}-\tfrac{1}{2}\mathbf{u},\mathbf{r},t)+m\mathbf{r}_0'\cdot(\boldsymbol{\nu}-\tfrac{1}{2}\mathbf{u})]\} . \tag{99}$$

For the purpose of coarse-grain averaging in $\mathbf{r}$ via integration with respect to $\mathbf{r}$ we Taylor-series expand in $\mathbf{u}$, keeping only the leading terms in J and the first two terms in S. The result is

$$P(\mathbf{r},t)=(m/h)^6\int d^3r_0\int d^3r_0'\int d^3\nu\int d^3u\,\psi(\mathbf{r}_0,0)\psi^*(\mathbf{r}_0',0)[J(\boldsymbol{\nu},\mathbf{r},t)]^{-1}$$
$$\times\exp\{(i/\hbar)[m\mathbf{u}\cdot[\mathbf{R}(\boldsymbol{\nu},\mathbf{r},t)-\tfrac{1}{2}(\mathbf{r}_0+\mathbf{r}_0')-m(\mathbf{r}_0-r_0')\cdot\boldsymbol{\nu}]\}$$
$$=(m/h)^3\int d^3r_0\int d^3r_0'\int d^3\nu\,\psi(\mathbf{r}_0,0)\psi^*(\mathbf{r}_0',0)[J(\boldsymbol{\nu},\mathbf{r},t)]^{-1}$$
$$\times[\exp(i/\hbar)m(\mathbf{r}_0'-\mathbf{r}_0)\cdot\boldsymbol{\nu}]\delta[\mathbf{R}(\boldsymbol{\nu},\mathbf{r},t)-\tfrac{1}{2}(\mathbf{r}_0+\mathbf{r}_0')] . \tag{100}$$

Define

$$f(\mathbf{v},\mathbf{r},t)$$
$$=(m/h)^3\int d^3r_0\int d^3r_0'\,\psi(\mathbf{r}_0,0)\psi^*(\mathbf{r}_0',0)$$
$$\times\exp[(i/\hbar)m\boldsymbol{\nu}\cdot(\mathbf{r}_0'-\mathbf{r}_0)]$$
$$\times\delta(\mathbf{R}(\boldsymbol{\nu},\mathbf{r},t)-\tfrac{1}{2}(\mathbf{r}_0+\mathbf{r}_0')) \tag{101}$$

and $\mathbf{v}(\boldsymbol{\nu},\mathbf{r},t)$ via (59) and (60), with $\mathbf{R}$ the initial position and $\boldsymbol{\nu}$ the initial velocity. Note that along the associated trajectory $\dot{\mathbf{R}}=\mathbf{0}$, $\dot{\boldsymbol{\nu}}=\mathbf{0}$. Equation (100) now reads

$$P(\mathbf{r},t)=\int d^3v\,f(\mathbf{v},\mathbf{r},t) , \tag{102}$$

where since f is a function of $\mathbf{R}$ and $\boldsymbol{\nu}$, it follows that when expressed in terms of $\mathbf{v},\mathbf{r},t$

$$0=\dot{\mathbf{f}}=\frac{\partial f}{\partial t}+\dot{\mathbf{r}}\cdot\nabla f+\dot{\mathbf{v}}\cdot\nabla_{\mathbf{r}}f$$
$$=\frac{\partial f}{\partial t}+\mathbf{v}\cdot\nabla f-\frac{1}{m}(\nabla W)\cdot\nabla_{\mathbf{v}}f . \tag{103}$$

Equation (103) is the well-known Vlasov equation,[13] but for a single electron. Equation (101) defines the Wigner distribution associated with $\psi(\mathbf{r}_0,0)$, as can be seen by introducing in (101) the new variables $\xi=\mathbf{r}-\mathbf{r}'$ and $\eta=\tfrac{1}{2}(\mathbf{r}+\mathbf{r}')$, in which event

$$f=(m/h)^3\int d^3\xi\,\psi(\mathbf{R}+\tfrac{1}{2}\xi,0)\psi^*(\mathbf{R}-\tfrac{1}{2}\xi\,0)e^{-im\mathbf{v}\cdot\xi/\hbar} . \tag{104}$$

