On approximations of the Schrödinger–Newton equation by harmonic potentials

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Abstract

The evolution of the, initially Gaussian, centre-of-mass wave-function for a homogeneous, spherical particle according to the Schrödinger–Newton equation can be approximated by a harmonic potential, if the wave-function is narrow compared to the size of the particle. Here, the validity of a previously proposed approximation of the Schrödinger–Newton equation is studied, where this is extended beyond the regime of narrow wave-functions, replacing the coupling constant of the harmonic potential by a function of the wave-function width. It turns out that such an extension beyond the narrow wave-function regime is not a good approximation for the self-gravitational evolution according to the Schrödinger–Newton equation.

1 Introduction

The evolution of the, initially Gaussian, centre-of-mass wave-function for a homogeneous, spherical particle according to the Schrödinger–Newton equation can be approximated by a harmonic potential, if the wave-function is narrow compared to the size of the particle. Here, the validity of a previously proposed approximation of the Schrödinger–Newton equation is studied, where this is extended beyond the regime of narrow wave-functions, replacing the coupling constant of the harmonic potential by a function of the wave-function width. It turns out that such an extension beyond the narrow wave-function regime is not a good approximation for the self-gravitational evolution according to the Schrödinger–Newton equation.

The Schrödinger–Newton equation,

\[ i\hbar \frac{\partial}{\partial t} \psi(t, \mathbf{r}) = \left( -\frac{\hbar^2}{2m} \nabla^2 - \frac{Gm^2}{|\mathbf{r} - \mathbf{r}'|} \right) \psi(t, \mathbf{r}), \tag{1} \]

is a nonlinear Schrödinger equation that includes a Newtonian self-gravitation interaction term. Its appearance is uncontroversial as an effective Hartree approximation for the mutual Newtonian interaction in a many-particle quantum state. In this context, it can be derived similar to the Gross–Pitaevskii equation \[1,3\] and has been already considered in the late 1960s in order to model the self-gravitation of Bosonic stars \[4\].

In the more recent past, the Schrödinger–Newton equation also gained attention as a more fundamental equation, i.e. a nonlinear modification of the non-relativistic one-particle quantum dynamics. Such a gravitational modification of the Schrödinger dynamics has been discussed as a hypothetical cause for spatial wave-function localisation \[5,7\], and also as a test case for the necessity to quantise the gravitational field \[8,12\].

While in the first sense, the Schrödinger–Newton equation is already an effective equation for a multi-particle system, in the latter sense, it can be generalised to the multi-particle equa-
an equation for the centre of mass [11]:

\[ i\hbar \partial_t \Psi(t, \mathbf{r}_1, \ldots, \mathbf{r}_N) = \left( -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V_g[\Psi] \right) \Psi(t, \mathbf{r}_1, \ldots, \mathbf{r}_N) \]  \hspace{1cm} (2a)

\[ V_g[\Psi](t, \mathbf{r}_1, \ldots, \mathbf{r}_N) = -G \sum_{i=1}^{N} \sum_{j=1}^{N} m_i m_j \int d^3r'_i \cdots d^3r'_N \frac{|\Psi(t, \mathbf{r}'_1, \ldots, \mathbf{r}'_N)|^2}{|\mathbf{r}_i - \mathbf{r}'_j|}, \]  \hspace{1cm} (2b)

where \( V_g \) denotes the gravitational potential, and \( \mathbf{r}_i \) are the coordinates, and \( m_i \) the masses of \( N \) particles. If a Born–Oppenheimer-like approximation scheme is applied, this can be reduced to an equation for the centre of mass [11]:

\[ i\hbar \frac{\partial}{\partial t} \psi(t, \mathbf{r}) = \left( -\frac{\hbar^2}{2m} \nabla^2 + V_g[\psi](t, \mathbf{r}) \right) \psi(t, \mathbf{r}) \]  \hspace{1cm} (3a)

\[ V_g[\psi](t, \mathbf{r}) = -G \int d^3r' \int d^3\mathbf{u} \int d^3\mathbf{v} \frac{|\psi(t, \mathbf{r}')|^2 \rho_c(\mathbf{u}) \rho_c(\mathbf{v})}{|\mathbf{r} - \mathbf{r}' - \mathbf{u} + \mathbf{v}|}. \]  \hspace{1cm} (3b)

Here \( \mathbf{r} \) is the centre-of-mass coordinate, \( \psi \) the centre-of-mass wave-function, and \( \rho_c \) the mass density of the many-particle system with respect to its centre of mass. One can see immediately that in situations where the mass distribution is point-like compared to the wave-function, equation (3) is well-approximated by equation (1).

