The Gross-Pitaevskii Equation
A Non-Linear Schrödinger Equation

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Abstract

Summary: The Gross-Pitaevskii equation, also called the non-linear Schrödinger equation, describes Bose-Einstein condensates in the low temperature regime. In what follows, students will learn how to use the NDSolve command of Mathematica to find some numerical solutions to this difficult differential equation. An online Mathematica notebook (*.nb file) is also available to download.

1 Introduction to Bose-Einstein Condensates

Bosons are integral spin particles; therefore, the Pauli exclusion principle does not apply, and more than one boson may occupy the same quantum state. This has important consequences on the thermodynamics of collections of bosons, which, instead of obeying Maxwell-Boltzmann statistics, obey the Bose distribution:

$$f^0(\epsilon_\nu) = \frac{1}{e^{(\epsilon_\nu - \mu)/kT} - 1}, \tag{1}$$

where $f^0(\epsilon_\nu)$ is the mean occupation number of the single-particle state ν; ϵ_ν is the energy associated with state ν; μ is the chemical potential ("the energy gained by the system as a result of the addition of a single particle at constant volume and entropy" [7]); k is the Boltzmann constant, and T is the temperature. Figure 1 shows the Bose distribution plotted for different values of the fugacity $\zeta \equiv \exp(\mu/kT)$.

For smaller values of T, such as $T \sim \mu$K or nK, the lesser energetic states become more populated. This is the rationale for creating Bose-Einstein condensates (BECs). Collections of bosons, such as alkalis, are trapped in a potential and cooled by either switching off the confining potential and allowing the collection of bosons to expand or by evaporative cooling. With both methods, only the coldest bosons undergo a phase transition into a single quantum state characteristic of the BEC.

Figure 2 shows a BEC experiment that uses the expansion method for cooling rubidium-87 atoms.

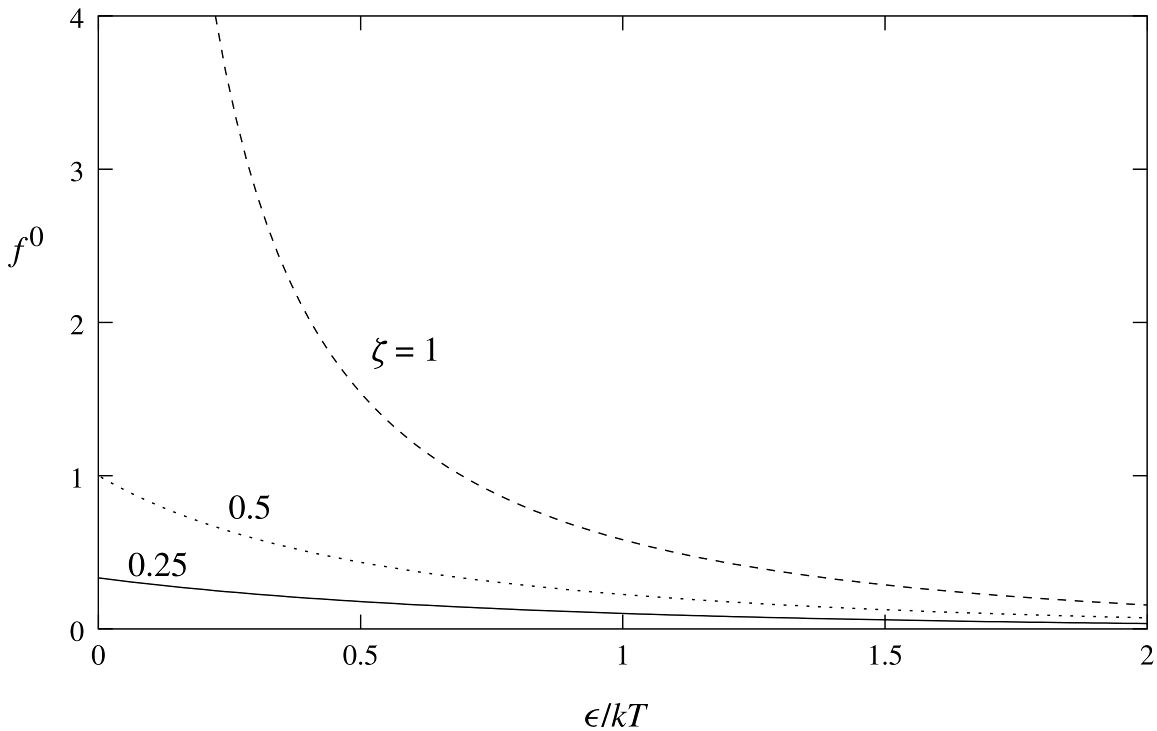

Figure 1: The Bose distribution (equation 1) for various values of the fugacity $\zeta \equiv \exp(\mu/kT)$ (figure courtesy [4])

