Gravitational instability via the Schrödinger equation

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Received 12 May 2006
Accepted 23 November 2006
Published 12 December 2006

Abstract. We explore a novel approach to the study of large-scale structure formation in which self-gravitating cold dark matter (CDM) is represented by a complex scalar field whose dynamics are governed by coupled Schrödinger and Poisson equations. We show that, in the quasi-linear regime, the Schrödinger equation can be reduced to the free-particle Schrödinger equation. We advocate using the free-particle Schrödinger equation as the basis of a new approximation method—the free-particle approximation—that is similar in spirit to the successful adhesion model. In this paper we test the free-particle approximation by appealing to a planar collapse scenario and find that our results are in excellent agreement with those of the Zeldovich approximation, provided care is taken when choosing a value for the effective Planck constant in the theory. We also discuss how extensions of the free-particle approximation are likely to require the inclusion of a time-dependent potential in the Schrödinger equation. Since the Schrödinger equation with a time-dependent potential is typically impossible to solve exactly, we investigate whether standard quantum-mechanical approximation techniques can be used, in a cosmological setting, to obtain useful solutions of the Schrödinger equation. In this paper we focus on one particular approximation method: time-dependent perturbation theory (TDPT). We elucidate the properties of perturbative solutions of the Schrödinger equation by considering a simple example: the gravitational evolution of a plane-symmetric density fluctuation. We use TDPT to calculate an approximate solution of the relevant Schrödinger equation and show that this perturbative solution can be used to successfully follow gravitational collapse beyond the linear regime, but there are several pitfalls to be avoided.
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Keywords: dark matter, cosmological perturbation theory, gravity

ArXiv ePrint: astro-ph/0605012

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1. Introduction

The local universe displays a rich hierarchical pattern of galaxy clustering that encompasses a vast range of length scales, culminating in rich clusters, super-clusters and filaments. However, the early universe was almost homogeneous with only slight temperature fluctuations seen in the cosmic microwave background radiation. Models of structure formation link these observations through the effect of gravity, relying on the fact
that small initially over-dense regions accrete additional matter as the universe expands (a mechanism known as gravitational instability). The growth of density perturbations via gravitational instability is well understood in the linear regime, but the nonlinear regime is much more complicated and generally not amenable to analytic solution. Numerical $N$-body simulations have led the way towards an understanding of strongly developed clustering. Although such calculations have been priceless in establishing quantitative predictions of the large-scale structure expected to arise in a particular cosmology, it remains important to develop as full an analytical understanding as possible. After all, simulating a thing is not quite equivalent to understanding it.

Analytical methods for studying the evolution of cosmological density perturbations fall into two broad classes (for a review see [1] and references therein). First there are techniques based on applying perturbation theory (PT) to a hydrodynamical description of self-gravitating cold dark matter (CDM). These Eulerian approaches range from simple first-order (linear) PT (e.g. [2]) through to higher-order approaches of vastly increased complexity (e.g. [3, 4]). First-order Eulerian PT (the so-called linearized fluid approach) has been the mainstay of structure formation theory for many decades, by virtue of its simplicity and its robustness on large scales where density fluctuations are very much smaller than the mean density. When extrapolated to smaller scales, it provides a useful indicative measure of clustering strength, but can lead to absurdities (such as a negative matter density) if taken too far. Alternatively, there are Lagrangian approaches in which the trajectories of individual CDM particles are perturbed, rather than macroscopic fluid quantities (e.g. [5]–[8]). Even first-order Lagrangian PT, the celebrated Zeldovich approximation [9], is capable of following the gravitational collapse of density perturbations into the quasi-linear regime, beyond the breakdown of linear Eulerian PT. Comparisons with full $N$-body calculations have shown that the Zeldovich approximation can successfully describe the quantitative morphology of the clustering pattern (e.g. [10]), as long as particle trajectories do not intersect. When particle trajectories cross (a phenomenon known as shell-crossing) the density field develops a formal singularity (known as a caustic). Since the Zeldovich approximation is purely kinematical, particles simply pass through the caustic and continue along their original trajectories. This leads to large-scale structure being rapidly ‘washed out’ in a manner not observed in $N$-body simulations. A simple extension of the Zeldovich approximation that overcomes this problem is the adhesion approximation [11]. In the adhesion approximation, particles move according to the Zeldovich approximation until trajectories intersect, but are assumed to ‘stick’ to each other when shell-crossing occurs. This sticking is achieved by including an artificial viscosity term in the equations of motion to mimic the action of the strong gravitational forces acting in the vicinity of a caustic. The adhesion model has proved very successful in explaining the pattern of large-scale structure observed in the universe; comparisons with $N$-body simulations have shown impressive agreement far into the nonlinear regime (e.g. [12]–[16]).

In this paper we explore a radically different approach to the study of large-scale structure formation based on a wave-mechanical description of self-gravitating CDM. Following a suggestion by Widrow and Kaiser [17], we transform the usual hydrodynamical equations of motion into a nonlinear Schrödinger equation coupled to a Poisson equation describing Newtonian gravity. The nonlinear Schrödinger equation is similar to the familiar linear Schrödinger of quantum mechanics, except for the presence of an extra term
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known as the *quantum pressure*. The reasoning behind this transformation is not new—in essence, it dates back to Madelung [18]—but it is quite neglected in cosmology. Coles [19] showed that the wave-mechanical approach provides a natural explanation of why the distribution function of density fluctuations, evolved from Gaussian initial conditions, should be close to the log-normal form that is observed. By studying the evolution of a one-dimensional sinusoidal density perturbation, Coles and Spencer [20] demonstrated that the wave-mechanical approach fares well in comparison with the Zeldovich approximation up until particle trajectories cross and that, when shell-crossing occurs, the wave-mechanical density field remains non-singular. Their work relied exclusively on numerical solutions of the Schrödinger equation; our objective here is to investigate how the Schrödinger–Poisson system can be solved by using approximation techniques instead. We show that, in an expanding universe, the Schrödinger equation can be reduced to the exactly solvable ‘free-particle’ Schrödinger equation by utilizing results from first-order Eulerian and Lagrangian PT. We advocate using the free-particle Schrödinger equation as the basis of a new approximation method—the *free-particle approximation*—that promises to be capable of evolving cosmological density perturbations into the quasi-linear regime. As we shall see, the free-particle approximation can essentially be thought of as an alternative to the adhesion model in which the viscosity term is replaced by the quantum pressure term. The performance of the new free-particle approximation is assessed, relative to the Zeldovich approximation, by considering a simple example of gravitational collapse. Particular attention is paid to elucidating the effect of the quantum pressure term since this has not been investigated previously. We also discuss how extensions of the free-particle approximation based on higher-order PT are likely to lead to a Schrödinger equation with a time-dependent potential that cannot be solved exactly. Consequently, we feel it is important to ascertain whether standard quantum-mechanical approximation techniques can be used, in a cosmological context, to obtain solutions of the Schrödinger equation with a time-dependent potential. In this work we concentrate on one particular approximation method: time-dependent perturbation theory (TDPT). Our goal is to investigate the properties of perturbative solutions of the Schrödinger equation in a cosmological setting; we perform our investigation by appealing to a simple gravitational collapse scenario. Although we restrict our attention to idealized examples in this work, the results we obtain will remain pertinent when the wave-mechanical method is applied to more general structure formation problems in the future.

The outline of this paper is as follows. First, in order to keep the paper as self-contained as possible, we briefly outline the basic theory of cosmological structure formation including the standard fluid approach, the Zeldovich approximation, the adhesion model, the wave-mechanical approach in general and the free-particle approximation in particular. Next, in section 3, we describe how the gravitational collapse of a plane-symmetric sinusoidal density perturbation can be modelled by using (i) the free-particle approximation and (ii) a perturbative solution of the Schrödinger equation with a time-dependent potential. We present our results in section 4 and conclude in section 5.

2. Cosmological structure formation

Observations suggest that there is approximately five times as much non-baryonic CDM in the universe as there is ordinary (luminous) matter. Consequently, large-scale
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structure formation is commonly studied by considering the gravitational amplification of fluctuations in the CDM distribution only. In standard treatments, collisionless CDM is assumed to be an ideal fluid with zero pressure (so-called dust) and the evolution equations for perturbations in the CDM fluid are obtained by linearizing the Einstein field equations about an expanding homogeneous and isotropic Friedmann–Robertson–Walker (FRW) cosmology (e.g. [21]–[23]). However, in this paper we will assume that the length scale of the perturbations is much smaller than the Hubble radius so that a Newtonian treatment is adequate (e.g. [2]).

2.1. The fluid approach

In an expanding universe, the Newtonian dynamical equations governing the evolution of fluctuations in a fluid of collisionless self-gravitating CDM can be written in the form:

\[
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{H} \mathbf{v} + \frac{1}{a} (\mathbf{v} \cdot \nabla_x) \mathbf{v} + \frac{1}{a} \nabla_x \Phi = 0,
\]

(1)

\[
\frac{\partial \delta}{\partial t} + \frac{1}{a} \nabla_x \cdot [(1 + \delta) \mathbf{v}] = 0,
\]

(2)

\[
\nabla_x^2 \Phi - 4\pi G \rho_{b,c} a^2 \delta = 0,
\]

(3)

where \( t \) is cosmological proper time and \( \mathbf{x} = \mathbf{x}(t) \) are comoving coordinates, related to physical coordinates \( \mathbf{r} \) via \( \mathbf{r} = a \mathbf{x} \). Here the scale factor \( a = a(t) \) has been normalized so that its value at the present epoch \( t_0 \) is \( a_0 = a(t_0) = 1 \). The Hubble parameter \( H = H(t) \) is defined by \( H \equiv \dot{a}/a \) where a dot denotes a derivative with respect to \( t \). The peculiar velocity field \( \mathbf{v} = \mathbf{v}(\mathbf{x}, t) \) is given by \( \mathbf{v} = a \mathbf{x} \) and the potential \( \Phi = \Phi(\mathbf{x}, t) \) is the peculiar Newtonian gravitational potential. The density contrast \( \delta = \delta(\mathbf{x}, t) \) is \( \delta = \rho/\rho_{b,c} - 1 \) where \( \rho = \rho(\mathbf{x}, t) \) is the CDM density field and \( \rho_{b,c} = \rho_{b,c}(t) \) is the CDM density in the homogeneous FRW background.

