Exercise 6. Quantum Monte Carlo simulation of a one-dimensional ideal Fermi gas in a harmonic trap.

Objective: Find ground-state properties of a one-dimensional trapped ideal Fermi gas in the presence of a harmonic confinement.

Theory

The Hamiltonian of N particles of mass m interacting with two-particle potential $V_2(|\mathbf{r}_i - \mathbf{r}_j|)$ and subjected to external field $V_1(\mathbf{r})$ is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i + \sum_{i=1}^{N}V_1(\mathbf{r}_i) + \sum_{i<j}V_2(|\mathbf{r}_i - \mathbf{r}_j|) \tag{1}$$

The time evolution of a quantum state is given by the Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \tag{2}$$

Here, we will be interested in the stationary solutions

$$\hat{H}\phi_n = E_n\phi_n, \quad n = 0, 1, \cdots \tag{3}$$

where ϕ_n are eigenfunctions and E_n are the corresponding eigenvalues. Our goal is to find the ground-state energy E_0 or provide the best approximation to it.

According to the *variational principle*, the variational energy E_{VMC} provides an upper bound to the ground-state energy E_0

$$E_{VMC} = \frac{\int \psi_T^*(\mathbf{R},\boldsymbol{\alpha})\hat{H}\psi_T(\mathbf{R},\boldsymbol{\alpha})\, d\mathbf{R}}{\int \psi_T^*(\mathbf{R},\boldsymbol{\alpha})\psi_T(\mathbf{R},\boldsymbol{\alpha})\, d\mathbf{R}} = \frac{\sum\limits_{n=0} c_n^2 E_n}{\sum\limits_{n=0} c_n^2} \geq E_0 \tag{4}$$

where we expanded the trial wave function over the basis of eigenfunctions (**??**), $\psi_T(\mathbf{R},\boldsymbol{\alpha}) = \sum\limits_{n=0} c_n\phi_n(\mathbf{R})$ and $\mathbf{R} = \{\mathbf{r}_1, \cdots, \mathbf{r}_N\}$ denotes a point in the phase space, $\boldsymbol{\alpha}$ denotes the set of variational parameters on which the trial wave function depends and which can be changed in order to minimize the variational energy. The equal sign is fulfilled ($E_{VMC} = E_0$) only if the trial wave function coincides with the ground state wave function, $\psi_T(\mathbf{R},\boldsymbol{\alpha}) = \phi_0(\mathbf{R})$.

In Quantum Mechanics, particles do not have a deterministic trajectory but rather their probability distribution is defined by the wave function of the system

$$p(\mathbf{R}) = |\psi(\mathbf{R})|^2. \tag{5}$$

If the wave function is known (or is approximated by an analytical or numerical trial wave function), probability distribution (**??**) can be sampled by the Metropolis algorithm.

On the contrary to a classical system, where the phase space contains both coordinates and velocities $\{\mathbf{r}_1, \cdots, \mathbf{r}_N; \mathbf{V}_1, \cdots, \mathbf{V}_N\}$, in the quantum case the phase space is smaller as momentum operator can be written as

$$\hat{\mathbf{p}} = -i\hbar\nabla \tag{6}$$

and the whole phase space can be chosen to be written in coordinate representation or in momentum representation. Another important difference is that there is no concept of deterministic trajectory and there is no analog of Newton's equations, thus molecular dynamics methods cannot be applied.

Integral for the energy (**??**) can be approximated by creating a Markov chain of length M $\{\mathbf{R}_1, \cdots, \mathbf{R}_M\}$ according to the probability $p(\mathbf{R}, \boldsymbol{\alpha})$ and calculating the average value over it

$$E_{VMC} = \frac{\int E_{loc}(\mathbf{R}, \boldsymbol{\alpha}) p(\mathbf{R}, \boldsymbol{\alpha})\, d\mathbf{R}}{\int p(\mathbf{R}, \boldsymbol{\alpha})\, d\mathbf{R}} \approx \frac{1}{M} \sum_{i=1}^{M} E_{loc}(\mathbf{R}_i, \boldsymbol{\alpha}) \tag{7}$$

Note that the correct normalization is obtained for *any* multiplicative constant in the trial wave function, i.e. calculations with $\psi_T \to C\psi_T$. Here the local energy is a function of coordinates and variational parameters

$$E_{loc}(\mathbf{R}, \boldsymbol{\alpha}) = \frac{1}{\psi_T(\mathbf{R}, \boldsymbol{\alpha})} \hat{H} \psi_T(\mathbf{R}, \boldsymbol{\alpha}) \tag{8}$$

For Hamiltonian (**??**) the local energy becomes

$$E_{loc}(\mathbf{R}, \boldsymbol{\alpha}) = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\Delta_i \psi_T(\mathbf{R}, \boldsymbol{\alpha})}{\psi_T(\mathbf{R}, \boldsymbol{\alpha})} + \sum_{i=1}^{N} V_1(\mathbf{r}_i) + \sum_{i<j} V_2(|\mathbf{r}_i - \mathbf{r}_j|) \tag{9}$$

