Particle Trajectories and the Perception of Classical Motion in the Free Propagation of Wave Packets.

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The free propagation in time of a normalisable wave packet is the oldest problem of continuum quantum mechanics. Its motion from microscopic to macroscopic distance is the way in which most quantum systems are detected experimentally. Although much studied and analysed since 1927 and presented in many text books, here the problem is re-appraised from the standpoint of semi-classical mechanics. Particular aspects are the emergence of deterministic trajectories of particles emanating from a region of atomic dimension and the interpretation of the wave function as describing a single particle or an ensemble of identical particles. Of possible wave packets, that of gaussian form is most studied due to the simple exact form of the time-dependent solution in real and in momentum space. Furthermore, this form is important in laser optics. Here the equivalence of the time-dependent Schrödinger equation to the paraxial equation for the propagation of light is demonstrated explicitly. This parallel helps to understand the relevance of trajectory concepts and the conditions necessary for the perception of quantum motion as classical.

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I. INTRODUCTION

The question of the relation of quantum to classical mechanics and the concomitant interpretation of the wave function can be traced to the dawn of wave mechanics. It is best discussed on the basis of continuum motion (originally called aperiodic motion). Already in the year 1926 in which he proposed a wave equation for material particles, Schrödinger realised the necessity to connect his description of particles by wave dynamics to that of classical motion. In a paper on the "Transition from micro- to macro-mechanics" [1] he showed that a wavepacket composed of harmonic oscillator functions (today called a coherent state) oscillates as a localised "particle". That is, he sought to demonstrate that a wave function can be assigned to a single atomic particle. In 1927 this proof was criticised by Heisenberg, also under the title "Transition from micro- to macro-mechanics" [2]. Although Schrödinger was thinking of bound states, Heisenberg showed the counter example of a freely-propagating gaussian wave packet which spreads as time progresses and so cannot describe a single particle. Even today, this spreading of a wave packet is presented in many text books as a hallmark of quantum behaviour inexplicable in classical mechanics.

However, also in 1927, Kennard [3] recognised that a gaussian wave packet contains infinitely many momentum components and, correctly using Born's statistical interpretation of the wave function, pointed out that these components will spread "like a charge of shot". Hence, wave function spreading corresponds to the expected classical behaviour of an *ensemble* of particles having an initial spread in momentum.

According to the statistical interpretation of a wave function $\Psi(\boldsymbol{r},t)$, the measurement of observables, position, momentum and energy of bound states can yield only the average, expectation values of these quantities. For bound states, modern imaging techniques can give indirectly the distribution $|\Psi(\boldsymbol{r},t)|^2$. Certain experiments, e.g. Compton scattering or fast electron scattering, image the corresponding bound momentum wave function distribution $|\tilde{\Psi}(\boldsymbol{p},t)|^2$. For continuum wave functions this imaging is performed more directly by measuring the projection $|\langle\, \boldsymbol{r} \mid \Psi \,\rangle|^2 = |\Psi(\boldsymbol{r},t)|^2$ of a wave packet on a detector at macroscopic distance. The momentum distribution $\tilde{\Psi}|^2 = |\langle\, \boldsymbol{p} \mid \Psi \,\rangle(\boldsymbol{p},t)|^2$ is inferred from times of flight. For this reason, since position and momentum distribution of particles can be measured by counting individual particles, the spatial and temporal propagation of continuum wave packets from a quantum zone of atomic dimension to a classical detector at macroscopic distance represents the simplest transition from quantum to classical behaviour.

The question of the identification of the component for fixed $\boldsymbol{p}$, defined mathematically from a Fourier transform, with a classically measured momentum (mass × velocity) was examined by Kemble in 1937 [4]. He showed that a measurement at *macroscopic* separation from the *microscopic* region of creation of the wave packet justifies the introduction of a classical velocity. More importantly, in a result referred to today as the "Imaging Theorem" (IT), he showed that the space wavefunction asymptotically assumes the form of the momentum wave function and the $\boldsymbol{r}$ coordinate of the wave function propagates in time according to the classical law $\boldsymbol{r}(t)$. This explains why particles move at macroscopic distances along classical trajectories.

The IT shows also that after propagation from microscopic to macroscopic positions and times, the semi-classical approximation to wave functions is justified. Since Kemble, the IT has been re-discovered and used spasmodically in scattering theory but developed in more detail quite recently. It has been suggested to embody the essence of the quantum to classical transition in that the wave function is preserved to asymptotic distances but the coordinates change along classical trajectories. This explains why experimenters can measure the manifestations of quantum entanglement whilst using classical trajectories to trace the motion of particles from microscopic collision complexes out to macroscopic detectors. The locus of points of constant measurement probability are classical paths described by the asymptotic wave function.

To bring aspects of the wave function more in line with the human experience of classical trajectories even at microscopic dimensions, Bohm [5] proposed an additional postulate, accompanying the Schrödinger equation solution $\Psi(\boldsymbol{r}, t)$, which leads to the definition of trajectories $\boldsymbol{r}(t)$ throughout *all space and time*. This does require a postulate since, although in classical mechanics a velocity arise as $d\boldsymbol{r}(t)/dt$, there is no such definition of a velocity in quantum mechanics. The plausible step of Bohm was to suggest such a connection, and hence a trajectory $\boldsymbol{r}(t)$ from integration of the velocity function, based upon a certain similarity of the equation of wave mechanics to that of classical mechanics.

There is now an enormous literature on Bohmian mechanics or "quantum trajectory" methods, extending to several volumes covering many aspects of quantum mechanics, see Refs.[6–11]. Here consideration is given to unbound particle motion as the simplest clear example of where well-defined trajectories occur classically. Of such motions, the free propagation of a gaussian wave packet, as first solved by Heisenberg [2] is the simplest. Although much-studied since that time, our aim is to throw some new light on the exact solution and on the approximate IT semi-classical solution with respect to the nature of the emergent trajectories.

At each fixed time the gaussian wave function is the ground state of the harmonic oscillator (HO) and it is shown that the energy, both potential and kinetic, of the HO figure prominently. The motion both from and to a minimum gauss wavepacket is considered and the precise correspondence to the optics text-book case of the focussing of a light beam with gaussian profile is demonstrated. Furthermore it is shown that the momentum-space gaussian wave function emerges naturally not only asymptotically but also along the Bohm trajectory.

In what follows, a smooth transition from Bohmian trajectories to the reality of the asymptotic classical trajectories is demonstrated. Whether or not one views the Bohm velocity and trajectories as "real" is left to the reader. The concept certainly has worth in so far as the "trajectory" does represent one aspect of the motion of the quantum wave. The construction of Bohmian trajectories simply follows the path of the normal vectors to the surfaces of constant action in the quantum wave function. This illuminates the behaviour of the wave function, in particular its phase development. The Bohm picture allows concepts familiar from classical mechanics to be applied to wave mechanics.

Indeed, the motion of wave fronts in quantum mechanics is equivalent to the propagation of the wave fronts of classical electromagnetic waves. Of course this connection can be traced all the way back to Hamilton, through Schrödinger and de Broglie, up to the present day [12]. An illuminating discussion of the analogy between classical mechanics and wave optics is given by Lanczos [13], see also the Refs. [10, 11]. We demonstrate explicitly the equivalence of the time-dependent Schrödinger equation (TDSE), as an approximation to the time-independent Schrödinger equation (TISE), and the paraxial approximation to the Helmholtz equation. This provokes one to examine further the approximate status of the TDSE.

The semi-classical limit of quantum mechanics is identical to the eikonal approximation in optics. The identification of particle classical trajectories in semi-classical wave mechanics is an exact parallel of the assignment of ray trajectories to light in wave optics. This analogy is explored in some detail, particularly with respect to gaussian laser beams, to illuminate further the concept of trajectories in quantum waves and rays in light waves.

The plan of the paper is as follows. In section II the propagation of quantum wave packets is described. The approximate semi-classical asymptotic form is derived. A result known as the "Imaging Theorem" (IT) connects the space wave function to the momentum wave function and justifies the introduction of a classical velocity. The IT is applied to the freely-moving gaussian wave packet.

In Bohmian mechanics, outlined in section III, a velocity is ascribed to all space and time points in the wave function. For a gaussian wave packet, an interpretation is given of the "quantum potential" and Gouy phase in terms of the instantaneous quantised harmonic oscillator state. It is demonstrated that the constant probability along a Bohm trajectory is explained by the IT result expressing this probability in terms of the invariant initial momentum space wave function. This constancy is shown to emerge from a time scaling of space coordinates along the trajectory.

In section IV the implications of wave packet spreading for the interpretation of the quantum to classical transition as applying to a single particle or only to an ensemble of particles is considered.

In section V the precise equivalence of the time-dependent Schrödinger equation (TDSE) as an approximation to the time-independent Schrödinger equation (TISE) and the paraxial equation as an approximation to the Helmholtz equation of classical optics, is proven.

In Section VI the focussing of laser beams is translated into a similar situation for quantum particle beams and this allows a simple criterion that a detection would be perceived as quantum or as classical motion of particles to be given. This is in complete analogy to the perception of wave or beam motion for light.

The results are summarised and commented in the Conclusions section VII.

II. WAVE FUNCTION PROPAGATION IN SPACE AND TIME

In solutions $\Psi(\boldsymbol{r},t)$ of the time-dependent Schrödinger equation (TDSE), the coordinates $\boldsymbol{r}$ and the time t are independent. By propagation, at each time t, the distribution of the wave function in the position $\boldsymbol{r}$ changes. This change can be calculated from the fundamental equation for wave function propagation, for simplicity assuming a time-independent Hamiltonian H,

$$|\,\Psi(t)\,\rangle = e^{-\frac{i}{\hbar}H(t-t')}\,|\,\Psi(t')\,\rangle \tag{1}$$

Projected into position space this gives the wave function propagation

$$\Psi(\boldsymbol{r},t) = \int K(\boldsymbol{r},t;\boldsymbol{r}',t')\,\Psi(\boldsymbol{r}',t')\,d\boldsymbol{r}', \tag{2}$$

where the space-time propagator K is simply

$$K(\boldsymbol{r},t;\boldsymbol{r}',t') = \langle\,\boldsymbol{r}\,|e^{-\frac{i}{\hbar}H(t-t')}|\,\boldsymbol{r}'\,\rangle. \tag{3}$$

The point to note here is that, for fixed time interval $t-t'$, "paths" beginning at all possible $\boldsymbol{r}'$ lead to the response at a given final position $\boldsymbol{r}$. This is acknowledged in the path integral formula for the evaluation of the kernel K [14], where all possible paths linking $\boldsymbol{r}'$ with $\boldsymbol{r}$ for motion in a fixed potential are taken into account.