In the opposite case, where the spatial wave-function can be considered narrow\(^1\) and the mass is distributed homogeneously over a sphere of radius \( R \), a good approximation to \( V_g \) is given by [11, 13]

\[ V_{\text{narrow}}[\psi](t, \mathbf{r}) = -\frac{G m^2}{R^3} \left( \frac{6}{5} \frac{R^2 - r^2}{2} + r \cdot \langle \psi \mid \mathbf{r} \mid \psi \rangle - \frac{\langle \psi \mid r^2 \mid \psi \rangle}{2} \right). \]  \hspace{1cm} (4)

The nonlinearity is still present, encoded in the expectation values. However, such an equation, that depends only on the first and second moments and is quadratic in \( \mathbf{r} \), can be shown to leave the shape of an initially Gaussian wave packet unchanged. Therefore, in the spherically symmetric case, the full (approximated) dynamics for a Gaussian wave packet are given by the time evolution of the width of the wave packet,

\[ \sigma(t) = \sqrt{\frac{2}{3} \langle \psi(t, \mathbf{r}) \mid r^2 \mid \psi(t, \mathbf{r}) \rangle}. \]  \hspace{1cm} (5)

While for a numerical analysis of equations (1) and (3) the wave-function must be simulated on a discretised grid of many points, for this quadratic approximation only the evolution of this one parameter \( \sigma(t) \) must be simulated. This significantly simplifies numerical simulations, and even allows for some analytical results which cannot be seen from the full equation.

The authors of [14, 15] try to make use of this simplification also for the case of a wide or intermediate wave packet. They propose a generalised gravitational potential

\[ V_g[\psi](t, \mathbf{r}) = \frac{k(\sigma(t))}{2} r^2 \]  \hspace{1cm} (6a)

with the function \( k(\sigma) \) given by

\[ k(\sigma) = \begin{cases} \frac{G m^2}{R^3} \left( 1 - \sqrt{\frac{3}{2}} \frac{9 \sigma}{63 R^2} + \sqrt{\frac{3}{2}} \frac{3 \sigma^3}{64 R^4} \right) & \text{if } \sigma^2 \leq \frac{8 R^2}{3} \\ \sqrt{\frac{3}{2}} \frac{4 G m^2}{9 \sigma^3} & \text{if } \sigma^2 > \frac{8 R^2}{3}. \end{cases} \]  \hspace{1cm} (6b)

\(^1\)If the single particles manifest a large spatial uncertainty this means narrow in comparison to the size of the whole \( N \)-particle system, while in a crystalline structure with well-localised atoms it means narrow compared to the distribution of a single atom, cf. the discussion in [13, 15].
However, apart from the obvious case of a narrow wave function, where it works well, this turns out not to be a good approximation for the Schrödinger–Newton dynamics. To demonstrate this, in this paper, a simulation of the evolution of the full equation (3) is compared to the evolution of $\sigma(t)$ with the results obtained for the approximation (6).

The reasoning behind the approximation (6) is discussed in the next section. In section 3, this approximation is compared to a numerical simulation of the full Schrödinger–Newton equation. The results are summed up and discussed in the last section.

