EFFECTS OF EXPANDING UNIVERSE IN THE SCHRÖDINGER-NEWTON APPROACH

SUBMITTED
BY

SRI DEVI WIJAYA

DIVISION OF PHYSICS & APPLIED PHYSICS
SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES

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Final Year Project - Effects of expanding universe in the Schrödinger-Newton approach

Sri Devi Wijaya

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Abstract

Our universe is expanding and this expansion accelerates. A way to model this experimental fact is to add the cosmological constant Λ to the Einstein's equations. Here we study the effect due to Λ to the already established Schrödinger-Newton equation proposed to describe gravitating quantum objects. A spherically symmetric Gaussian function is used in evaluating the possibilities of finding the concrete solution of Schrödinger-Newton equation, and the resulting wave-functions are obtained using Matlab programming software. The collapsed wave-functions are retrieved, and in agreement with the results found in [1]. We then proceed to adding the cosmological constant to the equation and observe no collapse behaviour in the wave-function for any mass. The rate of expansion of the wave-function increases much faster for microscopic particles and increases slower for more massive objects.

Contents

1 Introduction

Since the discovery of wave-particle duality of light, people started to see things differently. Then, added with the discovery that electrons do behave like a particle and a wave at the same time, the confusion began to accumulate. It was only in the early twentieth century that the confusion was resolved by Schrödinger, Heisenberg, and the others [2]. The discovery of quantum physics marks the beginning of modern physics together with Einstein's general relativity, and is also known as the golden age of twentieth century physics.

Quantum mechanics explains extremely well the behaviour of very small objects. The problem arises, however, when we want to describe the classical phenomena which incorporate massive objects. Massive objects, as far as our intuition is concerned, definitely do not behave like electrons. In contrast to quantum mechanics, classical physics such as Newtonian law of motion is verified to explain the macroscopic world well, at least to the non-relativistic approximation.

It is often perceived that since every macroscopic object is made of many microscopic atoms, we would be able to extend quantum mechanics to a macroscopic level and it must agree with the classical predictions, and also the Einstein's general relativity to be exact. However, there are only a few phenomena in the macroscopic domain where quantum mechanics seems to play a role. Such phenomena include superconductivity, flux quantization, or the Josephson effect [3]. Beyond that, quantum effects appear to be absent with the world around us. The most obvious sign of this can be seen from how a macroscopic object, like a ball always has a well defined position; while in quantum mechanics it is not the case. A free particle (a particle in the absence of any external forces) as pictured in quantum level, will have its position defined in terms of probability which means there is no way we are able to ascertain its position.

Another slightly less obvious case where the disagreement comes into view is when we look at the superposition of quantum objects. A few experimentations have confirmed the superposition principle in relatively large objects such as the double-slit experiments with buckyballs [4], the pizoelectric tuning fork experiment [5], or superposition of beryllium ion [6]. However, it is not clear how much larger objects could superpose and exist in several different states at the same time. If this were the case, we would be seeing an object at two different places at once, or even moving at two different directions at once, which do not really happen in our everyday experience.

One possible way to resolve the dispute is by considering the effect of gravitational interaction, i.e. to use the gravitational attraction to prevent the non-localisation of quantum objects. The idea later gave birth to a new equation called the Schrödinger-Newton equation, which was first brought up by Diosi [7] in 1985. Since then, a lot of work have been put to analyse the problem and obtain a possible solution to the equation, both numerically and analytically. It is, however, difficult to come up with an exact solution due to its highly non-linear property and hence numerical method is chosen to approach the problem. A comprehensive numerical work can be found in [8].

Some numerical studies have shown that resulting wave-function of the Schrödinger-Newton equation exhibits attraction property among different parts of the wave-function [9]. When the wave-function of the system is given by a single wave packet, this effect amounts to an inhibition of the free spreading of the wave packet, thus resulting in a self-focusing (or say, shrinking) of it for sufficiently high masses [9]. Moreover, two or more wave packets that are superposed at different locations will have their wave-functions to collapse to an average position, as how we understand the concept of centre of mass [10]. This is a good indication that Schrödinger-Newton equation could be a suitable avenue to connect quantum world with macroscopic world.

We therefore consider the Schrödinger-Newton equation as a reasonable alternative to solving the dispute between quantum and macroscopic worlds, and in this thesis extend its scope. It is a very well-known fact that our universe is expanding, and it was even observed to be expanding in accelerating manner modelled by the cosmological constant [11]. The question we pose is whether we would be able to see the effect of this expanding universe on the properties of the wave-function in Schrödinger-Newton approach. We will do this by adding cosmological constant into the derivation of the Schrödinger-Newton equation, and then solving the resulting dynamics numerically. We recover numerical method in [8] used to solve the Schrödinger-Newton equation, and then we add the cosmological effect Λ into the numerics. At the end of this thesis, limitations and improvements for this project are discussed.

2 Theory

2.1 Evolution of spherically symmetric Gaussian function in 3D

The numerical work in this thesis uses spherically symmetric Gaussian function as the initial condition, and the analytical derivation of the evolution of such function is given in the Appendix. The normalized wave-function at time zero can be written as

$$\psi(r,0) = \left(\frac{\alpha}{\pi}\right)^{3/4} \mathrm{e}^{-\alpha r^2/2} \tag{2.1.1}$$

where α is a parameter that determines the width of the function, and r is radius. This function is a spherically symmetric function, i.e. it only depends on time and the radial position, thus any angular derivatives in spherical coordinates vanish. This makes our analytical and numerical calculations easier as we only have to deal with one spatial component.

The time evolution of the free-particle Gaussian function in 3-dimension is

$$\psi(r,t) = (\pi\alpha)^{3/4}\left(\frac{\alpha m}{m+i\alpha\hbar t}\right)^{3/2} \exp\left(-\frac{\alpha m}{2(m+i\alpha\hbar t)}r^2\right) \tag{2.1.2}$$

where m is the mass of the object, and $\hbar$ is the Planck's constant. The analytical calculation will then be used to verify that our numerical method executes the correct results by comparing the output of the program as seen in Section 3.

Figure 1 shows the diagram of how the radial probability density spreads with time for free electron.

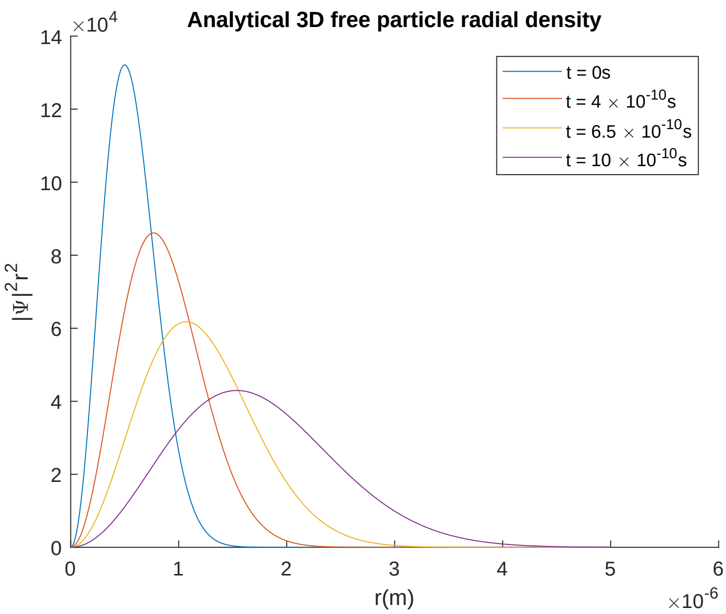


Figure 1: Spread of free particle radial probability density. Calculation is for an electron of mass $m = 9.109 \times 10^{-31}$kg.

We can see what happens to the probability density if we increase the mass of the particle. Figure 2 shows that the probability spreads more slowly for larger mass.

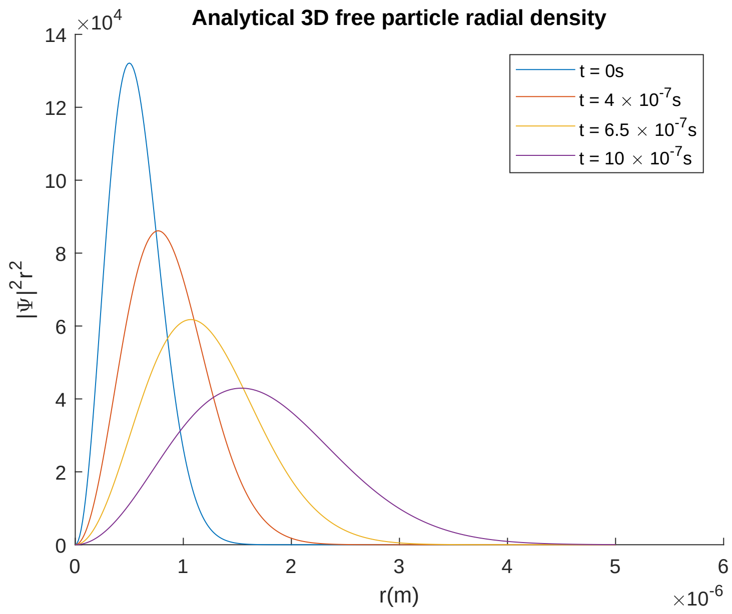


Figure 2: Spread of radial probability density for free particle of mass $m = 9.109 \times 10^{-28}$kg, which is near the mass of a proton. The wave-function of massive particles takes more time to spread quantum mechanically.

2.2 The Schrödinger-Newton equation

The Schrödinger -Newton equation introduced by Diosi [7] in 1984 for a single particle has the form:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + m\phi(\vec{r},t)\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{2.2.1}$$

where ∇^2 is the Laplacian in 3-dimension, ψ is the particle wave-function, and ϕ is the self-gravitating potential. The equation is a nonlinear Schrödinger equation with a non-local self-interacting term that depends on the probability of where the particle is found.