In the very simplest dynamics of *free* motion it is remarkable that the exact quantum kernel $K(\boldsymbol{r},t;\boldsymbol{r}',t')$ is identical to its semi-classical approximation [15]. Then the paths arising in the exact propagation of the wave function are restricted to those connecting $\boldsymbol{r}'$ with $\boldsymbol{r}$ which obey *classical* mechanics.

A. The Semi-classical Wave Function; Classical trajectories.

In this section the semi-classical (SC) wave function arising from propagation where the action function $S(\boldsymbol{r},t)$ has reached values much in excess of $\hbar$ is derived. It is shown that for the SC wave function a definite classical relation $\boldsymbol{r}(t)$ does emerge and defines a classical trajectory.

One begins with the exact propagation described by the integral equation (2),

For free motion the exact propagator kernel assumes its semi-classical form [15]

$$\begin{aligned} K(\boldsymbol{r},t;\boldsymbol{r}',t') &= \frac{1}{(2\pi i\hbar)^{3/2}}\left|\det\frac{\partial^2 S_c}{\partial\boldsymbol{r}\partial\boldsymbol{r}'}\right|^{1/2} e^{iS_c(\boldsymbol{r},t;\boldsymbol{r}',t')/\hbar} \\ &= \frac{1}{(2\pi i\hbar)^{3/2}}\left(\frac{d\boldsymbol{p}'}{d\boldsymbol{r}}\right)^{1/2} e^{iS_c(\boldsymbol{r},t;\boldsymbol{r}',t')/\hbar}, \end{aligned} \tag{4}$$

where now $S_c(\boldsymbol{r},t;\boldsymbol{r}',t')$ is the *classical* action in coordinate space and we define the initial classical momentum $\boldsymbol{p}' = \partial S_c/\partial\boldsymbol{r}'$. Since $\boldsymbol{r}$ and $t-t'$ are fixed but $\boldsymbol{r}'$ is variable then all momenta corresponding to given $\boldsymbol{r}'$ are possible. Thus, although the kernel describes classical motion, there is still an infinity of possible classical trajectories contributing to the $\boldsymbol{r}'$ integral of Eq. (2).

The second key approximation, which restricts severely the possible trajectories, is to consider propagation to a distance r which is large compared to the initial extent of the wave function in r'. This distance can still be very small on a macroscopic scale. Then, we consider the limit $\boldsymbol{r} \gg \boldsymbol{r}'$. In this limit one has $\boldsymbol{r}' \approx 0$, so that the action can be expanded around this point as

$$S_c(\boldsymbol{r},t;\boldsymbol{r}',t') \approx S_c(\boldsymbol{r},t;0,t') + \left.\frac{\partial S_c}{\partial\boldsymbol{r}'}\right|_0 \cdot \boldsymbol{r}'. \tag{5}$$

Specifying the initial momentum $\partial S_c/\partial\boldsymbol{r}'|_0 \equiv -\boldsymbol{p}'$, substitution in the integral Eq. (2) gives a Fourier transform and the result

$$\Psi(\boldsymbol{r},t) \approx (i)^{-3/2}\left(\frac{d\boldsymbol{p}'}{d\boldsymbol{r}}\right)^{1/2}\tilde{\Psi}(\boldsymbol{p}',t')\;e^{iS_c(\boldsymbol{r},t;0,t')/\hbar}, \tag{6}$$

where $\tilde{\Psi}(\boldsymbol{p}',t')$ is the *momentum-space* wavefunction of the initial, spatially-confined quantum system.

This equation is known as the Imaging Theorem (IT) approximation for the final wavefunction $\Psi(\boldsymbol{r},t)$ [16]. Actually, suitably generalised, it is valid for motion in arbitrary applied fields [17]. For the simple case of free motion, each final position $\boldsymbol{r},t$ along a single *classical* trajectory corresponds to a unique initial momentum $\boldsymbol{p}'$ emanating from $\boldsymbol{r}'=0, t'=0$ (we take the initial time to be zero).

For the free motion of a particle of mass m, one has the final momentum $m\boldsymbol{r}/t = \boldsymbol{p} = \boldsymbol{p}'$ and the van Vleck determinant [15] is

$$\frac{d\boldsymbol{p}}{d\boldsymbol{r}} = \left|\det\frac{\partial\boldsymbol{p}}{\partial\boldsymbol{r}}\right| = \left(\frac{m}{t}\right)^3. \tag{7}$$

The asymptotic wavefunction then is

$$\Psi(\boldsymbol{r},t) \approx \left(\frac{m}{it}\right)^{3/2} e^{imr^2/(2\hbar t)}\,\tilde{\Psi}(m\boldsymbol{r}/t). \tag{8}$$

Note that the classical action S_c implies the classical trajectory $\boldsymbol{r}(t) = \boldsymbol{p}t/m$ embedded in the quantum momentum-space wave function.

The probability of a particle to be located at fixed position $\boldsymbol{r}$ is equal to the probability that it was launched with fixed momentum $\boldsymbol{p}$. Then, from Eq. (6)

$$|\Psi(\boldsymbol{r},t)|^2\,d\boldsymbol{r}(t) = |\tilde{\Psi}(\boldsymbol{p})|^2\,d\boldsymbol{p} \tag{9}$$

showing that, although the wave function is preserved, the locus of points of constant detection probability is a classical trajectory. The sharper is $d\boldsymbol{r}(t)$ defined by the detector, the narrower is the detected momentum distribution $d\boldsymbol{p}$.

The IT approximate wave function, whose co-ordinates describe a classical trajectory, justifies the asymptotic dependence of the coordinates $\boldsymbol{r}$ and t and therefore the transformation $\Psi(\boldsymbol{r},t) \to \Psi(\boldsymbol{r}(t)) \propto \tilde{\Psi}(m\boldsymbol{r}/t)$ and the definition of a classical velocity $\boldsymbol{v} = \boldsymbol{r}/t$.

B. The freely-moving gaussian wave packet

In appendix A the time propagation of the initial wave packet, both in position and momentum space is considered. The time propagators in position, momentum and mixed position-momentum spaces are given and it is shown that, since the semi-classical propagators are exact, the coordinates of the propagators are connected by classical trajectories. The exact time-dependent functions for a gaussian wave packet are presented next.

In quantum mechanics it is accepted usually that calculations obtain equivalent results when carried out either in position or momentum space. Certain calculations are easier to perform in one or other space. First we consider free-particle propagation in momentum space which certainly is simpler than the propagation in configuration space. One can calculate the time-dependent momentum wave function from the propagator equation

$$\tilde{\Psi}(p,t) = \int \tilde{K}(p,t;p',0)\tilde{\Psi}(p',0)\,dp', \tag{10}$$

with momentum-space kernel

$$\tilde{K}(p,t;p',0) = \left(\frac{1}{2\pi\hbar}\right)^{1/2} e^{-\frac{i}{\hbar}\frac{p'^2}{2m}\,t}\,\delta(p-p'). \tag{11}$$

Then the propagating wave function has the form

$$\tilde{\Psi}(p,t) = \tilde{\Psi}(p,0)\,e^{-\frac{i}{\hbar}\frac{p^2}{2m}\,t} \tag{12}$$

That is, the initial momentum wave function is unchanged except for an acquired energy phase. This is valid for any normalisable initial wave packet.

Specifically for a gaussian one has

$$\tilde{\Psi}(p,t=0) = \left(\frac{\sigma^2}{\hbar^2\pi}\right)^{1/4} e^{-\sigma^2p^2/(2\hbar^2)}, \tag{13}$$

where $\hbar/\sigma$ is the width in momentum space. The time propagated wave function is

$$\begin{aligned}\tilde{\Psi}(p,t) &= \tilde{\Psi}(p,0)\,e^{-\frac{i}{\hbar}\frac{p^2}{2m}\,t} \\ &= \left(\frac{\sigma^2}{\hbar^2\pi}\right)^{1/4} e^{-\sigma^2p^2/(2\hbar^2)}\,e^{-\frac{i}{\hbar}\frac{p^2}{2m}\,t} \\ &\equiv \left(\frac{1}{\pi\tilde{\sigma}^2}\right)^{1/4} e^{-p^2/(2\tilde{\sigma}^2)}\,e^{-\frac{i}{\hbar}\frac{p^2}{2m}\,t}.\end{aligned} \tag{14}$$

Here we define the inverse momentum space width $\tilde{\sigma} \equiv \hbar/\sigma$ so that $\sigma\tilde{\sigma} = \hbar$ conforming to the uncertainty relation. As shown below, the parameter σ then is the wave packet width in configuration space.

Although given in many text books in complicated form, where the physical parameters m, σ and $\hbar$ are kept separately, the essential physics of the propagation can be subsumed in a single parameter. Already Heisenberg [2] recognised that one can define the characteristic parameter

$$T = \frac{m}{\hbar}\sigma^2 \tag{15}$$

with dimension of time. Then one can use it to define a dimensionless time $\tau \equiv t/T$. As will be shown, this parameter becoming larger than unity denotes the onset in time of classical trajectory behaviour, or alternatively the transition from wave to particle behaviour. Equally, it will emerge that it marks the transition from Bohmian trajectories to classical trajectories. In Optics, the equivalent parameter delineates near-field wave and far-field light ray spatial regions.

Peculiar to a gaussian is that both $\tilde{\Psi}(\boldsymbol{p},0)$ and the phase factor are exponentials involving p^2. This means that the exact momentum-space wave function Eq. (12) can be written in the compact form,

$$\tilde{\Psi}(p,t) = \left(\frac{1}{\pi\tilde{\sigma}^2}\right)^{1/4} e^{-\frac{p^2}{(2\tilde{\sigma}^2)}(1+i\tau)}. \tag{16}$$

Thus the only effect of time propagation is to introduce the complex time factor $(1+i\tau)$ into the exponent of the gaussian.

The configuration-space wave function can be derived from the propagation Eq. (2) with initial wave function

$$\Psi(x,t=0) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-x^2/(2\sigma^2)}, \tag{17}$$

or more simply as the Fourier transform (FT) of the momentum wave function Eq. (16). Then for $t>0$ the initial gaussian wavefunction propagates according to the exact form

$$\Psi(x,t) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} \frac{1}{(1+i\tau)^{1/2}} e^{-x^2/[2\sigma^2(1+i\tau)]}. \tag{18}$$

Again, comparison with the initial wave function of Eq. (17) shows that the only effect of time propagation is to introduce the imaginary factor $(1+i\tau)$ into the exponent of the gaussian.