It is straightforward to show (e.g. [2]) from the fluid equations (1)–(3) that, to first-order in Eulerian PT, density perturbations in the CDM fluid grow according to \( \delta = D \delta_i \) where \( \delta_i \) is the density contrast at some initial time \( t_i \) and the linear growth factor \( D = D(t) \) is the growing mode solution of

\[
\dot{D} + 2H \dot{D} - 4\pi G \rho_{b,c} D = 0,
\]

(4)

normalized so that \( D_i = D(t_i) = 1 \). The linear growth factor can then be used to write the fluid equations (1)–(3) in the alternative form:

\[
\frac{\partial \mathbf{u}}{\partial D} + (\mathbf{u} \cdot \nabla_x) \mathbf{u} + \frac{3 \Omega_c}{2 f^2 D} \mathbf{u} + \nabla_x \Theta = 0,
\]

(5)

\[
\frac{\partial \delta}{\partial D} + \nabla_x \cdot [(1 + \delta) \mathbf{u}] = 0,
\]

(6)

\[
\nabla_x^2 \Theta - \frac{3 \Omega_c}{2 f^2 D^2} \delta = 0,
\]

(7)

where the function \( f = f(D) \) is given by \( f \equiv \dot{D}/H D \) and \( \Omega_c = \Omega_c(D) \) is the familiar CDM density parameter: \( \Omega_c = 8\pi G \rho_{b,c}/3H^2 \). The gravitational potential \( \Theta = \Theta(\mathbf{x}, D) \) is related to the peculiar gravitational potential \( \Phi \) via \( \Theta = \Phi/a^2 \dot{D}^2 \). Similarly, the comoving
velocity field \( \mathbf{u} = \mathbf{u}(\mathbf{x}, D) \), defined by \( \mathbf{u} \equiv d\mathbf{x}/dD \), is obtained from the peculiar velocity \( \mathbf{v} \) by a simple rescaling: \( \mathbf{u} = \mathbf{v}/a D \). It is well known that linear Eulerian PT implies an irrotational velocity field: \( \mathbf{u} = -\nabla_x \phi \), where the velocity potential \( \phi = \phi(\mathbf{x}, D) \) is related to the gravitational potential \( \Theta \) via

\[
\phi = \frac{2 f^2 D}{3 \Omega_c} \Theta. \quad (8)
\]

The linearized fluid equations only provide an accurate description of gravitational instability in the linear regime \( \delta \ll 1 \). A considerably more powerful method than the linearized fluid approach is the Zeldovich approximation [9] which is capable of following the evolution of cosmological density perturbations into the quasi-linear regime \( \delta \sim 1 \).

### 2.2. The Zeldovich approximation

The Zeldovich approximation is a Lagrangian approach (formally first-order Lagrangian PT) in which individual particle trajectories are considered: the comoving Eulerian coordinate \( \mathbf{x} = \mathbf{x}(\mathbf{q}, D) \) of a particle initially located at a comoving Lagrangian coordinate \( \mathbf{q} \) is given by

\[
\mathbf{x} = \mathbf{q} + (D - 1) \mathbf{s}, \quad (9)
\]

where \( \mathbf{s} = \mathbf{s}(\mathbf{q}) \) is a time-independent vector field. Requiring that mass is conserved immediately leads to the following expression for the CDM density field in the Zeldovich approximation:

\[
\delta = \frac{(1 + \delta_i)}{J} - 1, \quad (10)
\]

where \( \delta_i = \delta_i(\mathbf{q}) \) is the initial density perturbation and \( J = J(\mathbf{q}, D) \) is the determinant of the Jacobian of the mapping (9) between Lagrangian and Eulerian coordinates. The density field (10) is known as the *continuity* density.

The Zeldovich approximation can also be formulated in Eulerian space by noting that (9) implies \( d\mathbf{u}/dD = 0 \) along a particle trajectory, provided particle trajectories do not intersect. Using the definition of the convective derivative \( d/dD = \partial/\partial D + \mathbf{u} \cdot \nabla_x \), it follows that the Zeldovich approximation corresponds to

\[
\frac{\partial \mathbf{u}}{\partial D} + (\mathbf{u} \cdot \nabla_x) \mathbf{u} = 0, \quad (11)
\]

in Eulerian space. Comparing (11) with the Euler equation (5) it is apparent that the Zeldovich approximation also guarantees an irrotational velocity field \( \mathbf{u} = -\nabla_x \phi \). We can then integrate (11) to obtain the so-called *Zeldovich–Bernoulli* [24] equation:

\[
\frac{\partial \phi}{\partial D} - \frac{1}{2} |\nabla_x \phi|^2 = 0, \quad (12)
\]

which possesses an analytical solution \( \phi = \phi(\mathbf{x}, D) \) of the form

\[
\phi = \phi_i - \frac{1}{2} (D - 1) |\mathbf{s}|^2, \quad (13)
\]

where \( \phi_i = \phi_i(\mathbf{q}) \) is the initial velocity potential and \( \mathbf{x} \) and \( \mathbf{q} \) are related by the mapping (9). As in the linearized fluid approach, the velocity potential \( \phi \) is related to the gravitational potential \( \Theta \) via (8) and thus the Poisson equation (7) implies

\[
\delta = D \nabla_x^2 \phi, \quad (14)
\]
which is known as the *dynamical* density field. In general, the continuity and dynamical density fields are not equivalent. However, in one dimension, the density fields (10) and (14) coincide and the Zeldovich approximation is an exact solution of the fluid equations as long as there is no shell-crossing (for a discussion, see [1] and references therein).

The Zeldovich approximation breaks down when particle trajectories cross since the mapping (9) from \( q \) to \( x \) is no longer unique. At a point where particle trajectories intersect, the velocity field becomes multi-valued, \( J \equiv 0 \) and the density field develops a formal singularity. The strong gravitational forces acting in the vicinity of the caustic should cause particles to be pulled towards it. However, since the Zeldovich approximation is kinematical, particles simply pass straight through the caustic and structure is rapidly ‘smeared out’ in an unphysical manner. The adhesion approximation [11] was specifically designed to tackle this shortcoming of the Zeldovich approximation.

### 2.3. The adhesion approximation

In the adhesion approximation, particles follow Zeldovich trajectories until shell-crossing occurs. However, when particle trajectories cross, the particles are assumed to ‘stick’ to each other. As a result, the singularities predicted by the Zeldovich approximation are regularized and stable structures are formed, rather than being ‘washed out’. Mathematically, the adhesion model is obtained from the Zeldovich approximation by including an artificial viscosity term in (11) so that:

\[
\frac{\partial u}{\partial D} + (u \cdot \nabla_x) u - \mu \nabla_x^2 u = 0,
\]

which is known as *Burgers’ equation* [25]. The constant \( \mu > 0 \) has dimensions of \( L^2 \) and can be thought of as a viscosity coefficient. A forcing term of the form \( \nabla_x \eta \), where \( \eta = \eta(x, D) \) is a random potential, can be included in Burgers’ equation to extend the adhesion model to the intergalactic medium (e.g. [26]). In the cosmologically relevant case of an irrotational velocity field \( u = -\nabla_x \phi \), (15) can be integrated to obtain

\[
\frac{\partial \phi}{\partial D} - \frac{1}{2} |\nabla_x \phi|^2 - \mu \nabla_x^2 \phi = 0.
\]

From a practical point of view, an attractive feature of Burgers’ equation (or, equivalently, (16)) is that it possesses an analytic solution. In the special case \( \mu \to 0 \) (known as the *inviscid* limit) a geometrical interpretation of the solution of Burgers’ equation can be used to determine the ‘skeleton’ of the large-scale structure present at any given time (e.g. [11,12,15]). In this limit the structures formed in the adhesion model are infinitely thin and the adhesion approximation reduces exactly to the Zeldovich approximation outside of mass concentrations. For finite values of \( \mu \), the viscosity term has an effect away from regions where particle trajectories cross and causes density perturbations to be suppressed on scales \( \lesssim \mu^{1/2} \) (e.g. [13]). The adhesion and Zeldovich approximations are then no longer identical outside of collapsing regions although, depending on the actual value of \( \mu \), they become similar at a certain distance.

The success of the adhesion model, relative to \( N \)-body calculations, has led to adhesive gravitational clustering becoming an important concept in the study of cosmological structure formation. Although the original motivation for the adhesion approximation
was purely phenomenological, it has recently been shown that, under certain simplifying assumptions, Burgers’ equation can be naturally derived from the coarse-grained equations of motion [27]–[31]. In these modern interpretations of the adhesion model, the regularizing parameter $\mu$ emerges, not as a (constant) viscosity coefficient, but rather as a (density-dependent) gravitational multi-stream coefficient, arising from the self-gravitation of a multi-stream system.

### 2.4. The wave-mechanical approach

An alternative approach to the study of large-scale structure formation was suggested by Widrow and Kaiser [17]. They proposed a wave-mechanical description of self-gravitating matter in which CDM is represented by a complex scalar field $\psi = \psi(x, D)$ whose dynamics are governed by coupled Schrödinger and Poisson equations (see [32] for a relativistic extension of the original Newtonian theory). In this section we give a pedagogical derivation of the wave-mechanical formalism in an expanding universe since this has not been presented in the literature previously.

We begin by assuming an irrotational velocity field $u = -\nabla_x \phi$. As discussed previously this is guaranteed to be the case in the linear and quasi-linear regimes and will remain so as long as there is no shell-crossing by Kelvin’s circulation theorem. The Euler equation (5) can then be integrated to obtain the Bernoulli equation

$$\frac{\partial \phi}{\partial D} - \frac{1}{2} |\nabla_x \phi|^2 - V = 0,$$

where the effective potential $V = V(x, D)$ depends on both the gravitational potential $\Theta$ and velocity potential $\phi$:

$$V = \Theta - \frac{3\Omega_c}{2f^2D} \phi.$$

(18)

The Bernoulli equation (17) can be combined with the continuity equation (6) by performing a Madelung transformation [18]

$$\psi = (1 + \delta)^{1/2} \exp\left(\frac{-i\phi}{\nu}\right),$$

(19)

where $\nu$ is a real parameter with dimensions of $L^2$. The wavefunction $\psi$ provides an elegant description of both density and velocity fields in a single complex function. Applying the Madelung transformation leads to the following coupled Schrödinger–Poisson system:

$$i\nu \frac{\partial \psi}{\partial D} = \left(-\frac{\nu^2}{2} \nabla_x^2 + V + P\right) \psi,$$

(20)

$$\nabla_x^2 \left[V - \frac{3\Omega_c}{2f^2D} \nu \arg(\psi)\right] - \frac{3\Omega_c}{2f^2D^2} (|\psi|^2 - 1) = 0,$$

(21)

where $P = P(x, D)$ is the so-called quantum pressure term, given by

$$P = \frac{\nu^2 \nabla_x^2 |\psi|}{2 |\psi|}.$$

(22)
If we neglect the quantum pressure term for the moment then we are left with the more familiar linear Schrödinger equation

$$i\nu \frac{\partial \psi}{\partial D} = \left( -\nu^2 \frac{\nabla^2}{2} + V \right) \psi.$$  \hspace{1cm} (23)

Inserting the Madelung transformation into (23) yields the usual continuity equation (6) and a modified Bernoulli equation of the form

$$\frac{\partial \phi}{\partial D} - \frac{1}{2} |\nabla_x \phi|^2 - V + P = 0,$$  \hspace{1cm} (24)

so the quantum pressure term appears in the fluid equations. This implies that we are free to drop the quantum pressure term from the nonlinear Schrödinger equation (20) and include it in the Bernoulli equation instead; this is the approach that we will adopt throughout this paper.

