# The Gross-Pitaevskii Equation

Ben Eller

circa 2017-2018, assignment for a course on PDEs

Quantum mechanical systems of many particles that move much slower than the speed of light in a vacuum ($c = 3 \times 10^8 \, \frac{\mathrm{m}}{\mathrm{s}}$) can be described by the many-body Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \hat{\mathcal{H}} \Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t). \tag{1}$$

$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t)$ is the many-body wavefunction which contains all the information about a system of $N$ generally interacting particles that have coordinates $\mathbf{r}_i$ at time $t$, and is the solution that we seek. $\hat{\mathcal{H}}$ is called the many-body Hamiltonian, and is a linear operator that represents the total energy of the system (kinetic plus potential). This can include external potentials imposed upon the system as well as interaction potentials between the different particles. For our purposes, Eq. (1) is a partial differential equation in $3N + 1$ independent variables. All the particles of the system are assumed to be identical bosons of mass $m$ (particles with integer valued intrinsic angular momentum, often called "spin"), and the Hamiltonian will take the form

$$\hat{\mathcal{H}} = \sum_{k=1}^{N} \left( \frac{-\hbar^2}{2m} \nabla_k^2 + V(\mathbf{r}_k) \right) + g \sum_{k=2}^{N} \sum_{j=1}^{k-1} \delta(\mathbf{r}_k - \mathbf{r}_j), \tag{2}$$

$\hbar = 1.055 \times 10^{-34}\,\mathrm{J{\cdot}s}$ being the reduced Planck's constant (pronounced "h-bar"). What we have here is a sum over single-particle operators that only act on the $k$-th particle plus a sum over distinct interacting pairs $(k, j)$. The single-particle operators are kinetic energy operators proportional to $\nabla_k^2$, and the external potential at position $\mathbf{r}_k$, $V(\mathbf{r}_k)$. The interaction between the particles has been assumed to be entirely due to contact forces in two-body collisions expressed as a Dirac delta-function $\delta(\mathbf{r}_k - \mathbf{r}_j)$ and characterized by a strength $g = 4\pi\hbar^2 a_s/m$, with $a_s$ being the $s$-wave scattering length which is a property of the particular atomic species. We cannot solve Eq. (1) exactly with this Hamiltonian (in fact we cannot in the vast majority of situations), however we can attempt to find stationary, approximate ground-state solutions using the variational method of quantum mechanics wherein we guess a trial form of the wavefunction with parameters we can vary to find the form that minimizes the expectation value of the energy (since we want the ground state). Since the many-body wavefunction for identical bosons obeys the condition $\Psi(..., \mathbf{r}_i, ..., \mathbf{r}_j, ..., t) = \Psi(..., \mathbf{r}_j, ..., \mathbf{r}_i, ..., t)$, an arbitrary number of bosons can occupy the same quantum state and we can take as our trial wavefunction $\Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t) = e^{-iEt/\hbar} \prod_{k''=1}^{N} \phi(\mathbf{r}_{k''})$, where $\phi$ is the single-particle ground state orbital. This form of the wavefunction would not work if the particles were fermions (particles with odd half-integer values of spin), since they obey an antisymmetric condition $\Psi(..., \mathbf{r}_i, ..., \mathbf{r}_j, ..., t) = -\Psi(..., \mathbf{r}_j, ..., \mathbf{r}_i, ..., t)$, a consequence of which is the Pauli exclusion principle that states that no two fermions can occupy the same quantum state. All of the atoms are assumed to be in the same state of the system $\phi$, and the wavefunction is symmetric under the interchange of two particles. By substituting our trial wavefunction into Eq. (1), multiplying both sides by $\prod_{k'=1}^{N} \phi^*(\mathbf{r}_{k'})$ and integrating over all the space-coordinates of the system, with $\int d^3R = \int d^3r_1 \int d^3r_2 ... \int d^3r_N$, we get the expectation value of the Hamiltonian