Indeed, from Eq. (16) and Eq. (18) one sees the expected conjugate similarity of momentum and configuration space wave functions. However, the apparently innocuous difference that the time factor $(1+i\tau)$ appears in the numerator of the exponent in Eq. (16) but in the denominator in Eq. (18) has a profound effect. It is the difference between a complex number z and the number $1/z = z^*/|z|^2$. This implies that the momentum wave function propagates form invariantly, only the phase factor varies with time. However, the space wave function spreads in time due to the extra factor $1/|z|^2 = (1+\tau^2)$ in the exponent. As time progresses the width of the wave packet increases. The preservation of normalisation during spreading is the reason for the extra normalisation factor $(1+i\tau)^{-1/2}$ in Eq. (18) compared to Eq. (16).

The complex normalisation factor $(1+i\tau)^{-1/2}$ in Eq. (18) can be written

$$(1+i\tau)^{-1/2} = (1+\tau^2)^{-1/2}\,\exp\left[-\frac{i}{2}\arctan\tau\right]. \quad (19)$$

The phase factor occurring corresponds exactly to what is known in the Optics of gaussian propagation as the Gouy phase [18]. Its physical meaning is explained below.

The IT condition emerges in the limit of large times. Large times corresponds to $\tau \equiv t/T \gg 1$. In this limit, putting explicitly $T = m\sigma^2/\hbar$, the exact wave function Eq. (18) has the asymptotic form

$$\begin{aligned}\Psi(x,t) \approx \left(\frac{\sigma^2}{\pi}\right)^{1/4} & \left(\frac{m}{i\hbar t}\right)^{1/2} \\ & \times e^{-[mx\sigma/(\sqrt{2}\hbar t)]^2} e^{imx^2/(2\hbar t)}.\end{aligned} \quad (20)$$

Substituting the classical condition $p = mx/t$ of the stationary phase approximation, valid asymptotically, one has the equivalent form

$$\begin{aligned}\Psi(x,t) &\approx \left(\frac{\sigma^2}{\hbar^2\pi}\right)^{1/4}\left(\frac{m}{it}\right)^{1/2} e^{-\sigma^2p^2/(2\hbar^2)} e^{\frac{i}{\hbar}\frac{p^2}{2m}t} \\ &= \left(\frac{m}{it}\right)^{1/2}\tilde{\Psi}(p,0)\,e^{\frac{i}{\hbar}\frac{p^2}{2m}t}.\end{aligned} \quad (21)$$

Hence, the space wave function is proportional to the momentum wave function Eq. (12). This is just the one-dimensional form of the IT of Eq. (6), with $p = mv = mx/t$ and $dp/dx = m/t$ for free motion. Note that the phase factor $i^{-1/2} = \exp(i\pi/4)$ is the asymptotic Gouy phase.

It must be emphasised that the introduction of an *asymptotic* classical velocity v is justified mathematically from the IT approximation and gives a large time classical connection $x(t) = vt$ between the quantum-mechanically independent coordinates x and t within the quantum wave function. The emergence of a classical velocity from a quantum mechanical momentum does not have to be postulated.

III. THE BOHMIAN TRAJECTORIES.

Following Bohm [5], as an additional postulate, a trajectory $\boldsymbol{r}(t)$ is defined and interpreted as that of a particle, or ensemble of particles, described by the wave function $\Psi(\boldsymbol{r},t)$ playing the role of a "pilot" wave. The development of Bohmian mechanics is given in great detail, for example in the lengthy volume of Holland [6]. A sketch of the derivation is as follows, reverting to three space dimensions.

First the wave function is written in amplitude-phase (also called polar) form

$$\Psi(\boldsymbol{r},t) = R(\boldsymbol{r},t)\,e^{\frac{i}{\hbar}S(\boldsymbol{r},t)}. \quad (22)$$

where R and S are real functions. Following Holland, with the momentum operator $\hat{\boldsymbol{p}} = -i\hbar\nabla$, a "local" momentum is defined as

$$\hat{\boldsymbol{p}}\Psi(\boldsymbol{r},t) = -i\hbar\nabla R\,e^{\frac{i}{\hbar}S(\boldsymbol{r},t)} + \nabla S\Psi(\boldsymbol{r},t). \quad (23)$$

Then the second term is used to define a real local velocity function

$$\dot{\boldsymbol{r}} = \boldsymbol{v}(\boldsymbol{r},t) \equiv \frac{1}{m}\nabla S(\boldsymbol{r},t). \quad (24)$$

The justification is to be found in the appearance of an equation of the same form as the Hamilton-Jacobi (HJ) equation of classical mechanics. This arises from substitution of this complex wavefunction in the TDSE for a single particle of mass m

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - i\hbar\frac{\partial}{\partial t}\right)\Psi(\boldsymbol{r},t) = 0 \quad (25)$$

and separation of real and imaginary parts leading to two coupled equations. The first is,

$$\frac{(\nabla S)^2}{2m} + V(\boldsymbol{r}) + Q(\boldsymbol{r},t) + \frac{\partial S}{\partial t} = 0, \quad (26)$$

reducing, for $Q = 0$ to the classical HJ equation. The additional term is the "quantum potential"

$$Q(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\left[\frac{\nabla^2 R}{R}\right]. \quad (27)$$

One notes that this potential, in direct analogy to the appearance of a centrifugal potential, is a fictitious potential arising from the kinetic energy part of the Hamiltonian operator.

The second equation is the continuity equation for the probability density with R^2 and flux $\boldsymbol{j} = (R^2\frac{\nabla S}{m})$,

$$\frac{\partial R^2}{\partial t} + \nabla\,.\left(R^2\frac{\nabla S}{m}\right) = 0. \quad (28)$$

The Bohmian trajectory $\boldsymbol{r}(t)$ is then calculated by integrating the velocity equation Eq. (24). This trajectory $\boldsymbol{r}(t)$ is viewed as a particle's "quantum" trajectory, deterministically connecting the initial $\boldsymbol{r}_i$ to the final $\boldsymbol{r}$. We emphasise, what is being designated a momentum function is simply the gradient ∇S of the phase of the quantum wavefunction. Important is that the direction of ∇S is the normal to the instantaneous wave front.

Refraining from philosophical questions as to the "reality" of such trajectories, we adopt a pragmatic standpoint within standard quantum mechanics. If one recognises that the function $\nabla S(\boldsymbol{r},t)$ gives the normal to the wave front surface at each space-time point, then one can plot the locus of such normal vectors. Knowledge of this locus provides useful insight into the quantum wave function and in this sense does not contradict standard quantum mechanics.

However, due to the quantum potential, even for free motion the Bohm trajectories do not agree with the classical ones (although the latter ones enter the semiclassical version of the propagator which is quantum mechanically exact). The relation between the two types of trajectories is investigated in more detail using a Gaussian initial wavefunction. It will turn out that the Bohm trajectories connect smoothly to those classical trajectories defined in a mathematically correct way in the IT wave function Eq. (8).

A. The Bohmian velocity and trajectories for a gaussian wave packet.

In polar form the exact space wave function Eq. (18) has the more complicated form

$$\Psi(x,t) = \frac{1}{[\pi\sigma^2(1+\tau^2)]^{\frac{1}{4}}} \exp\left[-\frac{i}{2}\arctan\tau\right] \times \exp\left[-\frac{x^2}{2\sigma^2(1+\tau^2)}\right] \exp\left[i\frac{x^2\,\tau}{2\sigma^2(1+\tau^2)}\right]. \tag{29}$$

The action function of this exact wave function is

$$S = \hbar\frac{x^2}{(2\sigma^2)}\frac{\tau}{(1+\tau^2)} - \frac{\hbar}{2}\arctan\tau. \tag{30}$$

The Bohmian velocity is postulated as

$$\dot{x} \equiv \frac{1}{m}\frac{\partial S}{\partial x} = \frac{x}{T}\frac{\tau}{(1+\tau^2)} \tag{31}$$

and can be written also as

$$\dot{x} = \frac{x}{t}\frac{\tau^2}{(1+\tau^2)}. \tag{32}$$

One recognises that asymptotically, when $\tau \gg 1$, then $|x/t|$ is the constant classical speed v which is positive.

The Bohmian velocity equation can be integrated over time to yield the Bohmian trajectory

$$x(t) = x_0(1+\tau^2)^{1/2} \tag{33}$$

where, to emphasise the zero of time on the trajectory, now we define $x(0) \equiv x_0$. To satisfy the large time limit of the classical trajectory $x(t) \approx \pm vt$ one has the condition $x_0 = \pm vT$, so that, for a fixed final momentum $p = \pm mv$, the trajectory has a fixed well-defined position at $t = 0$. Each trajectory, Bohmian and its classical asymptote, is then characterised solely by its final velocity $\pm v$ and the constant T.

The Bohmian trajectory equation can be written in the form

$$x(t) = \pm v(t^2 + T^2)^{1/2} \tag{34}$$

and the classical IT trajectory $x(t) = \pm vt$ is the $t \gg T$ limit. Note that the Bohmian trajectory has the $t = 0$ conditions, position $x_0 = \pm vT$ and the initial velocity $\dot{x}(0) = 0$ for all trajectories. By contrast the classical trajectories have the $t = 0$ conditions, position $x_0 = 0$ and constant classical velocity $v = p/m$ for the different trajectories.

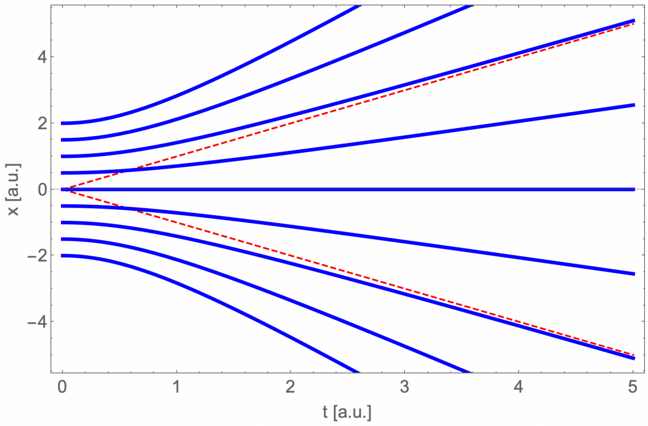

FIG. 1: The axes are in atomic units (a.u.). The continuous blue lines are the Bohmian trajectories $x(t)$ representing the spreading in one dimension (vertical axis) of a gaussian wavefunction for positive times. The horizontal axis is the time axis. The time constant is $T = 1$ a.u.. The trajectories are asymptotic to the IT straight-line $x = \pm vt$ classical trajectories which extrapolate back to $x = 0$. As example, the red dashed lines are the asymptotes for $v = \pm 1.0$.