The parameter $\nu$ appears in the Schrödinger equation in a manner analogous to the Planck constant in real quantum mechanics. However, the system we are considering here is entirely classical and thus $\nu$ is treated as an adjustable parameter that controls the quantum pressure term $P \propto \nu^2$ appearing in the Bernoulli equation (24). The quantum pressure term acts as a regularizing term in the fluid equations, preventing the generation of multi-stream regions and singularities in the density field when particle trajectories cross. This was demonstrated by Coles and Spencer [20] who used the wave-mechanical approach to follow the gravitational collapse of a one-dimensional sinusoidal density perturbation through shell-crossing. The effect of the quantum pressure is thus qualitatively similar to that of the term $\mu \nabla^2 \phi$ in the adhesion model and $\nu$ plays a similar role to the viscosity parameter $\mu$, in the sense that they are both approximations to a general gravitational multi-stream coefficient arising in collisionless systems. The link between the wave-mechanical approach and the adhesion approximation will be further discussed below. In the semi-classical limit $\nu \to 0$ we expect the effect of the quantum pressure term to be minimized and thus our wave-mechanical representation of self-gravitating CDM will approach the standard hydrodynamical description.

The main deficiency of the wave-mechanical approach described here is that it is based on the fluid equations and thus implicitly assumes the existence of a single fluid velocity at each point. Consequently, the Schrödinger–Poisson system is incapable of properly describing the formation of multi-stream regions. However, this is not an intrinsic problem of the wave-mechanical formalism, but is instead a consequence of the simple Madelung form of the wavefunction we have used. Widrow and Kaiser [17] showed that one can deploy more sophisticated representations of the wavefunction, such as the coherent-state formalism of Husimi [33], that allow for multi-streaming. The wave-mechanical approach can then be adapted to follow the full Vlasov evolution of the phase-space distribution function beyond the laminar flow regime [17,32,34]. These extensions are beyond the scope of this paper.

2.4.1. The free-particle approximation. The full Schrödinger–Poisson system cannot be solved analytically and so we must resort to either numerical or approximation methods; in this work we are concerned with the latter approach. The Schrödinger–Poisson system can be significantly simplified by using the fact that, to first order in Eulerian and Lagrangian
PT, the gravitational and velocity potentials are related via \( \phi = 2 f ^ 2 D \Theta / 3 \Omega_c \). In this case, it is evident from (18) that the effective potential \( V \) is identically zero and the Schrödinger equation (23) reduces to the exactly solvable free-particle Schrödinger equation

\[
\nu \frac{\partial \psi}{\partial D} = -\frac{\nu^2}{2} \nabla_x^2 \psi.
\]  

(25)

Accordingly, the Poisson equation (21) decouples from the Schrödinger equation and provides the following relationship between the amplitude and phase of the wavefunction:

\[
\nu \nabla_x^2 [\arg(\psi)] + \frac{1}{D}(|\psi|^2 - 1) = 0.
\]  

(26)

Inserting the Madelung transformation (19) into (25) and (26) we obtain

\[
\frac{\partial \phi}{\partial D} - \frac{1}{2} |\nabla_x \phi|^2 + \mathcal{P} = 0,
\]  

(27)

along with the continuity equation (6) and the familiar relation (14). The modified Bernoulli equation (27) looks like the adhesion approximation (16), except that the term \( \mu \nabla_x^2 \phi \) has been replaced by the quantum pressure \( \mathcal{P} \). Since the quantum pressure term cannot be written in a form proportional to \( \nabla_x^2 \phi \), we formulate an alternative to the adhesion model based on the free-particle Schrödinger equation (25) and the Poisson-like equation (26). We call this new approximation scheme the free-particle approximation. In appendix A we show that, in the semi-classical limit \( \nu \to 0 \), the free-particle approximation reduces to the Zeldovich approximation prior to shell-crossing. The quantum pressure term will then only become important in regions where particle trajectories intersect.

3. Examples of gravitational collapse using the Schrödinger equation

3.1. A simple test of the free-particle approximation

The free-particle approximation should be capable of following the evolution of density fluctuations into the quasi-linear regime. In order to verify this hypothesis, we test the free-particle approximation by appealing to a simple example: the gravitational collapse of a plane-symmetric density perturbation. The assumption of plane-symmetry implies that we are effectively considering a one-dimensional problem. This is advantageous since, in one dimension, the Zeldovich approximation provides an exact solution of the equations of motion until shell-crossing occurs. The performance of the new free-particle approximation can then be assessed relative to the exact Zeldovich solution. We will consider the case where the parameter \( \nu \) is finite (rather than \( \nu \to 0 \)) and investigate the effect of the quantum pressure term as \( \nu \) is varied. This is an important issue to address since the quantum pressure term is an integral part of the free-particle approximation (and, indeed, the wave-mechanical approach in general). For illustrative purposes we assume the plane-symmetric initial density perturbation \( \delta_i = \delta_i(x) \) is sinusoidal:

\[
\delta_i = \delta_a \cos \left( \frac{2\pi x}{d} \right),
\]  

(28)
where $d$ is the comoving period of the perturbation and $0 < |\delta_\lambda| \leq 1$ to ensure that the initial CDM density field is everywhere non-negative. The corresponding initial velocity potential perturbation is found from (26):

$$\phi_i = -\left(\frac{d}{2\pi}\right)^2 \delta_i.$$  

(29)

The one-dimensional free-particle Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial D} = -\frac{\nu^2}{2} \frac{\partial^2 \psi}{\partial x^2}$$  

must then be solved subject to the initial condition

$$\psi_i = (1 + \delta_i)^{1/2} \exp \left(\frac{-i\phi_i}{\nu}\right).$$  

(31)

with $\delta_i$ and $\phi_i$ given by (28) and (29), respectively. In order to simplify calculations we consider a large cubic volume of comoving side length $L$ equipped with periodic boundary conditions at each face. This is a construction commonly used in the study of cosmological structure formation; the limit $L \to \infty$ can always be taken as a final step. Furthermore, we divide the cubic volume into cells of side length $d$ (i.e. we set $L = Nd$, $N > 0$ an integer) since the initial density perturbation (28) is periodic with comoving period $d$.

### 3.1.1. Solution of the free-particle Schrödinger equation.

The solution of the free-particle Schrödinger equation in a static background cosmology is discussed in detail in appendix B.1. Rather than repeating the calculation for the case of an expanding background, it suffices to note that we can simply replace proper time $t$ by the linear growth factor $D$ in the solution obtained in appendix B.1. The solution of the free-particle Schrödinger equation (30) is then

$$\psi = \sum_n a_n \exp \left[\frac{-i(D - 1)E_n^{(0)}}{\nu}\right] \phi_n^{(0)},$$  

(32)

where $E_n^{(0)} = \nu^2 k_n^2 / 2$ and $k_n = 2n\pi / d$ is a comoving wavenumber. The (orthonormal) eigenfunctions $\phi_n^{(0)} = \phi_n^{(0)}(x)$ are of the form

$$\phi_n^{(0)} = \frac{1}{L^{3/2}} \exp (ik_n x)$$  

(33)

and the expansion coefficients $a_n$ are determined from

$$a_n = NL^2 \int_0^d \overline{\phi_n^{(0)}}(x) \psi_i(x) \, dx,$$  

(34)

where the overbar denotes complex conjugation and the initial wavefunction $\psi_i$ is given by (31). It follows from (33) that the expansion coefficients $a_n$ can be calculated simply by taking the Fourier transform of the initial wavefunction.
3.2. Beyond the free-particle approximation

The free-particle formalism provides an approximation to the full Schrödinger–Poisson system that is exactly solvable. The free-particle approximation is motivated by the fact that the effective potential $V$ appearing in the Schrödinger–Poisson system is zero to first order in both Eulerian and Lagrangian PT. Since the free-particle approximation is based on linear PT, a natural extension of the free-particle approximation could be constructed simply by including higher-order terms in PT. However, including higher-order terms in PT implies $V \neq 0$ in general (e.g. [3, 8]), leading to a time-dependent external potential in the Schrödinger equation (23). The Schrödinger equation with a time-dependent potential is typically impossible to solve analytically, so either a numerical or an approximate solution must be sought.

In light of the above comments, we feel it is important to investigate whether quantum-mechanical approximation methods can be used, in a cosmological context, to obtain useful solutions of the Schrödinger equation with a time-dependent potential. We will focus on time-dependent perturbation theory (TDPT) since this is one of the most widely used approximation schemes in quantum mechanics. Our aim is to elucidate the properties of perturbative solutions of the Schrödinger equation with a time-dependent potential in a cosmological setting. In particular, we wish to assess the effect of varying the parameter $\nu$ where we again assume that $\nu$ is finite. It is not our intention here to explicitly formulate a higher-order extension of the free-particle approximation; we leave this for future work. Instead we investigate perturbative solutions of the Schrödinger equation by considering a simple idealized scenario. We begin by rewriting the Schrödinger–Poisson system in a static background cosmology; the reason for this will become apparent.

In a static universe the scale factor is constant $a = a_0 = 1$ (i.e. $H = 0$) and the Friedmann equations imply that the universe is closed with a non-zero cosmological constant $\Lambda = 4\pi G \rho_{b,c}$. The Schrödinger–Poisson system can then be written in the form:

$$i\nu \frac{\partial \psi}{\partial t} = \left( -\frac{\nu^2}{2} \nabla_x^2 + \Phi \right) \psi,$$

$$\nabla_x^2 \Phi - 4\pi G \rho_{b,c} (|\psi|^2 - 1) = 0,$$

where comoving coordinates $x$ now coincide with physical coordinates $r$. The potential $\Phi$ is the peculiar gravitational potential and

$$\psi = (1 + \delta)^{1/2} \exp \left( \frac{-i\varphi}{\nu} \right),$$

where the peculiar velocity $v$ is the gradient of the velocity potential $\varphi = \varphi(x, t)$: $v = -\nabla_x \varphi$. Inserting the Madelung transformation (37) into (35) and (36) we obtain

$$\frac{\partial \varphi}{\partial t} - \frac{1}{2} |\nabla_x \varphi|^2 - \Phi + P = 0,$$

as well as the continuity equation (2) and the Poisson equation (3) in a static universe. The gradient of the modified Bernoulli equation (38) gives the Euler equation (1) in a static background, but with an extra term corresponding to the gradient of the quantum pressure $P$. It follows from the fluid equations (1)–(3) in a static background that, to first
order in Eulerian PT, the peculiar gravitational potential evolves according to $\Phi = D\Phi_i$, where $D = \exp\left([t - t_i]/\tau\right)$ and $\tau = 1/\Lambda^{1/2}$ is the characteristic timescale for the collapse of a density fluctuation. To first order in Lagrangian PT (i.e. the Zeldovich approximation) it is straightforward to show from (8) and (13) that, in a static universe, the gravitational potential $\Phi = \Phi(x, t)$ is given by

$$\Phi = D \left[ \Phi_i - \frac{1}{2} (D - 1) |v_i|^2 \right],$$

(39)

where $\Phi_i = \Phi_i(q)$ is the initial gravitational potential, $v_i = v_i(q)$ is the initial peculiar velocity field and the coordinates $x$ and $q$ are related by the mapping (9) with $s = \tau v_i$. Therefore, in a static background, we have a non-zero time-dependent potential appearing in the Schrödinger equation (35) to first order. This is in contrast to the expanding background case where we must include higher-order terms in PT to obtain $V \neq 0$ in the Schrödinger equation (23). Since our goal is to investigate perturbative solutions of the Schrödinger equation with a time-dependent potential, it will clearly be simpler to work in a static background as we can then use a first-order (rather than a cumbersome higher-order) expression for the potential. This is why we have assumed a static background cosmology.