Note that if we let ξ go into minus ξ, then f goes into its complex conjugate and hence must be real. Observe too that at t_0 one has $\mathbf{R}=\mathbf{r}$, $\boldsymbol{\nu}=\mathbf{v}$ whence it follows from (103) that

$$\int d^3v\,f=(m/h)^3\int d^3\xi\,\psi(\mathbf{r}-\tfrac{1}{2}\xi,0)\psi^*(\mathbf{r}-\tfrac{1}{2}\xi,0)\int d^3v\,e^{-im\mathbf{v}\cdot\xi/\hbar}$$
$$=(m/h)^3\int d^3\xi\,\psi(\mathbf{r}+\tfrac{1}{2}\xi,0)\psi^*(\mathbf{r}-\tfrac{1}{2}\xi,0)(2\pi)^3\delta(m\xi,\hbar)$$
$$=|\psi(\mathbf{r},0)|^2 \tag{105}$$

which is non-negative. Observe that in this development the Wigner distribution has emerged in a natural way.

For $t>t_0$ note that on using (63) and (104), and integrating over all $\mathbf{v}$, but an arbitrary finite domain in $\mathbf{r}$, one has

$$\int d^3r\int d^3v\,f=\int d^3R\int d^3v\,f$$
$$=(m/h)^3\int d^3R\int d^3\xi\int d^3V\int d^3\xi\,\psi(\mathbf{R}+\tfrac{1}{2}\xi,0)\psi^*(\mathbf{R}-\tfrac{1}{2}\xi,0)e^{-im\mathbf{u}\cdot\xi/\hbar} . \tag{106}$$

Suppose that for almost all values of $\mathbf{R}$ in the range of $\mathbf{R}$, the range in $\mathbf{u}$ can be taken to be effectively infinite. Then it follows directly that

$$\int d^3r\int d^3v\,f=\int d^3R\,|\psi(\mathbf{R},0)|^2 . \tag{107}$$

Thus although f itself need not be positive, its coarse-grained overage over $\mathbf{r}$ is non-negative.

Equation (85) has the disadvantage that more than one orbit can pass through a given point $\mathbf{r}$ at time t, which makes $\nabla J(\mathbf{v}_0,\mathbf{r},t)$ and $\nabla\nabla S(\mathbf{V}_0,\mathbf{r},t)$ singular on caustics.

Equation (84) has the advantage that the orbits in phase space never cross, and so if $W(\mathbf{r},t)$ is analytic, and $\psi(\mathbf{r},0)$ falls off exponentially as it does for a bound state, then J, S, and $\mathbf{a}_0$ are analytic functions of $\mathbf{r}$ and $\mathbf{v}$. To demonstrate this we note that when $\psi(\mathbf{r},0)$ falls off exponentially in $\mathbf{r}$, then a_0 as given by (81) possesses derivatives of arbitrarily high order with respect to $\mathbf{v}_0$, and hence is an analytic function of $\mathbf{v}_0$. Moreover, with $W(\mathbf{r},t)$ possessing arbitrarily high derivatives with respect to $\mathbf{r}$, Eqs. (59) and (60) can be differentiated arbitrarily with respect to $\mathbf{r}_0$ and $\mathbf{v}_0$, whence $\mathbf{r}$ and $\mathbf{v}$ and all derivatives thereof with respect to $\mathbf{r}_0$ and $\mathbf{v}_0$ exist and are constructed by integration of ordinary differential equations along trajectories. Thus $\mathbf{r}$, $\mathbf{v}$, J^2, and S are analytic functions of $\mathbf{r}_0,\mathbf{v}_0$.[14] This, as we shall now show, implies that they are analytic functions of $\mathbf{r}$ and $\mathbf{v}$.

