Mean Field Calculations for Bosons

In this section we will learn how the Mean Field (MF) approximation is defined and exploited to study a system of N interacting Bosons.
Let us consider the following Hamiltonian (in coordinate representation) of N identical Bosons:

$$\hat{H} = \sum_{i=1}^{N} \left\{ -\frac{\hbar^2}{2m} \nabla_i^2 + v_{ext}(r_i) \right\} + \sum_{i<j}^{N} v(r_{ij}).$$

Here we assume for simplicity that the problem has spherical symmetry, without loss of generality. The system is embedded in an external field v_{ext}. This is for instance a good representation of ultracold Bosonic atoms trapped by a laser.

We want to focus on the study of the system in the ground state (at $T = 0$). If we want to determine its properties, we need to solve the stationary states Schroedinger's equation for the lowest energy eigenstate:

$$\hat{H}\Psi_0 = E_0\Psi_0,$$

where the solution

$$\Psi_0 \equiv \Psi_0(\vec{r}_1 \ldots \vec{r}_N)$$

is a function that we cannot explicitly determine either analytically or numerically.

In the Mean Field Approximation we assume that the effect of the mutual interaction between particles can be replaced by an average interaction to which each of the constituents of the system is independently subjected.

More specifically, the MF approximation consists of finding a single particle effective Hamiltonian h_{eff}, whose solutions:

$$h_{eff}\varphi_i(\vec{r}) = \mu_i\varphi_i(\vec{r})$$

are such that

$$\Psi_0 = \hat{\mathcal{S}}\prod_{i=1}^{N}\varphi_i(\vec{r_i}),$$

where the operator $\hat{\mathcal{S}}$ symmetrizes the product under all the possible exchanges of the indices. Finding the correct expression of h_{eff} is as hard as solving the original problem. We will later discuss the very existence of this effective Hamiltonian.

The total energy of the system in the MF context would then be $E = \sum_{i=1}^{N}\mu_i$. It is straightforward to observe that, since we are interested in the ground state, the only option we have is to choose $\varphi_i = \varphi_0 \forall i$.

This means that the wavefunction will be:

$$\Psi_0(\vec{r}_1 \ldots \vec{r}_N) = \prod_{i=1}^{N} \varphi(\vec{r}_i),$$

where $\varphi \equiv \varphi_0$. The product is automatically symmetric under particle exchanges.

While finding the correct h_{eff} is substantially impossible, we can always resort to our friend, the variational principle. What we will do is to approximate the ground state with a product Ψ of single particle states, and find the best possible representation with a variational calculation. This means to consider the energy E as a functional $E[\varphi]$ of the only "variable" left in the game, the single particle function φ. We will then variate the energy with respect to φ and find the minimum, constrained to the normalization of φ:

$$\frac{\delta}{\delta\varphi}\left[E[\varphi] - \mu \int_V |\varphi(\vec{r})|^2 d\vec{r}\right] = 0$$

We now need to evaluate $E[\varphi]$. This is simply the expectation of the Hamiltonian $\langle \Psi | \hat{H} | \Psi \rangle$. The wavefunction Ψ is written as:

$$\Psi(\vec{r}_1 \ldots \vec{r}_N) = \prod_{i=1}^{N} \varphi(\vec{r}_i),$$

therefore:

$$E[\phi] = \int_V \cdots \int_V \varphi^*(\vec{r}_1) \cdots \varphi^*(\vec{r}_N) \times$$

$$\times \left\{ \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + v_{ext}(r_i) \right] + \sum_{i<j}^{N} v(r_{ij}) \right\} \varphi(\vec{r}_1) \cdots \varphi(\vec{r}_N) d\vec{r}_1 \cdots d\vec{r}_N .$$

The expression can be greatly simplified. Let us consider for instance the kinetic term:

$$T[\varphi] = \int_V \cdots \int_V \varphi^*(\vec{r}_1) \cdots \varphi^*(\vec{r}_N) \left(\sum_{i=1}^N -\frac{\hbar^2}{2m} \nabla_i^2 \right) \varphi(\vec{r}_1) \cdots \varphi(\vec{r}_N) d\vec{r}_1 \cdots d\vec{r}_N \,.$$