To proceed with our investigation, we now apply the wave-mechanical approach to a specific example of gravitational collapse. As before, we consider the evolution of a plane-symmetric sinusoidal density perturbation $\delta_i$ of the form (28). The corresponding initial peculiar gravitational potential is then found from the Poisson equation (36):

$$\Phi_i = -\left(\frac{d}{2\pi\tau}\right)^2 \delta_i,$$

(40)

and the initial peculiar velocity field is given by

$$v_i^2 = \left(\frac{d}{2\pi\tau}\right)^2 (\delta_n^2 - \delta_i^2),$$

(41)

which follows from (40) by noting that, in a static universe, the linear (Eulerian and Lagrangian) PT relation (8) implies the gravitational potential $\Phi$ and velocity potential $\varphi$ satisfy $\varphi = \tau \Phi$. The full one-dimensional Schrödinger equation we are aiming to solve is then

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\nu^2}{2} \frac{\partial^2}{\partial x^2} + \Phi\right) \psi,$$

(42)

where we use the first-order Lagrangian PT expression (39) for the gravitational potential $\Phi = \Phi(x, t)$ since this is exact in one dimension (up until shell-crossing occurs). The initial gravitational potential $\Phi_i = \Phi_i(q)$ and peculiar velocity $v_i = v_i(q)$ in (39) are given by (40) and (41), respectively. The Schrödinger equation (42) must be solved subject to the initial condition

$$\psi_i = (1 + \delta_i)^{1/2} \exp\left(\frac{-i\varphi_i}{\nu}\right),$$

(43)

where $\delta_i$ is given by (28) and $\varphi_i = \tau \Phi_i$. We again restrict our attention to a large cubic volume of side length $L$ equipped with periodic boundary conditions at each face. As before, the periodicity of the initial density perturbation suggests it will be convenient to partition the cubic volume into cubic cells of side length $d$ by writing $L = Nd$, $N > 0$ an integer.
3.2.1. Perturbative solution of the Schrödinger equation with a time-dependent potential. The Schrödinger equation (42) cannot be solved analytically; we have used TDPT to determine a second-order approximate solution instead. The details of the calculation are presented in appendix B.2. We summarize the main results here for reference. The perturbative solution was found to be

$$\psi = \sum_{j=0}^{2} \psi^{(j)},$$  \hspace{1cm} (44)$$

where the zeroth-order term $\psi^{(0)}$ is simply the solution of the free-particle Schrödinger equation ($\Phi \equiv 0$):

$$\psi^{(0)} = \sum_{n} a_{n} \exp \left[ \frac{-i(t - t_{i})E_{n}^{(0)}}{\nu} \right] \phi_{n}^{(0)},$$  \hspace{1cm} (45)$$

with $E_{n}^{(0)} = \nu^{2}k_{n}^{2}/2$ and $k_{n} = 2\pi n/d$. The eigenfunctions $\phi_{n}^{(0)}$ are of the form (33) and the expansion coefficients $a_{n}$ are found from (34) with the initial wavefunction $\psi_{i}$ now given by (43). The first-order term $\psi^{(1)}$ is

$$\psi^{(1)} = -i\frac{\delta_{a}}{8\pi^{2}\gamma} \sum_{n} a_{n} \sum_{m} I_{m,n} \phi_{m}^{(0)},$$  \hspace{1cm} (46)$$

where $\gamma = \nu\tau/d^{2}$ is a dimensionless parameter, $I_{m,n} = I_{m,n}(t)$ is defined by

$$I_{m,n} = \frac{1}{\tau} \int_{t_{i}}^{t} dt' \exp \left[ \frac{-i(t - t')E_{m}^{(0)}}{\nu} \right] \Phi_{m,n}(t') \exp \left[ \frac{-i(t' - t_{i})E_{n}^{(0)}}{\nu} \right],$$  \hspace{1cm} (47)$$

and the matrix elements $\Phi_{m,n} = \Phi_{m,n}(t)$ are given by

$$\Phi_{m,n} = D \left\{ \alpha \left[ J_{p}(2p\alpha) + \frac{3}{2} \sum_{s=\pm 2} J_{p+s}(2p\alpha) \right] + \left( \frac{\alpha^{2}}{2} - 1 \right) \sum_{s=\pm 1} J_{p+s}(2p\alpha) \right\},$$  \hspace{1cm} (48)$$

where $p = m - n$ is an integer, $\alpha = \alpha(t)$ is defined by $\alpha = \delta_{a}(D - 1)/2$ and the functions $J_{l}$ are Bessel functions of the first kind. The second-order term $\psi^{(2)}$ is given by

$$\psi^{(2)} = -\left( \frac{\delta_{a}}{8\pi^{2}\gamma} \right)^{2} \sum_{n} a_{n} \sum_{m} \sum_{l} \kappa_{l,m,n} \phi_{l}^{(0)},$$  \hspace{1cm} (49)$$

where $\kappa_{l,m,n} = \kappa_{l,m,n}(t)$ is defined by

$$\kappa_{l,m,n} = \frac{1}{\tau^{2}} \int_{t_{i}}^{t} dt' \int_{t_{i}}^{t'} dt'' \exp \left[ \frac{-i(t - t')E_{l}^{(0)}}{\nu} \right] \Phi_{l,m}(t') \exp \left[ \frac{-i(t' - t'')E_{m}^{(0)}}{\nu} \right] \times \Phi_{m,n}(t'') \exp \left[ \frac{-i(t'' - t_{i})E_{n}^{(0)}}{\nu} \right].$$  \hspace{1cm} (50)$$

In order to complete the perturbation expansion (44) of the wavefunction $\psi$, the integrals (47) and (50) must be evaluated numerically.
4. Results and discussion

We now analyse the gravitational collapse of the plane-symmetric sinusoidal density perturbation \((28)\) in (i) an expanding background, using the free-particle approximation, and (ii) a static background, using a perturbative solution of the Schrödinger equation with a time-dependent potential. In both cases the CDM density field is obtained from the amplitude of the wavefunction via \(\delta = |\psi|^2 - 1\) and compared with the linear growth law \(\delta = D \delta_\text{i}\) and the exact Zeldovich solution

\[
\delta = (1 + \delta_\text{i}) \left[ 1 - \left( D - 1 - \delta_\text{i} \right) \right]^{-1},
\]

which follows from (10) and (14). The evolution of the density fluctuation is followed up until particle trajectories cross which, from (51), occurs when the linear growth factor \(D = D_{\text{sc}} = 1 + 1/\delta_\alpha\). Hereafter we will assume, for illustrative purposes, that the amplitude of the initial density perturbation is \(\delta_\alpha = 0.01\), so that \(D_{\text{sc}} = 101\).

4.1. Planar collapse using the free-particle approximation

The (exact) solution of the one-dimensional free-particle Schrödinger equation \((30)\) is given by \((32)\). Upon introducing the dimensionless comoving coordinate \(\bar{x} = x/d\), we find that the free-particle solution depends solely on the dimensionless parameter \(\Gamma = \nu/d^2\), which we assume to be finite (as opposed to \(\Gamma \to 0\)). Recall that, in the semi-classical limit \(\Gamma \to 0\), the free-particle approximation coincides with the Zeldovich approximation before shell-crossing occurs (see appendix A). In one dimension this implies that the free-particle approximation will be exact in the limit \(\Gamma \to 0\) (provided there is no shell-crossing). This suggests that our numerical implementation of the free-particle approximation with finite \(\Gamma\) can be optimized by using the smallest possible value of \(\Gamma\). In practice there is a lower bound \(\Gamma_c\) on the value of \(\Gamma\) arising from the fact that we test the free-particle approximation on a discrete grid. Sampling at the Nyquist rate (the minimum possible sampling rate) requires that the phase change between two neighbouring grid points must be less than or equal to \(\pi\) radians. The phase of the initial wavefunction is proportional to \(1/\Gamma\) and so, as \(\Gamma\) approaches zero, the phase varies increasingly rapidly and the change in phase between two neighbouring grid points can exceed \(\pi\) radians. The phase is then insufficiently sampled and aliasing effects cause our free-particle method to break down. To avoid this problem we must choose \(\Gamma \geq \Gamma_c\); we expect the performance of the free-particle approximation to be optimal for \(\Gamma = \Gamma_c\). It is straightforward to show from \((31)\) that \(\Gamma_c = \delta_\alpha/2\pi^2 N_g\), where \(N_g\) is the number of grid points. We use \(N_g = 512\) so that \(\Gamma_c = 1 \times 10^{-6}\). We now investigate how the free-particle approximation, and in particular the quantum pressure term, behaves as \(\Gamma\) is decreased from a large value towards \(\Gamma = \Gamma_c\).

We begin by assuming \(\Gamma = 1\). The plots in the left-hand column of figure 1 show the evolution of the free-particle density field \(\delta = |\psi|^2 - 1\) in this case. The density field is only plotted in the interval \(0 \leq x \leq d\) since, by construction, the density field is periodic with comoving period \(d\). We can immediately see that the free-particle density field simply oscillates about the mean value \(\langle \delta \rangle = 0\) and there is no net growth of the initial density perturbation. We find that this oscillatory behaviour also persists for any \(\Gamma \geq 1\). This effect is caused by the quantum pressure term. Recall that the quantum pressure \(\mathcal{P}\) enters
Figure 1. Evolution of a plane-symmetric sinusoidal density perturbation in an expanding CDM-dominated universe. The amplitude of the initial density fluctuation is $\delta_a = 0.01$. The left-hand plots show the density fields obtained from the free-particle approximation (FP), the linearized fluid approach (LFA) and the Zeldovich approximation (ZA) at three different values of the linear growth factor. The parameter $\Gamma = 1$ in the free-particle approximation. The right-hand plots show the corresponding evolution of the magnitudes of the convective ($C$) and quantum pressure ($P$) terms, in units of $d^2$.

The free-particle formalism via the modified Bernoulli equation (27). Since $P \propto \nu^2 \propto \Gamma^2$, the parameter $\Gamma$ controls the size of the quantum pressure term relative to the convective term $C = C(x, D)$, defined by $C = -|\nabla_x \phi|^2/2$. The plots in the right-hand column of figure 1 compare the magnitudes of the quantum pressure and convective terms as a function of the linear growth factor. The quantum pressure term is the dominant term appearing in (27) at all times (except when it momentarily becomes zero as the density field passes through $\delta \equiv 0$). Therefore, the growth of the density perturbation appears to be inhibited by the large quantum pressure term. This is somewhat reminiscent of the adhesion approximation where the growth of fluctuations is suppressed on scales $\lesssim \mu^{1/2}$, leading to the large-scale structure distribution appearing ‘washed out’ for large $\mu$ [13]. However, even if the viscosity term is large, the density field in the adhesion model does...
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Figure 2. Evolution of a plane-symmetric sinusoidal density perturbation in an expanding CDM-dominated universe. The layout of the plots is as in figure 1; the only difference is that the parameter $\Gamma = 1.4 \times 10^{-3}$ in the free-particle approximation.

not display oscillatory behaviour; this is a peculiarity of the quantum pressure term. It is interesting to note that gas pressure in a baryonic fluid causes a qualitatively similar effect (e.g. [2]). If we were considering a baryonic fluid (rather than a pressureless fluid of CDM) then it would be necessary to account for the effects of gas pressure by including a classical pressure term in the Euler equation. Applying first-order Eulerian PT to the fluid equations then yields a characteristic length scale (the Jean’s length); any Fourier modes of the density field with a wavelength smaller than the Jean’s length undergo damped oscillation rather than growth. However, we must be careful not to directly compare the effects of the quantum pressure term to those of a classical pressure term since the origin and form of the two terms is very different.

