

Advanced Computational Physics - Exercise 3

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Mean Field methods

In class we have discussed the mean field approximation to the solution of the many-body problem. We are interested in computing some ground state properties of a system of N particles described by the generic Hamiltonian:

$$\hat{H} = \sum_{i=1}^N \left[-\frac{\hbar}{2m} \nabla_i^2 + V_{ext}(\vec{r}_i) \right] + \frac{1}{2} \sum_{i \neq j}^N v(\vec{r}_i, \vec{r}_j),$$

where $\vec{r}_1 \dots \vec{r}_N$ are the coordinates of our N particles, V_{ext} is some external field and v is the interaction potential. We have seen that the mean field approximation consists of assuming that the wave function (in coordinate space) can be written as a product of *single particle* functions:

$$\Psi(\vec{r}_1 \dots \vec{r}_N) = \mathcal{P}_{s,a}^{\hat{}} \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) \dots \phi_N(\vec{r}_N),$$

where

$$\hat{\mathcal{P}}_s = \frac{1}{\sqrt{N!}} \sum_{\hat{P}} \hat{P} \quad \text{for Bosons}$$

$$\hat{\mathcal{P}}_a = \frac{1}{\sqrt{N!}} \sum_{\hat{P}} (-1)^P \hat{P} \quad \text{for Fermions}$$

with \hat{P} all the elements in the permutation group for the N particles, and P the corresponding parity (even-odd). The problem is solved using once again the variational principle. One needs to minimize the expectation:

$$E_T = \langle \Psi | \hat{H} | \Psi \rangle$$

with respect to the set of single particle function used, with the constraint that the normalization of each of the ϕ_i is normalized, and that they constitute an orthonormal set.

We have studied two cases:

- For the many Boson case, we saw that the ground state is obtained by considering only one single particle function ϕ . The minimization of E_T leads to the so called Hartree equation. As an application we considered atoms interacting via a contact potential:

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

The variational procedure, and a change in units, lead to the so called *Gross-Pitaevskii* equation:

$$-\frac{1}{2} \frac{d^2}{dr^2} \phi(r) + \frac{1}{2} r^2 \phi(r) + Na \left(\frac{\phi(r)}{r} \right)^2 \phi(r) = \mu r$$

going on

- For the many Fermion case we first derived the so-called Hartree-Fock equations, and we then introduced the Density Functional Theory. In particular, we discussed the application to an alkali metal cluster, described within the so called jellium model, i.e. a model in which ions are substituted by a uniform positive charge distribution. I just want to remind that the energy density functional employed in a DFT calculation has the form:

$$E[\rho] = \sum_{i_{occ}} \int d\vec{r} \phi_i^*(\vec{r}) \left(-\frac{\hbar^2}{2m} \right) \nabla_i^2 \phi(\vec{r}) + \int d\vec{R} \rho(\vec{r}) v_{ext}(\vec{r}) +$$

$$\frac{1}{2} \int d\vec{r} \int d\vec{r}' \frac{\rho(\vec{r}) \rho(\vec{r}')}{|\vec{r} - \vec{r}'|} + E_{xc}[\rho(\vec{r})]$$

where the external potential is that of charged sphere of radius R_c and charge density $\rho_b = \frac{3}{4\pi r_s^3}$, with r_s is the *Wigner-Seitz radius*, and such that $\frac{4}{3}\pi R_c^3 \rho_b = N$, and N is the number of atoms (= number of the electrons for an alkali metal) in the cluster:

$$v_{ext}(r) = 2\pi\rho_b \begin{cases} \frac{1}{3}r^2 - R_c^2 & \text{for } r > R_c \\ -\frac{2}{3}\frac{R_c^3}{r} & \text{for } r < R_c \end{cases}$$

and E_{xc} is the exchange-correlation potential, which, in the Local Density Approximation (LDA) reads:

$$\int d\vec{r} \rho(\vec{r}) \epsilon_{xc}(\vec{r}),$$

with

$$\epsilon_{xc}(r) = -\frac{3}{4} \left(\frac{3}{\pi}\right)^{\frac{1}{3}} \rho(r)^{\frac{1}{3}} - \frac{0.44}{7.8 + \left(\frac{3}{4\pi\rho(r)}\right)}.$$

I remind here that we are using units in which $\hbar = e = m_e = 1$.

Questions

1. Maybe you did not pay attention to this fact, but if we try to solve the Gross-Pitaevskii equation or the Hartree-Fock equations by means of what we called the *variational method* (expansion of the solution on a basis), we are applying the variational theorem in two steps: the first leads us to the equations (energy is minimized with respect to the single particle functions) the second *in the solution of the equations* (by expanding the single particle functions on a basis). Try to prove that this "double" application of the variational theorem still provides an upper bound property for the ground state solution. The answer is not necessarily complicated, but it needs a sound justification. [10 points]
2. Draw a flowchart for the self-consistent solution of the mean field equations (both GP and HF). Explicitly consider the mixing procedure, i.e. the fact that at each step the new potential (depending on the wave function which is a solution of the equation) is given in terms of $v_{\text{new}} = \alpha v_{\text{new}} + (1 - \alpha)v_{\text{old}}$, with $\alpha \ll 1$. [5 points]
3. Solve the GP equation for the ground state of a gas of cold atoms ($l = 0$) by means of the Numerov algorithm (see exercise 1). As a criterion for convergence use the comparison between the energy computed a) directly from the functional and b) from the eigenvalue μ (remember, μ **is not** the energy!!!). Try to find solutions for $Na = 0.01, 0.1, 1, 10, 100$ and compare the resulting density to the non interacting particle case. Discuss how the convergence speed varies with the coupling parameters (e.g. by looking at value of α necessary to make the procedure converge). [25 points]
4. Solve the GP equation for $Na = -0.01, 0, 1, 1\dots$. How far can you push Na ? what happens if Na becomes too large? Try to give a physical explanation of your result. [10 points]
5. Consider now clusters of Na ($r_s/a_0 = 3.93$) or K ($r_s/a_0 = 4.86$). Derive the Kohn-Sham equations from the energy density functional given above. Consider clusters with $N=8$ and $N=20$, and write a flowchart for the code solving the KS equations. [10 points]

6. Reusing the code written for the GP equation, solve the KS equation for the two clusters named above (the first with $N = 8$ containing only 1s and 1p orbitals, the second with $N = 20$ containing 1s,1p,1d, and 2s orbitals). Pay attention to the degeneracy of the energy levels when constructing the density! [40 points]

And remember...

The combined results of several people working together is often much more effective than could be that of an individual scientist working alone.(John Bardeen)