The equation follows from the semiclassical gravity proposed by Møller [12] and Rosenfeld [13], which considers only quantization of only the matter field but gravitational field remains classical. In this theory, the Einstein's field equations in standard unit become

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = \frac{8\pi G}{c^4}\langle\psi|\hat{T}_{\mu\nu}|\psi\rangle \tag{2.2.2}$$

where $R_{\mu\nu}$ is the Ricci tensor, $g_{\mu\nu}$ is the metric tensor, R is the Ricci scalar, G is the Newton gravitational constant, ψ is the wave-function, and $\hat{T}_{\mu\nu}$ is the energy-momentum tensor. In this model, the right hand side of the original Einstein equation's energy-momentum tensor $\hat{T}_{\mu\nu}$ is replaced by its expectation value. The semiclassical approach has sparked many arguments that fundamental classical fields are incompatible with quantum mechanics, in the sense that they could be used to violate the uncertainty principle [14], but these arguments turn out to be inconclusive. These arguments are discussed more thoroughly in [8].

We will derive the gravitational potential from eq.(2.2.2) by making several assumptions:

1. We will treat gravity as a linearized theory, i.e. only linear contributions from the space-time metric will be considered. In this case, the metric tensor $g_{\mu\nu}$ is approximated as

$$g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu} \tag{2.2.3}$$

where $\eta_{\mu\nu}$ is the Minkowski metric, and $h_{\mu\nu}$ are small perturbations with $|h_{\mu\nu}| \ll 1$.

2. In the weak-field (Newtonian) limit, the $\hat{T}_{00}$ term is much larger than the rest of the terms in $\hat{T}_{\mu\nu}$, hence we will focus on the $\mu = 0$, $\nu = 0$ terms in our workings.

We can contract eq.(2.2.2) by multiplying all terms by $g^{\mu\nu}$ as follows

$$g^{\mu\nu}(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R) = \frac{8\pi G}{c^4} \langle\psi|g^{\mu\nu}\hat{T}_{\mu\nu}|\psi\rangle \tag{2.2.4}$$

which reduces to

$$G = R - \frac{1}{2}g^{\mu\nu}g_{\mu\nu}R = \frac{8\pi G}{c^4} \langle\psi|\hat{T}|\psi\rangle \tag{2.2.5}$$

Hence, for 4-dimensional metric (3 space and 1 time) we have $g^{\mu\nu}g_{\mu\nu} = 4$, giving

$$R = -\frac{8\pi G}{c^4} \langle\psi|\hat{T}|\psi\rangle \tag{2.2.6}$$

Substituting eq.(2.2.6) back to eq.(2.2.2) and rewriting, we get

$$R_{\mu\nu} = \frac{8\pi G}{c^4}\big(\langle\psi|\hat{T}_{\mu\nu}|\psi\rangle - \frac{1}{2} \langle\psi|g_{\mu\nu}\hat{T}|\psi\rangle \big) \tag{2.2.7}$$

By sssumption No. 2, and applying it to assumption No. 1 with $g^{\mu\nu} = \eta^{\mu\nu} - h^{\mu\nu}$ and $h_{00} = h^{00}$, we can write the $\mu = 0$, $\nu = 0$ term for eq.(2.2.3) as

$$\begin{aligned} g_{00} &= -1 + h_{00} \\ g^{00} &= -1 - h_{00} \end{aligned} \tag{2.2.8}$$

Recall that we obtain $\hat{T}$ from $g^{\mu\nu}\hat{T}_{\mu\nu}$ in eq.(2.2.4) to eq.(2.2.5), hence we have

$$\hat{T} = -\hat{T}_{00} \tag{2.2.9}$$

and by plugging this in to eq.(2.2.7) we get

$$R_{00} = \frac{4\pi G}{c^4} \langle\psi|\hat{T}_{00}|\psi\rangle \tag{2.2.10}$$

The next step is to find R_{00}. In general, the Ricci curvature (or the Ricci tensor) can be expressed in terms of the Christoffel symbols Γ by [15]

$$R_{\alpha\beta} = \frac{\partial\Gamma^{\gamma}_{\alpha\beta}}{\partial x^{\gamma}} - \frac{\partial\Gamma^{\gamma}_{\alpha\gamma}}{\partial x^{\beta}} + \Gamma^{\delta}_{\alpha\beta}\Gamma^{\delta}_{\gamma\delta} - \Gamma^{\gamma}_{\beta\gamma}\Gamma^{\delta}_{\beta\gamma} \tag{2.2.11}$$

Thus

$$R_{00} = \frac{\partial\Gamma^{\gamma}_{00}}{\partial x^{\gamma}} - \frac{\partial\Gamma^{\gamma}_{0\gamma}}{\partial x^{0}} + \Gamma^{\delta}_{00}\Gamma^{\delta}_{\gamma\delta} - \Gamma^{\gamma}_{0\gamma}\Gamma^{\delta}_{0\gamma} \tag{2.2.12}$$

The second term of the expression is a time derivative term, hence it vanishes assumed static fields. The third and fourth terms are also ignored because both are of order higher than one (Γ^2). Hence, we are only left with the first term. The explicit form of Christoffel symbols for linearized gravity is [16]

$$\Gamma^{\alpha}_{\beta\gamma} = \frac{1}{2}\eta^{\alpha\delta}\left(\frac{\partial h_{\delta\beta}}{\partial x^{\gamma}} + \frac{\partial h_{\delta\gamma}}{\partial x^{\beta}} - \frac{\partial h_{\beta\gamma}}{\partial x^{\delta}}\right) \tag{2.2.13}$$

Setting the term β and γ from eq.(2.2.13) to zero, and substituting it to eq.(2.2.12) taking only the first term, we have the following

$$R_{00} = \frac{1}{2}\frac{\partial}{\partial x^{\gamma}}\eta^{\gamma\delta}\left[\frac{\partial h_{\delta 0}}{\partial x^{0}} + \frac{\partial h_{\delta 0}}{\partial x^{0}} - \frac{\partial h_{00}}{\partial x^{\delta}}\right] \tag{2.2.14}$$

Dropping time derivative terms, only $\delta = 1, 2, 3$ contribute to non-trivial solution. For these choices of δ we see only diagonal terms of $\eta^{\mu\nu}$ contribute, hence we have the final expression

$$R_{00} = -\frac{1}{2}\left[\eta^{11}\frac{\partial}{\partial x^1}\left(\frac{\partial h_{00}}{\partial x^1}\right) + \eta^{22}\frac{\partial}{\partial x^2}\left(\frac{\partial h_{00}}{\partial x^2}\right) + \eta^{33}\frac{\partial}{\partial x^3}\left(\frac{\partial h_{00}}{\partial x^3}\right)\right] \tag{2.2.15}$$

Rewriting eq.(2.2.15) and relabeling the indexing, we have

$$R_{00} = -\frac{1}{2}\eta^{ij}\partial_i\partial_j h_{00} \tag{2.2.16}$$

for $i = j = 1, 2, 3$. The constant in eq.(2.2.8) vanishes upon differentiation. The term $h^{ij}\partial_i\partial_j$ is known as box operator in Minkowski space, but here it reduces to Laplacian operator since i and j have no time derivative term. As a result, we obtain the final equation

$$R_{00} = -\frac{1}{2}\nabla^2 h_{00} \tag{2.2.17}$$

Combining eq. (2.2.17) with eq.(2.2.10), we recover Poisson equation for gravitation as follows

$$\nabla^2\phi = \frac{4\pi G}{c^2}\langle\psi|\hat{T}_{00}|\psi\rangle \tag{2.2.18}$$

for the potential $\Phi = -\frac{c^2}{2}h_{00}$. In Newtonian limit, the right-hand-side of eq.(2.2.18) reduces to the mass density of a single particle

$$\langle\psi|\hat{T}_{00}|\psi\rangle = c^2 m|\psi|^2 \tag{2.2.19}$$

This follows from classical approximation that

$$\hat{T}_{00} = c^2\hat{\rho} \tag{2.2.20}$$

where $\hat{\rho}$ is the mass density operator which is expressed as

$$\hat{\rho} = m\,|\vec{r}\rangle\,\langle\vec{r}| \tag{2.2.21}$$

The density operator can be thought of as an operator that describes the quantum system of a particle, in place of the wave function. When we specify a state ψ, the integral $\langle\psi|\hat{\rho}|\psi\rangle$ gives the probability density of finding the particle at position $\vec{r}$ [17]. Hence eq.(2.2.18) becomes

$$\nabla^2\phi = 4\pi G m|\psi|^2 \tag{2.2.22}$$

and

$$\phi(\vec{r}, t) = -Gm\int d^3r'\,\frac{|\psi(\vec{r}', t)|^2}{|\vec{r} - \vec{r}'|} \tag{2.2.23}$$

Substituting eq.(2.2.23) to eq.(2.2.1) we have Schrödinger-Newton equation for spherically symmetric solutions

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\psi(r,t) - Gm^2\int r'^2 dr'\,\frac{|\psi(r',t)|^2}{|r - r'|}\psi(r,t) = i\hbar\frac{\partial}{\partial t}\psi(r,t) \tag{2.2.24}$$

Schrödinger-Newton equation can also be derived from the variational principle of the action [18]

$$\begin{aligned} S(\psi, \nabla\psi, \psi_t) &= \int\int dt\; d^3r\left[\frac{i\hbar}{2}(\psi^*\psi_t - \psi\psi_t^*) - \frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi + \frac{Gm^2}{2}\int d^3\,r'\,\frac{\psi'^*\psi'}{|\vec{r} - \vec{r}'|}\psi^*\psi\right] \\ &= \int\int dt\; d^3r\;\mathcal{L}(\psi, \nabla\psi, \psi_t) \end{aligned} \tag{2.2.25}$$

where ψ_t refers to derivative of ψ with respect to t, and $\mathcal{L}$ is the Lagrangian of the action. The Euler-Lagrange equation for this Lagrangian is

$$\frac{\partial \mathcal{L}}{\partial \psi_i} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\psi_i}}\right) - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla \psi} = 0 \tag{2.2.26}$$

where ψ_i is (ψ, ψ^*) and ψ^* is the complex conjugate of ψ. By substituting the Lagrangian in eq.(2.2.25), we will recover the Schrödinger-Newton equation for both ψ and ψ^*.