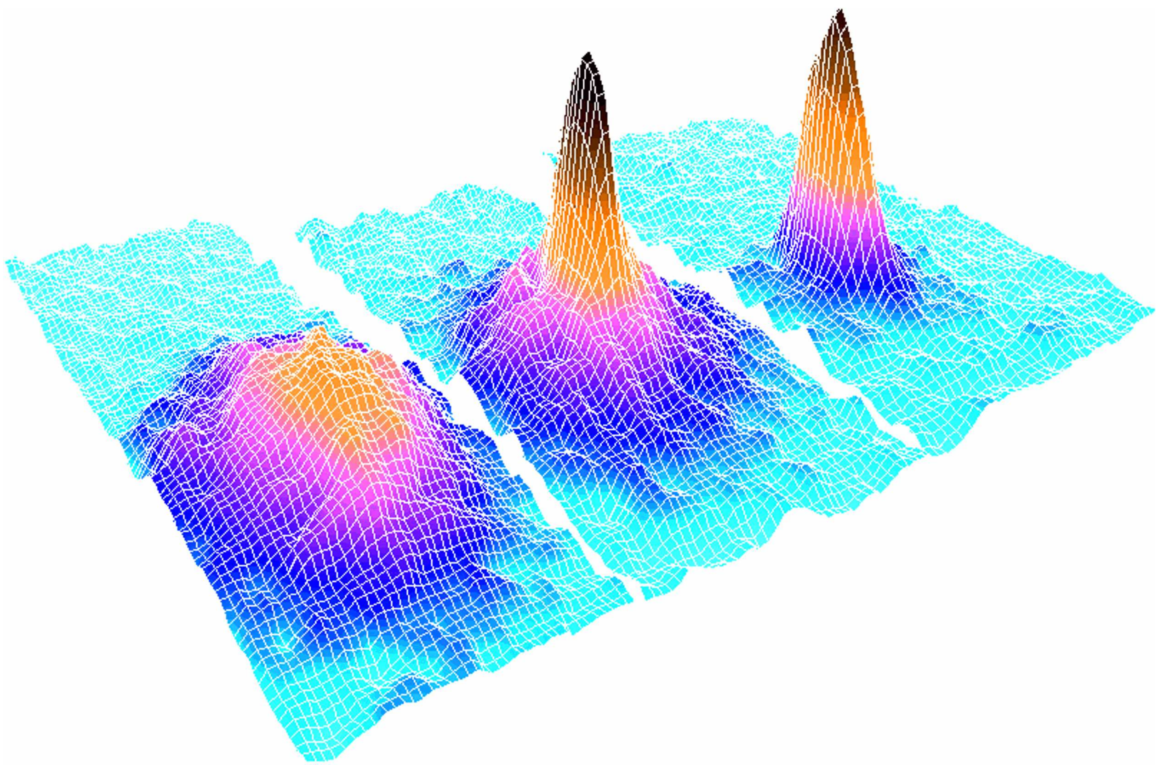

Figure 2: The 2-dimentional velocity distribution of rubidium-87 atoms in expansion method BEC experiment. The left frame corresponds to the distribution before condensation, and the other frames show the distribution after the bosons have cooled and condensed into a BEC. Only data from a 200×270 μm field of view centered on the condensate were used to make these velocity distributions. [1]

2 Derivation of the Gross-Pitaevskii Equation

The Gross-Pitaevskii (G-P) equation [3, 5] describes a zero-temperature BEC for which the scattering length between atoms, a, is smaller than the spacing between atoms. [4]

To derive[1] the G-P equation, we begin with the many-body Hamiltonian describing N interacting particles for the external potential V_{ext} and particle-particle interaction potential $V(\mathbf{r}-\mathbf{r}')$:

$$\hat{H} = \int d\mathbf{r}\ \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\ \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r}). \tag{2}$$