The quantum pressure $P \propto \Gamma^2$ should become less significant as $\Gamma$ is decreased. The left-hand column of figure 2 displays the free-particle density field as a function of the linear growth factor when $\Gamma = 1.4 \times 10^{-3}$. Figures 2(a) and (b) show that the free-particle density field evolves as expected up to $D = D_{sc}/2$, in the sense that matter flows towards initially over-dense regions. However, the growth rate of the over-densities is considerably less than that predicted by the exact Zeldovich solution. For $D > D_{sc}/2$, the over-densities in the free-particle density field cease to grow and actually begin to decay, leading to a
large discrepancy between the free-particle and Zeldovich approximation density fields at $D \approx D_{sc}$; see figure 2(c). This behaviour is counterintuitive; over-densities should continue to grow up until shell-crossing occurs as in first-order Eulerian and Lagrangian PT. The quantum pressure term $P$ again provides the explanation. The right-hand column of figure 2 shows the evolution of $|C|$ and $|P|$. We can see that the convective term initially dominates the quantum pressure term in the Bernoulli equation (27). This remains the case at early times, corresponding to when the free-particle approximation agrees well with the linearized fluid approach and the Zeldovich approximation. However, the quantum pressure quickly grows until, at $D \approx D_{sc}/2$, it is much larger than the convective term. The large quantum pressure term suppresses the gravitational collapse of the density perturbation, causing the over-densities to cease growing and subsequently decay.

The effect of the quantum pressure term is indeed less pronounced in the $\Gamma = 1.4 \times 10^{-3}$ case than in the $\Gamma = 1$ case. However, at late times it causes matter to flow away from over-dense regions in an unrealistic manner. We find that, when $\Gamma$ is reduced to $\Gamma \approx 1 \times 10^{-3}$, the quantum pressure never becomes large enough to cause the decay of over-densities and the initial density perturbation grows up until shell-crossing. However, the collapse of the fluctuation is still highly suppressed by the quantum pressure term in high-density regions and the free-particle approximation thus provides a poor match to the Zeldovich approximation in such regions. As $\Gamma \rightarrow \Gamma_c$, the suppression effect of the quantum pressure term diminishes and the agreement between the free-particle and Zeldovich approximations improves. The left-hand column of figure 3 shows the free-particle evolution of the initial density perturbation in the optimal case $\Gamma = \Gamma_c = 1 \times 10^{-6}$. At all values of the linear growth factor the free-particle approximation now provides an excellent match to the exact Zeldovich solution, even in over-dense regions. However, unlike the Zeldovich approximation, the free-particle approximation leads to a density field that remains well behaved at shell-crossing. The right-hand column of figure 3 shows the corresponding evolution of $|C|$ and $|P|$. It is immediately apparent that the convective term completely dominates the quantum pressure term at all values of the linear growth factor. Although the quantum pressure term is small, it is non-zero (because we are using a finite $\Gamma$) and thus will have some effect on the collapse of the density perturbation. However, this effect is negligibly small for $\Gamma = 1 \times 10^{-6}$.

4.2. Planar collapse using the Schrödinger equation with a time-dependent potential

In a static background the linear growth factor is given by $D = \exp[(t - t_i)/\tau]$. Upon introducing a dimensionless time coordinate $\bar{t} = (t - t_i)/\tau$ we find that, for $\delta_a = 0.01$, shell-crossing occurs when $\bar{t} = \bar{t}_{sc} = \ln(D_{sc}) \approx 4.6$. We now use the perturbative solution (44) of the one-dimensional Schrödinger equation with a time-dependent potential (42) to follow the gravitational collapse of the initial density perturbation (28) up to $\bar{t}_{sc}$. Observe that the perturbation expansion of the wavefunction depends on one dimensionless parameter: $\gamma = \nu \tau / d^2$, which we assume to be finite. As in the previous section, phase-aliasing effects impose a lower bound $\gamma_c$ on the value of $\gamma$ in practice. It follows from (43) that again $\gamma_c = \delta_a/2\pi^2 N_g = 1 \times 10^{-6}$. Based on the results of our test of the free-particle approximation, it is reasonable to suppose that the performance of the wave-mechanical approach will be optimized for $\gamma = \gamma_c$. Since the gravitational potential (39) appearing in (42) is exact in one dimension, we would expect the wave-mechanical density field to
agree well with that of the exact Zeldovich solution in this optimal case. Unfortunately, as we shall see, the situation is more complex when dealing with perturbative solutions of the Schrödinger equation. We now examine the behaviour of the TDPT solution of the Schrödinger equation as $\gamma$ is reduced from a large value towards $\gamma = \gamma_c$.

As a starting point we choose $\gamma = 1$. In this case we find that the wave-mechanical density field $\delta = |\psi|^2 - 1$ oscillates rapidly about $\langle \delta \rangle = 0$ and there is no overall growth of the initial density fluctuation (cf figure 1). In fact, the wave-mechanical approach leads to an oscillatory density field for any $\gamma > 1$. As in the previous section, this is due to the fact that the quantum pressure term is the dominant term in the Bernoulli equation (38) for all times up to shell-crossing. The quantum pressure $P \propto \nu^2 \propto \gamma^2$ and thus should become less influential as $\gamma$ is decreased. The evolution of the wave-mechanical density field for $\gamma = 0.1$ is shown in the left-hand column of figure 4. By comparing figure 4(a) with figure 4(b) we see that the initial over-densities begin to decay rather than grow; this is unphysical. However, at $\bar{t} \approx \bar{t}_{sc}/3$, the decay slows and halts and matter begins to move towards over-dense regions in the usual fashion up to $\bar{t} \approx \bar{t}_{sc}$. Since over-dense regions only begin to collapse after $\bar{t} \approx \bar{t}_{sc}/3$, the final wave-mechanical density field
Figure 4. Evolution of a plane-symmetric sinusoidal density perturbation in a static CDM-dominated universe. The amplitude of the initial density perturbation is $\delta_a = 0.01$. The left-hand plots show the density fields obtained from the wave-mechanical approach with a time-dependent potential (WM), the linearized fluid approach (LFA) and the Zeldovich approximation (ZA). The parameter $\gamma = 0.1$ in the wave-mechanical approximation. The right-hand plots show the corresponding evolution of the magnitudes of the convective ($C$), gravitational potential ($\Phi$) and quantum pressure ($P$) terms, in units of $d^2/\tau^2$.

is considerably more homogeneous than the density fields obtained from the linearized fluid approach and the Zeldovich approximation. The reason for this behaviour becomes apparent if we examine the relative sizes of the convective, gravitational potential and quantum pressure terms in (38). The plots in the right-hand column of figure 4 compare the time variation of $|C|$, $|\Phi|$ and $|P|$. At $\tilde{t} = 0$ the quantum pressure is the dominant term and subsequently causes the initial over-densities to decay. However, in a static background, the gravitational potential (39) grows rapidly with time and, at $\tilde{t} \approx \tilde{t}_{sc}/3$, dominates over the quantum pressure and convective terms. This corresponds to the time when the over-densities cease to decay and the gravitational collapse of the density fluctuation begins to proceed as expected. The gravitational potential then remains the dominant term up until shell-crossing occurs.

We find that, as the value of $\gamma$ is reduced further, the effect of the quantum pressure term indeed lessens. However, for $\gamma < 0.02$, the wave-mechanical approach exhibits
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Figure 5. Evolution of a plane-symmetric sinusoidal density perturbation in a static CDM-dominated universe. The left-hand plots are as in figure 4, except that the parameter $\gamma = 0.015$ in the wave-mechanical approximation. The right-hand plots show the corresponding evolution of the ratios $\chi_{1,0}$ and $\chi_{2,0}$ defined in the text.

rather unusual behaviour. For example, consider $\gamma = 0.015$ (note $\gamma \gg \gamma_c$); figure 5 illustrates the behaviour of the wave-mechanical approximation in this case. It is evident from figures 5(a) and (b) that the wave-mechanical approximation now provides a close match to the linearized fluid approach and the exact Zeldovich solution up to $\bar{t} \approx 2\bar{t}_{sc}/3$. However, at times close to shell-crossing, an over-density appears at $x = d/2$ (i.e. where the gravitational potential is at a maximum) in the wave-mechanical density field. This is clearly not realistic. To explain this, recall that the second-order perturbative solution of the Schrödinger equation (42) is

$$\psi = \sum_{j=0}^{2} \psi^{(j)},$$  \hspace{1cm} (52)

where $\psi^{(0)}$, $\psi^{(1)}$ and $\psi^{(2)}$ are given by (45), (46) and (49), respectively. In order for the perturbation expansion (52) to be valid we require the first-and second-order terms to be much smaller than the zeroth-order term. However, $\psi^{(1)} \propto 1/\gamma$ and $\psi^{(2)} \propto 1/\gamma^2$ so, for small values of $\gamma$, we anticipate that these terms will be large compared to $\psi^{(0)}$. To check
this we define a ratio
\[ \chi_{j,0} = \frac{|\psi^{(j)}|}{|\psi^{(0)}|}, \]
with \( j = 1, 2 \). We then require \( \chi_{1,0} \ll 1 \) and \( \chi_{2,0} \ll 1 \) for our perturbative solution to hold. The ratios \( \chi_{1,0} \) and \( \chi_{2,0} \) are shown as functions of time in the right-hand column of figure 5. At early times \( \chi_{1,0} \) and \( \chi_{2,0} \) are both small as they should be. However, they both grow with time until, at \( t \approx t_{sc} \), the first-and second-order terms in the perturbation expansion of the wavefunction are comparable to the zeroth-order term. A general feature is that the first-order term initially grows at a faster rate than the second-order term but, as the time of shell-crossing approaches, the second-order term begins to grow very rapidly and is soon comparable to the first-order term. The false over-density at \( x = d/2 \) then develops, suggesting that this is due to the onset of non-perturbative behaviour in the system. We find that, as \( \gamma \to \gamma_c \), the perturbative solution of the Schrödinger equation breaks down at progressively earlier times.

The development of non-perturbative behaviour is somewhat reminiscent of the onset of turbulence in a classical fluid. It is interesting to speculate that small values of \( \gamma \) could be linked to some form of turbulent behaviour in our hydrodynamical description of quantum mechanics, especially when we realize that \( \nu \) has dimensions of viscosity and that the dimensionless parameter \( 1/\gamma \) is similar to the Reynolds’s number appearing in classical fluid mechanics. Turbulence in classical fluids is associated with the formation of vortices which obviously does not occur in one-dimensional systems. Nevertheless the analogy is compelling. A possible explanation is that very small values of \( \gamma \) involve large angular frequencies in the phase of the wavefunction (which is proportional to \( 1/\gamma \)). To regain classical behaviour in the limit \( \gamma \to 0 \) the waves from which \( \psi \) is constructed must cancel exactly. Since the limit \( \gamma \to 0 \) involves waves of infinitely small wavelength, any finite perturbative calculation will find convergence impossible. A related but converse phenomenon arises in Eulerian fluids (i.e. fluids without intrinsic viscosity) when they are described in terms of a truncated spectrum [35].