The Bohmian trajectories are shown in Fig. 1 for a selection of initial values across the width of the gaussian centred at $x = 0$. One sees that all trajectories start out perpendicular to the x-axis indicating zero initial Bohm velocity. This is seen from Eq. (31) at $t = 0$. Initially the normal to the phase fronts of the gaussian wavefunction indeed are orthogonal to the spreading direction x. The difference between Bohm and the classical straight-line $x = \pm vt$ trajectories is clear. The Bohmian trajectories do not cross reflecting the single-valued property of the wave function. They are asymptotic to the straight-line classical trajectories, which all can be extrapolated back to the origin $x = 0$. This is in line with the expansion of the action around $\boldsymbol{r'} = 0$ of Eq. (5) which leads to the SC wave function of the IT approximation. From Fig. 1 one sees that the two Bohm trajectories beginning at $vT = \pm 1.0$ converge rapidly (for $T \approx 3.0$) to the IT straight-line classical trajectories for $v = \pm 1.0$. In line with the IT prediction, the distribution in space of $|\Psi(x,t)|^2$, when plotted as a function of $x/t = p/m$ for $\tau \gg 1$ i.e. for $t \gg T$, is exactly that of the momentum distribution $|\tilde{\Psi}(p, t = 0)|^2$ and does not change in time.

B. Quantum potential, Gouy phase and the harmonic oscillator.

The quantum potential is defined in terms of the amplitude $R(x,t)$ which from Eq. (29) can be written

$$R(x,t) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} \frac{1}{(1+\tau^2)^{1/4}}\, e^{-\frac{x^2}{(2\sigma^2)}\frac{1}{(1+\tau^2)}}. \tag{35}$$

From this expression the quantum potential is

$$\begin{aligned} Q(x,t) &= -\frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial^2 R}{\partial x^2} \\ &= -\frac{\hbar^2}{2m\sigma^4}\left[\frac{x^2}{(1+\tau^2)^2} - \frac{\sigma^2}{(1+\tau^2)}\right] \\ &= -\frac{m}{2T^2}\left[\frac{x^2}{(1+\tau^2)^2} - \frac{\sigma^2}{(1+\tau^2)}\right]. \end{aligned} \tag{36}$$

Some remarks on the description of this function as a "potential".

1) As noted already, its origin is the kinetic energy term in the Hamiltonian and so it is clearly a fictitious potential. In this picture, the Bohm velocity, analogous to the radial velocity, appears in only a part of the total kinetic energy.

2) Although dealing with free propagation under a constant Hamiltonian, the potential function Q is time-dependent.

3) The appearance of the second x-independent but time-varying contribution is unusual for a potential function. For fixed t it is a constant.

We clarify these aspects in that, first we recognise that at each fixed time, the spreading gaussian function is the ground state wave function of the harmonic oscillator (HO).

With $T = m\sigma^2/\hbar$ the function Q can be written

$$Q(x,t) = -\frac{m}{2T^2}\frac{x^2}{(1+\tau^2)^2} + \frac{\hbar}{2T}\frac{1}{(1+\tau^2)} \tag{37}$$

For fixed time t, the wave function is that of the ground-state HO with frequency

$$\omega(t) = \frac{1}{T}\frac{1}{(1+\tau^2)} \tag{38}$$

and in particular $\omega(0) = 1/T$ at time zero, which gives additional meaning to the constant T. Then the quantum potential takes the form

$$Q(x,t) = -\frac{1}{2}m\omega^2(t)\, x^2 + \frac{1}{2}\,\hbar\omega(t) \tag{39}$$

at each fixed time t. Of course this shows clearly that the quantum "potential" is indeed the difference of the oscillator potential energy and total energy, i.e. the *kinetic* energy of the instantaneous oscillator state. This form also shows that the mysterious x-independent second term in Q is simply the total energy of the oscillator.

Even more interesting, in appendix B it is shown that the x-independent term in the quantum potential, the HO eigenenergy, has its origin in the derivative of the Gouy phase contribution to the total action function S. The phase factor is the action from the integral of the adiabatic energy of the oscillator $E_0(t) \equiv \hbar\omega(t)/2$ in Eq. (39) i.e.

$$\begin{aligned} \exp\left(\frac{i}{\hbar}\int^t E_0(t')dt'\right) &= \exp\left(\frac{i}{2}\int^t \omega(t')dt'\right) \\ &= \exp\left(\frac{i}{2}\arctan\tau\right) \end{aligned} \tag{40}$$

which is exactly the Gouy phase of Eq. (29). Some authors have identified the Gouy phase with a geometric phase [19, 20]. It has been identified in ionised-electron wave packets [21] and a connection to Maslov phases [15] pointed out. Here we have shown its origin to be simply the dynamic adiabatic time-dependent energy phase of the time-dependent Schrödinger equation. This is a new interpretation of the Gouy phase in quantum mechanics.

C. The Wave Function along a trajectory.

The nature of the exact wave function along the Bohm trajectory $x(t)$ is striking in its simplicity. Substituting the trajectory $x(t) = x_0(1+\tau^2)^{1/2}$ into Eq. (29) gives the wave function

$$\begin{aligned} \Psi(x(t)) =& \frac{1}{[\pi\sigma^2(1+\tau^2)]^{\frac{1}{4}}}\exp\left[-\frac{i}{2}\arctan\tau\right] \\ &\times \exp\left[-\frac{x_0^2}{2\sigma^2}\right]\,\exp\left[i\frac{x_0^2\,\tau}{2\sigma^2}\right]. \end{aligned} \tag{41}$$

That is, the gaussian function has a *constant amplitude* along the trajectory. Furthermore, recognising that $x_0 = vT$, where v is the asymptotic constant classically velocity, this equation can be written in the form

$$\begin{aligned} \Psi(x(t)) =& \frac{1}{[\pi\sigma^2(1+\tau^2)]^{\frac{1}{4}}}\exp\left[-\frac{i}{2}\arctan\tau\right] \\ &\times \exp\left[-\frac{\sigma^2 p^2}{2\hbar^2}\right]\,\exp\left[\frac{i}{\hbar}\frac{p^2 t}{2m}\right], \end{aligned} \tag{42}$$

where $p^2 = (\hbar x_0^2/\sigma^2)^2 = (mv)^2$ is precisely the momentum variable appearing in the initial, but constant in time, gaussian momentum wave function $\tilde{\Psi}(p,0)$ of Eq. (12). The action phase factor is also that of the classical asymptotic trajectory. Proceeding further with the transformation, one can show that along the trajectory

$$\left(\frac{dp}{dx}\right)^{1/2} = \frac{\sigma}{\hbar^{1/2}}\,(1+\tau^2)^{1/4}. \tag{43}$$

Then the space wave function is

$$\Psi(x(t)) = \left(\frac{dp}{dx}\right)^{1/2}\exp\left[-\frac{i}{2}\arctan\tau\right]\tilde{\Psi}(p,0)\,\exp\left[\frac{i}{\hbar}\frac{p^2 t}{2m}\right]. \tag{44}$$

which is precisely of the IT form of Eq. (6). Thus we see the remarkable result that along the Bohm trajectory, the value of the coordinate space wave function is proportional to the *initial momentum space wavefunction* which propagates unchanged in time. The *asymptotic* form of the IT wave function is valid *for all times* but with the substitution $p = mv = mx/(t^2+T^2)^{1/2}$. It converts smoothly into the semi-classical wave function with $p = mv = mx/t$ for $t \gg T$.

Note that Eq. (44) shows that along the Bohm trajectory, the space wave function provides an image of the initial momentum wave function, as an extension of the IT to the near zone. Also, following Eq. (9) one sees from Eq. (44) that the probability

$$|\Psi(x,t)|^2\, dx(t) = |\tilde{\Psi}(p,0)|^2\, dp, \tag{45}$$

to locate a particle on the Bohmian trajectory and its classical IT extension, is a constant.

D. Time-scaling of Space; the Co-moving Frame.

In this section it is shown that the transition to a Bohm trajectory can be viewed as a time scaling of space. This gives a further meaning to the appearance of the Gouy phase.

The time-scaling of space coordinates is employed frequently in dynamics, not only in quantum mechanics [22, 23] but also in classical mechanics [24] and cosmology [25]. In the context of this paper it was employed by Solovev [22] to show the equivalence of free motion to harmonic oscillator motion in quantum mechanics. A thorough discussion of such time transformations in non-relativistic quantum mechanics is given by Takagi [26], who emphasised the transformation to a co-moving frame. In hydrodynamics such a transformation is described as going from the Euler frame to the Lagrange frame. Here we expose a novel connection of the time-scaling of space to the concept of Bohm trajectories and their classical asymptotes.

In the TDSE of free motion

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - i\hbar\frac{\partial\Psi}{\partial t} = 0 \tag{46}$$

we introduce new space and time coordinates,

$$q \equiv \frac{x}{a(t)} \qquad \bar{t} \equiv \int^t \frac{dt'}{a(t')^2}, \tag{47}$$

where $a(t)$ is dimensionless so that q and $\bar{t}$ retain their usual dimensions. Substitution in Eq. (46) gives the transformation

$$\Psi(x,t) = a^{-1/2}\exp\left(\frac{i}{2}a\dot{a}\, mq^2\right)\Phi(q,\bar{t}), \tag{48}$$

where Φ satisfies the TDSE of a harmonic oscillator (HO) with *time-dependent* frequency, i.e.

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}m\, a^3\ddot{a}\, q^2\right)\Phi = i\hbar\frac{\partial\Phi}{\partial\bar{t}}. \tag{49}$$

Note that the dot signifies differentiation w.r.t. t.

If, in recognition of the Bohm trajectory Eq. (33), we choose $a(t) = (1+\tau^2)^{1/2}$, where $\tau = t/T$, then we obtain the standard HO equation with a *time-independent* fixed frequency $\omega_0 = 1/T$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}m\,\omega_0^2\, q^2\right)\Phi = i\hbar\frac{\partial\Phi}{\partial\bar{t}}. \tag{50}$$

The solutions to Eq. (50) are the HO wavefunctions of which the ground state, with energy $E_0 = \frac{1}{2}\hbar\omega_0$, is

$$\Phi(q,\bar{t}) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4}\exp\left(-\frac{q^2}{2\sigma^2}\right)\exp\left(-\frac{i}{\hbar}E_0\bar{t}\right), \tag{51}$$

where the standard energy phase is $E_0\bar{t}/\hbar = \frac{1}{2}\omega_0\bar{t} = \frac{1}{2}\bar{t}/T = \frac{1}{2}\arctan\tau$, showing that the new time is simply proportional to the Gouy phase.

Hence, in the co-moving frame Φ is the fixed non-expanding gaussian, only space expands. This is exactly in line with our introduction of a complex space trajectory.

