Quantum Monte Carlo for Condensed Matter and Statistical Physics (M2)

TD session **3** F. Mezzacapo, T. Roscilde

General goal and rules of the TD sessions: *The TD sessions are fully hands-on namely, in every TD session you are supposed to write and test different parts of a Path Integral Monte Carlo computer code designed to estimate the physical properties of quantum systems, in some selected cases. You can write the code alone or in a two-people team. You should choose a programming language (C++, Fortran, etc.) and be able to plot your results (using e.g., Gnuplot, the plotting utilities of Matlab, etc.). We assume that you have a reasonable familiarity with at least one programming language.*

1 The model

We will consider the problem of two bosonic particles subjected to an external harmonic potential in one spatial dimension. The Hamiltonian, in the so-called harmonic oscillator natural units (see previous TD sheet), reads:

$$\mathcal{H} = \sum_{i=1}^{N} \left[\frac{1}{2} \frac{\partial^2}{\partial x_i^2} + v(x_i) \right], \text{ with } v(x) = \frac{1}{2}x^2 \text{ and } N = 2. \tag{1}$$

The above model, despite its simplicity, will allow us to investigate important quantum effects arising from particle indistinguishability and bosonic statistics.

2 The swap update

As we have seen in the last TD session, the problem of two distinguishable particles can be tackled after a few trivial modifications of the code used for the single particle case. The required minimal changes are basically related to the estimates of the observables, while the sampling strategy remains essentially unchanged. Conversely, to account for particle indistinguishability,

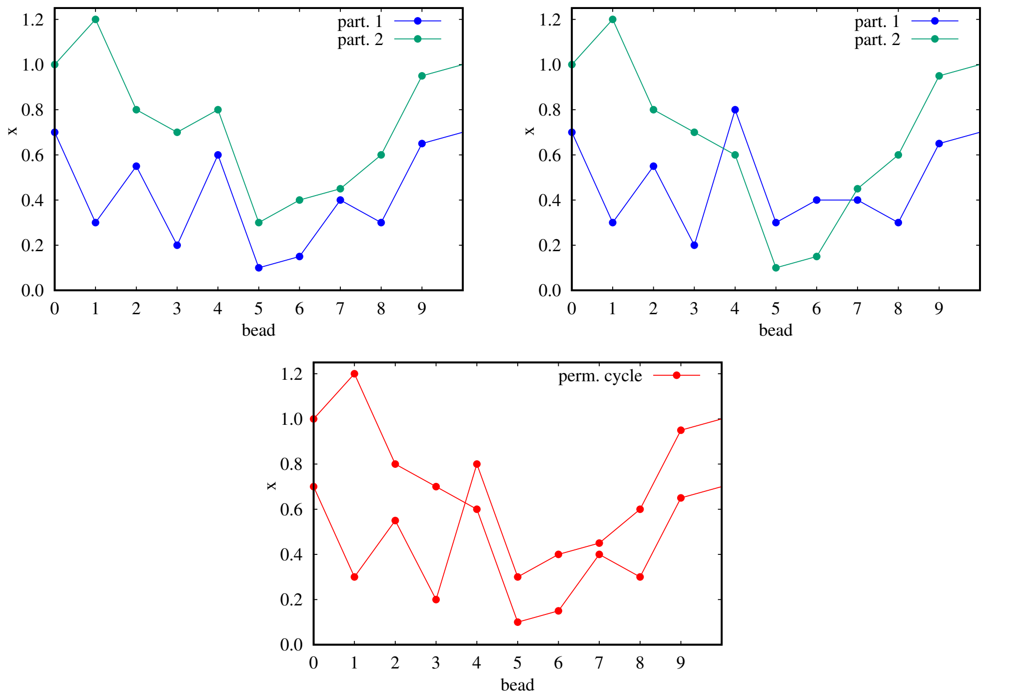

Figure 1: *Illustration of the swap update: Two distinct world lines of* $M = 10$ *beads (left panel) are involved in a permutation cycle after the acceptance of a swap update (middle panel). A subsequent swap destroys the cycle and the resulting world lines are again separate (right panel).*

we have to introduce an additional update known as the swap update. Here we will discuss a very basic implementation of this update.