2.2.1 Conservation laws for Schrödinger-Newton equation

Conservation laws in Schrödinger-Newton equation can be derived from the invariant properties of the action in eq.(2.2.25). In general, if an action is invariant under certain transformations, the conservation law holds [19]:

$$\frac{\partial}{\partial \xi_\nu}\left[\mathcal{L}\delta\xi_\nu - \frac{\partial \mathcal{L}}{\partial(\partial_\nu \psi_i)}\delta\psi_i\right] = 0 \tag{2.2.27}$$

where ξ_ν refers to (t, r, θ, ϕ), δ denotes infinitesimal translation and ψ_i refers to (ψ, ψ^*), holds. The action is invariant under phase, time, and space translations, which lead to the conservation of probability, energy, and momentum respectively. We will go through each of these below.

1. Phase transformation: $\psi \to \mathrm{e}^{i\theta}\psi$
   The action $S(\psi, \nabla\psi, \psi_t)$ is invariant under the phase transformation, i.e. $(S(\psi, \nabla\psi, \psi_t) = S(\mathrm{e}^{i\theta}\psi, \nabla \mathrm{e}^{i\theta}\psi, (\mathrm{e}^{i\theta}\psi)_t)$ of angle θ, as the exponential terms cancel with its conjugate. Hence, the following conservation law holds.

$$\partial_t|\psi|^2 + \nabla \cdot \{i(\psi\nabla\psi^* - \psi^*\nabla\psi)\} = 0 \tag{2.2.28}$$

   This leads to a conservation of the probability, and to be exact conservation of mass.

$$P = \int d^3r\ |\psi|^2 = constant \tag{2.2.29}$$

2. Time translation: $t \to t + \delta t$
   Similarly, it is obvious that the action is also invariant under time translation, hence the energy

$$E = \frac{\hbar^2}{2m}\int d^3r\ |\nabla\psi|^2 - \frac{Gm^2}{2}\int\int d^3r d^3r'\ \frac{|\psi'|^2}{|\vec{r} - \vec{r}'|}|\psi|^2 \tag{2.2.30}$$

   is conserved.

3. Space translation: $\vec{r} \to \vec{r} + \delta\vec{r}$
   Now, this one is a little tricky. We have to be aware of the definition of $|\vec{r} - \vec{r}'|$ in the potential. In our case, this term actually refers to the difference in spatial distance between two points within the mass distribution. Hence, when we translate the $\vec{r}$ by $\delta\vec{r}$, we are translating the whole system by that amount. In other words, this is similar to translating the inertial frame S in 1-dimension Galilean mechanics by Δx which leads us to a new inertial frame S'. This results in invariance of distance between two points. Therefore the action in eq.(2.2.25) is also invariant under spatial translation.
   This results in conservation law of momentum:

$$\vec{p} = i\int d^3r\ (\psi\nabla\psi^* - \psi^*\nabla\psi) = constant \tag{2.2.31}$$

Several other conservation laws can also be found using the same method, such as conservation of angular momentum and centre of mass.

2.2.2 Problems with Schrödinger-Newton equation

The mass distribution density $m|\psi(\vec{r})|^2$ is interpreted as the fraction of mass of particle found near point $\vec{r}$, in contrast with our understanding of probability density that describes how likely the particle is to be found at a point. Moreover, the particle in Schrödinger-Newton system is treated simultaneously as a point mass and as a mass distribution, which is another weird thing we find in the equation.

Following the problem above, [20] identified that the wave-function in Schrödinger-Newton equation is a collective variable of the whole system of N particles under mean-field approximation, with large N. It is also mentioned that the coupling of classical gravity with quantum matter is only meaningful under mean field approximation for large number of particles, and there is no such N- or single- particle system in Schrödinger-Newton system. An analogy of this problem is the Quantum Electrodynamics, which when used with the same approach as Schrödinger-Newton leads to incompetencies in describing elementary particle systems. This brings us to think whether we should really picture the equation as a single particle or many particle problem.

Moreover, we commonly know that conserved quantities in quantum mechanics can also be proven by taking the time derivative of expectation value. In other words, the following must hold

1. Conservation of normalization
$$\frac{d}{dt}\int d^3r\ |\psi|^2 = 0 \tag{2.2.32}$$
2. Conservation of expectation value of the momentum operator
$$\frac{d}{dt}\langle\psi|\hat{\vec{p}}|\psi\rangle = \frac{d}{dt}\int d^3r\ \psi^*\big(-i\hbar\nabla\big)\psi = 0 \tag{2.2.33}$$
3. Conservation of expectation value of the energy operator
$$\frac{d}{dt}\langle\psi|\hat{E}|\psi\rangle = \frac{d}{dt}\int d^3r\ \psi^*\left[-\frac{\hbar^2}{2m}\nabla^2\left(r^2\frac{\partial}{\partial r}\right) - Gm^2\int d^3r'\ \frac{|\psi'|^2}{|r-r'|}\right]\psi = 0 \tag{2.2.34}$$

Through a bit of work, it is possible to arrive at eqs.(2.2.32) and (2.2.34). On the other hand, conservation law of momentum operator leaves us with the following

$$\frac{d}{dt}\langle\psi|\hat{\vec{p}}|\psi\rangle \sim \langle\psi|\frac{\partial\phi}{\partial r}|\psi\rangle \tag{2.2.35}$$

as a result of Ehrenfest theorem that imposes external force from the gravitational potential. However, we are not are not able to show that the right-hand-side of eq.(2.2.35) is zero.

2.3 Schrödinger-Newton equation with cosmological constant

The cosmological constant Λ was always considered as zero, until the discovery of the accelerating universe. Nowadays, it is seen as a form of dark matter which acts as a type of anti-gravity that causes the accelerating universe.

The initial Einstein equation included a constant that was meant to prevent the universe from expanding until he removed it from the equation after knowing that the universe is expanding. We start with adding the constant to Einstein equation in eq.(2.2.2):

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R - \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4}\langle\psi|\hat{T}_{\mu\nu}|\psi\rangle \tag{2.3.1}$$

Using similar steps as in the previous section, we end up with

$$\nabla^2\Phi = \frac{4\pi G}{c^2}\langle\psi|T_{00}|\psi\rangle + \Lambda c^2 \tag{2.3.2}$$

We can obtain the expression for the potential by integrating the above equation assuming spherically symmetric solution which results in

$$\Phi(r,t) = -Gm \int r'^2 dr' \frac{|\psi(r',t)|^2}{|r-r'|} - \frac{1}{6}\Lambda c^2 r^2 \tag{2.3.3}$$

The cosmological constant Λ is known to have a positive value:

$$\Lambda = (1.36284 \pm 0.00028) \cdot 10^{-52}\text{m}^{-2} \tag{2.3.4}$$

according to [21]. This number is also expressed in other unit system: $\Lambda = 2.036 \cdot 10^{-35}\text{s}^{-2}$ as described in [22]. However, since we are using the standard unit, we will use Λ in eq.(2.3.4).

3 Numerical method

This research hugely follows the numerical method described in [8]. It will be discussed briefly here. The approach used in [8] is to discretize space and time and to find dynamics of Schrödinger-Newton equation by iteration. To begin with, we need to specify the convention to describe the steps used in the next few sections. For terms like u_j^n, the upper index is the time index and lower index is the spatial index, and it represents the solution at position $r = j\Delta r$ and time $t = n\Delta t$.

The numerical method can be summarized as:

1. Approximating the radial derivative at the origin using difference equation to be used in the next steps
2. Expanding the formal solutions of Schrödinger equation to obtain discretized expression of the solutions
3. Establishing a numerical method to generate the self-gravitating potential and stating the numerics problem explicitly
4. Using Matlab to process the numerics problem discussed above

3.1 Difference equation for the radial derivative

As mentioned in Section 2.1, we will omit all the angular terms in our derivation. Hence we are only left with the radial component of the Laplacian:

$$\nabla_r^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \tag{3.1.1}$$

We need to make an approximation because the above expression for Laplacian will produce singularity at the origin and we want to avoid this. Salzman [8] provided two methods to do this, but we will only discuss one of them here.

The central difference equation for second order derivative in 3-dimension is expressed as:

$$\nabla^2 f = \frac{f(x+dx)+f(x-dx)+f(y+dy)+f(y-dy)+f(z+dz)+f(z-dz)-2f(x)-2f(y)-2f(z)}{(dx+dy+dz)^2} \tag{3.1.2}$$

where $f(x+dx)$ means the value of f at $x+dx$ and dx is a small change in x. Taking the centre at the origin, we have

$$\nabla^2 f = \frac{f(dx)+f(-dx)+f(dy)+f(-dy)+f(dz)+f(-dz)-6f(0)}{dr^2} \tag{3.1.3}$$

The average of the equation as we rotate the axes N times for N approaching infinity is

$$\nabla^2 f = \frac{6(\bar{f}-f_0)}{dr^2} \tag{3.1.4}$$

where $\bar{f}$ is the mean value of f. Equation (3.1.4) is valid for Laplacian centered at the origin, and for spherical symmetric functions the equation becomes

$$\nabla^2 f = \frac{3[f(dr) - 2f(0) + f(-dr)]}{dr^2} \tag{3.1.5}$$

which reduces to

$$\nabla^2 f = 3\frac{\partial^2 f}{\partial r^2} \tag{3.1.6}$$

3.2 Discretization of Schrödinger equation

This section summarizes the steps and methods used in [8]. The first step of discretizing Schrödinger equation is by Taylor expanding the solutions to the equation (known also as forward time, centered space discretization):

$$\psi(r, \Delta t) = \mathrm{e}^{-i\hat{H}\Delta t/\hbar}\psi(r, 0) \tag{3.2.1}$$

into a discrete equation

$$\psi_j^{n+1} = \left(\hat{\mathbb{1}} - \frac{i\hat{H}\Delta t}{\hbar}\right)\psi_j^n \tag{3.2.2}$$

where $\hat{\mathbb{1}}$ is an identity operator. Unfortunately, this method is unconditionally unstable [1]. A numerically stable solution is given by the Cayley's form. We first translate the future wavefunction back in time [8]:

$$\mathrm{e}^{+i\hat{H}\Delta t/\hbar}\psi(r, \Delta t) = \psi(r, 0) \tag{3.2.3}$$

which by expanding we get

$$\psi_j^{n+1} = \left(\hat{\mathbb{1}} + \frac{i\hat{H}\Delta t}{\hbar}\right)^{-1}\psi_j^n \tag{3.2.4}$$

