Gravitationally induced inhibitions of dispersion according to a modified Schrödinger–Newton equation for a homogeneous-sphere potential

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Abstract
We modify the time-dependent Schrödinger–Newton equation by using a potential for a solid sphere suggested by Jäälkäinen (2012 Phys. Rev. A 86 052105) as well as a hollow-sphere potential. Compared to our recent paper (Giulini and Großardt 2011 Class. Quantum Grav. 28 195026) where a single point particle, i.e. a Coulomb potential, was considered, this has been suggested to be a more realistic model for a molecule. Surprisingly, compared to our previous results, inhibitions of dispersion of a Gaussian wave packet occur at even smaller masses for the solid-sphere potential, given that the width of the wave packet is not exceeded by the radius of the sphere.

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(Some figures may appear in colour only in the online journal)

1. Introduction

This paper is the third in a series of papers [1, 2] on the Schrödinger–Newton equation. This equation first appeared in the paper by Diósi [3], following earlier suggestions by [4]. It was considered in the context of gravity-induced quantum-state reduction by Penrose [5, 6], who also called it the Schrödinger–Newton equation, henceforth abbreviated SN equation. In our work, we regard this equation as a model for the interaction between a quantum-mechanical system and its own classical gravitational field. It has been demonstrated in [2] that the SN equation results as a non-relativistic limit from the Einstein–Klein–Gordon and Einstein–Dirac system. We refer to our earlier papers and references therein for further motivation, mathematical details and the discussions surrounding this equation.
In [1], we investigated the time-dependent SN equation:

\[ i\hbar \frac{\partial}{\partial t} \Psi(t, \vec{x}) = \left( -\frac{\hbar^2}{2m} \Delta + (\Phi * |\Psi|^2)(t, \vec{x}) \right) \Psi(t, \vec{x}), \]

with a potential term that is the spatial convolution of the absolute-value squared of the wavefunction with the Coulomb potential \( \Phi(\vec{r}) = -\frac{Gm^2}{r} \):

\[ (\Phi * |\Psi|^2)(t, \vec{x}) = -Gm^2 \int \frac{|\Psi(t, \vec{y})|^2}{|\vec{x} - \vec{y}|} d^3 y. \]

Our numerical and analytical consideration of the SN equation in [1] showed that inhibitions of dispersion due to the gravitational self-interaction occur at mass values of about \( 6.5 \times 10^9 \text{ u} \) for a given wave packet width of 0.5 \( \mu \text{m} \). This result was contrary to a previous one by Salzman and Carlip [7, 8], where inhibitions of dispersion were claimed to occur at mass values more than six orders of magnitude smaller, namely at \( m \approx 1600 \text{ u} \). Somewhat loosely, this behaviour of a wave packet initially shrinking in width was called a ‘collapse’ by Salzman and Carlip and we adopt this nomenclature.

As we pointed out in the summary of [2], more consideration has to be given to the question concerning the application of the SN equation to realistic systems, like molecules. In a recent paper [9], Jääskeläinen suggested that the gravitational self-interaction for a molecule should be modelled by the potential of a solid sphere of radius \( R \)

\[ \Phi(r) = \begin{cases} -\frac{Gm^2}{r} \frac{3}{2} - \frac{r^2}{2R^2}, & \text{if } r < R \\ -\frac{Gm^2}{r}, & \text{if } r \geq R, \end{cases} \]

which has to be put into equation (1) instead of the Coulomb potential.

Jääskeläinen points out that in our case, for a wave packet width of 0.5 \( \mu \text{m} \), the results obtained for this potential deviate from the results for the Coulomb potential for masses beyond \( 10^{10} \text{ u} \).

We will next briefly review the rationale behind such a modification and then turn to the quantitative changes it implies for our previous analysis [1]. For comparison, we will also consider the case of a hollow sphere.

### 2. How to separate the SN equation

In this section, we briefly discuss how a one-particle SN equation for the centre of mass is obtained by the separation from an \( N \)-particle SN equation, as claimed in [9].

