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:

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

where

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

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

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.

In this first exercise we limit ourselves to the case of Bosons.

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:

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

Questions

1. 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 wich 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]

2. Solve one iteration of the GP equation for the ground state of a gas of cold atoms ($\ell = 0$) by means of the Numerov algorithm (see exercise 1), using as a first guess for the solution the ground state of the confining harmonic well multiplied by the parameter $0 \leq \alpha \leq 1$. Discuss the evolution of the solutions with α. [15 points]

3. Implement the self-consistent procedure to fully solve the GP equation. 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). [40 points]

4. Solve the GP equation using the finite differences method (i.e. writing the equation in matrix form and diagonalizing). Compare and discuss the differences in the accuracy and execution speed between the two methods. [30 points]

5. Using either the Numerov algorithm or the finite differences method, repeat the calculation for negative values of a. What is the difference between the case of $a > 0$ and $a < 0$? How far can you go with $|a|$ and still obtain a stable solution?

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)