Roughly speaking, Cayley's form is the average of both forward and backward time evolution, i.e. we require that they agree halfway through the evolution:

$$\left[\hat{\mathbb{1}} + \frac{i\Delta t}{2\hbar}\right]\psi_j^{n+1} = \left[\hat{\mathbb{1}} - \frac{i\Delta t}{2\hbar}\hat{H}\right]\psi_j^n \tag{3.2.5}$$

Solving this equation we get:

$$\psi_j^{n+1} = \chi_j^n - \psi_j^n \tag{3.2.6}$$

where $\chi_j^n = \hat{Q}^{-1}\psi_j^n$ for $\hat{Q} = \frac{1}{2}\left(\hat{\mathbb{1}} + \frac{i\Delta t}{2\hbar}\hat{H}\right)$.

The explicit expression for $\hat{Q}$ operator can be formulated by using the difference equation for Laplacian in the Hamiltonian. The following are the expressions for three different cases:

1. For $j \neq 0, N-1$ (N refers to the point at infinity), we have:

$$\hat{Q}\chi_j^n = -KR\left(\frac{j-1}{j}\right)\chi_{j-1}^n + \frac{1}{2}[1 + PVg_j^n + 2KR]\ \chi_j^n - KR\left(\frac{j+1}{j}\right)\chi_{j+1}^n \tag{3.2.7}$$

where Vg is the gravitational potential and we have defined:

$$R = \frac{\Delta t}{(\Delta r)^2}, \quad K = \frac{i\hbar}{8m}, \quad P = \frac{i\Delta t}{2\hbar} \tag{3.2.8}$$

2. For $j = N-1$ (point before spatial infinity):

$$\hat{Q}\chi_{N-1}^n = -KR\left(\frac{N-2}{N-1}\right)\chi_{N-2}^n + \frac{1}{2}[1 + PVg_{N-1}^n + 2KR]\ \chi_{N-1}^n \tag{3.2.9}$$

[1] See [23] pg. 836 and 847

3. For $j = 0$ (point at the origin):

$$\hat{Q}\chi_0^n = \frac{1}{2}[1 + PVg_0^n + 12KR]\chi_0^n - 6KR\chi_1^n \tag{3.2.10}$$

Now, we can summarize the procedure for obtaining the solution for Schrödinger equation in a recursive order. Firstly, solve eq.(3.2.6) for all position component to get ψ_j^n. The new wave-function is obtained by subtracting the old wave-function by χ^n: $\psi^{n+1} = \chi^n - \psi^n$. By repeating these steps, we arrive at the solutions for a desired time.

For the numerics, we are going to build a Tridiagonal Matrix to contain all the variables and perform the Thomas Algorithm [2]. This matrix looks like:

$$\begin{pmatrix} b_0 & c_0 & & & & & \\ a_1 & b_1 & c_1 & & & & \\ & a_2 & b_2 & c_2 & & & \\ & & & \ddots & & & \\ & & & & a_{N-2} & b_{N-2} & c_{N-2} \\ & & & & & a_{N-1} & b_{N-1} \end{pmatrix}$$

where coefficients a_i, called super-diagonal are the coefficients of variable χ_{j-1}^n, b_i, called diagonal are the coefficients of χ_j^n, and c_i, called sub-diagonal are the coefficients of χ_{j-1}^n in eqs.(3.2.7), (3.2.9), and (3.2.10). We multiply this matrix into a general equation for solving eq.(3.2.6) as follows

$$\begin{pmatrix} b_0 & c_0 & & & & & \\ a_1 & b_1 & c_1 & & & & \\ & a_2 & b_2 & c_2 & & & \\ & & & \ddots & & & \\ & & & & a_{N-2} & b_{N-2} & c_{N-2} \\ & & & & & a_{N-1} & b_{N-1} \end{pmatrix} \begin{pmatrix} \chi_0 \\ \chi_1 \\ \chi_2 \\ \vdots \\ \chi_{N-1} \\ \chi_{N-1} \end{pmatrix} = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-2} \\ \psi_{N-1} \end{pmatrix} \tag{3.2.11}$$

We eliminate the super-diagonal elements in the matrix by performing multiplications and subtractions to the subsequent rows in the matrix. After re-defining the equations we end up with

$$\begin{pmatrix} B_0\chi_0 & + & c_0\chi_1 & & & & & & \\ & & B_1\chi_1 & + & c_1\chi_2 & & & & \\ & & & & B_2\chi_2 & + & c_2\chi_3 & & \\ & & & & & & \ddots & & \\ & & & & & & B_{N-2}\chi_{N-2} & + & c_{N-2}\chi_{N-1} \\ & & & & & & & & B_{N-1}\chi_{N-1} \end{pmatrix} = \begin{pmatrix} D_0 \\ D_1 \\ D_2 \\ \vdots \\ D_{N-2} \\ D_{N-1} \end{pmatrix}$$

where

$$B_i = b_i - \frac{a_i}{B_{i-1}}c_{i-1}, \quad D_i = d_i - \frac{a_i}{B_{i-1}}D_{i-1}, \quad i = 0, ..., N-1 \tag{3.2.12}$$

then we can obtain the solution ψ_i as

$$\psi_i = \frac{D_i - c_i\psi_{i+1}}{B_i} \tag{3.2.13}$$

for $i = N-1, ..., 0$. That is, we are working backwards from the last entry to the beginning. Note that this calculation is only for a time-step, thus to find the time evolution we have to repeat this a number of times.

[2]See Appendix C in [8]

3.3 Formulating the numerics for the self-gravitating potential

The gravitational potential in eq.(2.2.23) can be written as (assuming spherical symmetry) [8]:

$$\Phi(r,t) = -4\pi G m^2 \left(\frac{1}{r} \int_0^r r'^2 dr' |\psi(\vec{r}', t)|^2 + \int_r^\infty r' dr' |\psi(\vec{r}', t)|^2 \right) \tag{3.3.1}$$

where r is the position in space where the potential is computed. For numerical work, we can express the above equation into a pseudo-numerical code notation as follows:

$$\begin{aligned} V_j^n &= -4\pi G m^2 \left(\frac{1}{j\Delta r} \sum_{i=0}^{j-1} |\psi_i^n|^2 (i\Delta r)^2 \Delta r + \sum_{i=j}^{N-1} |\psi_i^n|^2 (i\Delta r)\Delta r \right) \\ &= -4\pi G m^2 (\Delta r)^2 \left(\frac{1}{j} \sum_{i=0}^{j-1} |\psi_i^n|^2 i^2 + \sum_{i=j}^{N-1} |\psi_i^n|^2 i \right) \end{aligned} \tag{3.3.2}$$

Equation (3.3.2) is rather easy to understand once we get used to the notation. In short, potential at point j is obtained by summing over all ψ_i for each time-step. Hence we need to have the wave-function to compute the potential.

To include the cosmological effect, we simply add the contribution term in eq.(2.3.3) into eq.(3.3.2) as the following

$$V_j^n = -4\pi G m^2 (\Delta r)^2 \left(\frac{1}{j} \sum_{i=0}^{j-1} |\psi_i^n|^2 i^2 + \sum_{i=j}^{N-1} |\psi_i^n|^2 i \right) + \frac{1}{6}\Lambda c^2 j^2 \tag{3.3.3}$$

3.4 Numerics with Matlab

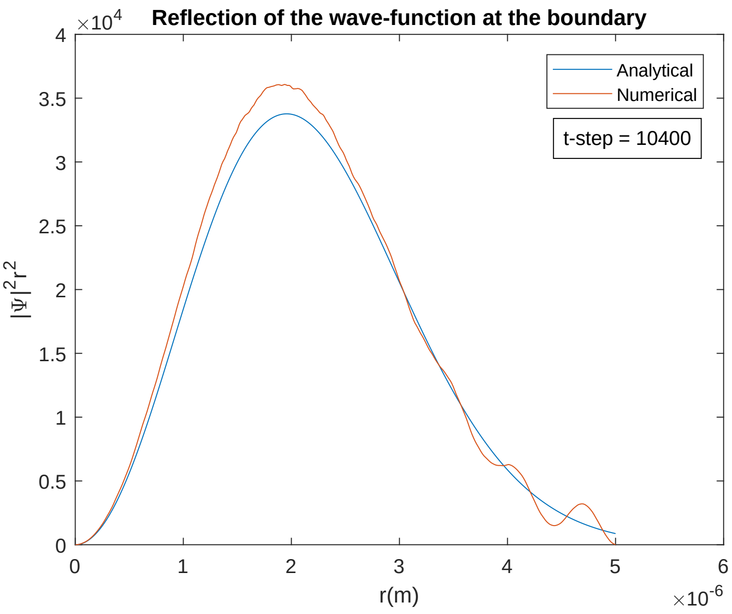
We are one step away from the results, we need to compile a program that can work out the numerical steps above. This has been done using Matlab. When working with Matlab, we have to take note that Matlab uses zero indexing sequence, hence the first element of a vector is labeled as $M(1,1)$. As most of our notations in the numerics equations involve zero indexing, then we have to shift one index forward. The complete Matlab program is attached in the Appendix.