To this end let $F(\mathbf{r}_0,\mathbf{v}_0)$ be any function analytic in $\mathbf{r}_0$ and $\mathbf{v}_0$. Then on using the chain rule

$$\left[\frac{\partial F}{\partial \mathbf{r}_0}\right]_{\mathbf{v}_0}=\left[\frac{\partial}{\partial \mathbf{r}_0}\mathbf{r}\right]\cdot\left[\frac{\partial F}{\partial \mathbf{r}}\right]_{\mathbf{v}}+\left[\frac{\partial}{\partial \mathbf{r}_0}\mathbf{v}\right]\cdot\left[\frac{\partial F}{\partial \mathbf{v}}\right]_{\mathbf{r}}, \tag{108}$$

$$\left[\frac{\partial F}{\partial \mathbf{v}_0}\right]_{\mathbf{r}_0}=\left[\frac{\partial}{\partial \mathbf{v}_0}\mathbf{r}\right]\cdot\left[\frac{\partial F}{\partial \mathbf{r}}\right]_{\mathbf{r}}+\left[\frac{\partial}{\partial \mathbf{v}_0}\mathbf{v}\right]\cdot\left[\frac{\partial F}{\partial \mathbf{v}}\right]_{\mathbf{r}}. \tag{109}$$

Let the 6×6 matrix formed by derivatives in Cartesian coordinates

$$\underline{\Delta}=\begin{bmatrix}\left[\dfrac{\partial}{\partial \mathbf{r}_0}\mathbf{r}\right]_{\mathbf{v}_0} & \left[\dfrac{\partial}{\partial \mathbf{r}_0}\mathbf{v}\right]_{\mathbf{v}_0}\\ \left[\dfrac{\partial}{\partial \mathbf{v}_0}\mathbf{r}\right]_{\mathbf{r}_0} & \left[\dfrac{\partial}{\partial \mathbf{v}_0}\mathbf{v}\right]_{\mathbf{r}_0}\end{bmatrix}. \tag{110}$$

Note that

$$\det\underline{\Delta}=\frac{\partial(\mathbf{r},\mathbf{v})}{\partial(\mathbf{r}_0,\mathbf{v}_0)}=1 \tag{111}$$

and that (108) and (109) can be written in the matrix form

$$\begin{bmatrix}\left.\dfrac{\partial F}{\partial \mathbf{r}_0}\right|_{\mathbf{v}_0}\\ \left.\dfrac{\partial F}{\partial \mathbf{v}_0}\right|_{\mathbf{r}_0}\end{bmatrix}=\underline{\Delta}\cdot\begin{bmatrix}\left.\dfrac{\partial F}{\partial \mathbf{r}}\right|_{\mathbf{v}}\\ \left.\dfrac{\partial F}{\partial \mathbf{v}}\right|_{\mathbf{r}}\end{bmatrix}. \tag{112}$$

But

$$\underline{\Delta}^{-1}=\underline{\Delta}^{a}/\det\underline{\Delta}=\underline{\Delta}^{a} \tag{113}$$

whence on inversion (112) yields

$$\begin{bmatrix}\left.\dfrac{\partial F}{\partial \mathbf{r}}\right|_{\mathbf{v}}\\ \left.\dfrac{\partial F}{\partial \mathbf{v}}\right|_{\mathbf{r}}\end{bmatrix}=\underline{\Delta}^{a}\begin{bmatrix}\left.\dfrac{\partial F}{\partial \mathbf{r}_0}\right|_{\mathbf{v}_0}\\ \left.\dfrac{\partial F}{\partial \mathbf{v}_0}\right|_{\mathbf{r}_0}\end{bmatrix}. \tag{114}$$

The right-hand side is a well-behaved function of $\mathbf{r}_0,\mathbf{v}_0$ and hence of $\mathbf{r},\mathbf{v}$. Thus $(\partial F/\partial \mathbf{r})_{\mathbf{v}}$ and $(\partial F/\partial \mathbf{v})_{\mathbf{r}}$ exist. Clearly iteration of this argument shows that all derivatives of F with respect to $\mathbf{r}$ and $\mathbf{v}$ exist.

