Machine Learning and Non Linear Schrodinger Equations

Huseyin T. Senyasa
(Dated: October 10, 2017)

...

I. GROSS-PITAEVSKII EQUATION

Since we are going to try to guess ground state energy for a given potential, we should first able to generate train data. To do that, we require analytic and numerical solutions for energy values.

Gross-Pitaevskii Equation is given as;

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar}{2m}\nabla^2\psi + V(r)\psi + g|\psi|^2\ \psi$$

The coefficient of the non-linear term determines the interaction type. If there is no interaction $g = 0$ and equation reduces the Schrodinger Equation. For repulsive interactions $g > 0$, and $g < 0$ for attractive.

Time Independent GPE

If the given potential is independent of time, GPE is separable and there are stationary solutions.

Stationary Solutions

When the potential is given, characteristic of the system is determined by non-linear term's coefficient, g as shown below. Symmetric harmonic potential is,

$$V(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$$

It is convenient to define characteristic length and interaction parameter (IP) to describe strength of the interactions which are given by respectively,

$$l_r = \sqrt{\frac{\hbar}{m\omega_r}}$$

$$\frac{Na_s}{l_r}$$

where a_s is s wave scattering length.

if $IP \gg 1$, it corresponds to strong repulsive interaction, $IP < 1$, weak interactions.

In no interaction case which means $g = 0$, GPE reduces to SE. This leads us to obtain well known harmonic potential solutions. Energy is given by,

$$E = \frac{3}{2}N\hbar\omega_r$$

In strong repulsive interaction, there is no analytic solution. We can obtain energy values by solving the GPE numerically or by approximation which is known as Thomas-Fermi approximation. Approximation requires negligence of the $\nabla^2\psi$ term. When the equation is solved and normalized condition is satisfied, energy is

$$E = \frac{5}{7}\mu N$$

and

$$\mu = \frac{\hbar\omega_r}{2}\left(\frac{15Na_s}{l_r}\right)^{\frac{2}{5}}$$

Reduction of Dimension

The shape of the condensate can be controlled by applied potential. When harmonic potential is symmetric, shape of the condensate is spherical but if we increase the ω_z component of the potential for fixed ω_y, ω_x, we can reshape it into pancake like shaped. In this case, condensate can be described by z component and system can be represented by 1D GPE which is given as,

$$\mu_{1D}\psi_z = \frac{-\hbar}{2m}\frac{d^2\psi}{dz^2} + V(z)\psi_z + g_{1D}|\psi_z|^2\ \psi_z$$

(ground state density is directly proportional to s wave scattering length, since g is function of s wave scattering length.)

(It also shows that for $g < 0$, system is not stable since density cannot be negative.)