The wave-function must satisfy boundary conditions at $r = 0$ and $r \to \infty$:

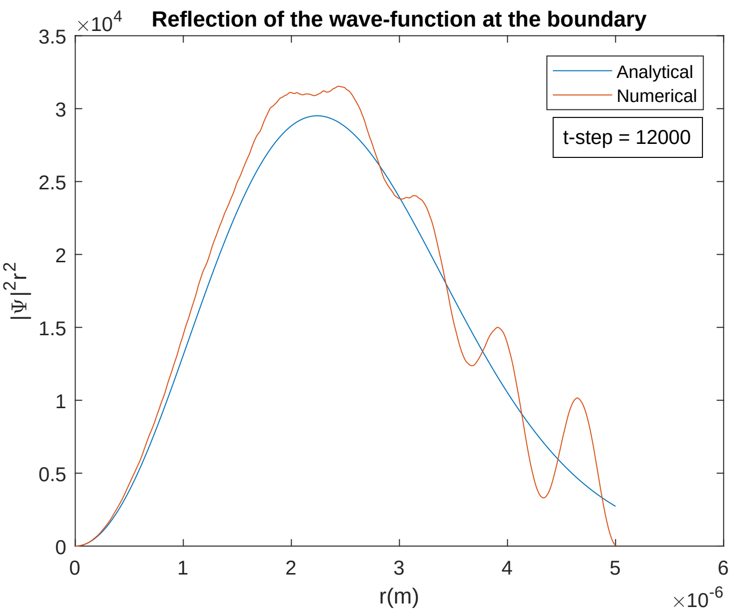
$$\psi(r = 0, r \to \infty) = 0 \tag{3.4.1}$$

The numerical infinity is chosen such that the wave-function at specific time t at point r is zero, and the time range must show a reasonable expansion to give a good view of the evolution when we go to Schrödinger-Newton system. In this thesis, we choose the evolution time limit such as the peak of the radial density decreases to about one third of the initial wave-function.

When we choose the point of numerical infinity that is not in accordance with the above requirement, we observe some slopes at the further end of the wave-function that are not found in the analytical graph. This is an effect of a wave-function reflected off numerical infinity, caused by Neumann boundary condition [8]. This can be seen more clearly in the following figures.



(a)



(b)

Figure 3: Effects of reflection at numerical infinity; comparison for two different time-steps, $m = 9.109 \times 10^{-31}$kg and numerical infinity at $r = 5 \times 10^{-6}$m.

The results of the numerics are very sensitive to the change in variable and the value of R in eq.(3.2.8). That is, we need to find the optimum value of the time-step and position-step, and it is found out that R is not a fixed number. Rather, its value varies for different mass. We compare our results by setting the gravitation to zero ($G = 0$), i.e. the free praticle case, with analytical evolution. A comparison diagram can be seen below.

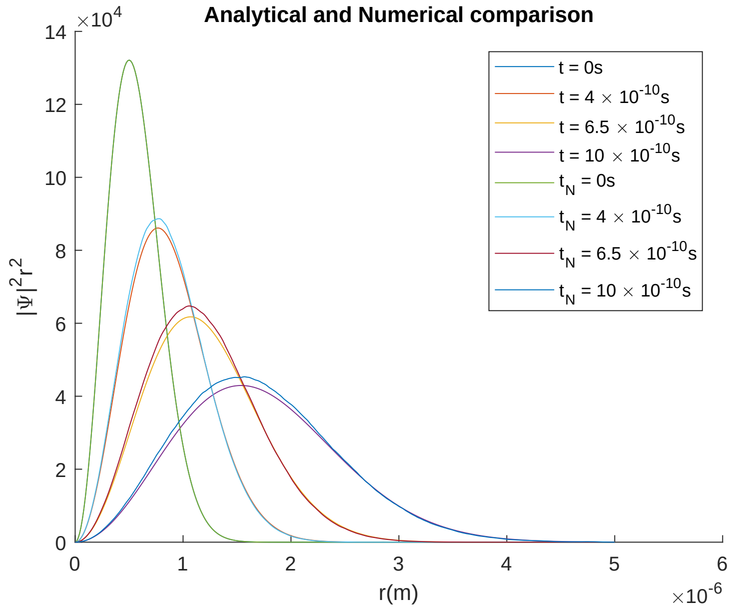


Figure 4: Comparison between numerical and analytical result for free electron. Gravitational constant is set to zero and the numerical infinity is at $r = 5 \times 10^{-6}$m.

The best fit is obtained for $R \simeq 456$, and the comparison is made for $m = 9.109 \times 10^{-31}$kg and $\alpha = 4 \times 10^{12}$, which corresponds to width of wave-function $1/\sqrt{\alpha} = 0.5$µm. The numerics can represent an accurate result as long as we maintain the discrepancies with analytical result whenever change of variables is made. A numerical discrepancy is pictured in the following figure.

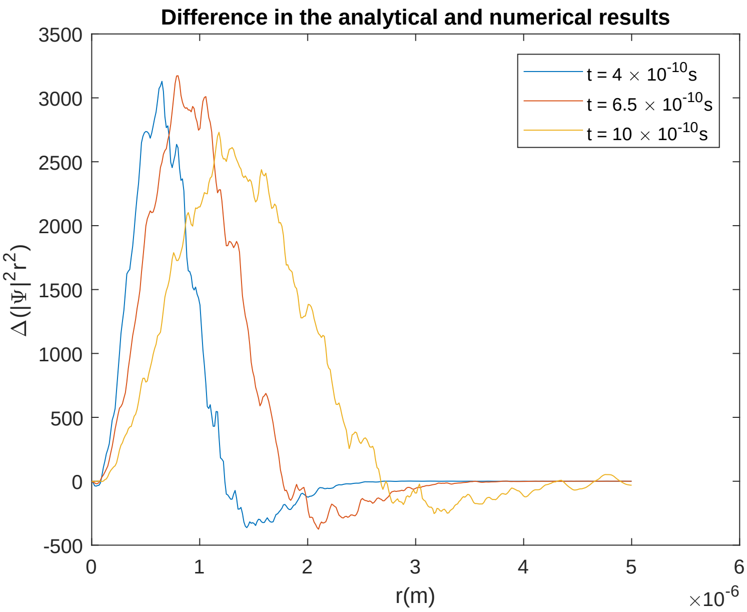


Figure 5: Imprecision plot for free particle in Fig.4. We maintain the discrepancy by comparing the result against analytical free particle for each mass.

4 Results

4.1 Schrödinger-Newton equation without Λ

We summarize the result as follows

1. For mass below 9.109×10^{-18}kg the spread of wave-function is indistinguishable from free particle.

2. Particles of masses between 9.109×10^{-18}kg and 3.109×10^{-17}kg are observed to spread slower in the Schrödinger-Newton regime than that of free particle.

3. The collapsed wave-function is observed in the range of mass from 5.109×10^{-17}kg to around 2.109×10^{-16}kg. Masses close to this range experience fluctuations which are described as chaotic behaviour of the wave-function in [8]. This behaviour is characterized by wave-functions having the tendency to collapse and spread at the same time.

4. For masses higher than 1.109×10^{-15}kg, the collapse does not appear anymore and the wave-function becomes stationary. We think that the collapse is not seen here because the time taken for the collapse to occur is beyond our numerical limit.

These results are in accordance with those obtained in [1].

The collapsed wave-function has interesting property where it rapidly falls towards the centre, as shown in the figure below.

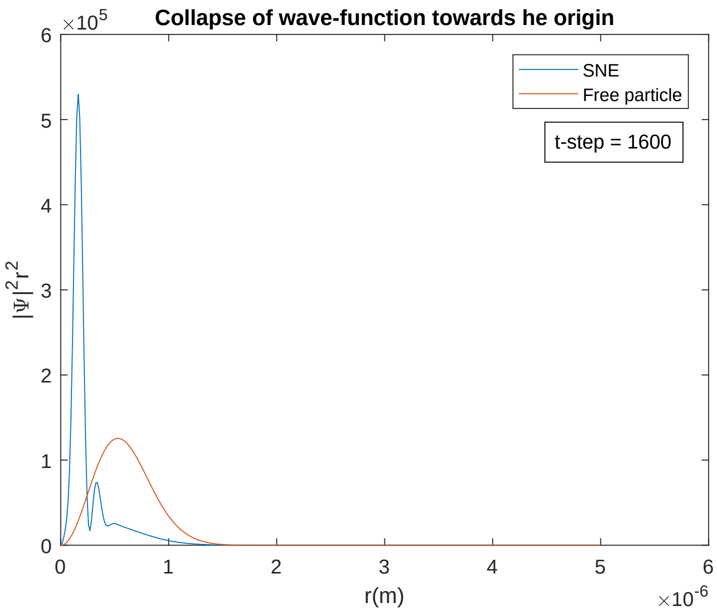
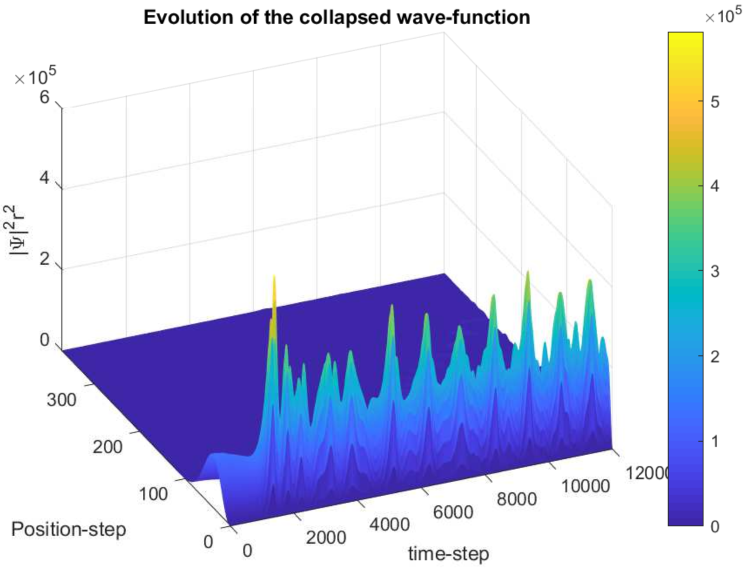
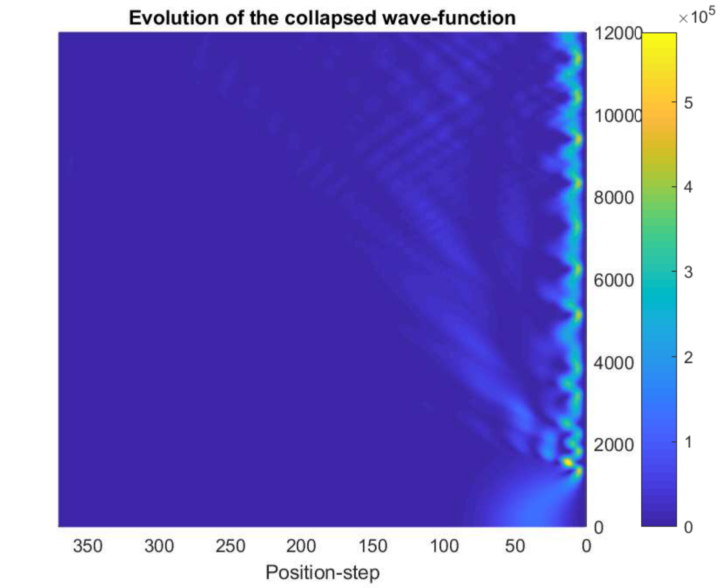