2 Wave packet width dynamics in quadratic approximation

To sum up the idea of the approximation (6), consider a general spherically symmetric Schrödinger equation which is quadratic in $r$:

$$i\hbar \frac{\partial}{\partial t}\psi(t, r) = -\frac{\hbar^2}{2m} r^2 \frac{\partial}{\partial r} \psi(t, r) + h(\sigma(t)) \psi(t, r) + \frac{k(\sigma(t))}{2} r^2 \psi(t, r). \tag{7}$$

This equation is nonlinear due to the implicit wave-function dependence of $h(\sigma(t))$ and $k(\sigma(t))$. If now we make the Gaussian ansatz

$$\psi(t, r) = \left(\frac{\pi \sigma(t)^2}{3} \right)^{-3/4} \exp \left( -\frac{r^2}{2\sigma(t)^2} - i r^2 \varphi_2(t) - i \varphi_0(t) \right) \tag{8}$$

for the wave-function, where the width $\sigma$, as well as the phases $\varphi_2$ and $\varphi_0$, are real-valued functions of time, and then we take the derivatives by $t$ and $r$, and insert them into equation (7), this yields the following closed system of three first order differential equations:

$$\frac{d}{dt} \sigma(t) = -\frac{2\hbar}{m} \sigma(t) \varphi_2(t) \tag{9a}$$

$$\frac{d}{dt} \varphi_0(t) = \frac{3\hbar}{2m \sigma(t)^2} + \frac{h(\sigma(t))}{h} \tag{9b}$$

$$\frac{d}{dt} \varphi_2(t) = -\frac{\hbar}{2m \sigma(t)^4} + \frac{2h \varphi_2(t)^2}{m} + \frac{k(\sigma(t))}{2h}. \tag{9c}$$

Taking the time derivative of equation (9a) and inserting (9c) yields a closed second order differential equation for the width:

$$\frac{d^2}{dt^2} \sigma(t) = \frac{\hbar^2}{m^2 \sigma(t)^3} - \frac{k(\sigma(t)) \sigma(t)}{m}. \tag{10}$$

Hence, the time evolution of the width of the Gaussian wave packet depends only on the width dependent coupling constant $k(\sigma)$. In particular, it also does not depend on the spatially constant potential $h(\sigma)$. For the narrow wave-function potential (4) we have

$$k(\sigma) = \frac{Gm^2}{R^3} = \text{constant.} \tag{11}$$

Now note that equation (7) possesses the conserved energy

$$E = \frac{\hbar^2}{2m} \int d^3x |\nabla \psi(t, r)|^2 + U(\sigma(t)), \tag{12}$$

if the potential $U$ satisfies

$$\frac{dU(\sigma(t))}{d\sigma(t)} = \frac{3}{2} \sigma(t) k(\sigma(t)). \tag{13}$$
For the standard harmonic oscillator potential, where $k$ is a constant, $U$ is simply the potential energy of the oscillator.

The authors of [14, 15] now use the potential between two identical homogeneous spheres of radius $R$ in distance $d$ [16],

$$\Phi_{\text{sphere}}(d) = -\frac{G m^2}{R} \times \left\{ \frac{6}{5} - \frac{2}{d^2} \frac{d^2}{R^2} + \frac{3}{7} \frac{d^3}{R^2} - \frac{1}{5} \frac{d^5}{R^5} \right\} \text{ for } d \leq 2R, $$

$$\Phi_{\text{sphere}}(d) = -\frac{G m^2}{d^2} \text{ for } d > 2R. $$

(14)

to justify the ansatz $U(\sigma) = \Phi_{\text{sphere}}(\sqrt{\langle r^2 \rangle})$, which results in equation (6b) for the function $k$.

Intuitively speaking, the particle moves in a time-dependent harmonic potential, whose coupling constant is tuned in such a way that the potential energy of the particle in the trap matches the gravitational potential energy between two particles, one sitting at the centre of the harmonic potential and the other one sitting at $\sqrt{\langle r^2 \rangle}$.