It is clear from the above discussion that there is a conflict to be faced when choosing an appropriate value of \( \gamma \). On the one hand, we wish to set \( \gamma = \gamma_c \) to ensure that the quantum pressure term is minimized. On the other hand, our perturbative solution of the Schrödinger equation becomes more stable as \( \gamma \) is increased. The best one can do in this situation is to compromise by selecting the smallest possible value of \( \gamma \) for which the perturbative solution of the Schrödinger equation remains physically reasonable over the timescales of interest. We denote this ‘optimal’ value by \( \gamma_o \). In the situation under consideration here, we find that \( \gamma_o = 0.02 \); the left-hand column of figure 6 shows the behaviour of the wave-mechanical density field in this case. We can see from figures 6(a) and (b) that the wave-mechanical approach is again in good agreement with the linearized fluid approach and the exact Zeldovich solution for times up to \( t \approx 2t_{sc}/3 \). Figure 6(c) shows that, at \( t \approx t_{sc} \), the wave-mechanical density field is well-behaved (in the sense that there is no unphysical over-density at \( x = d/2 \)) and agrees extremely well with the Zeldovich approximation in the vicinity of \( x = d/2 \). The wave-mechanical approach also leads to the formation of over-densities with \( \delta \approx 2.2 \) (i.e. in the quasi-linear regime). However, there is still a large discrepancy between the wave-mechanical and Zeldovich approximation density fields in high-density regions. This is partly attributable to the
Figure 6. Evolution of a plane-symmetric sinusoidal density perturbation in a static CDM-dominated universe. The layout of the plots is as in figure 5; the only difference is that the parameter $\gamma = 0.02$ in the wave-mechanical approximation.

fact that, although dominated by the gravitational potential term, the quantum pressure term is still non-negligible for $\gamma = 0.02$ and thus hinders the collapse of the density fluctuation. In addition, as shown by the plots in the right-hand column of figure 6, the ratios $\chi_{1,0}$ and $\chi_{2,0}$ grow with time, eventually becoming comparable to unity at $\bar{t} \approx \bar{t}_{sc}$. Consequently, our perturbative solution (44) of the Schrödinger equation is on the verge of failing completely at times close to shell-crossing.

5. Conclusion

In this paper we have proposed a new approximation method suitable for evolving cosmological density perturbations into the quasi-linear regime. This new method is based upon the free-particle Schrödinger equation and is thus called the free-particle approximation. We have seen that the free-particle approximation provides an alternative to the well-known adhesion model in which the viscosity term $\mu \nabla^2 \phi$ is replaced by the quantum pressure term $P$. The quantum pressure acts as a regularizing term that prevents the generation of density singularities when particle trajectories cross.
Therefore, in contrast to the Zeldovich approximation, the free-particle method does not fail catastrophically when shell-crossing occurs. The quantum pressure term is controlled by a free parameter $\nu$ which plays a similar role to the viscosity parameter $\mu$. We have shown that, in the semi-classical limit $\nu \to 0$, the free-particle approximation reduces to the Zeldovich approximation, provided there is no shell-crossing. The quantum pressure term will then only have an effect in multi-stream regions.

We have performed a simple test of the free-particle approximation by considering the gravitational collapse of a plane-symmetric sinusoidal density perturbation. The behaviour of the free-particle approximation has been examined for several different finite values of the parameter $\nu$ (or, equivalently, $\Gamma$ in the notation of section 4.1) in an attempt to elucidate the role of the quantum pressure term. We have found that, contrary to the $\nu \to 0$ case, the quantum pressure affects the free-particle approximation before shell-crossing occurs if $\nu$ is finite. In particular, the quantum pressure acts to suppress the gravitational collapse of density fluctuations; the degree of suppression depends on the actual value of $\nu$. For large values of $\nu$, the quantum pressure term completely dominates over the convective term in the modified Bernoulli equation (27) and the free-particle density field then simply oscillates about $\langle \delta \rangle = 0$. As the value of $\nu$ is decreased the effect of the quantum pressure term diminishes. When the value of $\nu$ is set to the smallest possible value $\nu_c$ allowed by our numerical implementation of the free-particle method, we find that the free-particle approximation provides an excellent match to the exact Zeldovich solution of the equations of motion, up until shell-crossing occurs. In this case the quantum pressure term is still non-zero, but is negligibly small in comparison with the convective term and thus has little effect before shell-crossing.

The success of the free-particle approximation in the simple example presented here suggests that this method promises to be a useful analytical tool for modelling the formation of large-scale structure in the universe. In a subsequent paper we will exhaustively test the free-particle approximation in a more cosmologically relevant scenario by appealing to a full $N$-body simulation [36].

The free-particle approximation is motivated by the fact that, to first order in Eulerian and Lagrangian PT, the effective potential $V$ appearing in the full Schrödinger–Poisson system is zero. In future work it may prove desirable to go beyond the free-particle approximation by including higher-order terms in PT. We anticipate that any such extension of the free-particle approximation will, in general, lead to a Schrödinger equation with a time-dependent potential that cannot be solved exactly. Instead, either numerical or approximation methods must be deployed. In this work we have examined whether TDPT is a suitable technique for constructing approximate solutions of the Schrödinger equation in a cosmological setting. We have performed our investigation by appealing to a simple model where the universe is assumed to be static. In this case the gravitational potential $\Phi$ appearing in the Schrödinger–Poisson system is non-zero to first order in both Eulerian and Lagrangian PT. We use first-order Lagrangian PT (which is exact in one dimension) to calculate $\Phi$ in the Schrödinger equation for the case of a plane-symmetric sinusoidal density perturbation. A perturbative solution of the resulting Schrödinger equation was then found by applying second-order TDPT. To elucidate the properties of this perturbative solution we have studied the behaviour of the wave-mechanical approximation as the (finite) parameter $\nu$ (or $\gamma$ in the notation of section 4.2) is varied. For large values of $\nu$ the quantum pressure term $P$ is the
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dominant term in the modified Bernoulli equation (38) and again acts to inhibit the gravitational collapse of the density fluctuation. On the other hand, we have seen that the perturbation expansion of the wavefunction breaks down for small values of $\nu$, leading to the formation of an unphysical over-density where the gravitational potential is at a maximum. Therefore, in order to optimize the performance of our perturbative wave-mechanical approach, we must be satisfied with choosing the smallest possible value of $\nu$ for which the TDPT solution of the Schrödinger equation remains physically sensible over the timescales of interest. In this optimal case we find that the wave-mechanical approach is capable of evolving the density perturbation into the quasi-linear regime, but provides a poor match to the exact solution in over-dense regions.

In summary, we have shown that TDPT is a viable means of calculating approximate solutions of the Schrödinger equation in a cosmological context, provided extreme care is taken in choosing $\nu$. Although we have only considered a simple example, we believe that the issues we have highlighted regarding perturbative solutions of the Schrödinger equation will remain pertinent in more general situations. Thus our work promises to be useful in the future when constructing more sophisticated alternatives to the free-particle approximation.

Acknowledgments

CJS would like to thank PPARC for the award of a studentship that made this work possible. We also thank the anonymous referee for helpful comments.

Appendix A. Path integral solution of the free-particle Schrödinger equation in the semi-classical limit

The solution $\psi = \psi(x, D)$ of the free-particle Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial D} = -\frac{\nu^2}{2} \nabla_x^2 \psi \quad (A.1)$$

can be written in the form

$$\psi = \int U(x, D; q, 1) \psi_i(q) \, d^3q, \quad (A.2)$$

where $\psi_i = \psi_i(q)$ is some initial wavefunction and $U = U(x, D; q, 1)$ is the free-particle propagator. In the path integral formulation of quantum mechanics, the propagator involves a sum over all possible spacetime paths connecting the points $(q, 1)$ and $(x, D)$. The path integral expression for the free-particle propagator is a standard result, see [37] for example. In the case at hand the free-particle propagator is given by

$$U = \frac{1}{[2\pi i\nu(D-1)]^{3/2}} \exp \left[ \frac{i|x - q|^2}{2\nu(D-1)} \right] \quad (A.3)$$

and so the wavefunction (A.2) becomes

$$\psi = \frac{1}{[2\pi i\nu(D-1)]^{3/2}} \int \exp \left[ \frac{i|x - q|^2}{2\nu(D-1)} \right] \psi_i(q) \, d^3q. \quad (A.4)$$
Inserting the Madelung form

$$\psi_i = (1 + \delta_i)^{1/2} \exp \left( \frac{-i\phi_i}{\nu} \right)$$

(A.5)
of the initial wavefunction into (A.4) then yields

$$\psi = \frac{1}{[2\pi i \nu (D - 1)]^{3/2}} \int [1 + \delta_i(q)]^{1/2} \exp \left( \frac{i}{\nu} \left[ \frac{|x - q|^2}{2(D - 1)} - \phi_i(q) \right] \right) \, d^3q.$$  \hspace{1cm} (A.6)

Recall that we are interested in the solution of the free-particle Schrödinger equation in the semi-classical limit $\nu \rightarrow 0$. The exponent appearing in (A.6) is complex and so the integrand will be a rapidly oscillating function of $q$ in the limit $\nu \rightarrow 0$. The dominant contribution to the integral in (A.6) will then be from points where the phase varies least rapidly with $q$, i.e. at stationary points. This method of evaluating the integral in (A.6) is referred to as the method of stationary phase. Before proceeding, we first rewrite the exponent in (A.6) by introducing a function $S = S(x; D; q, 1)$ of the form

$$S = \frac{|x - q|^2}{2(D - 1)} - \phi_i.$$  \hspace{1cm} (A.7)