Figure 6: Collapse of wave-function towards the origin observed for $m = 8.109 \times 10^{-17}$kg, plotted against the free particle solution.

Wave-function in the collapse regime behaves in a fluctuative way, but on average we see that wave-function's tendency to shrink happens almost all the time. The following shows evolution of wave-function under the collapse regime.



(a) The peaks of the radial density fluctuates with time.



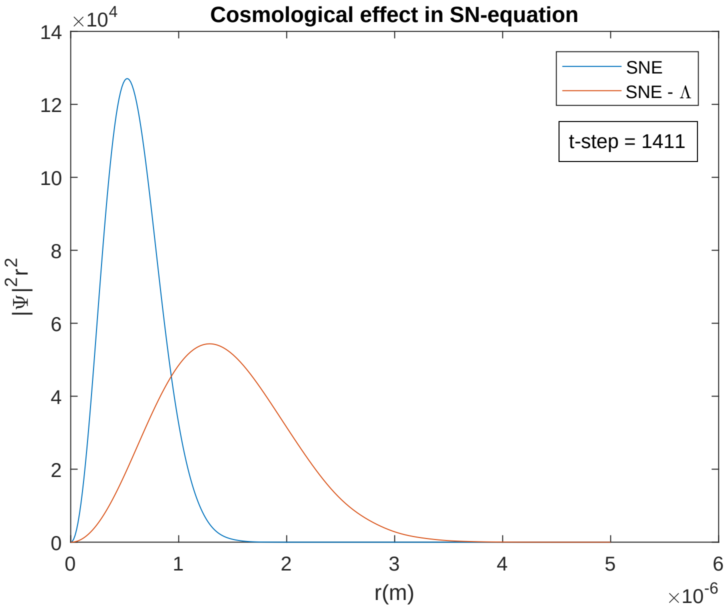
(b) The wave-function starts to collapse at approximately t-step = 1600 which is about $t = 10866$s.

Figure 7: Evolution of the collapsed wave-function for $m = 8.109 \times 10^{-17}$kg.

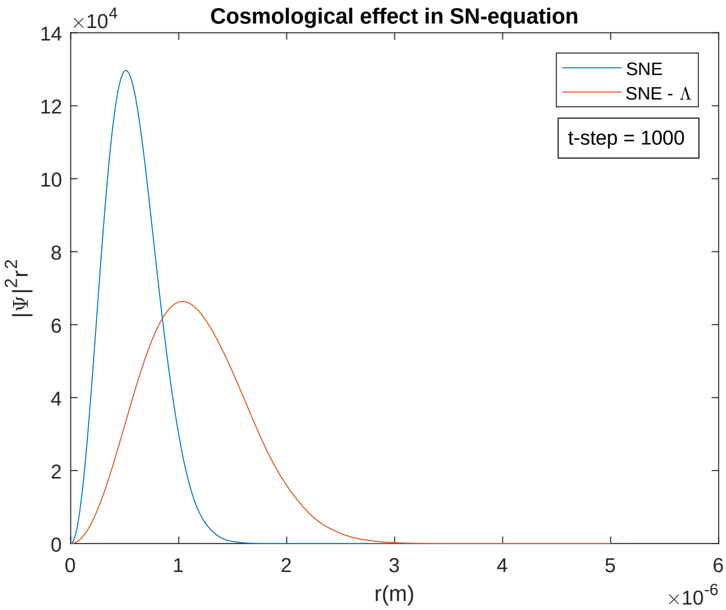
4.2 Schrödinger-Newton equation with Λ

Anti-gravity makes the wave-function spread much faster, in contrast with the self-gravitating force. We suppose that microscopic objects experience more impact from the cosmological constant, hence spreading at much faster rate. Our numerics is bound to a certain time limit and can not capture changes for much smaller masses.

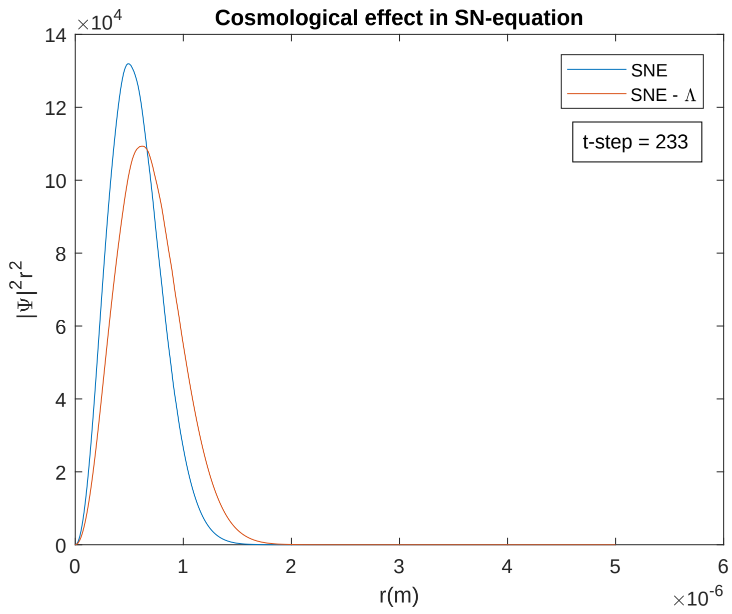
Within the same time-frame, rate of expansion reduces with increasing mass as seen in the following figures


Cosmological effect in SN-equation
SNE
SNE - Λ
t-step = 1411
$|\Psi|^2 r^2$
$\times 10^4$
r(m)
$\times 10^{-6}$

(a)


Cosmological effect in SN-equation
SNE
SNE - Λ
t-step = 1000
$|\Psi|^2 r^2$
$\times 10^4$
r(m)
$\times 10^{-6}$

(b)



(c)

Figure 8: Effect of cosmological constant in Schrödinger-Newton equation for (a) $m = 8.109 \times 10^{-21}$kg, (b) $m = 1.109 \times 10^{-20}$kg, and (c) $m = 5.109 \times 10^{-20}$kg at $t = 0.958$s. The wave-function evolves much rapidly in a decreasing rate with increasing mass.

The cosmological effect in Schrödinger-Newton equation also introduces no collapse behaviour in the wave-function. We investigate the masses within collapse regime in Section 4.1 and find that instead of collapsing, the wave-function behaves just like free particle with greater evolution rate.

5 Conclusions

Anti-gravity effect generated by Λ in the Schrödinger-Newton equation induces no collapse behaviour, in contrast with the self-gravitating force. The wave-function expands more rapidly with cosmological contribution as compared to the Schrödinger-Newton case alone. We also find that the increase in expansion rate decreases as the mass gets heavier.

These results do not surprise us, since from our understanding of Λ as a form of anti-gravity, it will speed up the evolution of the wave-function. In this thesis, we have proven that the cosmological constant contribution to Schrödinger-Newton equation indeed affects the wave-function in this way.

The numerical work that we perform in this research has several limitations, to the extend that improving it would give more accurate and better results. As mentioned in Section 4.1, collapse of wave-function is not seen beyond certain mass is due to the limits on our programme. Specifically, by increasing the number of iterations, position and time range, the collapse can probably be seen in larger mass scale. Therfore, future research should be improving on this.

Acknowledgement

Thank you to Professor Paterek Tomasz for the guidance and supervising this research, Matthew Lake for giving valuable inputs and suggestions, and Kelvin for his ideas and help in writing up the evolution of Gaussian function in Appendix A.