Indeed, for this choice of scaling function $a(t) = (1+\tau^2)^{1/2}$, one has $q = x/a = x_0 = vT$. Then, transforming back to the laboratory frame using Eq. (48), gives

$$\begin{aligned}\Psi(x,t) =& \frac{1}{[\pi\sigma^2(1+\tau^2)]^{\frac{1}{4}}}\exp\left[-\frac{i}{2}\arctan\tau\right] \\ &\times\exp\left[-\frac{x_0^2}{2\sigma^2}\right]\exp\left[i\frac{x_0^2\,\tau}{2\sigma^2}\right].\end{aligned} \tag{52}$$

which is precisely Eq. (41). Then the IT equations Eq. (42) and Eq. (44) follow also.

Also a further interpretation of the Gouy phase, which has the simple form $\frac{1}{2}$ arctan (τ) has emerged. On the one hand it appears as the adiabatic energy integral Eq. (40). On the other hand it provides exactly the transformation to a frame coinciding with the Bohm trajectory through the definition of a new time $\bar{t} \equiv T$ arctan (t/T).

The connection between quantum wave mechanics and Optics is the subject of the next Section. In particular, the two-dimensional TDSE is shown to be identical to the paraxial wave equation of optics. Hence the results obtained for the propagation of quantum wave packets apply equally to the propagation of laser light beams.

IV. THE SPREADING OF WAVE PACKETS

The question of the spreading of wave packets turns out to be a prime example of the difference between the single-particle (SP) interpretation of the wave function and the “ensemble” view that the wave function applies only to the statistical properties of many particles and cannot be assigned to a single particle [27, 28].

The SP picture is presented in very many quantum text books. Since, in assigning the wave function to a single particle, the spreading of the wave function does not correspond to a localised particle, then the spreading is seen as non-classical i.e. a purely quantum effect .

We consider the quantum to classical transition on the basis of gaussian wave packet propagation and spreading represented by the Bohmian trajectories of Fig. 1. Important is that the condition $t < T$ delineates the "quantum" region where the quantum potential is non-zero and the opposite $t > T$ region is where the quantum potential tends to zero and the trajectories become classical.

In the SP picture, the suppression of "quantum" spreading is seen as essential to the localisation of a single classical particle. For example, in Ref. [29], macroscopic values of mass 1 gram and size $\sigma = 1\mu$m are assumed to show that, for times $t \ll m\sigma^2/\hbar = T$ which are of the order of 10^{35}a.u. (greater than the age of the universe), a single particle has a wave packet which retains its width. Hence, since the wave packet centre obeys Ehrenfest's theorem, it is assumed that an observation would conclude that the particle moves classically.

With reference to Fig. 1 one sees that for $\tau \ll 1.0$ or $t \ll T$ the particles move on trajectories almost parallel to the time axis. Since the width in real space is macroscopic, the width in momentum space is very small, in the example $\approx 10^{-5}$ a.u.. However, this extremely small width in momentum space confines particles to a Bohmian trajectory with almost zero velocity in the x direction i.e. a trajectory $x(t) \approx 0$. This one particular Bohm trajectory coincides with the straight-line classical trajectory. Since it is the trajectory of the centre of the wave packet, this single trajectory is straight-line classical as dictated by the Ehrenfest theorem for free motion.

For convenience we have chosen a wave packet whose centre does not move in the x direction. Were one to choose a centre with momentum p_0 then the classical SP limit would have particles confined to the straight-line trajectory $x(t) = p_0 t/m$. The SP classical criterion is valid for all t in the limit $T \to \infty$. Note however that the region $t < T$ is precisely the *quantum wave* region.

By contrast, in the ensemble interpretation adopted here, the spreading is viewed as a simple consequence of the initial distribution of momenta in the x direction. The spreading simply mirrors the fact that an ensemble of classical particles with different velocities spreads in time.Then the classical transition is more general in that every trajectory, independent of the particle mass, becomes classical for some $t > T$. On an atomic scale, the large time t implies large distance x where the action function has values much in excess of $\hbar$. In this region the IT wave function is valid and describes a *classical* ensemble of trajectories with different velocities emanating from $x = 0$, as shown in Fig. 1. Hence in the ensemble picture the condition $t > T$ for the quantum to classical transition is precisely the *opposite* of the condition assumed in the SP picture.

To put it simply, in the SP picture the wave packet spreading in seen as non-classical as it delocalises the wave function assigned to a *single particle*. In the ensemble picture the spreading is seen as the epitome of the classical dynamics of an *ensemble* of particles with different momenta, embedded within the delocalised quantum wave function.

A general condition for the transition to classical motion is that the action function S assumes values everywhere greater than $\hbar$. For a gaussian wave packet one can show that, for the SP picture "classical condition" $t < T$, the action is approximately $\hbar\, t/T$ which does not fulfil the classical requirement. For the ensemble picture criterion, $t > T$, the action becomes $S \approx (1/2)mv^2\, t$ which is larger than $\hbar$ everywhere (except along the centroid Ehrenfest trajectory $v = 0$!). Hence the accepted text-book SP explanation of the quantum to classical transition would appear questionable.

V. WAVE, RAY AND PARTICLE PICTURES

It is interesting that the mathematics of the quantum to classical transition of particle wave mechanics is identical to that of the wave to beam transition in electrodynamics. In electrodynamics the transition from wave to beam or ray picture begins with the eikonal approximation to the Helmholtz equation. For a single field component $\Psi(\boldsymbol{r})$, the Helmholtz equation reads

$$[\nabla^2 + k^2(\boldsymbol{r})]\, \Psi(\boldsymbol{r}) = 0, \tag{53}$$

where $k = \; k_0\, n = \Omega n/c$ with refractive index $n(\boldsymbol{r})$, velocity of light c and light frequency Ω. The TISE has the same form but with $k^2 = 2m(E - V(\boldsymbol{r}))/(\hbar^2)$, with total energy E and potential $V(\boldsymbol{r})$. The analogy becomes an identity if one defines, for light, the free momentum $p = \hbar\Omega/c$. For particles, the asymptotic free momentum is $p = (2mE)^{1/2}$. Then in both cases one has $k(\boldsymbol{r}) = p\, n(\boldsymbol{r})/\hbar$ where for particles the dimensionless "refractive index" is $n(\boldsymbol{r}) \equiv (1 - V(\boldsymbol{r})/E)^{1/2}$. Also in both cases the wavelength is $\lambda(\boldsymbol{r}) = 2\pi/k(\boldsymbol{r})$.

Substitution of the polar expression

$$\Psi(\boldsymbol{r}, t) = R(\boldsymbol{r}, t)\, e^{iS'(\boldsymbol{r},t)} \tag{54}$$

into the Helmholtz Eq. (53), where R and the dimensionless phase S' are real functions, and taking the real part gives, for both particles and light, the simple equation

$$(\nabla S')^2 = k^2(\boldsymbol{r}) + \frac{\nabla^2 R}{R}. \tag{55}$$

One recognises the emergence of the term of equivalent form to the "quantum potential" on the right side of this equation.

For light it is customary to define a phase $S = S'/k_0$ to give the exact equation

$$(\nabla S)^2 = n(\boldsymbol{r})^2 + \frac{1}{k_0^2}\frac{\nabla^2 R}{R} \tag{56}$$

For particles it is usual to define an action phase as $S = \hbar S'$ to give the analogous equation

$$(\nabla S)^2 = 2m(E - V(\boldsymbol{r})) + \hbar^2 \frac{\nabla^2 R}{R}, \tag{57}$$

the time-independent form of Eq. (26).

For light, the transition to ray optics is made by neglect of the second term on the right in Eq. (56). This "eikonal" approximation is often justified by saying that $k_0 \to \infty$ or correspondingly the wavelength goes to zero. Of course k_0 is fixed, more accurate is to say that R is slowly varying so that $\frac{\nabla^2 R}{R}$ is small. Alternatively n^2 is everywhere much bigger than the term $\frac{1}{k_0^2}\frac{\nabla^2 R}{R}$ which can be dropped.

In complete analogy, for particles the transition to a classical trajectory is made by neglect of the quantum potential in Eq. (57) to give the classical Hamilton-Jacobi equation. For particles, the classical limit is often expressed as $\hbar \to 0$, although $\hbar$ is a fixed constant. Again more accurate is to say that the slowly varying function R implies that the quantum potential is everywhere small and can be neglected. Alternatively the classical limit is where the kinetic energy $(E - V)$ everywhere far exceeds the quantum potential $\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$.

The eikonal approximation for light is synonymous with Fermat's principle of least path for light rays. The Hamilton-Jacobi equation for particles is synonymous with Hamilton's principle of least action for particle trajectories. The analogy between light and particle dynamics becomes even more striking when one recognises that the IT of quantum mechanics gives the result that the asymptotic space wavefunction of Eq. (6) is proportional to the initial momentum wavefunction. For light, the Fraunhofer diffraction pattern at large distance from a slit is proportional to the Fourier transform to wave number (momentum) space of the slit function, see Ref. [30].

It should be remarked that traditionally in Optics, the ray picture is used only where the eikonal approximation to Eq. (56) is justified, just as here the classical action to define a classical trajectory is used only when the quantum potential can be neglected. In this asymptotic zone the Hamiltonian formulation of ray propagation is well-developed [31]. When the full equation Eq. (56) is applicable one speaks of the wave regime. The analogue of defining Bohmian trajectories in the wave regime is rarely used in Optics, rather wave fronts are drawn. However, an extension of the trajectory picture to describe electromagnetic waves in all of space, equivalent to Bohmian mechanics for the Schrödinger equation, has been suggested [32].

In the next section the similarity of light and particle dynamics is extended further by showing the equivalence of the paraxial approximation of the Helmholtz equation to the TDSE of quantum mechanics.

A. The paraxial approximation of Optics

In the paraxial approximation one considers light travelling in the z direction as a plane wave to give

$$\Psi(\boldsymbol{r}) = \psi(\boldsymbol{r})\, e^{ikz}, \tag{58}$$

where ψ is a slowly varying function of z and we consider for the moment a constant k. Substitution in the Helmholtz equation Eq. (53) and neglect of the second derivative with respect to z, gives the paraxial equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + 2ik\,\frac{\partial\psi}{\partial z} = 0. \tag{59}$$

In the particle case, one takes Eq. (53) as the TISE of quantum mechanics. Then the paraxial equation follows from the same approximation of slowly-varying $\psi(\boldsymbol{r})$ in the z direction. For particles we multiply Eq. (59) by $-\hbar^2/(2m)$ to write the paraxial equation in the form,

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}\right) - i\frac{\hbar^2 k}{m}\,\frac{\partial\psi}{\partial z} = 0 \tag{60}$$

The key step in deriving a TDSE is when the variable z can be treated as a *classical variable* $z(t)$ with a corresponding *classical velocity* $\dot{z}(t) \equiv v_z$. Then in Eq. (60) one puts $\hbar k/m = p_z/m = v_z = \partial z/\partial t$, so that the paraxial equation becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}\right) - i\hbar\,\frac{\partial\psi}{\partial t} = 0 \tag{61}$$

which is the TDSE for motion in two dimensions.

