Computational Physics
Exercise 4

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Variational Monte Carlo for superfluid ^{4}He

Noble gases at $T \sim 0$K display substantial deviations from the classical behavior. He isotopes remain liquid at any temperature, and for a temperature of about 2.17K, ^{4}He (a Boson) shows a transition to a superfluid state. ^{3}He has quite different properties due to its Fermionic nature, but it also displays a superfluid like transition at a temperature ~ 2.5mK (quite lower). Zero-temperature liquid ^{4}He can be reasonably approximated by a collection of N point-like particles occupying the ground state of an Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} v(r_{ij}),$$

where r_{ij} is the interatomic distance, and v is the Lennard-Jones potential:

$$v(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^1 2 - \left(\frac{\sigma}{r}\right)^6\right].$$

The parameters for He (independent of the mass) are $\epsilon = 10.22$K and $\sigma = 0.2556$nm. Liquid ^{4}He shows a saturation property, i.e. it has a finite density when no external pressure is applied. This density is experimentally found at about 21.86nm^{-3} (i.e. particles per cubic nanometer).

We want to find a theoretical estimation of the saturation density for this model and compare it to the experimental value.

The employed method will be Variational Monte Carlo. Since we need to use a finite number of particles to study a homogeneous and isotropic liquid, we will use the approximation of periodic boundary conditions, as

discussed in class. The trial wavefunction is the minimal form satisfying the cusp condition and the symmetry properties of the system:

$$\Psi_T(\vec{r}_1 \ldots \vec{r}_N) = \exp\left[-\frac{1}{2}\sum_{i<j}^{N}\left(\frac{b}{r_{ij}}\right)^5\right],$$

where b is the only variational parameter.

1. Write down the explicit expressions for the local kinetic energy both written as (shorthand notation) $-\hbar^2/2m \int \Psi_T \nabla^2 \Psi_T dR$ and $-\hbar^2/4m[\int \Psi_T \nabla^2 \Psi_T dR - \int \nabla\Psi_T \nabla\Psi_T dR]$ as discussed in class. [5 points]

2. Work out the constant $\hbar^2/2m$ when using ϵ as energy unit and σ as length unit. Use the ^{4}He mass expressed in a.m.u.. [5 points]

3. Build up a routine placing 32 atoms on a face centered cubic lattice containing 2×2×2 elementary cells, each one defined by the vectors $(0,0,0), (1/2,1/2,0), (0,1/2,1/2), (1/2,0,1/2)$. Set the lattice constant in such a way that the density becomes $n = n_0$, where n_0 is the experimental saturation point. This will be your starting configuration. [15 points]

4. Build the VMC code using the Metropolis algorithm to sample $|\Psi_T|^2$, and estimate the energy of the 32 particles in the periodic box at the experimental saturation density. Minimize the energy with respect to the parameter b, and report the optimal value found (use the units suggested in point 2!). Compare the kinetic energy computed the two ways.

5. Repeat the previous analysis for two densities above and two densities below n_0. Do not exceed an interval ±5% (the energy is very sensitive to density!). Determine your value of the saturation density and compare it to the experimental one (the two value are not identical, but reasonably close).