Appendix A Analytical solution to the time evolution of spherically symmetric Gaussian function (by: Kelvin)

The Hamiltonian of a free particle of mass m moving in 3-Dimension reads:

$$\hat{\mathcal{H}} = \frac{\hat{p_x}^2}{2m} + \frac{\hat{p_y}^2}{2m} + \frac{\hat{p_z}^2}{2m} \tag{A.0.1}$$

By using the method of separation of variables, the eigenfunction of the Hamiltonian can be written as a product of three eigenfunctions, each of which is a function of a single variable.

$$\begin{aligned}\phi_{k_x,k_y,k_z}(x,y,z) &= \left(\frac{1}{\sqrt{2\pi}}e^{ik_x x}\right)\left(\frac{1}{\sqrt{2\pi}}e^{ik_y y}\right)\left(\frac{1}{\sqrt{2\pi}}e^{ik_z z}\right)\\ \phi_{\vec{k}}(\vec{\chi}) &= \frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\cdot\vec{\chi}}\end{aligned} \tag{A.0.2}$$

where $\vec{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}$ and $\vec{\chi} = x\hat{x} + y\hat{y} + z\hat{z}$. Any arbitrary wave function $\psi(\vec{\chi})$ can be expressed in the momentum eigenstates which reads:

$$\psi(\vec{\chi}) = \int_{-\infty}^{\infty} \tilde{\psi}(\vec{k})\phi_{\vec{k}}(\vec{\chi})\mathrm{d}^3k \tag{A.0.3}$$

Multiplying equation (20) with the conjugate if the momentum eigenfunction $\phi^*_{\vec{k'}}(\vec{\chi})$ and integrate over the whole space gives:

$$\int_{-\infty}^{\infty} \phi^*_{\vec{k'}}(\vec{\chi})\psi(\vec{\chi})\mathrm{d}^3\chi = \int_{-\infty}^{\infty} \phi^*_{\vec{k'}}(\vec{\chi})\int_{-\infty}^{\infty} \tilde{\psi}(\vec{k})\phi_{\vec{k}}(\vec{\chi})\mathrm{d}^3k\mathrm{d}^3\chi \tag{A.0.4}$$

$\tilde{\psi}(\vec{k})$ is independent of χ,

$$\begin{aligned}\int_{-\infty}^{\infty} \phi^*_{\vec{k'}}(\vec{\chi})\psi(\vec{\chi})\mathrm{d}^3\chi &= \int_{-\infty}^{\infty} \tilde{\psi}(\vec{k})\left(\int_{-\infty}^{\infty} \phi^*_{\vec{k'}}(\vec{\chi})\phi_{\vec{k}}(\vec{\chi})\mathrm{d}^3\chi\right)\mathrm{d}^3k\\ &= \int_{-\infty}^{\infty} \tilde{\psi}(\vec{k})\left(\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} e^{i(\vec{k}-\vec{k'})\cdot\vec{\chi}}\mathrm{d}^3\chi\right)\mathrm{d}^3k\\ &= \int_{-\infty}^{\infty} \tilde{\psi}(\vec{k})\delta\left(\vec{k}-\vec{k'}\right)\mathrm{d}^3k\\ \int_{-\infty}^{\infty} \phi^*_{\vec{k'}}(\vec{\chi})\psi(\vec{\chi})\mathrm{d}^3\chi &= \tilde{\psi}(\vec{k'})\end{aligned} \tag{A.0.5}$$

Hence, we have the following relationship between $\psi(\vec{\chi})$ and $\tilde{\psi}(\vec{k})$ which reads:

$$\tilde{\psi}(\vec{k}) = \int_{-\infty}^{\infty} \psi(\vec{\chi})e^{-i\vec{k}\cdot\vec{\chi}}\mathrm{d}^3\chi \tag{A.0.6}$$

$$\psi(\vec{\chi}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} \tilde{\psi}(\vec{k})e^{i\vec{k}\cdot\vec{\chi}}\mathrm{d}^3k \tag{A.0.7}$$

From now on, we shall assume our wave function $\psi(\vec{\chi}) = \psi(r)$ is spherically symmetric. We also introduce spherical coordinates such that the z-axis is along the $\vec{k}$ vector ($|\vec{\chi}| = r$, $|\vec{k}| = k$) and calculate

$$\begin{aligned}
\tilde{\psi}(\vec{k}) &= \int_{-\infty}^{\infty} \psi(r) e^{-i\vec{k}\cdot\vec{\chi}} \mathrm{d}^3\chi \\
&= \int_0^{\infty} \mathrm{d}r \int_0^{\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \; \psi(r) e^{-ikr\cos\theta} r^2 \sin\theta \\
&= 2\pi \int_0^{\infty} \mathrm{d}r \; r^2 \psi(r) \int_0^{\pi} \mathrm{d}\theta \; e^{-ikr\cos\theta} \sin\theta \\
&= 4\pi \int_0^{\infty} \mathrm{d}r \; r^2 \psi(r) \frac{\sin(kr)}{kr} \\
\tilde{\psi}(k) &= \frac{4\pi}{k} \int_0^{\infty} r \sin(kr) \psi(r) \mathrm{d}r
\end{aligned} \tag{A.0.8}$$

where we have used

$$\int_0^{\pi} \mathrm{d}\theta \; e^{-ikr\cos\theta} \sin\theta = -\int_1^{-1} e^{-ikru} \mathrm{d}u = \left[\frac{e^{-ikru}}{ikr}\right]_1^{-1} = 2\frac{\sin(kr)}{kr} \tag{A.0.9}$$

Similarly, for $\psi(\vec{\chi})$:

$$\begin{aligned}
\psi(\vec{\chi}) &= \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \tilde{\psi}(\vec{k}) e^{i\vec{k}\cdot\vec{\chi}} \mathrm{d}^3 k \\
&= \frac{1}{(2\pi)^3} \int_0^{\infty} k^2 \mathrm{d}k \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \mathrm{d}\theta \; \tilde{\psi}(k) e^{ikr\cos\theta} \\
&= \frac{1}{(2\pi)^3} \int_0^{\infty} \frac{4\pi}{r} k \sin(kr) \tilde{\psi}(k) \mathrm{d}k \\
\psi(r) &= \frac{1}{2\pi^2 r} \int_0^{\infty} k \sin(kr) \tilde{\psi}(k) \mathrm{d}k
\end{aligned} \tag{A.0.10}$$

Consider a particle of mass m with a localized initial wavefunction which is a Gaussian with width $\alpha^{-1/2}$.

$$\psi(r,0) = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{4}} e^{-\alpha r^2/2} \tag{A.0.11}$$

The question is then how does this wave function evolve in time? Similar to the previous section, the general idea is to express the initial wave function $\psi(r,0)$ in terms of the momentum eigenfunctions of the free particle and find out how it evolves since we know how the eigenfunctions evolve in time. Let us begin with finding $\tilde{\psi}(k)$ for this wave function. From equation (A.0.8), we have:

$$\begin{aligned}
\tilde{\psi}(k) &= \frac{4\pi}{k} \int_0^{\infty} r \sin(kr) \psi(r) \mathrm{d}r \\
&= \frac{4\pi}{k} \left(\frac{\alpha}{\pi}\right)^{\frac{3}{4}} \int_0^{\infty} r \sin(kr) e^{-\alpha r^2/2} \mathrm{d}r
\end{aligned} \tag{A.0.12}$$

Now, we need to solve the following integral:

$$I = \int_0^{\infty} r \sin(kr) e^{-\alpha r^2/2} \mathrm{d}r \tag{A.0.13}$$

Integrate by parts using

$$\begin{aligned}
u &= \sin(kr) & \mathrm{d}v &= r e^{-\alpha r^2/2} \mathrm{d}r \\
\mathrm{d}u &= k\cos(kr)\mathrm{d}r & v &= \frac{1}{2}\int e^{-\alpha r^2/2} \mathrm{d}\left(r^2\right) \\
& & &= -\frac{1}{\alpha} e^{-\alpha r^2/2}
\end{aligned}$$

Hence,

$$\int_0^\infty r\sin(kr)e^{-\alpha r^2/2}\mathrm{d}r = \left[-\frac{1}{\alpha}\sin(kr)e^{-\alpha r^2/2}\right]_0^\infty + \frac{k}{\alpha}\int_0^\infty \cos(kr)e^{-\alpha r^2/2}\mathrm{d}r$$
$$I = \frac{k}{\alpha}\int_0^\infty \cos(kr)e^{-\alpha r^2/2}\mathrm{d}r \tag{A.0.14}$$

Notice that the integrand is an even function and therefore, we can rewrite I as follows:

$$\begin{aligned} I = \frac{k}{2\alpha}\int_{-\infty}^\infty \cos(kr)e^{-\alpha r^2/2}\mathrm{d}r &= \frac{k}{2\alpha}\int_{-\infty}^\infty \frac{1}{2}\left(e^{ikr}+e^{-ikr}\right)e^{-\alpha r^2/2}\mathrm{d}r \\ &= \frac{k}{4\alpha}\int_{-\infty}^\infty \left(e^{-\frac{\alpha r^2}{2}+ikr}+e^{-\frac{\alpha r^2}{2}-ikr}\right)\mathrm{d}r \\ &= \frac{k}{4\alpha}\left(2\sqrt{\frac{2\pi}{\alpha}}\;e^{-k^2/2\alpha}\right) \end{aligned}$$
$$I = \int_0^\infty r\sin(kr)e^{-\alpha r^2/2}\mathrm{d}r = \frac{k}{\alpha}\sqrt{\frac{\pi}{2\alpha}}\;e^{-k^2/2\alpha} \tag{A.0.15}$$

Substituting I into equation (A.0.12) gives:

$$\tilde{\psi}(k) = \frac{4\pi}{k}\left(\frac{\alpha}{\pi}\right)^{\frac{3}{4}}\left(\frac{k}{\alpha}\sqrt{\frac{\pi}{2\alpha}}\;e^{-k^2/2\alpha}\right) = 2\sqrt{2}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}e^{-k^2/2\alpha} \tag{A.0.16}$$

From equation (A.0.10) and equation (A.0.16), the wave function at an arbitrary time t reads:

$$\psi(r,t) = \frac{1}{2\pi^2 r}\int_0^\infty k\sin(kr)\tilde{\psi}(k)e^{-\frac{E}{\hbar}t}\mathrm{d}k \tag{A.0.17}$$
$$\begin{aligned} &= \frac{1}{2\pi^2 r}\int_0^\infty k\sin(kr)\left[2\sqrt{2}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\exp\left(-\frac{k^2}{2\alpha}\right)\right]\exp\left(-i\frac{E}{\hbar}t\right)\mathrm{d}k \\ &= \frac{\sqrt{2}}{\pi^2 r}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\int_0^\infty k\sin(kr)\exp\left[-\left(\frac{k^2}{2\alpha}+i\frac{\hbar k^2}{2m}t\right)\right]\mathrm{d}k \\ &= \frac{\sqrt{2}}{\pi^2 r}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\int_0^\infty k\sin(kr)\exp\left[-\left(\frac{m+i\alpha\hbar t}{2\alpha m}\right)k^2\right]\mathrm{d}k \\ &= \frac{\sqrt{2}}{\pi^2 r}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\int_0^\infty k\sin(kr)\exp\left[-\frac{\alpha'}{2}k^2\right]\mathrm{d}k \qquad \text{where} \qquad \alpha' = \frac{m+i\alpha\hbar t}{\alpha m} \end{aligned}$$