This is the sum of N integrals of the form:

$$\int_V \cdots \int_V \varphi^*(\vec{r}_1) \cdots \hat{\varphi}^*(\vec{r}_i) \cdots \varphi^*(\vec{r}_N) \varphi(\vec{r}_1) \cdots \hat{\varphi}(\vec{r}_i) \cdots \varphi(\vec{r}_N) d\vec{r}_1 \cdots \hat{d\vec{r}_i} \cdots d\vec{r}_N \times$$

$$\times \int_V \varphi^*(\vec{r})_i \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right) \varphi(\vec{r}_i) d\vec{r}_i \,,$$

where the ˆ symbol indicates a missing factor in the product. The integral above reduces to a product of N independent integrals. Assuming that φ is normalized, all of them are $= 1$, but for the one involving the index i.

content...We can simplify even more. Since we are integrating over the various $\vec{r}_i$, we can arbitrarily exchange the indices within the integral. This means that the kinetic term will become a sum of integrals that are all equal, and we can drop the dependence on the particle index, obtaining:

$$T[\varphi] = N \int_V \varphi^*(\vec{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \varphi(\vec{r}) d\vec{r}.$$

We can repeat the same argument for the external potential, that becomes:

$$V_{ext}[\varphi] = N \int_V \varphi^*(\vec{r}) v_{ext}(r) \varphi(\vec{r}) d\vec{r} = N \int_V |\varphi(\vec{r})|^2 v_{ext}(\vec{r}) d\vec{r}.$$

The two–body interaction can also be treated in the same way. One immediately realizes that it is more convenient to avoid the double counting by considering all possible pairs regardless of the index order, and then divide the sum by 2. This yields an expression very similar to the previous ones:

$$V_{int}[\varphi] = \frac{N(N-1)}{2} \int_V \int_V |\varphi(\vec{r})|^2 |\varphi(\vec{r'})|^2 v(|\vec{r} - \vec{r'}|) d\vec{r} d\vec{r'} .$$

The energy functional is the sum of these three terms:

$$E[\varphi] = T[\varphi] + V_{ext}[\varphi] + V_{int}[\varphi].$$

At this point we realize that rather than requiring the normalization of φ to be constrained, one could constrain that the total number of particles N is conserved.

The one-body density operator of an N-body system is defined as:

$$\hat{\rho}(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r_i}).$$

it is easy to prove that:

$$\langle \Psi | \hat{\rho} | \Psi \rangle = N |\varphi(\vec{r})|^2 \equiv \rho(\vec{r}),$$

which easily translates into:

$$\int_V \rho(\vec{r}) d\vec{r} = N.$$

This can be used as an alternative constraint in the minimization of the energy.

The energy can be written as a functional of the density ρ in the form:

$$E[\rho] = \int_V \varphi(\vec{r})^* \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \varphi(\vec{r}) d\vec{r} + \int_V \rho(\vec{r}) V_{ext}(r) d\vec{r} +$$

$$+ \frac{N-1}{2N} \int_V \rho(\vec{r}) \rho(\vec{r'}) v(|\vec{r} - \vec{r'}|) d\vec{r} d\vec{r'}.$$

We are eventually ready for the minimization! Given the form of the expectation of the kinetic energy, it is more convenient to variate the functional with respect to φ^*, rather than φ:

$$\frac{\delta}{\delta \varphi^*} \left[E[\rho] - \mu \int_V \rho(\vec{r}) d\vec{r} \right] = 0.$$

The result of the variation is the following equation:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r})+v_{ext}(r)\varphi(\vec{r})+\frac{N-1}{N}\left[\int_V \rho(\vec{r'})v(|\vec{r}-\vec{r'}|)d\vec{r'}\right]\varphi(\vec{r})=\mu\varphi(\vec{r}),$$

which is called the Hartree Equation. It has the form of a Schroedinger equation for the single particle wavefunction:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r})+v_{eff}[\vec{r},\rho(\vec{r})]\varphi(\vec{r'})=\mu\varphi(\vec{r}),$$

but with an effective potential that depends on the density, hence by the solution of the equation itself! This implies that the techniques to solve the equation have to be somehow modified with respect to the standard ones.