The operator of the potential energy is diagonal in coordinate space and its calculation is trivial. On the other hand operator of momentum (**??**) is non-diagonal and as a consequence, the calculation of the kinetic energy in Eq. (**??**) requires evaluation of the second derivative. Alternatively, a second estimator for the kinetic energy can be obtained by performing integration by parts,

$$-\int \psi^* \nabla^2 \psi \, d\mathbf{R} = -\psi^* \nabla \psi|_\Omega + \int |\nabla \psi|^2 \, d\mathbf{R} \tag{10}$$

where Ω denotes the limits of integration. Typically, for a trapped system, the wave function vanishes at large distances, $\psi|_\Omega = 0$, while for a system in periodic boundary conditions, $\nabla\psi|_\Omega = 0$ so that the wave function is periodic. As a result, the corresponding contribution vanishes.

The presence of two independent estimators for the kinetic energy is a very powerful tool to check if the code contains an error, as their derivation does not imply any specific shape of the trial wave function. The estimators will differ if

1. Metropolis method is not implemented correctly and the generated probability distribution is incorrect

2. first derivative of the trial wave function is not implemented correctly

3. second derivative of the trial wave function is not implemented correctly

A typical choice for the trial wave function is a pair product form

$$\psi_T(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \prod_{i=1}^{N} f_1(\mathbf{r}_i) \prod_{j<k}^{N} f_2(|\mathbf{r}_j - \mathbf{r}_k|), \tag{11}$$

where $f_1(r)$ is the one-body term that takes into account the presence of the external field and $f_2(r)$ are the two-body correlation terms, known also as Jastrow terms.

If $f_1(r)$ or $f_2(r)$ decay fast (e.g. in an exponential form), it is convenient to express the wave function as

$$\psi_T(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \exp\left\{ \sum_{i=1}^{N} u_1(\mathbf{r}_i) + \sum_{j<k}^{N} u_2(|\mathbf{r}_j - \mathbf{r}_k|), \right\} \tag{12}$$

where $u_1(r) = \ln f_1(r)$ and $u_2(x) = \ln f_2(x)$.

The drift force is defined as a vector corresponding to the gradient acting on particle i:

$$\vec{F}_i(\mathbf{R}) = \frac{\nabla_i \Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} = \frac{f'(\vec{r}_i)}{f(\vec{r}_i)} \frac{\vec{r}_i}{|\vec{r}_i|} + \sum_{k \neq i}^{N} \frac{f_2'(|\vec{r}_i - \vec{r}_k|)}{f_2(|\vec{r}_i - \vec{r}_k|)} \frac{\vec{r}_i - \vec{r}_k}{|\vec{r}_i - \vec{r}_k|} = \tag{13}$$

$$= u_1'(\vec{r}_i) \frac{\vec{r}_i}{|\vec{r}_i|} + \sum_{k \neq i}^{N} u_2'(|\vec{r}_i - \vec{r}_k|) \frac{\vec{r}_i - \vec{r}_k}{|\vec{r}_i - \vec{r}_k|} \tag{14}$$

Differentiating the trial wave function one finds the expression for the kinetic energy contribution to the local energy,

$$E_{kin}^{loc}(\mathbf{R}) = \frac{\hbar^2}{2m} \left\{ \sum_{i=1}^{N} E_1^{loc}(\vec{r}_i) + 2 \sum_{j<k}^{N} E_2^{loc}(|\vec{r}_j - \vec{r}_k|) - \sum_{i=1}^{N} [\vec{F}_i(\mathbf{R})]^2 \right\}, \tag{15}$$

where the one-body contribution to the local energy is

$$E_1^{loc}(r) = -\frac{f_1''(r)}{f_1(r)} + \left(\frac{f_1'(r)}{f_1(r)} \right)^2 = -u_1''(r) \tag{16}$$

and the two-body contribution is

$$E_2^{loc}(r) = -\frac{f_2''(r)}{f_2(r)} - \frac{(D-1)}{r} \frac{f_2'(r)}{f_2(r)} + \left(\frac{f_2'(r)}{f_2(r)} \right)^2 = -u_2''(r) - \frac{(D-1)}{r} u_2'(r) \tag{17}$$

where $D = \{1; 2; 3\}$ is the system dimensionality.

Alternatively, the kinetic energy can be estimated by calculating the average of the square of the drift force, i.e.

$$E_{kin,drift}^{loc}(\mathbf{R}) = \frac{\hbar^2}{2m} \sum_{i=1}^{N} [\vec{F}_i(\mathbf{R})]^2 \tag{18}$$

Note that the square of the drift force is calculated as one of the ingredients of the direct estimator (see the last term in Eq. (**??**)).