Equation 2 is given in the second quantization, a way of quantizing classical fields. $\hat{\Psi}^\dagger(\mathbf{r})$ and $\hat{\Psi}(\mathbf{r})$ are called boson field operators; they create and annihilate particles, respectively, at position $\mathbf{r}$. If $|0\rangle$ denotes the state of the vacuum, i.e., the state with zero particles, then $\hat{\Psi}^\dagger(\mathbf{r})|0\rangle$ produces the state with one particle at $\mathbf{r}$. Likewise, $\hat{\Psi}(\mathbf{r})|0\rangle = |0\rangle$. These states comprise Fock space. Boson creation and annihilation operators, $a^\dagger_\alpha$ and a_α respectively, are in Fock space, too. For the single-particle state indexed by α, the operators obey the following equations and commutation relations:

$$a^\dagger_\alpha \mid n_0, n_1, \ldots, n_\alpha, \ldots\rangle = \sqrt{n_\alpha + 1} \mid n_0, n_1, \ldots, n_\alpha + 1, \ldots\rangle, \tag{3}$$

$$a_\alpha \mid n_0, n_1, \ldots, n_\alpha, \ldots\rangle = \sqrt{n_\alpha} \mid n_0, n_1, \ldots, n_\alpha - 1, \ldots\rangle, \tag{4}$$

$$\left[a_\alpha, a^\dagger_\beta\right] = \delta_{\alpha,\beta}, \left[a_\alpha, a_\beta\right] = 0, \left[a^\dagger_\alpha, a^\dagger_\beta\right] = 0, \tag{5}$$

where the eigenvalues of the number operator $\hat{n}_\alpha = a^\dagger_\alpha a_\alpha$, which counts how many particles are in a particular state, are n_α.

Separating a boson field operator into wave function and annihilation operator components yields

$$\hat{\Psi}(\mathbf{r}) = \sum_\alpha \Psi_\alpha(\mathbf{r}) a_\alpha, \tag{6}$$

and expressing $\hat{\Psi}(\mathbf{r})$ in the Heisenberg representation of time dependent operators yields

$$\hat{\Psi}(\mathbf{r}, t) = \Phi(\mathbf{r}, t) + \hat{\Psi}'(\mathbf{r}, t). \tag{7}$$

$\Phi(\mathbf{r}, t) \equiv \langle\hat{\Psi}(\mathbf{r}, t)\rangle$ is called the order parameter or "wave function of the condensate" [2] and $\hat{\Psi}'(\mathbf{r}, t)$ can be interpreted as a perturbation on that condensed state. With the Heisenberg equation,

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r}, t) = [\hat{\Psi}, \hat{H}], \tag{8}$$

which gives the time dependence of an operator, one can express the time evolution of the field operator $\hat{\Psi}(\mathbf{r}, t)$ using Equation 2 for $\hat{H}$ in the Heisenberg representation as

$$\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r}, t) = \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + \int d\mathbf{r}'\hat{\Psi}^\dagger(\mathbf{r}', t)V(\mathbf{r}'-\mathbf{r})\hat{\Psi}(\mathbf{r}', t)\right]\hat{\Psi}(\mathbf{r}, t). \tag{9}$$

The G-P equation describes the evolution of $\Phi(\mathbf{r}, t)$ and, consequently, of the condensate density $n_0(\mathbf{r}, t) = |\Phi(\mathbf{r}, t)|^2$. The G-P equation assumes:

[1] I derive the G-P equation according to [2]. For the original derivations, see [3, 5].

1. $\hat{\Psi}'(\mathbf{r},t)$ is negligible, so $T \sim 0$ and $\hat{\Psi}(\mathbf{r},t) \approx \Phi(\mathbf{r},t)$.
2. The potential represents a "contact interaction"

$$V(\mathbf{r}' - \mathbf{r}) = g\delta(\mathbf{r}' - \mathbf{r}), \tag{10}$$

   where

$$g \equiv \frac{4\pi\hbar^2 a}{m}, \tag{11}$$

   with a being the scattering length. [4]
3. Inter-particle spacing is much larger than a.

Plugging Equation 10 into Equation 9 gives the G-P equation:

$$i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Phi(\mathbf{r},t)|^2\right)\Phi(\mathbf{r},t). \tag{12}$$

The term $g|\Phi(\mathbf{r},t)|^2$ is the non-linear term.