IV. THE SURFACE-STATE ELECTRON PROBLEM

It is instructive to apply the GFI method to the SSE problem for which, in the absence of an external perturbation, the initial-value problem can be solved exactly. The associated Schrödinger equation is

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+W\psi\ , \tag{115}$$

where

$$W(x)=-\frac{e^2}{\epsilon x} \tag{116}$$

and ϵ is the dielectric constant of the layer of liquid helium to which the electron is bound by its image force. The conditions on the solutions are

$$\psi(0,t)=0\ , \tag{117}$$

$$\int dx\,|\psi(x,t)|^2=1\ , \tag{118}$$

and the range in x is zero to infinity.

It is convenient to introduce the Laplace transform

$$F(H,x)=\int_0^\infty dt\,\psi(x,t)\exp(iHt/\hbar)\ , \tag{119}$$

where $\mathrm{Im}H>0$. Then (116)–(118) imply

$$\frac{\hbar^2}{2m}\frac{d^2F}{dx^2}+\left[H+\frac{e^2}{\epsilon x}\right]F=i\hbar\psi(x,0)\ ,$$
$$F(H,0)=0,\quad F(H,\infty)=0\ . \tag{120}$$

Define

$$H=|H|\,e^{i\theta}\ , \tag{121}$$

$$\lambda=(-8mH/\hbar^2)^{1/2}=|8mH/\hbar^2|^{1/2}\exp[\tfrac{1}{2}i(\theta-\pi)]\ , \tag{122}$$

$$y=\lambda x\ , \tag{123}$$

$$\kappa=2me^2/\hbar^2\epsilon\lambda\ . \tag{124}$$

Then (120) is carried into

$$\frac{d^2F}{dy^2}+\left[-\frac{1}{4}+\frac{\kappa}{y}\right]F=-\frac{i\psi(x,0)\hbar}{4H}\ . \tag{125}$$

Let $M_{\kappa,1/2}(y)$ and $W_{\kappa,1/2}(y)$ be the Whittaker functions.[15,16] In the upper half H plane these have the asymptotic behavior

$$\Gamma(1-\kappa)M_{\kappa,1/2}(y)=y^{-\kappa}e^{y/2}\left[1+\frac{\kappa(\kappa+1)}{y}+\frac{\kappa(\kappa+1)^2(\kappa+2)}{2y^2}+\cdots\right], \tag{126}$$

$$W_{\kappa,1/2}(y)=y^{\kappa}e^{y/2}\left[1-\frac{\kappa(\kappa-1)}{y}+\frac{\kappa(\kappa-1)^2(\kappa-2)}{2y^2}+\cdots\right]. \quad (127)$$

Moreover, $M_{\kappa,1/2}$ is an entire function of y, while $W_{\kappa,1/2}$ has a logarithmic singularity at $y=0$. It is then readily established by the method of variation of parameters that the solution of (125) satisfying the boundary conditions is

$$F(H,x)=\frac{i\lambda\Gamma(1-\kappa)\hbar}{4H}\left[W_{\kappa,1/2}(\lambda x)\int_0^x dx'\,M_{\kappa,1/2}(\lambda x')\psi(x',0)+M_{\kappa,1/2}(\lambda x)\int_x^\infty dx'\,W_{\kappa,1/2}(\lambda x')\psi(x',0)\right]. \quad (128)$$

In terms of F the desired solution is

$$\psi(x,t)=\int_C \frac{dH}{\hbar}e^{-iHt/\hbar}F(H,x)\,, \quad (129)$$

where the Bromwich inversion contour C is a straight line in the complex H plane parallel to the real axis and traversed from left to right. Now the singularities of F are simple poles at $1-\kappa=0,-1,-2,\ldots$, associated with $\Gamma(1-\kappa)$, and a branch point at $H=0$ associated with the logarithmic singularity of $W_{\kappa,1/2}$. In terms of H the poles occur for

$$H=-\frac{me^4}{2n^2\hbar^2\epsilon^2},\quad \text{where } n=1,2,3,\ldots, \quad (130)$$

the energies of the hydrogenic discrete levels. If we choose a branch cut along the positive real H axis and evaluate (129) by deformation of the contour into the lower half H plane, there results an expression which is a sum over the discrete levels associated with the poles and an integral along the real axis associated with the continuum.