From this intuitive picture it is already evident what could go wrong with such an approximation, if applied to the self-gravitational potential in the Schrödinger–Newton equation. For the case of a narrow wave-function, the gravitational potential within the particle is, in fact, a harmonic potential, as is also indicated by the approximation (4). However, in the wide wave-function case, where the mass density is well approximated by a delta distribution, the gravitational potential for a Gaussian wave-function of width $\sigma$ is

$$V_g(r) = -\frac{G m^2}{r} \text{ erf} \left( \frac{r}{\sigma} \right),$$

(15)

where erf is the Gauss error function. While this can be approximated by a quadratic function for small $r$, for $r \gg \sigma$ we have

$$V_g(r) = -\frac{G m^2}{r} + O \left( \frac{1}{r^2} \right).$$

(16)

Therefore, for the full Schrödinger–Newton equation, contrary to the approximation (6), the part of the wave-function at positions $r > \sigma$ will not see a quadratic potential, not even as an approximation, but a Coulomb-like potential. From the evolution according to the full Schrödinger–Newton equation one expects a weaker response to gravity than the approximation (6) suggests.

The quadratic approximation also cannot cover the long-time behaviour of the wave-function, at least for the case of a wide wave-function. In this case, the Schrödinger–Newton equation becomes approximately the one-particle equation [1], for which it has been shown [17], that for a positive total energy,

$$E = \int d^3r \frac{\hbar^2}{2m} \left| \nabla \psi(t, r) \right|^2 - \frac{1}{2} G m \int d^3r d^3r' \left| \psi(t, r) \right|^2 \left| \psi(t, r') \right|^2 \left| r - r' \right| > 0, $$

(17)

the second moment, $\langle r^2 \rangle$, is unbound. Hence, if the mass is not too large, $\sigma(t)$ will tend to infinity, while it would remain finite for all times according to equation (10) with (6b).

In order to get a better picture of when the quadratic potential with width dependent coupling constant provides a good approximation to the full Schrödinger–Newton equation, we compare it with a numerical evolution of the full equation in the next section.

3 Comparison with numerical evolution of the full Schrödinger–Newton equation

We want to compare equation (10) for a particle, which is modelled by a homogeneous sphere, with the dynamics of the wave-function width for the full Schrödinger–Newton equation. Therefore, we consider the full equation [3], i.e. we apply the Born–Oppenheimer type, but no further
approximations. This equation can be solved numerically, using the same Crank–Nicolson algorithm that was applied in [9, 18]. The only difficulty is to calculate the potential $V_g$ in every time step. For this purpose, the homogeneous-sphere potential was simplified analytically to a one-dimensional integral, cf. appendix A. We then calculate the width $\sigma(t)$ of the numerically obtained wave-function according to equation (5), regardless of the shape of the resulting wave-function.

Note that the Schrödinger–Newton equation is invariant under a rescaling \[ m \rightarrow \mu m, \quad t \rightarrow \mu^{-5} t, \quad r \rightarrow \mu^{-3} r, \quad \psi(t, r) \rightarrow \mu^{9/2} \psi(\mu^{5} t, \mu^{3} r). \] (18)

This scaling law makes it convenient to express lengths, masses, and times in the following units, depending on the width $\sigma_0$ of the initial wave-function: \[ [l] = \sigma_0, \quad [m] = 1 \text{ m.u.} = \left( \frac{\hbar^2}{G \sigma_0} \right)^{1/3}, \quad [t] = 1 \text{ t.u.} = \left( \frac{\sigma_0^5}{G \hbar} \right)^{1/3}. \] (19)

Expressed in these units, all statements become independent of the choice of the initial width of the wave-function. Self-gravitational effects start to become significant for masses around 1 m.u.

Figure 1 shows the evolution of the width of a narrow wave-function ($\sigma_0/R = 0.1$). For masses of 2 m.u. and above, there is a significant difference between the free evolution and the Schrödinger–Newton equation, while the simulation of the full Schrödinger–Newton equation is in good agreement with the harmonic potential approximation, as expected.