Hereafter we will write $S = S(q)$ for brevity since the integral in (A.6) is over $q$ only. At stationary points $\bar{q}$ of the phase we then have $S_{,m}(\bar{q}) = 0$, where $S_{,m}$ denotes $\partial S/\partial q_m$, leading to

$$x = \bar{q} + (D - 1)s(\bar{q}),$$  \hspace{1cm} (A.8)

with the time-independent vector field $s = s(q)$ defined by $s = -\nabla_q \phi_i$. In what follows we assume that, for a given value $D$ of the linear growth factor, there is one and only one stationary point $\bar{q}$ satisfying (A.8) for each $x$. This is tantamount to assuming the absence of shell-crossing. We now Taylor-expand the function $S$ about the stationary point $\bar{q}$:

$$S(q) \approx S(\bar{q}) + \frac{1}{2} \sum_{m=1}^{3} \sum_{n=1}^{3} (q_m - \bar{q}_m) S_{,mn}(\bar{q}) (q_n - \bar{q}_n),$$  \hspace{1cm} (A.9)

where $S_{,mn}$ denotes $\partial^2 S/\partial q_m \partial q_n$ and we have used the fact that $S_{,m}(\bar{q}) = 0$. Inserting (A.9) into (A.6) and changing variables to $p = q - \bar{q}$ we obtain

$$\psi = \frac{[1 + \delta_i(\bar{q})]^{1/2}}{[2\pi i \nu (D - 1)]^{3/2}} \exp \left[ \frac{i}{\nu} S(\bar{q}) \right] \int \exp \left[ -\frac{1}{2} p^T \mathbf{M}(\bar{q}) p \right] \, d^3p,$$  \hspace{1cm} (A.10)

where the superscript $T$ denotes a transpose and $\mathbf{M}(\bar{q})$ is a complex symmetric matrix whose elements are $M_{mn}(\bar{q}) = -iS_{,mn}(\bar{q})/\nu$. The three-dimensional Gaussian integral in (A.10) can be evaluated using standard techniques:

$$\int \exp \left[ -\frac{1}{2} p^T \mathbf{M}(\bar{q}) p \right] \, d^3p = \left[ (2\pi)^3 M(\bar{q}) \right]^{-1/2},$$  \hspace{1cm} (A.11)

where $\mathcal{M}(\bar{q})$ is the determinant of $\mathbf{M}(\bar{q})$. In order for (A.11) to hold we require $\mathcal{M}(\bar{q}) \neq 0$; this condition is satisfied before shell-crossing occurs. To see this, first note that (A.7) implies $S_{,mn}(\bar{q}) = J_{mn}(\bar{q})/(D - 1)$ where $J_{mn}(\bar{q}) = \delta_{mn} + (D - 1)s_{m,n}(\bar{q})$ and $\delta_{mn}$ is the
Kronecker delta. The real symmetric matrix \( \mathbf{J}(\bar{q}) \) with elements \( J_{mn}(\bar{q}) \) is then simply the Jacobian matrix of the Zeldovich approximation evaluated at the stationary point \( \bar{q} \). It follows that

\[
\mathcal{M}(\bar{q}) = \frac{i}{\nu(D-1)^3} J(\bar{q}),
\]

where \( J(\bar{q}) \) is the determinant of the Jacobian matrix \( \mathbf{J}(\bar{q}) \). Since \( J(\bar{q}) \) is non-zero up until shell-crossing occurs, then so is \( \mathcal{M}(\bar{q}) \). We can then substitute (A.12) and (A.11) into (A.10) to obtain

\[
\psi = \left[ 1 + \frac{\delta_i(\bar{q})}{J(\bar{q})} \right]^{1/2} \exp \left[ \frac{i}{\nu} S(\bar{q}) \right].
\]

Comparing (A.13) with the Madelung transformation we see that, in the limit \( \nu \to 0 \), the CDM density field \( \delta = \delta(x, D) \) in the free-particle approximation is given by

\[
\delta = \frac{1 + \delta_i(\bar{q})}{J(\bar{q})} - 1
\]

and the velocity potential \( \phi = \phi(x, D) \) follows from (A.7):

\[
\phi = \Phi_i(\bar{q}) - \frac{1}{2}(D-1)|\mathbf{s}(\bar{q})|^2,
\]

where \( x \) and \( \bar{q} \) satisfy (A.8). The expressions (A.14) and (A.15) are identical to those obtained in the Zeldovich approximation; see (10) and (13). Therefore we have shown that, prior to shell-crossing (i.e. while there is a one-to-one correspondence between \( x \) and \( \bar{q} \)), the free-particle approximation reduces to the Zeldovich approximation in the semi-classical limit \( \nu \to 0 \).

Appendix B. Perturbative solution of the one-dimensional Schrödinger equation with a time-dependent potential

We have used the wave-mechanical approach to study the gravitational evolution of a plane-symmetric sinusoidal density perturbation in a static universe. The appropriate one-dimensional Schrödinger equation to be solved was

\[
i\nu \frac{\partial \psi}{\partial t} = \left( -\frac{\nu^2}{2} \frac{\partial^2}{\partial x^2} + \Phi \right) \psi,
\]

with an external gravitational potential \( \Phi = \Phi(x, t) \) of the form

\[
\Phi = D \left[ \Phi_i - \frac{1}{2}(D-1)v_i^2 \right],
\]

where \( \Phi_i = \Phi_i(q) \) is the initial gravitational potential, \( v_i = v_i(q) \) is the initial velocity field and Eulerian coordinates \( x \) are related to Lagrangian coordinates \( q \) by the Zeldovich mapping \( x = q + \tau(D-1)v_i \) with \( D = \exp[(t - t_i)/\tau] \). For an initial density perturbation \( \delta_i = \delta_i(q) \) of the form \( \delta_i = \delta_i \cos(2\pi q/d) \) we have

\[
\Phi_i = -\left( \frac{d}{2\pi\tau} \right)^2 \delta_i
\]
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\[ v^2_i = \left( \frac{d}{2\pi \tau} \right)^2 \left( \delta_a^2 - \delta_i^2 \right). \]  

(B.4)

We now describe how to construct a second-order perturbative solution of the Schrödinger equation (B.1) using TDPT. To begin with, note that (B.1) is written in the position representation. It can be written in a more general form without referring to a particular basis as

\[ i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \]  

(B.5)

where \(|\psi(t)\rangle\) is a general ket representing the state of the physical system at time \(t\) and \(\hat{H}(t)\) is the time-dependent total Hamiltonian. In order to solve (B.5) using PT it is convenient to split the total Hamiltonian according to

\[ \hat{H}(t) = \hat{H}_0 + \hat{\Phi}(t) \]  

where \(\hat{H}_0 = \hat{P}^2/2\) is the free-particle Hamiltonian (with \(\hat{P}\) the momentum operator) and \(\hat{\Phi}(t)\) is the time-dependent potential (B.2) in operator form. Before continuing to develop a perturbative solution of (B.5) we first describe how to solve the free-particle Schrödinger equation

\[ i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}_0|\psi(t)\rangle. \]  

(B.6)

B.1. The free-particle Schrödinger equation

The solution \(|\psi(t)\rangle\) of the general free-particle Schrödinger equation (B.6) is obtained from the initial state ket \(|\psi_i\rangle = |\psi(t_i)\rangle\) via

\[ |\psi(t)\rangle = \hat{U}_0(t,t_i)|\psi_i\rangle, \]  

(B.7)

where \(\hat{U}_0(t,t_i)\) is a unitary operator, known as the free-particle time-evolution operator, obeying

\[ i\hbar \frac{d}{dt} \hat{U}_0(t,t_i) = \hat{H}_0 \hat{U}_0(t,t_i). \]  

(B.8)

The free-particle Hamiltonian \(\hat{H}_0\) is independent of time and so we can directly integrate (B.8) to find that

\[ \hat{U}_0(t,t_i) = \exp \left[ -\frac{i(t - t_i)\hat{H}_0}{\hbar} \right]. \]  

(B.9)

The initial state ket \(|\psi_i\rangle\) can be expanded in terms of orthonormal eigenkets \(|n^{(0)}\rangle\) of \(\hat{H}_0\) as

\[ |\psi_i\rangle = \sum_n a_n |n^{(0)}\rangle, \]  

(B.10)

where \(a_n = \langle n^{(0)}|\psi_i\rangle\) and the eigenkets \(|n^{(0)}\rangle\) satisfy the general time-independent free-particle Schrödinger equation

\[ \hat{H}_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle. \]  

(B.11)
In order to determine the eigenvalues $E_n^{(0)}$ and the eigenkets $|n^{(0)}\rangle$ we must solve the eigenvalue problem (B.11). To do this it is convenient to first rewrite it in the position representation:

$$-\frac{\nu^2}{2} \frac{d^2 \phi_n^{(0)}}{dx^2} = E_n^{(0)} \phi_n^{(0)}, \quad \text{(B.12)}$$

where $\phi_n^{(0)} = \phi_n^{(0)}(x)$ are the eigenfunctions, defined by $\phi_n^{(0)} = \langle x | n^{(0)} \rangle$. Introducing $k_n^2 = 2E_n^{(0)}/\nu^2$ we find that the solutions to (B.12) are of the form

$$\phi_n^{(0)} = \frac{1}{L^{3/2}} \exp(ik_n x), \quad \text{B.13}$$

where $k_n = 2n\pi/L$, $n$ an integer, since we are considering a cubic volume of side length $L$ equipped with periodic boundary conditions at each face. The pre-factor $1/L^{3/2}$ comes from the requirement that the eigenfunctions are normalized.

The solution of the free-particle Schrödinger equation (B.6) follows upon inserting the time-evolution operator (B.9) and the initial ket expansion (B.10) into (B.7). In the position representation we find

$$\psi = \sum_n a_n \exp \left[ -i(t - t_i) E_n^{(0)} \right] \phi_n^{(0)}, \quad \text{B.14}$$

where $\psi = \langle x | \psi(t) \rangle$, $E_n^{(0)} = \nu^2 k_n^2/2$ and the eigenfunctions $\phi_n^{(0)}$ are given by (B.13). The expansion coefficients $a_n = \langle n^{(0)} | \psi_i \rangle$ are found from

$$a_n = L^2 \int_0^L \phi_n^{(0)}(q) \psi_i(q) \, dq, \quad \text{B.15}$$

where $\psi_i = \langle q | \psi_i \rangle$ and an overbar denotes complex conjugation. As discussed previously, we divide the cubic volume into cells of side length $d$ by setting $L = Nd$, $N > 0$ an integer. We can then write (B.15) as

$$a_n = L^2 \sum_{j=0}^{N-1} \int_{jd}^{(j+1)d} \phi_n^{(0)}(q) \psi_i(q) \, dq. \quad \text{B.16}$$

Performing a change of variable $q' = q - jd$ leads to

$$a_n = L^2 \int_0^d \phi_n^{(0)}(q') \psi_i(q') \, dq' \sum_{j=0}^{N-1} \exp(-ijk_n d), \quad \text{B.17}$$

where we have used (B.13) along with the fact that the initial Madelung wavefunction $\psi_i = (1 + \delta_i)^{1/2} \exp(-i\varphi_i/\nu)$ is periodic with period $d$. However,

$$\sum_{j=0}^{N-1} \exp(-ijk_n d) = N\delta_{n,pN}, \quad \text{B.18}$$

where $p$ is an integer, and thus the coefficients $a_n$ are given by

$$a_n = NL^2 \int_0^d \bar{\phi_n^{(0)}}(q') \psi_i(q') \, dq' \quad \text{B.19}$$

where the eigenfunctions $\phi_n^{(0)}$ are given by (B.13), but with $k_n = 2n\pi/d$. It follows from (B.19) that the expansion coefficients are simply found by taking the Fourier transform of the initial wavefunction.
B.2. The Schrödinger equation with a time-dependent potential

Our aim now is to perturbatively solve the Schrödinger equation (B.5) with a time-dependent Hamiltonian of the form $\hat{H}(t) = \hat{H}_0 + \hat{\Phi}(t)$ where the potential is given by (B.2) in the position representation. As before, the solution $|\psi(t)\rangle$ of the Schrödinger equation is related to the initial ket $|\psi_i\rangle$ via

$$|\psi(t)\rangle = \hat{U}(t, t_i)|\psi_i\rangle,$$

where the time-evolution operator obeys

$$i\hbar \frac{d}{dt} \hat{U}(t, t_i) = \hat{H}(t)\hat{U}(t, t_i).$$

The previously determined eigenkets $|n^{(0)}\rangle$ of the free-particle Hamiltonian $\hat{H}_0$ form an orthonormal set and so we may expand the initial state ket $|\psi_i\rangle$ as in (B.10) with the expansion coefficients $a_n = \langle n^{(0)}|\psi_i\rangle$ given by (B.19). In order to determine the state ket $|\psi(t)\rangle$ at a time $t$, it is clear from (B.20) that we require an expression for the time-evolution operator $\hat{U}(t, t_i)$. Since the Hamiltonian now depends explicitly on time, we can no longer simply integrate (B.21) to obtain an expression for the time-evolution operator as we did in the free-particle case. The strategy in such a situation is to seek an approximate expression for the time-evolution operator. We now describe how this may be achieved by using TDPT.