This is simply an example of the general derivation of the TDSE from the TISE in higher dimension, see Ref. [33], when one or more of the quantum variables can be treated classically. Here, the z coordinate becomes the time i.e. the classical longitudinal motion of the particle in the z direction provides its own clock for the quantum motion in the transverse direction.

In this connection one notes that the plane wave $\exp(ikz) = \exp(ipz/\hbar)$ is already of SC form since $\partial S/\partial z = p$, the classical HJ condition. Interestingly, the paraxial form of the two-dimensional Helmholtz equation is seen clearly as an approximation in Optics. However, the equivalent two-dimensional TDSE is viewed as *exact* in quantum mechanics, although it is stressed in Ref. [33] that, because of the classical nature of time, the TDSE of Eq. (61) is an *approximation* to the full TISE in a higher number of space dimensions.

B. Equivalence of the Paraxial Equation and the TDSE.

The IT limit is asymptotic and the time T is the natural limit defining the edge of the quantum wave zone. The Bohmian trajectories are defined where the quantum potential is still non-negligible. In terms of wave fronts, the Bohmian trajectories describe the change in the direction of the normal to the instantaneous wave front. The asymptotic classical constant velocity corresponds to the wave fronts becoming locally almost plane, as for a plane wave.

We have shown already that the paraxial equation of Optics (60) and the TDSE of quantum mechanics are

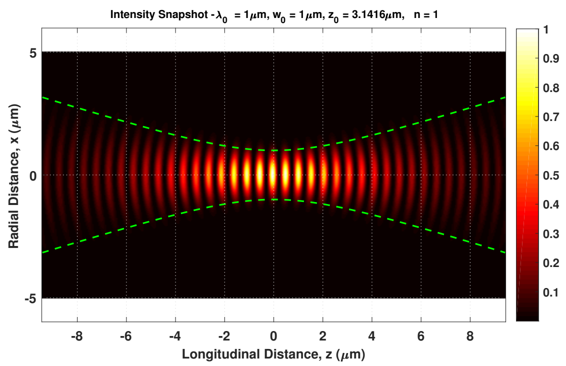

FIG. 2: The wave fronts of a gaussian light beam focussed at $z = 0$. The dashed lines follow the beam waist i.e. the path of equal intensity at $1/e^2$ of the maximum. Figure reproduced courtesy of Prof. E. Glytsis.

equivalent mathematically. The gaussian beam in optics is much studied as the typical output of a laser. The wave fronts of such a beam are shown in Fig. 2. One notes the macroscopic scale of distance compared to the atomic units of Fig. 1. In laser gaussian beams one considers two transverse dimensions x, y. Here for purposes of illustration it is simpler to restrict to one x dimension. The corresponding scalar electric field with wave number k can be written [18],

$$\begin{aligned} E \propto \left(\frac{W_0}{W(z)}\right)^{1/2} \exp\left(-\frac{x^2}{W^2(z)}\right) \\ \times \exp\left(-i\frac{kx^2}{2R(z)} + \frac{i}{2}\arctan\left(\frac{z}{z_0}\right)\right). \end{aligned} \tag{62}$$

Here, z_0 is called the Rayleigh range and is the distance after which the asymptotic straight-line ray approximation begins to become valid. The width of the beam is given by $W(z)$ with

$$W(z) = W_0 \left(1 + \frac{z^2}{z_0^2}\right)^{1/2} \tag{63}$$

where W_0 is the minimum width of the beam, see the dashed lines on Fig. 2. It is usual to define this "waist" of the beam corresponding to the locus of the amplitude being $(1/e)$ of its maximum.

By comparison of Eq. (62) with Eq. (29) one has the equivalence between optics and quantum mechanics in the correspondences $z_0 \to T$ and

$$\begin{aligned} W_0^2 \to 2\sigma^2, \quad \tau \to z/z_0, \\ \text{and} \quad W^2(z) \to 2\sigma^2(1+\tau^2). \end{aligned} \tag{64}$$

Furthermore, the Rayleigh range can be written $z_0 = k\sigma^2$, the analogue of $T = (m/\hbar)\sigma^2$ in quantum mechanics

The phase $\arctan(z/z_0)$ in Eq. (62), which is the Gouy phase, appears in the quantum time-dependent wavefunction in the equivalent form as $\arctan(t/T) \equiv \arctan(\tau)$, see Eq. (29).

The function

$$R(z) = \frac{z_0^2}{z}\left(1 + \left(\frac{z}{z_0}\right)^2\right) \tag{65}$$

gives the radius of curvature of the beam fronts. The action phase function from Eq. (62), neglecting the x-independent Gouy phase, is given as $S = kx^2/(2R(z))$.

Then the analogue of the Bohm velocity dx/dt is defined as

$$\frac{dx}{dz} \equiv \frac{1}{k}\frac{\partial S}{\partial x} = x\,\frac{z}{(z^2+z_0^2)}. \tag{66}$$

This can be integrated to give the trajectory

$$x(z) = x_0\left(1 + \left(\frac{z}{z_0}\right)^2\right)^{1/2} \tag{67}$$

which is identical to the quantum Bohm trajectory Eq. (33) with z/z_0 replacing $\tau = t/T$.

Asymptotically, the wave fronts become essentially spherical but locally almost planar. This is the region where in Optics the eikonal approximation becomes valid allowing the definition of a straight-line ray of light. The equation of this straight line is $x = (k_x/k)\,z$, where k_x is the wave number in the x transverse direction. Hence, from the asymptotic $z \gg z_0$ limit of Eq. (67) one has $x_0 = k_x\sigma^2$.

If one plots the optics Bohm trajectories or stream lines, as in Fig. 1 for particles, each trajectory intercepts the $z = 0$ axis at x_0. The beam waist shown in Fig. 2 is just one example of a Bohm trajectory with $x_0 = \sqrt{2}\sigma \equiv W_0$. That the Bohm trajectories can be defined for the paraxial Helmholtz equation has been shown already in Ref. [32], where the trajectories were calculated numerically. In Optics the equivalence of Bohm trajectories are not drawn usually, rather in books on wave optics e.g. Ref. [18], it is customary to depict wave fronts (lines of constant phase) spreading in the z direction, as shown in Fig. 2.

Clearly however, were one to connect the normals to the wave fronts, one would reproduce the Bohm trajectories. Exactly as in the quantum case, it is shown in appendix C that the wave function along a Bohm trajectory is of the IT form, i.e. is proportional to the invariant FT of the x wave function to k_x space. Asymptotically the IT $t \gg T$ result of quantum mechanics is just the well-known Fraunhofer diffraction $z \gg z_0$ limit of Optics. Along a Bohm trajectory in the quantum case, the probability is conserved. Along a Bohm trajectory in Optics the intensity is conserved.

Some authors [19, 20] have argued that the Gouy phase is a topological or geometric phase. In the TDSE, here a different interpretation of the Gouy phase as the adiabatic-energy phase of the fixed-time quantised gaussian state has been derived. This extends also to the paraxial optics equation. Then it can be shown that, for fixed z, the eigenvalue of the transverse gaussian "cavity" is simply given by the expectation value of the transverse wave number

$$< k_x^2(z) > \quad = \frac{1}{\sigma^2\left(1+(\frac{z}{z_0})^2\right)} \tag{68}$$

Then the Gouy phase is obtained as the integral of this adiabatic eigenvalue

$$\phi = \frac{1}{z_0}\int^z \frac{dz'}{\left(1+(\frac{z'}{z_0})^2\right)} = \arctan\left(\frac{z}{z_0}\right) \tag{69}$$

since $z_0 = k\sigma^2 = kW_0^2/2$. This corresponds to the result of Ref. [34] who showed that the Gouy phase is the integral of the expectation value of k_x^2. For a gaussian this expectation value is simply proportional to the eigenvalue.

The aspect that the Gouy phase of gaussian beams has its origin in the finite extent of the wave packet at the focus has been pointed out in Optics already [35, 36]. In Ref. [36] it is shown to be related to the difference between the wave-front path (in quantum mechanics the Bohm trajectory) and the straight-line ray motion (in quantum mechanics the classical trajectory) as light traverses the focus, see Fig. 2. In Ref. [35] and Ref. [34] the Gouy phase is attributed to the transverse spatial confinement of the wave profile.

This establishes the one-to-one correspondence between the TDSE and the paraxial equation of Optics for the propagation of a gaussian beam. It has been suggested that Bohm trajectories can be identified as the paths of photons in an interference experiment [37]. From the demonstrated equivalence of paraxial equation and TDSE, the paths of constant high intensity for light will indeed mirror the Bohm trajectories of constant high probability for particles. Hence the tracks seen [37] are the single-photon onset of near-field "Talbot carpet" patterns well-known in grating diffraction. An illustration of such interference patterns and associated Bohm trajectories for massive particles is given in Ref. [38].

VI. PROPAGATION FROM NEGATIVE TIMES; BEAM FOCUSSING FOR MASSIVE PARTICLES.

In Fig. 3 the time reversal invariance of the wave packet propagation has been used to plot also the Bohm trajectories beginning at large negative times and converging to the fixed gaussian at zero time. Then the trajectories diverge to positive times as shown. This is the quantum version of the gaussian beam focussing which is shown in Fig. 2. It is readily achieved as the gaussian beam output of a laser in Optics [18] as has been presented in the previous section. Sadly, such a focussing free particle wave packet would be difficult to achieve. Apart from the preparation, unlike photons which hardly interact,

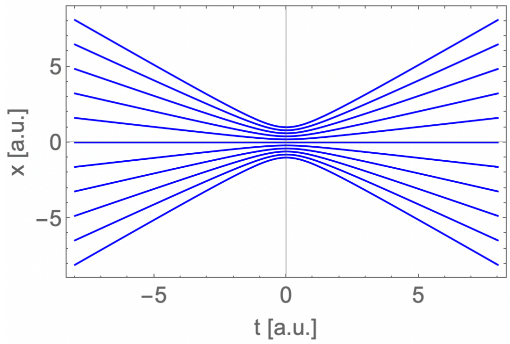

FIG. 3: The Bohmian trajectories $x(t)$ representing the focussing in one dimension (vertical axis) of a gaussian wave function with time increasing from left to right. The time constant is $T = 1.0$. The axes are in atomic units (a.u.).

material particles compressed to microscopic separations always interact.