Model

The Hamiltonian of N ideal fermions of mass m confined to a one-dimensional harmonic oscillator with frequency ω is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2}{2}\sum_{i=1}^{N} x_i^2 \tag{19}$$

The ground-state energy of a single particle, $N = 1$, in the 1D oscillator, is non-zero, $E_0 = \hbar\omega/2$, due to quantum fluctuations, contrarily to the classical case with zero minimal energy at $T = 0$.

It is convenient to choose oscillator length $a_{ho} = \sqrt{\hbar/m\omega}$ as the unit of length and $\hbar\omega$ as the unit of energy. With this choice, one can recover the limits of vanishing interaction potential $\lambda \to 0$. The Hamiltonian in dimensionless units reads as

$$\hat{\tilde{H}} = -\frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} \tag{20}$$

The wave function of an ideal Fermi gas can be constructed as a Slater determinant,

$$\psi(x_1, ..., x_N) = \begin{vmatrix} \varphi_0(x_1) & \varphi_0(x_2) & \cdots & \varphi_0(x_N) \\ \varphi_1(x_1) & \varphi_1(x_2) & \cdots & \varphi_1(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{N-1}(x_1) & \varphi_N(x_2) & \cdots & \varphi_{N-1}(x_N) \end{vmatrix} \tag{21}$$

in such a way that interchanging positions of two particles $x_i \to x_j$, $x_j \to x_i$ is equivalent to interchanging two columns, and the determinant changes its sign $\psi \to -\psi$. This correctly reproduces antisymmetric Fermi Dirac statistics. If two Fermions have the same positions, $x_i = x_j$, the wave function vanishes, $\psi = 0$, according to the Pauli exclusion principle.

For the ground-state wave function, the single-particle orbitals are chosen as the eigestates of a single-particle ($N = 1$ problem),

The wave function of the ground state can be written explicitly

$$\psi(x_1, ..., x_N) = (-1)^{\mathcal{P}}\prod_{i<j}|x_i - x_j|\prod_k e^{-\frac{1}{2}x_k^2} \tag{22}$$

where the parity factor is $(-1)^{\mathcal{P}} = \text{sign}(\prod_{i>j}(z_i - z_j))$ for fermions.

The ground-state energy per particle is

$$\frac{E}{N} = \frac{1}{2}N\hbar\omega. \tag{23}$$

Notice, that local quantities (for example, density profile, pair distribution function, etc.) rely on the absolute value of the wave function, $|\psi(\mathbf{R})|^2$, so that the parity factor becomes irrelevant, $|(-1)^{\mathcal{P}}|^2 = 1$, and can be omitted in the Metropolis algorithm.

Algorithm

1. generate a random initial configuration
2. make a loop over Monte Carlo iterations
3. move the point $\mathbf{R} \to \mathbf{R}'$ in the phase space. for example, each particle can be displaced according to a random flat ($r_i \to r_i + (2\xi - 1)A$, where A is the amplitude) or Gaussian ($r_i \to r_i + \xi$) distribution
4. accept or reject the move according to the Metropolis algorithm. For example, throw a random number $\xi \in (0, 1)$ and accept the move if $p(\mathbf{R}')/p(\mathbf{R}) > \xi$.
5. accumulate the local energy and its square ($energy := energy + local\_energy; energy2 = energy2 + local\_energy * local\_energy$); density profile;

6. after $Niter$ iterations are done, estimate the mean energy ($\langle E\rangle \approx energy/Niter$), its variance: $\sigma_E^2 = \langle E^2 - \langle E\rangle^2\rangle \approx energy2/Niter - (energy/Niter) * *2$ and its statistical error $\varepsilon_E = \sigma_E/\sqrt{N_{uncorr}}$ where N_{uncorr} is the number of uncorrelated measurements.

Task

1. calculate the density profile for

   I) $N = 1$ particle

   II) $N = 10$ particles

   III) $N = 100$ particles

   Note that for a single particle, the Fermi statistics does not play a role, and Hamiltonian (**??**) describes a free harmonic oscillator, with energy $E = \hbar\omega/2$ and the density profile given by a Gaussian. As more fermions are added, Pauli exclusion principle comes into play and Friedel oscillations should be visible. For many particles, the Local Density Approximation can be used, leading to a semicircular density profile, $n_{LDA}(r) = \sqrt{2N/\pi^2}\sqrt{1 - r^2/R_{TF}^2}$, with the Thomas-Fermi radius R_{TF} related to the chemical potential $\mu = N\hbar\omega$ according to $\mu = mR_{TF}^2/2$. The LDA approximation is valid when $R_{TF} \gg a_{ho}$, i.e. when $\mu \gg \hbar\omega$

2. calculate the direct estimator for the kinetic energy as given by Eq. (**??**). Verify that the local energy is constant, meaning that the trial wave function coincides with the ground-state wave function.

3. calculate the drift-force estimator for the kinetic energy, as given by Eq. (**??**). Verify that the average of this estimator indeed gives the correct energy for the kinetic energy.