

The Hamiltonian operator for the continuous Fermi–Hubbard model is:

$$\hat{H} = -\frac{1}{2} \sum_{l=1}^N \nabla_l^2 + h \sum_{l=1}^N (\cos^2(\pi x_l/L) + \cos^2(\pi y_l/L)) + \sum_{l=1}^{N_\uparrow} \sum_{m=1}^{N_\downarrow} \frac{g}{\pi s^2} e^{-\frac{(\mathbf{r}_l^\uparrow - \mathbf{r}_m^\downarrow)^2}{s^2}}$$

Here, we use  $N_\uparrow = N_\downarrow = 72$  fermions in  $14 \times 14$  lattices as an example.

Using the file in1.txt to run the code for PIMD simulation. In the terminal, the input is “./prog in1.txt out1.txt”. In this case, the simulation result is saved in out1.txt after finishing the MD steps.

We interpret the meaning of the parameters in in1.txt as follows. For continuous Fermi–Hubbard model, see “Samples/Fast PIMD Hubbard” in our codes.

Seed 2 (the random initialization, we may change the number to give different random initialization)

Na 72 (the particle number in  $N_\uparrow$ )

Nb 72 (the particle number in  $N_\downarrow$ )

P 40 (the number of beads for each particle)

insteps 2000000 (the number of MD steps for thermal equilibrium)

MDsteps 1000000 (the number of MD steps for importance sampling)

T 3.0 (the temperature)

vi 1 ( $\xi$  for the fictitious identical particles)

site 14 ( $14 \times 14$  lattices)

L 1.0 (L in  $\hat{H}$ )

h 1.0 (h in  $\hat{H}$ )

g 1 (g in  $\hat{H}$ )

s 0.5 (s in  $\hat{H}$ )