The difference between classical and quantum behaviour is illustrated in Fig. 4. There only a pair of classical and Bohmian trajectories for the asymptotic velocities $\pm v = 1.0$ is shown. The classical trajectories are the straight-line classical trajectories passing through the origin and crossing there. By contrast, the corresponding pair of Bohmian trajectories do not cross and simply diverge from each other for $|t| < T$.

This figure illustrates also the scaling of the time (and hence the distance z) by the constant $T = m\sigma^2/\hbar$. If T becomes smaller by the extent σ becoming smaller, then the classical trajectory is valid over more of time and space. Were the gaussian that of nuclei, rather than atoms, then the semi-classical IT wave function would be valid after distance of the order of tens of femto-metres.

The trajectories of Fig. 4 look remarkably like Landau-Zener avoided crossings between the "diabatic" classical trajectories $x(t) = \pm vt$, which cross at $t = 0, x = 0$ and the "adiabatic" Bohmian trajectories $x(t) = \pm v(t^2 + T^2)^{1/2}$, which have an avoided crossing of magnitude $2vT$ there. For free motion the classical trajectories have fixed velocity $\pm v$ which is preserved through the crossing. However, the Bohmian trajectories change their character from $\pm vt$ to $\mp vt$ as they traverse the avoided crossing.

The non-crossing can be explained from the single-valued nature of the wavefunction, preventing the normals to the wave front having two values at the same point. In the Bohmian interpretation it is attributed to the quantum force becoming relevant as the wave packet shrinks to atomic dimensions. This acts to repel the classical trajectories to prevent them crossing at $x = 0$. In-

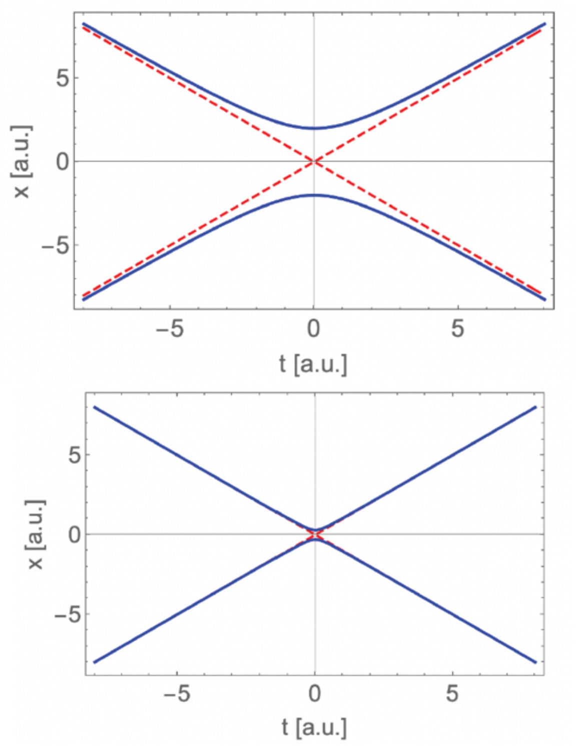

FIG. 4: Two Bohmian trajectories $x(t)$ representing the focussing in one dimension (vertical axis) of a gaussian wavefunction with time proceeding from left to right. The straight lines are the asymptotic classical trajectories for $\pm v = \pm 1.0$ a.u.. The upper panel is for $T = 2$ a.u. The lower panel is for $T = 0.3$ a.u.. The axes are in atomic units (a.u.).

deed, it is simple to show that the quantum force, defined as $F = -\partial Q/\partial x$, when integrated over all time gives exactly the momentum change of $2mv$. One can view the change of momentum as indicating a quantum "pressure" preventing the compression of the wave function to zero extent.

The sole physical parameter deciding quantum or classical character is $T = m\sigma^2/\hbar$. That is, apart from the mass, it is the spatial extent σ of the wavepacket at $t = 0$ which decides when the classical trajectories emerge. This is in line with the semi-classical IT approximation where the $x \approx 0$ assumption clearly corresponds to the $\sigma \to 0$ limit.

Hence, the quantum to classical transition is illuminated by considering the limit that the initial position wave function shrinks to a point. This is the limit that $\sigma \to 0$ and correspondingly that $T \to 0$, i.e. the extent of the quantum wave function goes to zero. The limit of the gaussian of Eq. (17) is, up to a normalisation constant, a delta function. Substituting a delta function $\delta(x')$ in Eq. (A1) gives simply

$$\Psi(x,t) = K(x,t;0,0) = \left(\frac{1}{2\pi\hbar}\right)^{1/2} \left(\frac{m}{it}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2t}x^2}. \tag{70}$$

If one recognises that the Fourier transform of the initial delta function gives the momentum wavefunction equal to a constant i.e. $\tilde{\Psi}(p,0) = \left(\frac{1}{2\pi\hbar}\right)^{1/2}$ then one has, valid for all x, t,

$$\Psi(x,t) = \left(\frac{m}{it}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2t}x^2}\,\tilde{\Psi}(p,0). \tag{71}$$

Furthermore, one sees that, with the phase $S = mx^2/(2t)$ one has the classical condition $p = dS/dx = mx/t$. Then writing the phase factor as $\frac{i}{\hbar}\frac{m}{2t}x^2 = \frac{i}{\hbar}\frac{p^2}{2m}t$ exactly the IT result of Eq. (21) is obtained. Thus as the spatial wavefunction shrinks to a point, as one might expect, the asymptotic IT result is valid everywhere. Up to a normalisation constant, the space and momentum wavefunctions (see Eq. (12)) are identical in form. For $T \to 0$ the trajectories for all times $t > T$ are the classical ones of the lower panel of Fig. 4.

What happens as T grows from zero is that it corresponds simply to the introduction of a complex time $t \to t - iT$. That is the *exact* space wave function becomes, now restoring the correct normalisation

$$\Psi(x,t) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} \frac{iT^{1/2}}{(t-iT)^{1/2}} \exp\left(\frac{i}{\hbar}\frac{m}{2(t-iT)}x^2\right). \tag{72}$$

This is of the same form as the wavefunction propagating from a delta function Eq. (70) but now with complex time. Putting $T = m\sigma^2/\hbar$ and $\tau = t/T$ it is readily confirmed that this form corresponds to Eq. (18) and the polar form Eq. (29).

Hence, the departure of the wavefunction from its asymptotic semi-classical form and definition of a classical trajectory, can be viewed as a transformation from time t to an extended time $(t^2 + T^2)^{1/2}$, the passage of time slows. Its mathematical realisation is in the time scaling of position as given in section III D.

VII. CONCLUSIONS

The free motion of a normalisable wave packet, exemplary of gaussian form, has been analysed. In standard quantum mechanics, only the expectation values, averages over the wave packet components, of the observables energy, momentum and position are defined. For spreading wave packets, these mean values have little significance. Hence, particularly for the constant momentum components of a free wave packet, it is tempting to assign physical meaning to the individual components. This is achieved by the stationary phase approximation of the IT for asymptotic propagation. Then it emerges that the constant p value in the momentum wave function can be put equal to the classical momentum $p = mx/t$ in the space wave function. A classical trajectory is defined within the quantum wave function.

The classical trajectory is the locus of the normal to the constant action wave fronts. The probability of detection is constant along these trajectories. The extrapolation of these properties into the non-asymptotic near-field region has been shown to give loci synonymous with the proposed particle trajectories of Bohmian mechanics.

Behaving as a classical ensemble, each p component of the wave function corresponds to a different trajectory and at a given fixed time these different p trajectories all cross at the origin, at a single point in space. The essence of quantum mechanics is that the ensemble spatial wave function is of finite extent and the necessity of quantisation leads to an effective non-compressibility of space to a point.

The precise equivalence of the TDSE to the paraxial equation of Optics has been shown with concomitant equivalence of time or space propagation of light waves. Hence the Bohm trajectories are equivalent to the well-known near-field patterns of light diffraction.

The main results of this study of the free propagation of a gaussian quantum wave function can be summarised as follows:

A) There is a one-to-one correspondence with the propagation of gaussian light beams in Optics. The photon tracks along lines of constant light intensity, both in near and far field zones, are just the particle Bohm trajectories of the equivalent TDSE. All the results listed below apply equally well, suitably translated, to the space and momentum (wave number) gaussian wave functions of the paraxial equation of Optics.

B) The Bohmian and classical trajectories are defined solely by the constant asymptotic velocity v and the time parameter $T = m\sigma^2/\hbar$, where σ is the $t = 0$ width of the wave function. Unique classical trajectories begin at $x = 0$ at time zero. Unique Bohm trajectories begin at finite $x_0 = vT$ at time zero.

C) The semi-classical wave function of the Imaging Theorem (IT) justifies defining a classical trajectory for $t \gg T$. The Bohmian trajectories connect smoothly to these asymptotic trajectories.

D) The exact wave function in momentum space propagates with constant amplitude and a classical action phase. We have shown that the exact *spatial* wave function along the Bohmian trajectory is proportional to this invariant momentum function with the relation $p = mx(t)/(t^2 + T^2)^{1/2} = mv$. Asymptotically this becomes the IT wave function with the interpretation $p = mx/t = mv$. Along the whole trajectory, the proportionality factor is the square root of the classical density of states (Van Vleck) factor.

E) The invariance of the wave function along the Bohm trajectory and its classical extension arises from a time-scaling of the position coordinate i.e. a transition to the co-moving frame. For a gaussian the Gouy phase provides the dimensionless time scaling function. The "time dilation" of space coordinates represents the difference between the finite extent of the wave function and the point convergence of the classical trajectories.

F) The Bohmian trajectory, and its extension the classical trajectory, comprise the locus of points of equal measurement probability. In Optics these are the stream lines of constant intensity.

G) The time propagation of the gaussian can be viewed as the adiabatic propagation of the HO eigenstate. At any fixed time, the quantum potential function $Q(x,t)$ arises from the kinetic energy as the difference between the fictitious potential function, $m\omega^2(t)/2$, and the instantaneous quantised energy, $\hbar\omega(t)/2$, of the localised wave packet.

H) The Gouy phase corresponds to the adiabatic energy phase of the instantaneous HO ground state energy $E(t) = \hbar\,\omega(t)/2$, i.e.

$$\exp\left(\frac{i}{\hbar}\int^t E(t')dt'\right) = \exp\left(\frac{i}{2}\int^t \omega(t')dt'\right).$$

This gives rise to the position-independent contribution to the quantum potential.