Consider the \( N \)-particle SN equation

\[ i\hbar \dot{\Psi}_N(\vec{r}^N) = \left[ -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \Delta_{i} + V_{\text{EM}}(\vec{r}^N) + U_{\text{G}}[\Psi_N(\vec{r}^N)] \right] \Psi_N(\vec{r}^N), \]

\[ V_{\text{EM}}(\vec{r}^N) = \sum_{i=1}^N \sum_{j=1}^{i-1} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}, \]

\[ U_{\text{G}}[\Psi_N(\vec{r}^N)] = -G \sum_{i=1}^N \sum_{j=1}^N m_i m_j \int \frac{|\Psi_N(\vec{r}^N)|^2}{|\vec{r}_i - \vec{r}_j|} dV^N \]

\[ = -G \sum_{i=1}^N \sum_{j=1}^N m_i m_j \int \frac{P_j(\vec{r}_j)}{|\vec{r}_i - \vec{r}_j|} d^3 r_j. \]
Here, \( \vec{r}_i^N \) indicates the set of all \( N \) coordinates \( \vec{r}_i \), \( m_i \) the mass of the \( i \)th particle and \( \Delta r_i \) is the Laplacian with respect to the \( i \)th coordinate. By \( P_i \), we denote the \( i \)th marginal distribution that one obtains by integrating \( |\Psi_N(\vec{r}_i^N)|^2 \) over all \( (N - 1) \) factors \( \mathbb{R}^3 \) that parametrize the positions of all particles except the \( i \)th.

The intuitive picture underlying the gravitational potential term \( U_G \) is as follows: Each particle is under the influence of a Newtonian gravitational potential that is sourced by an active gravitational mass density to which each particle contributes proportional to its probability density in position space as given by the marginal distribution of the total wavefunction:

\[
\rho_{\text{mat}}(\vec{x}) = \sum_{j=1}^{N} m_j P_j(\vec{x}) = \sum_{j=1}^{N} m_j \int |\Psi_N(\vec{r}_j^N)|^2 \delta(\vec{r}_j - \vec{x}) \, dV^N. \tag{7}
\]

Although each particle lives in its own copy of \( \mathbb{R}^3 \), they all ‘feel’ the same matter density \( \rho_{\text{mat}} \). In particular, the self-interaction of each particle with its own field is included.

The gravitational interaction of all \( N \)-particles is then given by

\[
U_G[\Psi_N(\vec{r}_i^N)] = -G \sum_{i=1}^{N} \int \frac{m_i \rho_{\text{mat}}(\vec{x})}{|\vec{r}_i - \vec{x}|} \, d^3x \]

\[
= -G \sum_{i=1}^{N} \sum_{j=1}^{N} \int \frac{m_i m_j P_j(\vec{x})}{|\vec{r}_i - \vec{x}|} \, d^3x. \tag{8}
\]

Note that this is the \( N \)-particle SN equation as stated by Diósi [3], which is different from that given by Jääskeläinen [9]. In [9], the mutual gravitational interactions are said to be negligible compared to electromagnetic interactions and only the diagonal terms of \( U_G \) are considered. But in situations where the width of the individual marginal distributions is large compared to the mutual distances of their centres, these contributions are of the same order of magnitude as the diagonal terms.

We emphasize that in this treatment, there is a twofold difference between the electromagnetic and gravitational interactions of the particles. First, self-interactions of particles with their own electromagnetic field are not considered. Second, whereas the electromagnetic interaction is local, the gravitational interaction is non-local in the sense explained above. It is this non-locality that is responsible for a non-trivial contribution of the overall gravitational field to the dynamics of the centre of mass.

We now introduce the centre of mass coordinates

\[
\vec{r} = \frac{\sum_{i=1}^{N} m_i \vec{r}_i}{M}, \quad M = \sum_{i=1}^{N} m_i, \quad \vec{p}_i = \vec{r}_i - \vec{r} \quad (i = 0, \ldots, N - 1) \tag{9}
\]

and make the separation ansatz \( \Psi_N(\vec{r}_i^N) = (m_N/M)^{3/2} \psi(\vec{r}) \chi(\vec{r}_i^{N-1}) \), where the prefactor comes from the integral measure and allows us to normalize all wavefunctions to 1. Then, \( V_{\text{EM}} \) only depends on the relative coordinates \( \vec{p}_i \).

Substituting the separation ansatz into expression (6), \( U_G \) can be written as

\[
U_G \approx -G \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} m_i m_j \int \frac{|\psi(\vec{r})|^2 |\chi(\vec{p}_i^{N-1})|^2 \, d^3\rho_i \cdots d^3\rho_{N-1} \, d^3\vec{r}}{|\vec{r} + \vec{p}_i - \vec{p}_j|}, \tag{10}
\]

where we assumed \( N \) to be a large number, such that all terms involving the \( N \)th particle can be neglected. They give only \( (2N - 1) \) out of \( N^2 \) contributions. Let