This changes in the intermediate regime ($\sigma_0/R = 1$, see figure 2), and even more for a wide wave-function ($\sigma_0/R = 10$, see figure 3). While both the simulation and the approximation...
Figure 2: Evolution of the width of an initially Gaussian wave packet in the intermediate regime ($R = \sigma_0$). The dotted line represents the behaviour according to the free Schrödinger equation without gravity, the solid line is the solution of equation (10) with the coupling constant (6b), and the error-bar dots show the result of the full numerical analysis (the error given by the standard deviation of an average over multiple data points).
Figure 3: Evolution of the width of an initially Gaussian wave packet in the wide wave-function regime ($R = 0.1 \sigma_0$). The dotted line represents the behaviour according to the free Schrödinger equation without gravity, the solid line is the solution of equation (10) with the coupling constant $6b$, and the error-bar dots show the result of the full numerical analysis (the error given by the standard deviation of an average over multiple data points).
show oscillations, the simulated results oscillate with a significantly lower frequency and a much smaller amplitude. Also the centre of the oscillations, corresponding to the stationary ground state of the Schrödinger–Newton equation, is closer to the initial width of the wave-function than the centre of the harmonic oscillations.

Figure 4 indicates that at least in the wide wave-function regime the wave-function does not remain a Gaussian at all. Instead, the probability density accumulates on the surface of the particle. This is the behaviour one would intuitively expect for the gravitational potential of a homogeneous sphere, whose minimum is at the surface. While the gravitational potential inhibits dispersion outside the radius of the sphere, gravity is too weak to compensate the quantum mechanical spreading inside the sphere. The centre of mass of a molecule, according to the Schrödinger–Newton equation, is most likely found on its surface.

Up to this point, we conclude that the approximation (6) with width dependent coupling is only a good approximation in the narrow wave-function regime. Figure 5 shows how this approximation compares to the approximation (4) with constant coupling (dotted line in the figure). In the narrow wave-function regime, both are good approximations. A significant difference between the two approximations can only be seen for larger times (figure 5), where the approximation with width dependent coupling shows a smaller deviation from the numerical result. In the intermediate (figure 5), and even more in the wide wave-function regime (figure 5), the approximation with width dependent coupling is obviously much closer to the result of the numerical evolution. However, in this regime, both approximations show a high deviation from the numerical result.

4 Conclusion

The purpose of this paper was an examination of the proposal to approximate the Schrödinger–Newton equation for a spherical homogeneous particle by a harmonic potential with wave packet width dependent coupling [14, 15]. In such a potential, an initially Gaussian wave packet remains Gaussian and the Schrödinger–Newton equation can be reduced to a one-parameter equation for the wave-packet width. Such an approximation can decrease computation times for numerical simulations considerably.

However, for a centre-of-mass wave-function which is wide compared to the particle radius, the gravitational potential is essentially Coulomb-like, and therefore, a quadratic potential cannot provide a good approximation. This has been confirmed by comparison with a numerical evolution of the full Schrödinger–Newton equation.
On the other hand, in the case of a narrow wave-function, the gravitational potential is indeed approximately quadratic. In this case, the approximation works well, as is also indicated by the comparison with the full numerical evolution. The direct comparison of the approximation with width dependent coupling and the much simpler approximation with an ordinary harmonic potential with constant coupling shows, however, that in this regime the latter works also very well.

In conclusion, although conceptually interesting, the approximation (6) is only of marginal practical value to simulate the dynamics of a Gaussian wave packet. Instead, the quadratic approximation (4) turns out to be useful for simplified calculations, both numerically and analytically, in the narrow wave-function regime. Conversely, the numerical evolution of the Schrödinger–Newton equation (1), as performed in [9, 19], cannot be easily circumvented in the wide wave-function regime.

Even more difficult is the intermediate regime where \( \sigma_0 / R \approx 1 \). In this regime, neither the quadratic approximation nor the one-particle equation (1) can provide a good description of the evolution of the centre of mass. The simulation of the full many-particle centre-of-mass equation (3), used in section 3, is necessary to get reliable results.

The numerical analysis shows that, in the narrow wave-function regime, the deviation between both approximations, and the deviation of the approximations to the numerical results, are comparable. Hence, the approximation with width dependent coupling—or rather the comparison of both approximations—could be helpful in providing an indicator of how good both approximations still are after a given period of time.