$$E[\phi^*] = \int d^3R \left( \prod_{k'=1}^{N} \phi^*(\mathbf{r}_{k'}) \right) \sum_{k=1}^{N} \left( \frac{-\hbar^2}{2m} \nabla_k^2 + V(\mathbf{r}_k) \right) \left( \prod_{k''=1}^{N} \phi(\mathbf{r}_{k''}) \right)$$
$$+ g \int d^3R \left( \prod_{k'=1}^{N} \phi^*(\mathbf{r}_{k'}) \right) \sum_{k=2}^{N} \sum_{j=1}^{k-1} \delta(\mathbf{r}_k - \mathbf{r}_j) \left( \prod_{k''=1}^{N} \phi(\mathbf{r}_{k''}) \right). \tag{3}$$

We can separate off the wavefunctions not participating in the sums and write

$$E[\phi^*] = \int d^3R \sum_{k=1}^{N} \left( \prod_{k' \neq k}^{N} \phi^*(\mathbf{r}_{k'}) \phi(\mathbf{r}_{k'}) \right) \phi^*(\mathbf{r}_k) \left( \frac{-\hbar^2}{2m} \nabla_k^2 + V(\mathbf{r}_k) \right) \phi(\mathbf{r}_k)$$
$$+ g \int d^3R \sum_{k=2}^{N} \sum_{j=1}^{k-1} \left( \prod_{k' \neq k \neq j}^{N} \phi^*(\mathbf{r}_{k'}) \phi(\mathbf{r}_{k'}) \right) \phi^*(\mathbf{r}_k) \phi^*(\mathbf{r}_j) \delta(\mathbf{r}_k - \mathbf{r}_j) \phi(\mathbf{r}_k) \phi(\mathbf{r}_j). \tag{4}$$

Now we can use the fact that the many-body wavefunction is normalized and therefore satisfies

$$\int d^3R \, \Psi^*(\mathbf{r}_1, ..., \mathbf{r}_N) \Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = 1, \tag{5}$$

and the properties of the Dirac delta-function to reduce Eq. (4) to

$$E[\phi^*] = \sum_{k=1}^{N} \int d^3r_k \phi^*(\mathbf{r}_k) \hat{h}_k \phi(\mathbf{r}_k)$$
$$+ g \sum_{k=2}^{N} \sum_{j=1}^{k-1} \int d^3r_k \phi^*(\mathbf{r}_k) \phi^*(\mathbf{r}_k) \phi(\mathbf{r}_k) \phi(\mathbf{r}_k), \tag{6}$$

where $\hat{h}_k = \left( \frac{-\hbar^2}{2m} \nabla_k^2 + V(\mathbf{r}_k) \right)$. We can swap the sums in Eq. (6) for a factors of $N$ and $N(N-1)/2$ respectively, since all the particles have the same wavefunction, leaving us with

$$E[\phi^*] = N \int d^3r \left( \phi^*(\mathbf{r}) \hat{h} \phi(\mathbf{r}) + \frac{g}{2}(N-1) \phi^{*2}(\mathbf{r}) \phi^2(\mathbf{r}) \right). \tag{7}$$

Now what we want to do is add in the constraint that $G[\phi^*] = \int d^3r \phi^* \phi - 1 = 0$, and find the form of $\phi$ that yields a stationary value of $E[\phi^*] - \lambda G[\phi^*]$, where $\lambda$ is a Lagrange multiplier. This can be accomplished by allowing either $\phi$ or $\phi^*$ to vary arbitrarily. Here we vary $\phi^*$, and denoting this variation by $\delta\phi^*$ we have

$$0 = (E[\phi^* + \delta\phi^*] - E[\phi^*]) - \lambda(G[\phi^* + \delta\phi^*] - G[\phi^*])$$
$$= \Bigg( \int d^3r \Big( (\phi^*(\mathbf{r}) + \delta\phi^*(\mathbf{r})) \hat{h} \phi(\mathbf{r}) + \frac{g}{2}(N-1)(\phi^*(\mathbf{r}) + \delta\phi^*(\mathbf{r}))^2 \phi^2(\mathbf{r}) \Big) \tag{8}$$
$$- \int d^3r \left( \phi^*(\mathbf{r}) \hat{h} \phi(\mathbf{r}) + \frac{g}{2}(N-1) \phi^{*2}(\mathbf{r}) \phi^2(\mathbf{r}) \right) \Bigg)$$
$$- \lambda \Bigg( \int d^3r (\phi^*(\mathbf{r}) + \delta\phi^*(\mathbf{r})) \phi(\mathbf{r}) - 1 - \int d^3r \phi^*(\mathbf{r}) \phi(\mathbf{r}) + 1 \Bigg) \tag{9}$$