In order to demonstrate the relationship of the GFI solution and (129) it is convenient to use in place of the asymptotic representations (126) and (127) their WKB counterparts, viz., if

$$\mu=(1-4\kappa/y)^{1/2} \quad (131)$$

one employs

$$\Gamma(1-\kappa)M_{\kappa,1/2}(y)\sim\mu^{-1/2}\exp\left[\tfrac{1}{2}\int dy\,\mu\right], \quad (132)$$

$$W_{\kappa,1/2}(y)\mu^{-1/2}\sim\exp\left[-\tfrac{1}{2}\int dy\,\mu\right]. \quad (133)$$

It is readily verified that (132) and (133) agree with (126) and (127) through terms of order $1/y$. If we use the asymptotic forms (132) and (133), Eq. (129) leads to

$$\psi(x,t)=\frac{1}{h}\int_C dH\int_0^\infty dx'[v(H,x)v(H,x')]^{-1/2}\psi(x',0)\exp\left[\frac{i}{\hbar}\left[\int_{\inf(x,x')}^{\sup(x,x')}dx''\,v(H,x'')-Ht\right]\right]\times\left[1+\frac{2me^2}{\hbar^2\epsilon}\left[\frac{\hbar^2}{8mH}\right]^{3/2}\left[\frac{1}{x^2}+\frac{1}{(x')^2}\right]+\cdots\right], \quad (134)$$

where the terms indicated by dots are higher order in $1/H$. Thus if

$$K(x,x',t)=\frac{1}{h}\int_C dH[v(H,x)v(H,x')]^{-1/2}\exp\left[\frac{i}{\hbar}\left[\int_{\inf(x,x')}^{\sup(x,x')}dx''\,v(H,x'')-Ht\right]\right] \quad (135)$$

it follows on using the convolution theorem that

$$\psi(x,t)=\int_0^\infty dx'\,\psi(x',0)K(x,x',t)+\int_0^\infty dx'\int_0^t dt'\,\psi(x',0)K(x,x',t')\frac{e^2}{8h\epsilon}\left[\frac{\hbar(t-t')}{2m}\right]^{1/2}\left[\frac{1}{x^2}+\frac{1}{(x')^2}\right]+\cdots. \quad (136)$$

The leading term in (136) is a good approximation when

$$\frac{e^2t}{8\hbar\epsilon x^2}\left[\frac{\hbar t}{2m}\right]^{1/2}\ll 1\,. \quad (137)$$

Let us keep only the leading term in (136). Since there are no singularities in the upper half H plane of the integrand the contour C can be deformed into the real H axis and

$$\psi(x,t)=\frac{1}{h}\int_0^\infty dx'\int_{-\infty}^\infty dH\,\psi(x',0)[v(H,x)v(H,x')]^{-1/2}\exp\left[\frac{i}{\hbar}\left[\int_{\inf(x,x')}^{\sup(x,x')}dx''\,mv(H,x'')-Ht\right]\right]. \quad (138)$$

It follows from definition (122) that on the real H axis approached from above that

$$v(H,x)=\begin{cases} \left|\dfrac{2}{m}\left[H+\dfrac{e^2}{\epsilon x}\right]\right|^{1/2}, & H>\dfrac{e^2}{\epsilon x} \\ i\left|\dfrac{2}{m}\left[H+\dfrac{e^2}{\epsilon x}\right]\right|^{1/2}, & H<-\dfrac{e^2}{\epsilon x}. \end{cases} \tag{139}$$