Let us consider two particles 1 and 2, and the corresponding world lines

$$\begin{aligned} \boldsymbol{x}_1 &\equiv x_{1,0}, \cdots, x_{1,M-1} \text{ (with } x_{1,M} \equiv x_{1,0}) \text{ and} \\ \boldsymbol{x}_2 &\equiv x_{2,0}, \cdots, x_{2,M-1} \text{ (with } x_{2,M} \equiv x_{2,0}). \end{aligned} \tag{2}$$

The attempt of a swap update consists in randomly selecting a bead k (with $k \neq 0$) and proposing a new configuration $\boldsymbol{x}^{new} \equiv \{\boldsymbol{x}_1^{new}, \boldsymbol{x}_2^{new}\}$ such that

$$\begin{aligned} \boldsymbol{x}_1^{new} &\equiv x_{1,0}, \cdots, x_{1,k-1}, x_{2,k}, \cdots, x_{2,M-1} \text{ (with } x_{1,M}^{new} \equiv x_{2,0}) \text{ and} \\ \boldsymbol{x}_2^{new} &\equiv x_{2,0}, \cdots, x_{2,k-1}, x_{1,k}, \cdots, x_{1,M-1} \text{ (with } x_{2,M}^{new} \equiv x_{1,0}). \end{aligned} \tag{3}$$

Figure 1 illustrates the effect of two consecutive swap updates on a given two-particle configuration. Starting from two separate world lines (each comprising $M = 10$ beads) a swap has the effect of "gluing" them in a permutation cycle (middle panel). In this peculiar configuration one can come back to a given initial bead following the path only after having visited all the beads of the the two particles. The permutation cycle disappears after the acceptance of a second swap which leads to a configuration where each world line is again a distinct imaginary-time-periodic entity (right panel).

2.1

Implement the swap update explained above and add it to your code. After this, you should be able to investigate the physics of the Hamiltonian in Eq. (1) in the case of distinguishable, or indistinguishable bosonic particles. You may organize the sampling making use of the following strategy for a global update:

```
for (j = 0; j < N_s; j++)
{
  Randomly select a bead k (with k ≠ 0);
  Extract a random number ϵ uniformly distributed in [0,1];
  If (ϵ < THR) {Propose_swap;}
  else {Propose_displacement;}
  Perform Metropolis acceptance/rejection test;
}
new configuration obtained;
```

In the above pseudo-code N_s is the number of single updates proposed (you can set, for example, $N_s = \alpha MN$ with $\alpha = 0.5 - 1.0$), THR is a real number in $[0, 1]$ which determines the probability of proposing a swap or a displacement single update (see previous TD sheet). Test your code by computing for our two-particle model the energy per particle at an inverse temperature $\beta = 0.5$. Compare your result with the exact one: $e^{ex}_{Bs}(\beta = 0.5) = 1.8527$.

3 Bose vs. Boltzmann I: Energy

In the following we will investigate the effects of particle indistinguishability and bosonic statistics on the properties of model Eq. (1). In particular we will compare results when particles are Bosons or Boltzmannons. In the former case they are indistinguishable, in the latter distinguishable (and obeying the Boltzmann distribution).

3.1

Estimate the energy per particle for $\beta \in [0.3, 1.9]$ in the case of two identical bosons. Plot your results and compare them with the exact expression:

$$e^{ex}_{Bs}(\beta) = \frac{1}{4}\left(\frac{1}{\tanh(\beta/2)} + \frac{2}{\tanh(\beta)} - 1\right). \tag{4}$$

In order to visualize how the energy per particle changes when the bosonic statistics is taken into account you can also plot:

$$\Delta e(\beta) = \frac{e_{Bl}(\beta) - e_{Bs}(\beta)}{e_{Bl}(\beta)}, \tag{5}$$

where e_{Bl} is the energy per particle when the indistinguishability is not considered i.e., when particles are Boltzmannons. You can estimate e_{Bl} by running simulations without the swap updates as in the first TD sessions or using the exact expression (given in the previous TD sheet), to save time.

4 Bose vs. Boltzmann II: Pair distribution function

The pair distribution function is defined as:

$$g(r) = \mathcal{G}\sum_{j=1}^{M} \delta(r_j - r) \tag{6}$$

where $r_j = |x_{1,j} - x_{2,j}|$ and $\mathcal{G}$ is a constant fixed by the normalization condition $\sum_r g(r)dr = 1$. The pair distribution function can be estimated as an histogram analogously to the probability distributions introduced in Sec. 5 of the previous TD sheet.

4.1

Estimate $g(r)$ for a pair of bosons and a pair of boltzmannons at $\beta = 0.5$. Plot the two data sets. What is the main difference?