Points G) and H) refer to the HO ground state wave packet but, suitably generalised, apply equally to the higher (Hermite-Gauss) eigenstates. Indeed they should apply to any normalisable packet of finite spatial extent.

In conclusion, an analysis of the oldest problem of quantum continuum dynamics, the free propagation of a gaussian wave packet, has been given. The asymptotic SC form of the wave function, as emerging from the IT approximation justifies the introduction of a classical trajectory. The Bohmian trajectory, defined over all space and time, merges smoothly into the IT classical asymptote.

The Bohmian trajectory is here viewed as the locus of wave front normals, as in Optics. That the spatial wave function is proportional to the constant momentum wave function along a trajectory re-habilitates momentum space in the discussion of trajectories for the case of gaussians. However, in the sense that the quantum potential can be viewed as a fictitious potential function arising from the kinetic energy, the Bohm picture is appealing in that our understanding and language of classical motion can be translated into quantum mechanics. Then the well-known concepts of velocity, force, trajectory etc. can be applied in the quantum domain.

The departure of the wave function from its asymptotic semi-classical form and definition of a classical trajectory, can be viewed as a transformation from time t to an extended time $(t^2 + T^2)^{1/2}$, the passage of time slows. Its mathematical realisation is in the time scaling of position as given in section III D. The classical ensemble has all particles crossing at a point. Since it is maintained here that time arises from a space coordinate, the quantum behaviour can be seen as the finite incompressibility of space to a point. It is tempting to view this incompressibility as arising from the fictitious quantum potential, shown to be of instantaneous harmonic form.

The analysis of the classical limit has made plain that the wave function belongs to an ensemble of particles and should not be be taken as describing the deterministic motion of a single particle.

It should be made clear also as to what is implied here by the asymptotic quantum to classical transition. Classical variation of position and momentum variables appear always within the shroud of the semi-classical wave function. Hence, whether an observer perceives classical or quantum motion depends upon the resolution of the measurement. The spatial wave function oscillates in space and time due to the action phase. In low resolution one measures trajectories, in high resolution wave patterns. This is again in direct analogy to light. In low resolution one observes rays and sharp boundaries of obstacles, in high resolution wave diffraction patterns.

In this sense, the world is always quantum. Even without external de-cohering interactions which interrupt phase propagation, our perception of it through imprecise observation leads to the validity of a classical description. A more extensive defence of this point of view is to be found in Ref. [28].

VIII. ACKNOWLEDGEMENTS

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Appendix A: Free Propagators in Coordinate and Momentum Space

Taking initial time as zero, the time-dependent propagating wave function is given by

$$\Psi(x,t) = \int K(x,t;x',0)\Psi(x',0)\,dx', \tag{A1}$$

where the position coordinate $x(t=0) \equiv x'$. For free propagation to point (x,t) the kernel is given by

$$K(x,t;x',0) = \left(\frac{1}{2\pi\hbar}\right)^{1/2}\left(\frac{m}{it}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2t}(x-x')^2}. \tag{A2}$$

One can also consider time propagation of the initial wavefunction in momentum space, to a final position (x,t). This gives the alternative form

$$\Psi(x,t) = \int \bar{K}(x,t;p',0)\tilde{\Psi}(p',0)\,dp', \tag{A3}$$

with mixed kernel

$$\bar{K}(x,t;p',0) = \left(\frac{1}{2\pi\hbar}\right)^{1/2} e^{\frac{i}{\hbar}(p'x-p'^2\frac{t}{2m})}. \tag{A4}$$

Finally, one can calculate the time-dependent momentum wave function

$$\tilde{\Psi}(p,t) = \int \tilde{K}(p,t;p',0)\tilde{\Psi}(p',0)\,dp', \tag{A5}$$

with momentum-space kernel

$$\tilde{K}(p,t;p',0) = \left(\frac{1}{2\pi\hbar}\right)^{1/2} e^{-\frac{i}{\hbar}\frac{p'^2}{2m}t}\,\delta(p-p'). \tag{A6}$$

Since for free propagation, the phase in the expressions for the kernels is the classical action (in units of $\hbar$) we have, from Eq. (A2), the classical definition

$$\frac{\partial S}{\partial x} = m(x-x')/t \equiv p. \tag{A7}$$

Similarly, from Eq. (A4), we have

$$\frac{\partial \bar{S}}{\partial x} = p' = p \quad \text{and} \quad \frac{\partial \bar{S}}{\partial p'} = x - p't/m = x' \tag{A8}$$

and from Eq. (A6),

$$\frac{\partial \tilde{S}}{\partial p} = \frac{\partial \tilde{S}}{\partial p'} = p't/m. \tag{A9}$$

These are the expected classical relations for free propagation, although the wave functions resulting from the semi-classical propagators are still fully quantum mechanical.

Appendix B: Properties along a Bohmian Trajectory

Consider a transition from a fixed origin $\boldsymbol{r}$ to an instantaneous origin $\boldsymbol{r}(t)$ with velocity $\dot{r}(t)$. Defining the probability

$$P(\boldsymbol{r},t) = |\Psi(\boldsymbol{r},t)|^2\,d\boldsymbol{r} = |\Psi(\boldsymbol{r}(t))|^2\,d\boldsymbol{r}(t) \tag{B1}$$

along the trajectory, one has

$$\begin{aligned}\frac{\partial P}{\partial t} &= \left(\frac{\partial}{\partial t}|\Psi(\boldsymbol{r}(t))|^2\right)d\boldsymbol{r} + |\Psi(\boldsymbol{r}(t))|^2\,\dot{r} \\ &\equiv \left(\frac{\partial \rho}{\partial t}\right)d\boldsymbol{r} + \rho\,\boldsymbol{v}.\end{aligned} \tag{B2}$$

From the continuity equation Eq. (28), with $\rho = R^2$,

$$\frac{\partial \rho}{\partial t} + \nabla.\rho\frac{\nabla S}{m} = 0 \tag{B3}$$

Hence, if we choose the Bohmian trajectory with $\dot{r} = v = \nabla S/m$, we obtain by substitution in Eq. (B2),

$$\frac{dP}{dt} = -\nabla.\rho\,\boldsymbol{v}\,d\boldsymbol{r} + \rho\,\boldsymbol{v} = 0, \tag{B4}$$

so that the probability is constant along a Bohmian trajectory.

The time derivative of the action of Eq. (30) taken along the trajectory is

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial x}\,\dot{x}. \tag{B5}$$

This gives,

$$\begin{aligned}\frac{dS}{dt} &= \frac{\hbar x^2}{2T\sigma^2}\,\frac{1-\tau^2}{(1+\tau^2)^2} + \frac{\hbar x^2}{T\sigma^2}\,\frac{\tau^2}{(1+\tau^2)^2} - \frac{1}{2}\hbar\omega(t)\\ &= \frac{\hbar x^2}{2T\sigma^2}\,\frac{1}{(1+\tau^2)} - \frac{1}{2}\hbar\omega(t)\\ &= \frac{\hbar x_0^2}{2T\sigma^2} - \frac{1}{2}\hbar\omega(t) = \frac{1}{2}mv^2 - \frac{1}{2}\hbar\omega(t).\end{aligned} \tag{B6}$$

The second term, the eigenenergy of the HO, comes from the time derivative of the Gouy phase. One can also show, as must be, that $dS/dt = -Q(x,t)$ along the trajectory. Then the energy along the Bohm trajectory is just that of the classical free particle minus the instantaneous eigenenergy from the Gouy phase.

Appendix C: Wave Function along a Bohmian Trajectory in Optics

For convenience here the notation of Ref. [39] is followed, except that the gaussian width W_0 is replaced by the equivalent $\sqrt{2}\sigma$. The wave function in wave number variable k_x is given in Ref. [39] (only one transverse dimension is considered here) as,

$$\tilde{\psi}(k_x) = \sqrt{2}\sigma \exp\left(-\frac{\sigma^2}{2}\,k_x^2\right). \tag{C1}$$

Note that the normalisation assumed here is different from the equivalent quantum momentum wave function of Eq. (13). The space wave function is given by the FT from the wave number wave function,

$$\begin{aligned}\psi(x,z) &= (2\pi)^{-1/2}\int \tilde{\psi}(k_x)\exp\left(ik_x x - i\frac{k_x^2}{2k}\,z\right)dk_x\\ &= 2\pi\frac{\sigma^{1/2}}{(\sigma^2+i(z/k))^{1/2}}\exp\left[-\frac{x^2}{2(\sigma^2+i(z/k))}\right].\end{aligned} \tag{C2}$$

Note that the factor $(\sigma^2+i(z/k)) = \sigma^2(1+(z/z_0))$, when Eq. (C2) can be seen as the optics equivalent of the quantum Eq. (18). Indeed if now the definition $\tau \equiv z/z_0$ of a dimensionless "distance" is made, up to an insignificant constant normalisation, these two wave functions become identical. Then all results of section III C for the wave function along a Bohm trajectory apply equally to the Optics case.

In particular Eq. (41) is valid in the form

$$\begin{aligned}\psi(x(z)) =& \pi^{1/2}\frac{1}{[\sigma^2(1+\tau^2)]^{\frac{1}{4}}}\exp\left[-\frac{i}{2}\arctan\tau\right]\\ &\times\exp\left[-\frac{x_0^2}{2\sigma^2}\right]\exp\left[i\frac{x_0^2\,\tau}{2\sigma^2}\right].\end{aligned} \tag{C3}$$

but now with $\tau = z/z_0$ and $x_0 = k_x\sigma^2$. Performing this substitution one obtains

$$\begin{aligned}\psi(x(z)) =& \pi^{1/2}\frac{1}{[\sigma^2(1+(z/z_0)^2)]^{\frac{1}{4}}}\exp\left[-\frac{i}{2}\arctan(z/z_0)\right]\\ &\times\exp\left[-\frac{\sigma^2}{2}k_x^2\right]\exp\left[i\frac{k_x^2}{2k}z\right],\end{aligned} \tag{C4}$$

with $k_x = (x(z)/\sigma^2)\,(1+\tau^2)^{-1/2}$ along the trajectory. That is, as in the quantum case, the form of the wave number (momentum) wave function propagates unchanged along a Bohmian "stream line". Hence, the intensity of the wave within the cone $dx(z)$ is constant, corresponding to conservation of probability, Eq. (45), of the quantum case. The asymptotic $z \gg z_0$ form can be obtained by evaluation of the FT Eq. (C2) in SPA. The point of stationary phase is seen to be the straight ray condition $k_x = (k/z)x$. The result, the asymptotic form of Eq. (C4), is the well-known Fraunhofer diffraction limit corresponding to the IT approximation Eq. (21) in the quantum case.

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