II. EXAMPLE: VARIATIONAL MONTE CARLO (VMC) OF LIQUID HELIUM (BOSONS)

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A. Properties of liquid helium

Helium is the lightest element of the noble gases and has two stable isotopes, ^{4}He which is compost out of an even number of fermions (2 protons, 2 neutrons, 2 electrons), the ^{4}He atom behaves as boson, and ^{3}He which behaves as fermion due to its odd number of fermionic constituents. At low temperatures, helium fluids show effects due to the quantum nature of the motion and of the quantum statistics of the atoms. A precise microscopic description of helium is still challenging.

Pair potential and kinetic energy The effective pair potential between two helium atoms is phenomenologically described by a Lennard-Jones 12-6 potential

$$v^{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{1}$$

where r is the distance between them, $\epsilon = 10.22K$, and $\sigma = 2.566A$. (More accurate potentials are known under the name Aziz potential.) In contrast to classical fluids, the kinetic energy is not directly given in terms of the temperature, and introduces a second energy scale, $t = \hbar^2/(2m\sigma^2)$. For ^{4}He, we have $\hbar^2/2m = 6.02KA^2$ and $t \simeq 0.9K$, and $\hbar/2m = 8.03KA^2$ for ^{3}He leads to $t \simeq 1.2K$. At zero pressure, the equilibrium density of liquid ^{4}He is $\rho\sigma^3 = 0.365$, slightly higher than that of ^{3}He with $\rho\sigma^3 = 0.274$. In reduced units, where distances are measured in σ and energies in ϵ, the total Hamiltonian writes

$$\begin{aligned} H &= K + V & (2) \\ K &= -\lambda \sum_i \nabla_i^2, \quad V = \sum_{i<j} v^*(r_{ij}) & (3) \end{aligned}$$

with $\lambda = \hbar^2/(2m\sigma^2\epsilon) \simeq 0.0895$ for ^{4}He and $\lambda = 0.119$ for ^{3}He.

B. Variational wavefunction

In the following we will (first) consider only the bosonic liquid, ^{4}He. For a given many-particle wavefunction $\Psi_T(\mathbf{R})$, we want to evaluate the energy expectation value

$$\begin{aligned} E_T &= \frac{\int d\mathbf{R}\, \Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R})}{\int d\mathbf{R}\, |\Psi_T(\mathbf{R})|^2} & (4) \\ &= \int d\mathbf{R}\, p(\mathbf{R}) E_L(\mathbf{R}) & (5) \\ \pi(\mathbf{R}) &= \frac{|\Psi_T(\mathbf{R})|^2}{\int d\mathbf{R}\, |\Psi_T(\mathbf{R})|^2} & (6) \\ E_L(\mathbf{R}) &= \frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} & (7) \end{aligned}$$

and E_T is always an upper bound for the ground state energy E_0. The simplest bosonic wavefunction (upon normalization) is $\Psi_T(\mathbf{R}) = 1$, however, the potential energy diverges, so the bound is not useful. In order to obtain some more meaningful bound, the next simplest wavefunction writes

$$\Psi_T(\mathbf{R}) = \prod_{i<j} f(r_{ij}) \tag{8}$$

where $f(r)$ is some function which vanishes for $r \to 0$.

Jastrow wavefunction. There is a general theorem that the ground state wavefunction has no nodes, and we can choose it to be positive everywhere, so that it is confinient to rewrite the wavefunction in the form

$$\Psi_T(\mathbf{R}) = \exp[-U] \tag{9}$$

$$U = \sum_{i<j} u(r_{ij}) \tag{10}$$

which is known as Jastrow wavefunction. The Jastrow potential $u(r)$ must be choosen such that $u(r \to 0) \to +\infty$, and $u(r \to \infty) = 0$.

Local energy. The local energy is then expressed as

$$E_L(\mathbf{R}) = \lambda \sum_i \left[\sum_i \nabla_i^2 U - \sum_i (\nabla_i U)^2 \right] + V(\mathbf{R}) \tag{11}$$

so we need to calculate $v(r)$, $u(r)$, $u_\alpha(r) = \partial u(r)/\partial r_\alpha$, and $u_{\alpha\beta}(r) = \partial^2 u(r)/\partial r_\alpha \partial r_\beta$ for each pair of distance r_{ij}, the greek indices are for the spatial dimension.

Periodic boundary conditions. To describe the bulk behavior, we use periodic boundary conditions, and adapt the potential to vanish for distances larger than $r_c \leq K/2$ in order to apply the nearest image convention. We use

$$\tilde{v}(r) = v^*(r) - v^*(r_c), \quad r \leq r_c \tag{12}$$

In addition, in contrast to classical systems, we have to consider the boundary conditions for the wavefunction, too. Since the variational bound, $E_T \geq E_0$, only applies for continous wavefunctions with continuous first derivatives, we have to assure that $u(r)$, and $u'(r)$ vanishes for $r \geq r_c$, in order to use the image convention also for evaluating U. Vanishing potential and first derivatives at r_c can be assured using

$$\tilde{u}(r) = u(r) + u(2r_c - r) - 2u(r_c), \quad r \leq r_c \tag{13}$$

Monte Carlo evaluation. The probability $\pi(\mathbf{R}) \sim |\Psi_T(\mathbf{R})|^2 = \exp[-2U]$ cannot be created directly for many particles. We construct it via a Markov chain using the Metropolis algorithm. At each Monte-Carlo step, we propose to move some or all particles. For later purposes it is convinient to use a gaussian a-priori probability to displace the configuration $\mathbf{R}_{old}$ to a new one $\mathbf{R}_{new}$, for example, moving all N particles, we use

$$A(\mathbf{R}_{old} \to \mathbf{R}_{new}) = (4\pi\lambda\tau)^{-dN/2} \exp\left[-\frac{(\mathbf{R}_{new} - \mathbf{R}_{old})^2}{4\lambda\tau} \right] \tag{14}$$

The typical displacement per particle is $\sim \sqrt{\lambda\tau}$, and in order not to violate detailed balance, we have to take τ sufficiently small so that the displacement is always smaller than $L/2$. The move will be accepted with a probability

$$p(\mathbf{R}_{old} \to \mathbf{R}_{new}) = \min\left[1, \frac{\pi(\mathbf{R}_{new}) A(\mathbf{R}_{new} \to \mathbf{R}_{old})}{\pi(\mathbf{R}_{old}) A(\mathbf{R}_{old} \to \mathbf{R}_{new})} \right] \tag{15}$$

which in our case simplifies to

$$p(\mathbf{R}_{old} \to \mathbf{R}_{new}) = \min\left[1, \frac{\pi(\mathbf{R}_{new})}{\pi(\mathbf{R}_{old})} \right] = \min\left[1, e^{-2[U(\mathbf{R}_{new}) - U(\mathbf{R}_{old})]} \right] \tag{16}$$

Compared to a Monte Carlo simulation of a classical fluid, the Jastrow potential $2U$ in the quantum system plays a similar role as the interaction potential βV in the classical case.

Optimization. Since we do not know the ground state wavefunction exactly, we have to parametrize the potential $u(r)$ and optimize the trial energy obtained by the Monte Carlo evaluation by variation of the variational parameters. In general, we will have a non-linear function to optimize, which is a difficult problem by itself. Here, we will just use a very simple parametrization

$$u(r) = a r^{-b} \tag{17}$$

and determine roughly a and b.