**Figure 5:** Comparison of the approximations (6) and (4) with constant coupling \( k(\sigma) \). As before, the solid line is the solution of equation (10) with the \( \sigma \)-dependent coupling (6b), and the error-bar dots show the result of the full numerical analysis. The dotted line now represents the solution of equation (10) with the constant coupling (11). All plots are for a mass of 100 m.u.
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Appendix

A Numerical calculation of the self-gravitational potential

In a spherically symmetric situation, the self-gravitational potential is

\[
V_g(t,r) = -G \int d^3r' \left| \psi(t,r') \right|^2 I(r-r')
\]

\[
= -2\pi G \int_0^\infty dr' \left| r'^2 \psi(t,r') \right|^2 \int_{-1}^1 du I \left( \sqrt{r^2 + r'^2 - 2rr'} u \right)
\]

\[
= -2\pi G \int_0^\infty dr' \left| r'^2 \psi(t,r') \right|^2 \int_{|r-r'|}^{r+r'} dw \frac{w}{r'r'} I(w)
\]

\[
= -\frac{2\pi G}{r} \left[ \int_0^r dr' r f(r,r') \left| \psi(t,r') \right|^2 + \int_r^\infty dr' r f(r',r) \left| \psi(t,r') \right|^2 \right],
\]

(A.1)

where we substituted \( w^2 = r^2 + r'^2 - 2rr'u \), and defined

\[
f(a,b) = \int_{a-b}^{a+b} dw \, w I(w).
\]

(A.2)

For the mass density of a homogeneous sphere,

\[
I(\mathbf{d}) = \int d^3u \, d^3v \frac{\rho_c(u) \rho_c(v-\mathbf{d})}{|u-v|}
\]

\[
= \frac{m^2}{R} \times \begin{cases} \frac{6}{5} - 2 \left( \frac{d}{2R} \right)^2 + \frac{3}{2} \left( \frac{d}{2R} \right)^3 - \frac{1}{5} \left( \frac{d}{2R} \right)^5 & \text{for } d \leq 2R, \\ \frac{d}{2} & \text{for } d > 2R, \end{cases}
\]

(A.3)

we obtain

\[
f(a,b) = \frac{m^2}{R^6} \times \begin{cases} p(a,b) & \text{for } a-b \leq a+b \leq 2R, \\ q(a,b) & \text{for } a-b \leq 2R \leq a+b, \\ 2bR^6 & \text{for } 2R \leq a-b \leq a+b, \end{cases}
\]

(A.4)
with the polynomials

\[
p(a, b) = -\frac{a^6 b}{80} - \frac{a^4 b^3}{16} + \frac{3}{8} a^4 b R^2 - a^3 b R^3 - \frac{3 a^2 b^5}{80} + \frac{3}{4} a^2 b^3 R^2 - a b^3 R^3 + \frac{12}{5} a b R^5 - \frac{b^7}{560} + \frac{3 b^5 R^2}{40}
\]

\[
q(a, b) = \frac{a^7}{1120} - \frac{a^6 b}{160} + \frac{3 a^5 b^2}{160} - \frac{3 a^5 R^2}{80} - \frac{a^4 b^3}{32} + \frac{3}{16} a^4 b R^2 + \frac{a^4 R^3}{8}
\]

\[
+ \frac{3 a^3 b^4}{32} - \frac{3}{8} a^3 b^2 R^2 - \frac{1}{2} a^3 b R^3 - \frac{3 a^2 b^5}{160} + \frac{3}{8} a^2 b^3 R^2 + \frac{3}{4} a^2 b^2 R^3
\]

\[
- \frac{3 a^2 R^5}{5} + \frac{a b^6}{160} - \frac{3}{16} a b^4 R^2 - \frac{1}{2} a b^3 R^3 + \frac{6}{5} a b R^5 + a R^6 - \frac{b^7}{1120} + \frac{3 b^5 R^2}{80} + \frac{b^4 R^3}{8} - \frac{3 b^2 R^5}{5} + b R^6 - \frac{18 R^7}{35}.
\]

(A.5) (A.6)

The polynomials \( p \) and \( q \) are quite lengthy, but numerically much easier to handle than a numerical integration would be. We use equations (A.1) and (A.4)–(A.6) for the numerical calculation of \( V_g \).

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