The time-independent form results from substituting $\Phi(\mathbf{r},t) = \phi(\mathbf{r})\exp(-i\mu t/\hbar)$ into Equation 12:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + g\phi^2(\mathbf{r})\right)\phi(\mathbf{r}) = \mu\phi(\mathbf{r}). \tag{13}$$

3 Numerical Simulations

Equation 12, the G-P equation, can approximately be solved by neglecting the kinetic energy term. This is the Thomas-Fermi approximation [4]. Here, however, we use *Mathematica* to solve the time independent G-P equation numerically for various external potentials $V_{\text{ext}}(\mathbf{r})$, which I assume to be two-dimensional and cylindrically symmetric. I imposed the boundary conditions that $\phi(0.01) = 1$ and $\phi(10) = 0$; these were the only boundary conditions that obtained converging numerical solutions, and they help ensure the solution for the wave function can be normalized. To make the numerics simpler, I set $\hbar^2/m\mu = U_0 = 1$. This is the *Mathematica* numerical integration command that I ran:

$$\text{NDSolve}\left[\left\{-\frac{\hbar^2\left(\frac{\partial_{\{r,2\}}(r\phi[r])}{r} + V_{\text{ext}}[r]\phi[r] + r^2 g\phi[r]^2\right)}{2m} == \phi[r],\right.\right.$$
$$\left.\phi[0.01] == 1, \phi[10] == 0\right\}, \phi, \{r, 0.1, 10\}]$$

Shown in Figure 3 for various potentials is $|\phi(r)|^2$, the density of the condensate wave function $\phi(r)$. We can see that, for most potentials, they are in qualitative agreement with column density versus radial component (z) of Figure 4.

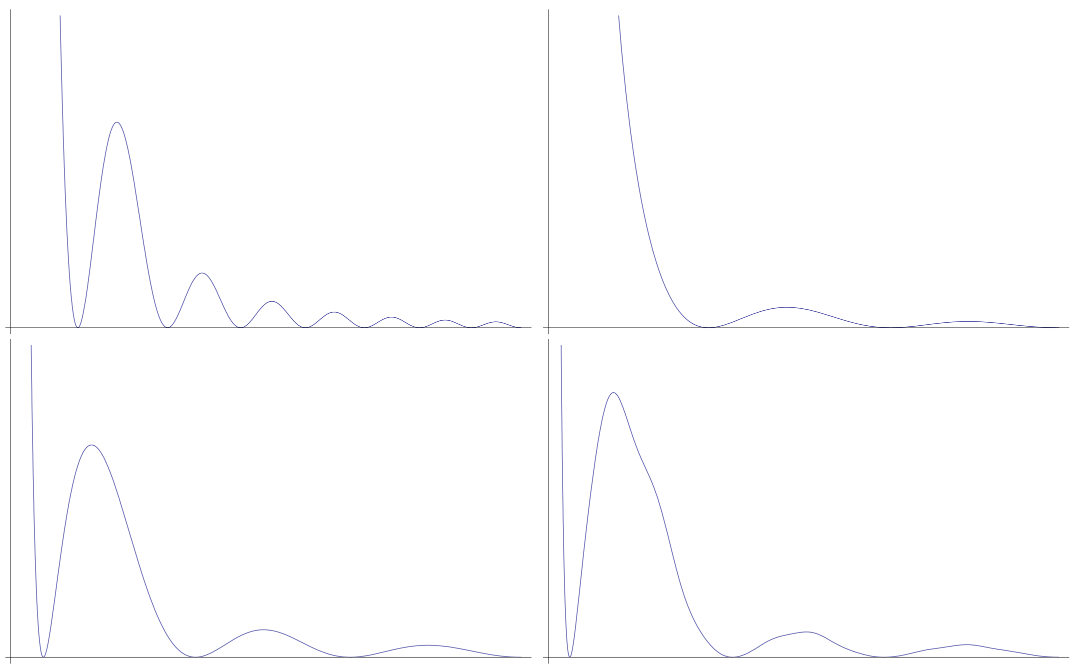

Figure 3: The top left plot shows the BEC column density (ordinate) versus radial distance r from the center of the BEC upon which a cylindrically-symmetric potential $V_{\mathrm{ext}}(r) \propto +r$ acts. The top right shows the BEC column density for $V_{\mathrm{ext}}(r) \propto +1/r$; bottom left, for $V_{\mathrm{ext}}(r) \propto +\exp(-1/r)$; and bottom right, for $V_{\mathrm{ext}}(r) \propto \sin(2\pi r)$.