Keeping only terms linear in $\delta\phi^*$ we see that (with $\phi^*\phi = |\phi|^2$)

$$\int d^3r\ \delta\phi^* \left\{ N \left( \hat{h}\phi + g(N-1)|\phi|^2\phi \right) - \lambda\phi \right\} = 0. \tag{10}$$

Since the $\delta\phi^*$ are arbitrary, we can conclude that $\phi(\mathbf{r})$ must satisfy the equation

$$\left( \frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g(N-1)|\phi|^2 \right)\phi = \mu\phi. \tag{11}$$

Equation (11) is known as the time-independent Gross-Pitaevskii equation (GPE), and we have defined $\mu = \lambda/N$ which is still unknown. We have used the definition $\hat{h} = \left( \frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right)$ here since Eq. (11) is how the equation is typically written in the literature. The factor of $N-1$ shows up because it was assumed that there is a definite number $N$ of atoms in the condensate. Another way to derive the time-independent GPE is to take as a trial wavefunction a coherent superposition of ground states with different numbers of atoms. Doing so will result in a factor of $N$ rather than $N-1$, however it corresponds to the average number of atoms instead. We note that the single-particle wavefunction $\phi$ is related to the condensate wavefunction $\Phi$ used in the body of this thesis in the following way, $\Phi = \sqrt{N}\phi$, and therefore the condensate wavefunction is normalized so that $\int d^3r|\Phi|^2 = N$. If we multiply both sides of the GPE by $\phi^*$ and integrate over all space, we get a formula for $\mu$:

$$\mu = \int d^3r \left( \phi^*\hat{h}\phi + g(N-1)|\phi|^4 \right). \tag{12}$$

Considering the energy functional (7), we can compute the chemical potential $\partial E/\partial N$ and show that (since the entropy and volume are fixed):

$$\frac{\partial E}{\partial N} = \int d^3r \left( \phi^*\hat{h}\phi + g(N-1/2)|\phi|^4 \right). \tag{13}$$

We see that Eqs. (12) and (13) are the same if $N >> 1$, and conclude that in this limit we can interpret $\mu$ as the chemical potential of the condensate, i.e. the energy required to add another particle to it. Solutions of Eq. (11) and the determination of the chemical potential from Eq. (12) for a given external potential $V(\mathbf{r})$ yield an equilibrium mean-field approximate form of the wavefunction that all particles in the system share. A time-dependent GPE can be found as well via the action principle [1]

$$\delta \int_{t_1}^{t_2} L(\phi, \phi^*, t)\, dt = 0 \tag{14}$$

with the Lagrangian (for large $N$)

$$\begin{aligned} L(\phi, \phi^*, t) = \int d^3r \Bigg[ & \frac{i\hbar}{2}\left( \phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t} \right) - \\ & \left( \frac{\hbar^2}{2m}|\boldsymbol{\nabla}\phi|^2 + V(\mathbf{r})|\phi|^2 + (gN/2)|\phi|^4 \right) \Bigg]. \end{aligned} \tag{15}$$

There are a number of books on this subject, such as Refs. [1] and [2]. There are many more, but these are complete works that cover all the basics and more in-depth topics of BEC, and are a good start for the interested reader.

## References

[1] C. J. Pethick and H. Smith, *Bose–Einstein Condensation in Dilute Gases*, Cambridge University Press, 2nd edition, 2008.

[2] L. Pitaevskii and S. Stringari, *Bose–Einstein Condensation and Superfluidity*, Oxford University Press, 2016.