Toolbox tutorial-Quantun Monte Carlo

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Task I Monte Carlo generator for classical gas

Consider a box system contained large number of ^{85}Rb with mass $m = 85m_0$ at room temperature T, where m_0 is the atom mass unit. The kinetic energy of the system E_k follows the probability density function

$$f(E_k) = 2\left(\frac{1}{k_B T}\right)^{3/2} \sqrt{\frac{E_k}{\pi}} e^{-\frac{E_k}{k_B T}} \tag{1}$$

In this exercise, we will compute the expectation value of E_k directly from Eq. 1 with the Monte Carlo method.

1. We know that the function $f(E_k)$ has the maximum

$$f\left(\frac{k_B T}{2}\right) = 2\sqrt{\frac{1}{\pi k_B T}} E_k^{3/2} e^{-1/2}. \tag{2}$$

Based on this information, we can use the accept-reject method to generate the random values of E_k. In the code "toolbox-QMC-1", we try to generate $N_{par} = 20000$ particles in the range $[0, 10k_B T]$ and plot it in a histogram to be compared with Eq. 1. Please finish the missing line and make the code work.

2. Based on the results of question 1, compute the expectation value for E_k

$$\langle E_k \rangle = \int E_k f(E_k) dE_k \tag{3}$$

And show it satisfy $\langle E_k \rangle = 1.5 k_B T$

3. **(To be finished at home after the 1st class)** Repeating the step 1 and 2 for $N_{exp} = 900$ times with particle number $N_{par} = 400$ in each experiment, and you can get N_{exp} number of $\langle E_k \rangle$ values. Proof that these $\langle E_k \rangle$ should follows a Gaussian distribution with standard deviation $\sigma_{\langle E_k \rangle}$. Set σ_f the standard deviation of $f(E_k)$, how much is the ratio $\sigma_f / \sigma_{\langle E_k \rangle}$?

Task II Superfluid to Mott insulator transition in 2D Bose-Hubbard model

We consider a 2D Bose-Hubbard model which Hamiltonian writes

$$\mathcal{H} = -J \sum_{j,j'} \left(\hat{b}_j^\dagger \hat{b}_{j'} + \text{H.c.} \right) + \sum_j \left[\frac{U}{2} \hat{b}_j^\dagger \hat{b}_j^\dagger \hat{b}_j \hat{b}_j - \mu \hat{n}_j \right] \tag{4}$$

where j is the index of the lattice site, j' is always the nearest neighbour of j,$\hat{b}_j^\dagger$ and $\hat{b}_j$ are the bosonic creation and annihilation operators on lattice site j, and $\hat{n}_i = \hat{b}_j^\dagger \hat{b}_j$ is the site occupation operator. The pre-factor of the three terms are the tunneling J, interaction

strength U and chemical potential μ. With the PIMC techniques and worm algorithm, one can compute the superfluid fraction of the system and capture the superfluid to Mott insulator transition. In this exercise, based on the ALPS packages, we will try to study this phase transition.

1. Install the ALPS correctly on your laptop and run the code "toolbox-QMC-2". For all the later calculations, we fix system size $L = 5$, interaction $U = 1.0$ and chemical potential $\mu = 0.5$. **(Note: please complete this task before the 2nd class)**

2. We fix $T = 0.1$ in this question. For the two tunneling values $t_1 = 0.01$ and $t_2 = 0.09$, scan the iteration numbers $N_{iter} = [500, 1000, 5000, 10000, 20000, 50000, 80000]$ and discuss what you find.

3. Choose a proper value of N_{iter}. Now, we scan the quantity "THERMALIZATION" by $N_{th} = [0, 20, 50, 100, 500, 1000, 2000]$. Just whether the current value of N_{th} is the good choice.

4. Scan the curve $f_s - t$ for three different temperatures $T_1 = 0.1$, $T_2 = 0.5$ and $T_3 = 1.0$. Comment.

5. For all the parameters set in the QMC calculations, which are technique and which are physical? In practice, if we want to study a physical properties of the system, what is the order of scanning the parameters?

Task III Correlation function for 1D Bose-Hubbard chain

In this task, we focus on a 1D Bose-Hubbard chain and its Hamiltonian is simply the 1D version of Eq. 4. Thanks to the worm algorithm, we can compute the first order correlation function, which is defined as s defined by

$$g^{(1)}(x, x') = \langle \hat{\psi}^\dagger(x)\hat{\psi}(x') \rangle. \tag{5}$$

To be more specific, in the worm code, we compute $g^{(1)}(x) = \int dx' g^{(1)}(x', x' + x)$. In 1D system, this function will decay algebraically $g^{(1)}(x) \sim x^{-\alpha}$ with $\alpha = 1/2K$ at large distance. In the regime $n \leq 1$ and $U/J \gg 1$, the Luttinger parameter K writes $K \simeq 1 + \frac{4J}{\pi U} sin(\pi n)$.

1. Run the code "Task3-1", check the status of $g^{(1)}(x)$ at large distance.
2. How to cure the problem to observe a clean tail of $g^{(1)}(x)$?