The solution of the Hartree equation needs what is called a self-consistent procedure. This means that one starts from a guess for the solution φ, thereby allowing to evaluate the part of the potential depending on ρ (also called the Hartree potential). Then the equation is solved, and the solution used to re-evaluate the Hartree potential, and so on until convergence is reached.

How can we declare convergence? In the process the eigenvalue μ will change, and it is possible to monitor its change at each step. When after n interations $|\mu_n - \mu_{n+1}| < \epsilon$, where ϵ is some threshold to be decided beforehands, the calculation can be stopped.

here is another important way to check convergence. Suppose that we want to compute the energy of the system. This can be done in two ways.

1. Evaluate the energy functional $E[\varphi]$ for the current φ.
2. If we take the Hartree equation, multiply by $\varphi(\vec{r})$ on the left and integrate, we obtain:

$$\mu = T[\varphi] + V_{ext}[\varphi] + 2V_{int}[\varphi] \Rightarrow E[\varphi] = \mu - V_{int}[\varphi].$$

The two estimates of the energy are different unless φ is equal to the correct, converged solution. We can use the difference of the two estimates of the energy in 1. and 2. as convergence criterion.

The Gross-Pitaevskii equation

The physics of trapped bosonic atoms is well described by an Hamiltonian in which the external potential v_{ext} is harmonic, and the interaction is a so called contact potential. A contact potential is good to reproduce the properties of a very diluted system, in which the short-range detail of the particle-particle interaction is irrelevant, and the only physically relevant quantity is the scattering length a.
This potential is conveniently expressed as:

$$v_{ext}(\vec{r}, \vec{r}') = \frac{4\pi\hbar^2 a}{m}\delta(\vec{r} - \vec{r}').$$

If we substitute the potentials in the Hartree equation we obtain:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r}) + \frac{m\omega^2 r^2}{2}\varphi(\vec{r}) + \frac{4\pi\hbar^2 a}{m}\left[\int_V \rho(\vec{r'})\delta(\vec{r} - \vec{r'})d\vec{r'}\right]\varphi(\vec{r}) = \mu\varphi(\vec{r}),$$

where we have taken $\frac{N-1}{N} \sim 1$.

Since the confining potential has spherical symmetry we can express the solution expanding in spherical harmonics.

Assuming that we are looking for the irrotational ground state, we can limit ourselves to the $\ell = 0$ state:

$$\phi(\vec{r}) = \frac{R^{0,0}(r)}{r} \cdot \frac{1}{\sqrt{4\pi}}.$$

Integrating over the angles in the Hartree potential, and remembering that

$$\delta(\vec{r} - \vec{r'}) = \frac{1}{4\pi r^2}\delta(r - r'),$$

the equation becomes ($R \equiv R^{0,0}$):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}R(r) + \frac{m\omega^2 r^2}{2}R(r) + \frac{\hbar^2 aN}{m}\left\{\int_V \left[\frac{R(r')}{r'}\right]^2 \delta(r - r')dr'\right\}R(r) = \mu R(r).$$

Now it is convenient to rescale the coordinates with respect to the harmonic oscillator length $a_{HO} = \sqrt{\frac{\hbar}{m\omega}}$, and define $\tilde{r} = r/a_{HO}$. This transforms the Hartree equation into:

$$-\frac{\hbar\omega}{2}\frac{d^2}{d\tilde{r}^2}R(\tilde{r}) + \frac{\hbar\omega\tilde{r}^2}{2}R(\tilde{r}) + \hbar\omega\left(\frac{a}{a_{HO}}\right)N\left[\frac{R(\tilde{r})}{\tilde{r}}\right]^2 R(\tilde{r}) = \mu R(\tilde{r}).$$

Now we can divide by $\hbar\omega$ (meaning that we are using that as energy units), and finally obtain a fully adimensional equation:

$$-\frac{1}{2}\frac{d^2}{d\tilde{r}^2}R(\tilde{r}) + \frac{\tilde{r}^2}{2}R(\tilde{r}) + \left(\frac{a}{a_{HO}}\right)N\left[\frac{R(\tilde{r})}{\tilde{r}}\right]^2 R(\tilde{r}) = \mu R(\tilde{r})$$

This is known as the Gross-Pitaevskii equation.