B.2.1. Time-dependent perturbation theory. In this work we have exclusively used a description of quantum dynamics known as the Schrödinger picture. However, TDPT solutions of the Schrödinger equation with a time-dependent potential are most easily constructed by appealing to another equivalent description of quantum dynamics known as the interaction picture. A general state ket in the interaction picture $|\psi(t)\rangle^{(I)}$ is related to the state ket in the Schrödinger picture $|\psi(t)\rangle$ by

$$|\psi(t)\rangle^{(I)} = \hat{U}_0^\dagger(t, t_i)\hat{U}(t, t_i)|\psi(t)\rangle,$$

where the free-particle time-evolution operator $\hat{U}_0(t, t_i)$ is given by (B.9) and a dagger denotes the adjoint. The superscript (I) will be used throughout to denote quantities in the interaction picture. Note that $|\psi_i\rangle^{(I)} = |\psi_i\rangle$ and so the interaction and Schrödinger picture state kets initially coincide. In the interaction picture it is straightforward to show that a general state ket evolves according to:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle^{(I)} = \hat{\Phi}^{(I)}(t)|\psi(t)\rangle^{(I)},$$

where $\hat{\Phi}^{(I)}(t) \equiv \hat{U}_0^\dagger(t, t_i)\hat{\Phi}(t)\hat{U}_0(t, t_i)$ is the perturbing potential in the interaction picture. It is apparent from (B.23) that the time evolution of a state ket in the interaction picture is determined solely by $\hat{\Phi}^{(I)}(t)$. The objective is to determine a perturbation expansion for the time-evolution operator $\hat{U}(t, t_i)$ in the Schrödinger picture. This is best achieved by first finding a perturbation expansion for the time-evolution operator in the interaction picture. In this picture a time-evolution operator $\hat{U}^{(I)}(t, t_i)$ can be defined by

$$|\psi(t)\rangle^{(I)} = \hat{U}^{(I)}(t, t_i)|\psi_i\rangle^{(I)}.$$
Substituting (B.24) into (B.23) it is clear that \( \hat{U}^{(1)}(t, t_1) \) obeys

\[
\text{i} \frac{\text{d}}{\text{d}t} \hat{U}^{(1)}(t, t_1) = \hat{\Phi}^{(1)}(t) \hat{U}^{(1)}(t, t_1),
\]

where this equation must be solved subject to the initial condition \( \hat{U}^{(1)}(t_1, t_1) = I \) with \( I \) the identity operator. Observe that equation (B.25), together with the appropriate initial condition, is equivalent to the integral equation

\[
\hat{U}^{(1)}(t, t_1) = I - \frac{\text{i}}{\nu} \int_{t_1}^{t} \hat{\Phi}^{(1)}(t') \hat{U}^{(1)}(t', t_1) \, \text{d}t'.
\]

The integral equation (B.26) provides a convenient means of determining a perturbation expansion for \( \hat{U}^{(1)}(t, t_1) \). By iteration we find that

\[
\hat{U}^{(1)}(t, t_1) = I - \frac{\text{i}}{\nu} \int_{t_1}^{t} \text{d}t' \hat{\Phi}^{(1)}(t') - \frac{1}{\nu^2} \int_{t_1}^{t} \text{d}t' \int_{t_1}^{t} \text{d}t'' \hat{\Phi}^{(1)}(t') \hat{\Phi}^{(1)}(t''),
\]

to second order. To find the corresponding time-evolution operator \( \hat{U}(t, t_1) \) in the Schrödinger picture, first note that \( |\psi(t)\rangle^{(1)} = \hat{U}^{(1)}(t, t_1) |\psi_0\rangle = \hat{U}^{(1)}(t, t_1) |\psi_1\rangle \) since the state kets in the interaction and Schrödinger pictures coincide at \( t = t_1 \). Using the definition (B.22) it follows that

\[
|\psi(t)\rangle = \hat{U}_0(t, t_1) \hat{U}^{(1)}(t, t_1) |\psi_1\rangle.
\]

Upon comparison with (B.20) it is immediately clear that the time-evolution operator in the Schrödinger picture \( \hat{U}(t, t_1) \) is related to \( \hat{U}^{(1)}(t, t_1) \) via

\[
\hat{U}(t, t_1) = \hat{U}_0(t, t_1) \hat{U}^{(1)}(t, t_1).
\]

Multiplying (B.27) by \( \hat{U}_0(t, t_1) \), inserting \( \hat{\Phi}^{(1)}(t) = \hat{U}_0^\dagger(t, t_1) \hat{\Phi}(t) \hat{U}_0(t, t_1) \) and using the following property of the time-evolution operator: \( \hat{U}_0(t, t_1) \hat{U}_0^\dagger(t', t_1) = \hat{U}_0(t, t_1) \hat{U}_0(t_1, t') = \hat{U}_0(t, t') \) then gives

\[
\hat{U}(t, t_1) = \sum_{j=0}^{2} \hat{U}_j(t, t_1),
\]

to second order, where \( \hat{U}_0(t, t_1) \) is given by (B.9),

\[
\hat{U}_1(t, t_1) = -\frac{\text{i}}{\nu} \int_{t_1}^{t} \text{d}t' \hat{U}_0(t, t') \hat{\Phi}(t') \hat{U}_0(t', t_1)
\]

and

\[
\hat{U}_2(t, t_1) = -\frac{1}{\nu^2} \int_{t_1}^{t} \text{d}t' \int_{t_1}^{t'} \text{d}t'' \hat{U}_0(t, t') \hat{\Phi}(t') \hat{U}_0(t', t'') \hat{\Phi}(t'') \hat{U}_0(t'', t_1).
\]

The second-order expression for the time-evolution operator (B.30) can be inserted into (B.20) along with the initial ket expansion (B.10) to give the following approximate solution of the Schrödinger equation (B.5):

\[
|\psi(t)\rangle = \sum_{j=0}^{2} |\psi^{(j)}(t)\rangle,
\]
where

$$|\psi^{(l)}(t)\rangle = \sum_{n} a_n \hat{U}_j(t, t_i) |n^{(0)}\rangle,$$

(B.34)

with $\hat{U}_0(t, t_i)$, $\hat{U}_1(t, t_i)$ and $\hat{U}_2(t, t_i)$ given by (B.9), (B.31) and (B.32), respectively. In the position representation the zeroth-order term $\psi^{(0)} = \langle x | \psi^{(0)}(t) \rangle$ is simply the solution (B.14) of the free-particle Schrödinger equation discussed earlier. Since the eigenfunctions $\phi_{n}^{(0)}$ and the matrix elements $\Phi_{m,n}$ of the free-particle Hamiltonian are independent of time, we may write the first-order term $\psi^{(1)} = \langle x | \psi^{(1)}(t) \rangle$ as

$$\psi^{(1)} = -\frac{i}{\nu} \sum_{n} a_n \sum_{m} J_{m,n} \phi_{m}^{(0)},$$

(B.35)

where $J_{m,n} = J_{m,n}(t)$ is defined by

$$J_{m,n} = \int_{t_i}^{t} \frac{d t'}{t_i} \exp \left[ \frac{-i(t - t') E_{m}^{(0)}}{\nu} \right] \phi_{m,n}(t') \exp \left[ \frac{-i(t' - t_i) E_{n}^{(0)}}{\nu} \right],$$

(B.36)

and the matrix elements $\Phi_{m,n}(t) = \langle m^{(0)} | \hat{\Phi}(t) | n^{(0)} \rangle$ are given by

$$\Phi_{m,n} = L^2 \int_{0}^{L} \frac{dx}{\phi_{m}^{(0)}(x)} \Phi(x, t') \phi_{n}^{(0)}(x) dx.$$

(B.37)

In order to calculate the matrix elements $\Phi_{m,n}$, we first use the Zeldovich approximation $x = q + \tau(D - 1) v_{i}$ to change to Lagrangian coordinates $q$. Inserting $\Phi$ from (B.2) and using (B.13) then leads to

$$\Phi_{m,n} = \frac{1}{L} \int_{0}^{L} \frac{D}{\phi_{m}^{(0)}(q)} \left[ \Phi_{1}(q) - \frac{1}{2}(D - 1) v_{i}^{2}(q) \right] \exp(-i k_{p} q) \exp(-i k_{p} \tau(D - 1) v_{i}(q))$$

$$\times J(q, t') dq,$$

(B.38)

where $k_{p} = k_{m} - k_{n}$ and the Jacobian determinant $J = \partial x / \partial q = 1 + \tau(D - 1) dv_{i} / dq$. Upon substituting $\Phi_{1}$ and $v_{i}$ from (B.3) and (B.4) we obtain, after a lengthy calculation,

$$\Phi_{m,n} = \frac{\delta_{a}}{2} \left( \frac{d}{2\pi \tau} \right)^{2} D \left\{ \alpha \left[ J_{p}(2p\alpha) + \frac{3}{2} \sum_{s=\pm 1} J_{p+s}(2p\alpha) \right] + \left( \frac{\alpha^{2}}{2} - 1 \right) \sum_{s=\pm 1} J_{p+s}(2p\alpha) \right\},$$

(B.39)

where $p = m - n$ is an integer, $\alpha = \alpha(t)$ is defined by $\alpha = \delta_{a}(D - 1) / 2$ and

$$J_{l}(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(i l \theta) \exp(-i x \sin(\theta)) d\theta,$$

(B.40)

are Bessel functions of the first kind. In a similar manner we find that the second-order term $\psi^{(2)} = \langle x | \psi^{(2)}(t) \rangle$ is given by

$$\psi^{(2)} = -\frac{1}{\nu^{2}} \sum_{n} a_n \sum_{m} \sum_{l} K_{l,m,n} \phi_{l}^{(0)},$$

(B.41)
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where $K_{l,m,n} = K_{l,m,n}(t)$ is defined by

$$K_{l,m,n} = \int_{t_i}^{t_f} dt' \int_{t_i}^{t_f} dt'' \exp \left[ -\frac{i(t - t')E_{l}^{(0)}}{\nu} \right] \Phi_{l,m}(t') \exp \left[ -\frac{i(t' - t'')E_{m}^{(0)}}{\nu} \right]$$

and the matrix elements $\Phi_{l,m}(t) = \langle l(0)|\hat{\Phi}(t)|m(0)\rangle$ and $\Phi_{m,n}(t) = \langle m(0)|\hat{\Phi}(t)|n(0)\rangle$ are obtained from (B.39).

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