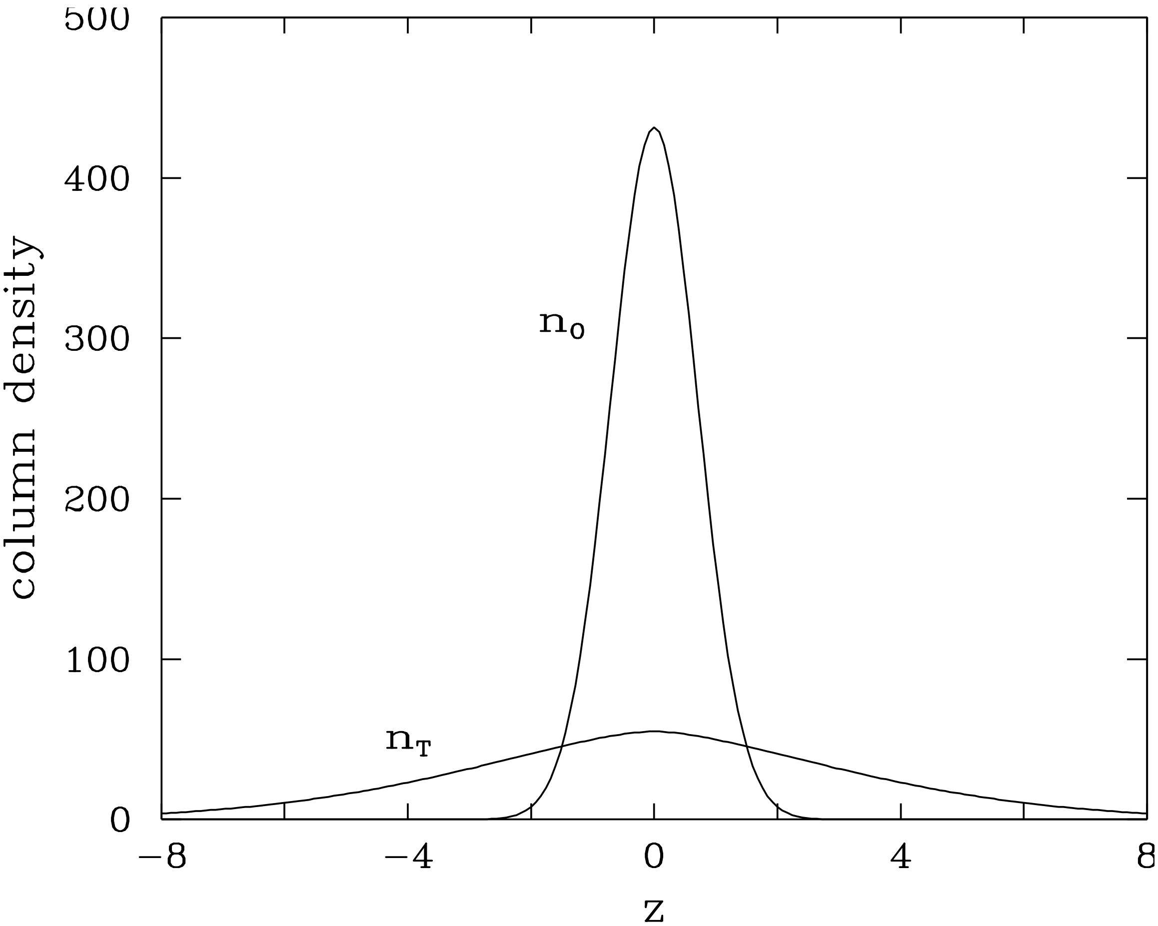

Figure 4: Column density versus radial component (z) of BEC in a harmonic oscillator potential. n_{T} and n_0 are the thermal and condensed (BEC) contributions, respectively, to the column density. (figure courtesy [2])

4 Conclusion

Bose-Einstein condensates, which the Gross-Pitaevskii equation governs in the low temperature regime, offer interesting experiments for one to perform in quantum mechanics. Among these are experiments for understanding the small anisotropies in BECs, or the formation of vortices (e.g., [6]). There are "cosmological experiments" (e.g., [7]) that try to draw a connection between the anisotropies in the universe, as seen by the Big Bang's leftover cosmic microwave background (CMB) radiation, and the anisotropies in superfluid ^{4}He, the nucleus of which is a boson. They can do this even though the early universe was very dense and hot and BECs are dilute and very cold.

References

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