3 All contributions can be considered of the same order of magnitude. Otherwise, just choose the particle that yields the smallest contribution as the \( N \)th particle.
be the marginal distribution of the relative wavefunction \( \chi \) for the \( i \)th particle and rename the integration variable \( \vec{\rho}_i \) to \( \vec{\rho}'_i \). Then, in the above approximation,

\[
U_G = -G \int |\psi(\vec{r}')|^2 \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} m_i \int \frac{m_j P^i_{rel}(\vec{\rho}')}{|\vec{r}' + \vec{\rho}_i - \vec{r}' - \vec{\rho}'_j|} \, d^3 \rho \, d^3 \rho'.
\]  

Now note that \( m_j P^i_{rel} = \rho^\text{mat}_j \) is simply the matter density of the \( j \)th particle relative to the centre of mass. We can therefore substitute the inner integral with the gravitational potential of the \( j \)th particle, which is

\[
\phi_j(\vec{r}) = -GM \int \frac{\rho_j^\text{mat}(\vec{y})}{|\vec{r} - \vec{y}|} \, d^3 y.
\]  

We then obtain

\[
U_G = \int |\psi(\vec{r}')|^2 \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \frac{m_j}{M} \phi_j(\vec{r}' + \vec{\rho}_i - \vec{r}') \, d^3 r'.
\]  

If now we assume that the extent of the molecule is much smaller than the width of the wavefunction, such that the wavefunction does not change much over a distance \(|\vec{\rho}|\), i.e. \( |\psi(\vec{r}' - \vec{\rho}_i)|^2 \approx |\psi(\vec{r}')|^2\), we can neglect the shift by \( \vec{\rho}_i \). The sum over all \( m_i \) then just yields the total mass \( M \) and the one-particle potentials \( \phi_j \) sum up to yield the full gravitational potential \( \Phi \). We finally obtain

\[
U_G[\psi(\vec{r})] = \int |\psi(\vec{r}')|^2 \Phi(\vec{r}' - \vec{r}) \, d^3 r'.
\]  

The SN equation (4) then separates into the ordinary electromagnetic multi-particle Schrödinger equation for the relative coordinates, for which the solution is taken to be given by the present lump of matter, and the SN equation (1) for the centre of mass wavefunction \( \psi(\vec{r}) \) with the modified gravitational potential \( \Phi \) for the matter at hand.

3. Results

3.1. Solid-sphere potential

We study the evolution of the spherically symmetric SN equation making use of the same numerical methods used in [1], simply replacing the potential by the solid-sphere potential (3). All results refer to an initial Gaussian wave packet

\[
\Psi(r, t = 0) = (\pi a^2)^{-3/4} \exp \left( -\frac{r^2}{2a^2} \right)
\]  

with a width of \( a = 0.5 \mu m \).

First, we look at the evolution of wave packets if the density of the solid sphere corresponds to the density of either lithium (534 kg m\(^{-3}\)) or osmium (22 610 kg m\(^{-3}\)), cf [9]. To illustrate the results, the radius within which 90% of the probability density are contained is plotted against time in figure 1 for several masses. In addition to the results for the density of lithium (Li) and osmium (Os), the results for the SN equation with the Coulomb potential obtained in [1] are also plotted.

For all masses considered, the modified potential results in an even faster collapsing wave packet. The shrinking behaviour also sets in for smaller masses, namely for \( 5 \times 10^9 \) u, the modified solution shrinks, while the SN equation solution is still spreading for this mass.
Figure 1. This plot shows the radius $r_{90}$ within which 90% of the probability lie plotted against time for several masses for the SN equation with Coulomb potential (SN) and with a solid-sphere potential for both the density of lithium (Li) and osmium (Os).

To obtain a better impression of this behaviour, let us take a look at the effect that the radius of the solid-sphere potential has on the mass for which the collapsing behaviour of the wave packet sets in. We thus ask the following question: given a sphere of radius $R$, what mass $m_c$ do we have to distribute homogeneously ‘within’ this sphere for a collapse of the wave packet to take place?

In [1], we found that for a 0.5 $\mu$m wave packet, a collapse is observed for masses of about $6.5 \times 10^9$ u and higher. In figure 2, this critical mass value is plotted depending on the radius of the solid sphere.

For small radii of several nanometres, this critical mass reduces to about two-thirds of the value obtained in [1] and it stays smaller than this value until the size of the solid sphere exceeds the width of the wave packet significantly. There seems to be an extremal value somewhere in between 20 and 100 nm.

3.2. $R > 0$ not lead to a diminishment of the collapse mass?

The behaviour described in the previous paragraph seems peculiar, as naively one would expect the gravitational field to be the weaker, and therefore the collapse mass to be the higher, the larger the solid-sphere radius obtains. But the ascertained radius dependence of the collapse mass becomes more comprehensible by an analysis of the total energy value of the SN equation.