This implies that if

$$I=\int_{\inf(x,x')}^{\sup(x,x')} dx''\, v(H,x'') \tag{140}$$

then

$$I=\int_{\inf(x,x')}^{\sup(x,x')} dx''\,|v(H,x'')|$$

$$=\int_{\inf(x,x')}^{-e^2/\epsilon H} dx''\,|v(H,x'')| \tag{140'}$$

$$+i\int_{-e^2/\epsilon H}^{\sup(x,x')} dx''\,|v(H,x'')| \tag{140''}$$

$$=i\int_{\inf(x,x')}^{\sup(x,x')} dx''\,|v(H,x'')|\ , \tag{140'''}$$

Eqs. (140′), (140″), and (140‴) following, respectively, from

$$-\frac{e^2}{\sup(x,x')}<H\ ,$$

$$-\frac{e^2}{\epsilon\inf(x,x')}<H<\frac{e^2}{\epsilon\sup(x,x')}\ ,$$

$$H<-\frac{e^2}{\epsilon\inf(x,x')}\ .$$

The condition that the phase in (138) be stationary is

$$t=\int_{\inf(x,x')}^{\sup(x,x')} dx''\frac{1}{v(H,x'')}$$

$$=\int_{\inf(x,x')}^{\sup(x,x')} dx''\frac{1}{|v(H,x'')|},\quad -\frac{e^2}{\epsilon\sup(x,x')}<H$$

$$=\int_{\inf(x,x')}^{-e^2/\epsilon H} dx''\frac{1}{|v(H,x'')|}-i\int_{-e^2/\epsilon H}^{\sup(x,x')} dx''\frac{1}{|v(H,x'')|},\quad \frac{e^2}{\epsilon\inf(x,x')}<H<\frac{e^2}{\epsilon\sup(x,x')}$$

$$=-i\int_{\inf(x,x')}^{\sup(x,x')} dx''\frac{1}{|v(H,x'')|},\quad H<-\frac{e^2}{\epsilon\inf(x,x')}\ . \tag{141}$$

Equation (141) is an implicit equation for that value of $H=H(x,x',t)$ which corresponds to the stationary point. Since t is real the stationary point can occur only for $H>-e^2/\epsilon\sup(x,x')$. The value of the second derivative of the phase with respect to H is

$$\frac{1}{\hbar}\frac{\partial}{\partial H}\int_{\inf(x,x')}^{\sup(x,x')} dx''\frac{1}{v(H,x'')}=-\frac{1}{\hbar}\int_{\inf(x,x')}^{\sup(x,x')} dx''\frac{1}{mv(H,x'')^3}\ . \tag{142}$$

Thus in the limit $\hbar\to 0$, on using the method of stationary phase, (138) implies

$$\psi(x,t)=\frac{1}{h}\int_0^{\infty} dx'\int_{-\infty}^{\infty} dH\,\psi(x',0)[v(\hat{H},x)v(\hat{H},x')]^{-1/2}$$
$$\times\exp\left[\frac{i}{\hbar}\left[\int_{\inf(x,x')}^{\sup(x,x')} dx''\,mv(\hat{H},x'')-\hat{H}t+\tfrac{1}{2}(H-\hat{H})^2\frac{\partial}{\partial\hat{H}}\int_{\inf(x,x')}^{\sup(x,x')} dx''\frac{1}{v(\hat{H},x'')}\right]\right]\ . \tag{143}$$

In order to construct the GFI counterpart solution note that since $H=\frac{1}{2}mv^2-e^2/\epsilon x$ is a constant of the motion one can write

$$v=\left[\frac{2}{m}\left[H+\frac{e^2}{\epsilon x}\right]\right]^{1/2}=v(H,x)\;; \tag{144}$$

$$t=\int_{x_0}^{x}dx''\frac{1}{v(H,x'')}\;, \tag{145}$$

$$v_0=\left[\frac{2}{m}\left[H+\frac{e^2}{\epsilon x_0}\right]\right]^{1/2}. \tag{146}$$

These equations then determine H, x_0, and v_0 implicitly as functions of v_0, x, and t. The action obeys

$$\dot{S}=\tfrac{1}{2}mv^2+\frac{e^2}{\epsilon x}=mv^2-H \tag{147}$$

whence

$$\begin{aligned}S&=mv_0x_0+\int_0^t dt'\,mv^2-Ht'\\&=mv_0x_0+\int_{x_0}^{x}dx''\,mv(H,x'')-Ht\;.\end{aligned} \tag{148}$$

