Determination of Scattering Length of Bose-Hubbard Model by Quantum Monte Carlo Simulations[1]

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The Bose-Hubbard model is the simplest non-trivial model for interacting boson system. It is widely believed that, in the dilute limit, the model is equivalent to the continuous model characterized by a single parameter, i.e., the s-wave scattering length. However, there has been no quantitative estimation of the scattering length in the unit of lattice constant. In the ISSP supercomputer project of SY2017, we aim at establishing the quantitative correspondence between the lattice model and the continuous-space model.

Here, the Bose-Hubbard model defined as

$$H = -t \sum_{(ij)} (b_i^\dagger b_j + \text{h.c.}) - \mu \sum_i b_i^\dagger b_i,$$

which is compared in our project to

$$H = \int d\mathbf{x} \phi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \phi(\mathbf{x}) + \int d\mathbf{x} d\mathbf{x}' \phi^\dagger(\mathbf{x}') \phi^\dagger(\mathbf{x}) V(\mathbf{x}' - \mathbf{x}) \phi(\mathbf{x}) \phi(\mathbf{x}')$$

with

$$V(\mathbf{x}) \equiv \begin{cases} \infty & (|\mathbf{x}| \le a_s) \\ 0 & (|\mathbf{x}| > a_s) \end{cases}$$

We carried out Monte Carlo simulation on the Bose-Hubbard model in dilute region, $10^{-3} < na^3 < 10^{-1}$. We used our original package DSQSS[2], which can be downloaded from the GITHUB and can be used under GPL license. We varied the system size L and the inverse temperature β to confirm that the result does not depend on these parameter beyond the statistical error, i.e., our result can be identified with those at zero temperature in the thermodynamic limit.

Figure 1 is our result compared with the analytical predictions made by Lee, Huang and Yang [3]. From this comparison we estimated the s-wave scattering length in the unit of the lattice constant as $a_s/a = 0.315$.

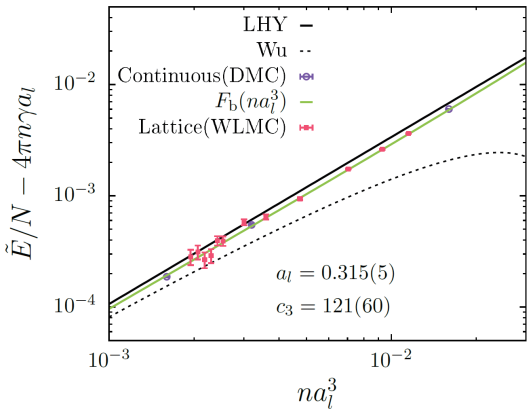

Figure 1: The correction in the normalized energy. The three curves labeled as "LHY", "Wu", and "F_b" represent the analytical prediction up to the first correction, up to the second correction and the third (logarithmic) correction, respectively. The open symbols labeled as "Continuous" are the results of the diffusion Monte Carlo for the continuous-space model whereas the closed symbols are for the present calculation of the lattice system.

[1] This report is based on A. Masaki-Kato, Y. Motoyama and N. Kawashima (unpublished).
[2] https://github.com/qmc/dsqss/wiki
[3] T. D. Lee, K. Huang and C. N. Y. Yang Phys. Rev. 106, 1135 (1957).