4 But note that the gravitational interaction is always weighted with the probability density of the Gaussian wave packet whose width is always fixed to 0.5 $\mu$m.

5 As the separation in section 2 only holds for small radii compared to the extent of the wave packet, the results for larger radii have to be regarded with some scepticism, anyway.
We performed a similar analysis in section 3.2 of [1] where we indicated the total energy for the SN wave packet:

\[ E = T + \frac{1}{2} V = \frac{\hbar^2}{2m} \int d^3x |\nabla \psi(t, \vec{x})|^2 + \frac{1}{2} \int d^3x |\psi(t, \vec{x})|^2 U(t, \vec{x}), \]

\[ (17) \]

where \( U(t, \vec{x}) = (\Phi * |\Psi|^2)(t, \vec{x}) \).

Harrison et al [10] pointed out that for the SN equation, a collapse can only be observed if the total energy is positive. The second time derivative of the second moment \( \ddot{Q} = \int \dot{x}^2 |\psi|^2 \) is given by

\[ \ddot{Q} = \frac{1}{m} \left( 4T - 2 \int d^3x |\psi(t, \vec{x})|^2 \dot{x} \cdot \vec{\nabla}U(t, \vec{x}) \right) \]

\[ (18) \]

for an arbitrary potential \( U \). If the potential fulfils a Poisson equation \( \Delta U \sim |\psi|^2 \), it takes the form

\[ 6 \]
\[\dot{Q} = \frac{1}{m} (4T + V) = \frac{1}{m} (4\mathcal{E} - V),\]  \hspace{1cm} (19)

which is strictly positive for positive energy.

Although this relation does not hold for the modified potentials, the mass value for which the total energy equals zero might nevertheless provide an insight into the qualitative behaviour of the equation. We thus plot this mass value \(m_0\) against the radius \(R\) of the solid sphere in figure 3. As one can see, this mass value indeed decreases significantly within the width of the wave packet and starts to increase only when the radius of the solid sphere exceeds this width.

Thus, qualitatively the behaviour of the zero-total-energy mass value coincides with the behaviour of the collapse mass.

### 3.3. Hollow-sphere potential

At least for the experimental situation of interferometry with fullerene molecules, it seems a more realistic model to consider a hollow-sphere potential

\[\Phi(r) = \begin{cases} 
-\frac{Gm^2}{R}, & \text{if } r < R \\
-\frac{Gm^2}{r}, & \text{if } r \geq R 
\end{cases}\]  \hspace{1cm} (20)

instead of the solid-sphere potential (3). Let us therefore repeat the analysis from section 3.1 for the potential (20).

The result is plotted in figure 4. As one can see, the collapse mass does not decrease but remains almost constant as long as the radius of the hollow sphere does not exceed the wave packet width. For larger radii, the collapse mass increases fast.

This can also be understood if, again, we look at the total energy (see figure 5). Contrary to the solid sphere, \(m_0\) for the hollow sphere converges against the SN value for \(R \to 0\) and compared to the solid-sphere value (dotted line), it only decreases very weakly before increasing for radius values above the width of the wave packet.
4. Conclusion

If one does not take the simpler point of view we took in [1] and models large molecules by a point-particle SN equation, and instead assumes the modified equation given in [9] to provide a more realistic description for such molecules, our results confirm that there are indeed deviations between both equations, as Jääskeläinen suggested.

However, whereas one naively might expect that a smaller matter density leads to a weaker gravitational interaction and therefore to a behaviour that is closer to the free Schrödinger equation, our results show that the converse is true. As long as the radius of the solid-sphere
potential does not significantly exceed the extent of the wave packet, the effect of inhibitions of dispersion is even increased compared to the unmodified SN equation. The analysis of the total energy given in section 3.2 provides an insight why this somewhat peculiar behaviour shows up.

Such an increase of the effect cannot be observed for the hollow-sphere potential, but there is also no significant decrease, as long as the radius of the hollow sphere does not exceed the extent of the wave packet.

The question why there should be a self-gravitational interaction while there is no electromagnetic self-interaction term present in the Schrödinger equation remains an issue that should be addressed (cf the discussion in [2]). This issue arises even more distinctly in the analysis given in section 2 of this paper, where the gravitational interactions are treated differently to the electromagnetic ones.

We conclude that taking into account the finite extent of the source in the way suggested in [9] does not lead to an attenuation of the effect of inhibitions of dispersion as discussed in [1]. The prospects for an experimental verification of self-gravitation of quantum systems in future molecular interferometry experiments remain unchanged.

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