Thus the GFI solution of the SSE problem is

$$\psi(x,t)=\frac{m}{h}\int dx'\int dv_0\,\psi(x',0)[J(v_0,x,t)]^{-1/2}\times\exp\left[\frac{i}{\hbar}\left[\int dx''\,mv(H,x'')-Ht+mv_0(x_0-x')\right]\right]. \tag{149}$$

Moreover, in this one-dimensional case

$$\begin{aligned}J=\frac{\partial(v_0,x)}{\partial(v,x)}&=\frac{\partial(v_0,x)}{\partial(H,x)}\frac{\partial(H,x)}{\partial(v,x)}\\&=\left[\frac{\partial(H,x)}{\partial(v_0,x)}\right]^{-1}\frac{\partial(H,x)}{\partial(v,x)}\\&=\left|\left[\frac{\partial H}{\partial v}\right]_x\Big/\left[\frac{\partial H}{\partial v_0}\right]_x\right|\end{aligned} \tag{150}$$

whence

$$J=mv\Big/\left[\frac{\partial H}{\partial v_0}\right]_x. \tag{151}$$

Now on using the results of (85) *et seq.* it follows that the first derivative of the phase with respect to v_0 is $m(x_0-x')/h$, and that the second derivative is

$$\frac{m}{\hbar}\left[\frac{\partial x_0}{\partial v_0}\right]_x=\frac{m}{\hbar}\left[\frac{\partial x_0}{\partial H}\right]_x\left[\frac{\partial x}{\partial v_0}\right]_x. \tag{152}$$

Thus if the stationary-phase point $x_0=x'$ is away from a caustic, on using the principle of stationary phase, (149) leads to

$$\psi(x,t)=\frac{m}{h}\int_0^\infty dx'\int_{-\infty}^{\infty}dv_0\,\psi(x',0)\left|\left[\frac{\partial H}{\partial v_0}\right]_x\frac{1}{mv(H,x)}+\cdots\right|^{1/2}\times\exp\left\{\frac{i}{\hbar}\left[\int_{x'}^{x}dx''\,mv(H,x'')-Ht+\tfrac{1}{2}m(v_0-v')^2\left[\frac{\partial x_0}{\partial H}\right]_x\left[\frac{\partial H}{\partial v_0}\right]_x+\cdots\right]\right\}, \tag{153}$$

where after all derivatives have been taken one sets $H=\hat{H}$, where $\hat{H}(x,x',t)$ is given by (143), and $v'=v(\hat{H},x')$. But if we take the derivative of (145) with respect to H at fixed x there results, on using (140) with x' replaced by x_0,

$$\begin{aligned}\frac{\partial x_0}{\partial H}&=v_0\frac{\partial}{\partial H}\int_{x_0}^{x}dx''\frac{1}{v(H,x'')}\bigg|_{x_0=x'}\\&=v'\int_{\inf(x,x')}^{\sup(x,x')}dx''\frac{1}{|v(H,x'')|}\;.\end{aligned} \tag{154}$$

It then follows on evaluating the integrals in (142) and (153) that the two expressions are equal. Thus the GFI solution corresponds to the short-time asymptotic solution. Note that (143) holds even near the caustics where $v(H,x)=0$, suggesting that the stationary-phase approximation gives a uniformly valid result.

V. CONCLUSIONS

The method of generalized Fourier integrals has been shown to provide a semiclassical approximation to the solution of the time-dependent one-particle Schrödinger equation for the case of localized wave functions. For problems such as the ionization of Rydberg states by external radio-frequency fields where one is primarily interested in knowing whether the electron is no longer localized near the nucleus and a spatially coarse-grained value of $P=|\psi(\mathbf{r},t)|^2$ is adequate, it is then sufficient to solve a classical Vlasov equation for the Wigner distribution function f and compute $P=\int d^3v\, f$. The technique provides a short-time solution which may, however, be valid long enough to establish for example that ionization has taken place. The method fails if the systems of rays developed to generate the solution display in the course of time sufficiently dense sets of caustics.

The method should generalize to many-body problems where almost all the particles are in the classical limit and permit their treatment by the methods of classical particle mechanics and classical statistical mechanics. Possible applications are the derivation of one-particle kinetic equations and the treatment of atomic processes in dense plasmas.

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