Applying equation (A.0.15) to solve the integral gives us:

$$\begin{aligned} \psi(r,t) &= \frac{\sqrt{2}}{\pi^2 r}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\left[\frac{r}{\alpha'}\sqrt{\frac{\pi}{2\alpha'}}\exp\left(-\frac{r^2}{2\alpha'}\right)\right] \\ &= \frac{\sqrt{2}}{\pi^2 r}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\left[r\frac{\alpha m}{m+i\alpha\hbar t}\left(\frac{\pi\alpha m}{2(m+i\alpha\hbar t)}\right)^{\frac{1}{2}}\exp\left(-\frac{\alpha m}{2(m+i\alpha\hbar t)}r^2\right)\right] \\ &= \frac{\sqrt{2}}{\pi^2 r}\left(\frac{\pi}{\alpha}\right)^{\frac{3}{4}}\left[\frac{\sqrt{\pi}r}{\sqrt{2}}\left(\frac{\alpha m}{m+i\alpha\hbar t}\right)^{\frac{3}{2}}\exp\left(-\frac{\alpha m}{2(m+i\alpha\hbar t)}r^2\right)\right] \end{aligned}$$
$$\psi(r,t) = (\pi\alpha)^{-\frac{3}{4}}\left(\frac{\alpha m}{m+i\alpha\hbar t}\right)^{\frac{3}{2}}\exp\left(-\frac{\alpha m}{2(m+i\alpha\hbar t)}r^2\right) \tag{A.0.18}$$

This wave function leads to a radial probability density of:

$$
\begin{aligned}
\rho(r,t) &= r^2\psi^*(r,t)\psi(r,t) \\
&= r^2(\pi\alpha)^{-\frac{3}{2}}\left[\left(\frac{\alpha^2 m^2}{(m-i\alpha\hbar t)(m+i\alpha\hbar t)}\right)^{\frac{3}{2}}\exp\left(-\frac{\alpha m}{2(m-i\alpha\hbar t)}r^2\right)\exp\left(-\frac{\alpha m}{2(m+i\alpha\hbar t)}r^2\right)\right] \\
&= r^2(\pi\alpha)^{-\frac{3}{2}}\left(\frac{\alpha^2 m^2}{m^2+\alpha^2\hbar^2 t^2}\right)^{\frac{3}{2}}\exp\left(-\frac{\alpha m^2}{m^2+\alpha^2\hbar^2t^2}r^2\right) \\
&= r^2\beta\exp\left(-\gamma r^2\right)
\end{aligned}
$$

where we have used:

$$
\beta = (\pi\alpha)^{-\frac{3}{2}}\left(\frac{\alpha^2m^2}{m^2+\alpha^2\hbar^2t^2}\right)^{\frac{3}{2}} \qquad \gamma = \frac{\alpha m^2}{m^2+\alpha^2\hbar^2t^2}
$$

The peak probability density r_p (the position where the particle is most likely to be found) can be found by taking

$$
\begin{aligned}
\frac{\partial\rho(r,t)}{\partial r} &= 0 \\
2r_p\beta\exp\left(-\gamma r_p^2\right) + r_p^2\beta\exp\left(-\gamma r_p^2\right)(-2\gamma r_p) &= 0 \\
2r_p\beta\exp\left(-\gamma r_p^2\right) &= 2\gamma r_p^3\beta\exp\left(-\gamma r_p^2\right) \\
r_p &= \sqrt{\frac{1}{\gamma}} \\
r_p &= \alpha^{-1/2}\left(1+\frac{\alpha^2\hbar^2}{m^2}t^2\right)^{\frac{1}{2}} \qquad \text{(A.0.19)}
\end{aligned}
$$

which "accelerates" outward at a rate:

$$
\begin{aligned}
a_{out} = \ddot{r_p} &= \frac{\partial}{\partial t}\left[\frac{\partial}{\partial t}\left(\alpha^{-1/2}\left(1+\frac{\alpha^2\hbar^2}{m^2}t^2\right)^{\frac{1}{2}}\right)\right] \\
&= \frac{\partial}{\partial t}\left[\alpha^{3/2}\frac{\hbar^2}{m^2 t}\left(1+\frac{\alpha^2\hbar^2}{m^2}t^2\right)^{-\frac{1}{2}}\right] \\
&= \left[\alpha^{3/2}\frac{\hbar^2}{m^2}\left(1+\frac{\alpha^2\hbar^2}{m^2}t^2\right)^{\frac{1}{2}} - \left(1+\frac{\alpha^2\hbar^2}{m^2}t^2\right)^{-\frac{1}{2}}\alpha^{7/2}\frac{\hbar^4}{m^4}t^2\right]\left(1+\frac{\alpha^2\hbar^2}{m^2}t^2\right)^{-1} \\
&= \frac{1}{\alpha r_p^2}\left(\alpha^{3/2}\frac{\hbar^2}{m^2}\alpha^{1/2}r_p - \alpha^{-1/2}\frac{1}{r_p}\alpha^{7/2}\frac{\hbar^4}{m^4}t^2\right) \\
&= \alpha\frac{\hbar^2}{m^2 r_p} - \alpha^2\frac{\hbar^4}{m^4 r_p^3}t^2 \\
&= \alpha\frac{\hbar^2}{m^2 r_p}\left(1-\alpha\frac{\hbar^2}{m^2 r_p^2}t^2\right) \\
&= \alpha\frac{\hbar^2}{m^2 r_p}\left[1-\frac{1}{r_p^2}\left(r_p^2-\frac{1}{\alpha}\right)\right] \\
\ddot{r_p} &= \frac{\hbar^2}{m^2 r_p^3} \qquad \text{(A.0.20)}
\end{aligned}
$$

Appendix B Matlab programme

B.1 Analytical Free Particle

```
%******************************Constants*********************************
h_bar = 6.626E−34;           %Planck constant, J.s
m = 9.109e−31;               %mass of particle, kg

%******************************Parameter*********************************
alpha = 4E12;                %determines the width of the wave−function
N = 370;                     %position−steps
Nt = 12000;                  %tiime−steps
r = linspace(0,5e−6,N)';     %the position range

t = linspace(0,15E−10,Nt);
Psi_t_a = zeros(N,Nt);

%***********************Evolution of wave−function***********************
for l = 1:N
    for k = 1:Nt
        Psi_t_a(l,k) = (pi*alpha)^(−3/4)*(alpha*m/(m+1i*alpha*h_bar*t(k)))^(3/2).*...
        exp(−alpha*m/(2*(m+1i*alpha*h_bar*t(k))).*(r(l)^2));
    end
end
```

B.2 Numerical

Parameters and Constants

The parameters used are true value (not scaled).

```
%******************************Parameters********************************
alpha = 4e12;                    %define the width
N = 370;                         %number of position−step
Nt = 12000;                      %number of time−step
j = linspace(0,5e−6,N)';         %the position range
dr = j(2)−j(1);                  %the position−step
n = linspace(0,4.15e1,Nt);       %the time range
dt = n(2)−n(1);                  %the time−step

%*******************************Constants********************************
G = 6.674E−11;                   %Gravitational constant in m^3kg−1s−2
%G = 0;
m = 4.109e−20;                   %Mass of electron in kg
h_bar = 6.626E−34;               %Planck constant in J.s
e = 1.6e−19;                     %Electric charge in Coulomb
c = 3E8;                         %speed of light
Lambda = 1.36E−52;               %Cosmological constant
c1 = (alpha/pi)^(3/4);           %constant for Psi_0
c2 = −4*pi*G*(m*dr)^2;           %constant for Vg_0
R = dt/(dr^2);
K = 1i*h_bar/(8*m);
P = 1i*dt/(2*h_bar);
```

The self-gravitating potential

This program is to compute the numerical self-gravitating potential, and the cosmological constant is chipped in Line 63.

```
for i = 0:N-1
    if i==0
        f1 = 0;
        f2 = sum(Psi(1:N,k).*conj(Psi(1:N,k)).*(0:N-1)');
        Vg(1,k) =  c2*f2;
    else
        f1 = sum(Psi(1:i,k).*conj(Psi(1:i,k)).*(0:i-1)'.^2);
        f2 = sum(Psi(i+1:N,k).*conj(Psi(i+1:N,k)).*(i:N-1)');
        Vg(i+1,k) =  c2*(1/i*f1+f2) - Lambda/6*c^2*(i+1)^2;
    end
end
```

The Tridiagonal Matrix

Diagonal vector

```
Dv(1) = 0.5*(1+P*Vg(1,k)+12*K*R);
Dv(2:N) = 0.5*(1+P*Vg(2:N,k)+2*K*R);
```

Super-diagonal vector

```
Superdv = zeros(N,1);
for i = 2:N
   Superdv(i) = -K*R*(i-1)/(i);
end
```

Subdiagonal vector

```
Subdv = zeros(N,1);
Subdv(1) = -6*K*R;
for i = 2:N-1
   Subdv(i) = -K*R*(i+1)/(i);
end
```

Getting the wavefunction

```
B(1) = Dv(1);
D(1) = Psi(1,k);
for i = 2:N
    B(i) = Dv(i)-Superdv(i)*Subdv(i-1)/B(i-1);
    D(i) = Psi(i,k)-Superdv(i)*D(i-1)/B(i-1);
end
x(N,k) = D(N)/B(N);
for i = N-1:-1:1
    x(i,k) = (D(i)-Subdv(i)*x(i+1,k))/B(i);
end

Psi(:,k+1) = x(:,k) - Psi(:,k);
```

The k is the number of iteration in time.

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