Theoretical Physics Workshop and Summer school in Svit, Slovakia
8^{th}-15^{th} September 2013
Introduction to Path Integral Monte Carlo methods, by Jakub Imriška

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Exercise 1:
Single particle in a 1-dimensional space in a harmonic potential

The task is to simulate a single particle in a harmonic 1-dimensional potential

$$\hat{\mathrm{H}} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega(n + \frac{1}{2}) \tag{1}$$

at finite inverse temperature β and to reproduce the exactly known total energy

$$E(\beta) = \frac{\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2}. \tag{2}$$

For convenience we set $\hbar = 1$, $\omega = 1$, $m = 1$, $k_B = 1$. We assume M Trotter slices, e.g. finite inverse temperature $\beta \equiv M\tau$.

Follow these steps:

- Implement the Metropolis algorithm with local updates
- Implement the measurement of energy and measurement of the average distance from the potential minumum; alternatively measure the histogram of the probability distribution of the particle position in realspace
- Invent a new type of update, find the acceptance rate and implement it
- Debug your program, check $E(\beta)$ using the provided table

β	1.0	2.0	4.0	5.0	10.0
$E(\beta)$	1.08198	0.656518	0.518657	0.506784	0.500045

  Provide a reliable error estimate either using the binning analysis or by checking that the error estimate does not change if you double the number of sweeps in between measurements while keeping the total number of measurements fixed.

- Check the discretization error ΔE for $\beta = 20$ as a function of $M = 25, 50, 100, 200$

Some reasonable values for the simulation: $\beta = 10$; $M = 100$; number of thermalization sweeps (1 sweep = M attempts of local updates): 20000; total number of sweeps: 300000; 1 measurement each 100 sweeps if using only local updates, with global moves once per 100 updates.

Set the radius of the (Gaussian) random displacement of the updates such that the acceptance probability is not close to 0 or to 1.

Low-temperature checks[1]:

- The mean radius of the ground state is $\langle r\rangle \equiv \int \mathrm{d}x\ |\Psi_{n=0}(x)|^2\,|x| = \sqrt{\frac{\hbar}{\pi m\omega}} \approx 0.5642$.
- The ground state wave function is $\Psi_{n=0}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$. In order to do a fair probability distribution comparison, you have to compute the appropriately binned ground state probabilities $p(a,b) = \int_a^b \mathrm{d}x\,|\Psi_{n=0}(x)|^2 = \frac{1}{2}\mathrm{erf}(a,b)$, and compare those with the measured histogram.

[1] Since the gap of our system is equal to $\hbar\omega$, the low-temperature physics shall be accessible for $T = \frac{1}{\beta} \ll \hbar\omega$.

Exercise 2:
Two interacting spinless bosons in a 1-dimensional space in a harmonic potential

The task is to simulate a 2 interacting (indistinguishable) spinless bosons in a harmonic 1-dimensional potential

$$\hat{\mathrm{H}} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 - \lambda\,|x_1 - x_2| \tag{3}$$

at finite inverse temperature β and to obtain the total energy.[2]

Follow these steps:

- Are the operators $\hat{T}$, $\hat{V}$ bounded from below for any λ?
- Modify your program from Ex.1 for 2 distinguishable particles (no permutations)
- Perform checks for $\lambda = 0$ to reproduce the known energy per particle $E(\beta)$ given in Eq.(2) for the 2 non-interacting (distinguishable) particles
- Implement an update corresponding to the change of permutation
- Debug your program: perform check of the non-interacting case ($\lambda = 0$) for 2 bosons; the exact total energy is

  $$\frac{E^0_{\text{2bosons}}(\beta)}{2} = \frac{\hbar\omega}{4}\left[-1 + 3\coth(\beta\hbar\omega) + \frac{1}{\sinh(\beta\hbar\omega)}\right]. \tag{4}$$

  For further check we employ an approximation to get some reference values: we truncate the 2-particle bosonic basis such that we set an upper bound on the non-interacting energy part.[3] This finite temperature perturbative approach works well for low temperatures and small λ. Check using the table below.

		$E(\beta)/2$ for non-interacting truncation level					precise
β	λ	$0\hbar\omega$	$1\hbar\omega$	$2\hbar\omega$	$3\hbar\omega$	$4\hbar\omega$	$E(\beta)/2$
5.0	0.0	0.5	0.50335	0.50344	0.50344	0.50344	0.50344
	0.1	0.46011	0.46345	0.46270	0.46273	0.46270	?
	0.25	0.40026	0.40361	0.39785	0.39800	0.39794	?
	0.5	0.30053	0.30388	0.27632	0.27698	0.27720	?
	1.0	0.10106	0.10440	−0.04270	−0.04037	−0.05065	?
2.0	0.0	0.5	0.55960	0.58900	0.59494	0.59657	0.59692
	0.1	0.46011	0.51971	0.55073	0.55731	0.55933	?
	0.25	0.40026	0.45987	0.48947	0.49732	0.50059	?
	0.5	0.30053	0.36013	0.37236	0.38320	0.39112	?
	1.0	0.10106	0.16066	0.04609	0.06656	0.07434	?

- Check dependence on M

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[2] Note that the interaction part of the Hamiltonian ($-\lambda\,|x_1 - x_2|$) reflects the Gauss law in 1-dimensional space. The interaction is repulsive for $\lambda > 0$.

[3] Truncation at non-interacting excitation of $3\hbar\omega$ would for instance mean that we consider Hilbert space spanned on these 2-particle states: $|0,0\rangle$, $\frac{1}{\sqrt{2}}(|1,0\rangle + |0,1\rangle)$, $\frac{1}{\sqrt{2}}(|2,0\rangle + |0,2\rangle)$, $|1,1\rangle$, $\frac{1}{\sqrt{2}}(|3,0\rangle + |0,3\rangle)$, $\frac{1}{\sqrt{2}}(|2,1\rangle + |1,2\rangle)$.

Exercise 3 (optional homework session):
Two interacting spinless fermions in a 1-dimensional space in a harmonic potential

The task is to simulate a 2 interacting (indistinguishable) spinless fermions in a harmonic 1-dimensional potential

$$\hat{\mathrm{H}} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 - \lambda\,|x_1 - x_2| \tag{5}$$

at finite inverse temperature β and to obtain the total energy.

Modify your program from Ex.2 for 2 bosons to 2 fermions:

- Add measurement of average sign
- Instead of accumulation of an observable A accumulate $A \cdot \mathrm{sign}$
- Use Jackknife analyses to obtain the thermodynamic average $\langle A \rangle = \frac{\langle A \cdot \mathrm{sign} \rangle}{\langle \mathrm{sign} \rangle}$
- Debug your program: perform check of the non-interacting case ($\lambda = 0$) for 2 fermions; the exact total energy is

$$\frac{E^0_{\mathrm{2fermions}}(\beta)}{2} = \frac{\hbar\omega}{4}\left[1 + 3\coth(\beta\hbar\omega) + \frac{1}{\sinh(\beta\hbar\omega)}\right]. \tag{6}$$

  For further check we employ an approximation to get some reference values: we truncate the 2-particle fermionic basis such that we set an upper bound on the non-interacting energy part.[4] This finite temperature perturbative approach works well for low temperatures and small λ. Check using the table below.

		$E(\beta)/2$ for non-interacting truncation level				precise
β	λ	$0\hbar\omega$	$1\hbar\omega$	$2\hbar\omega$	$3\hbar\omega$	$E(\beta)/2$
5.0	0.0	1.0	1.00335	1.00344	1.00344	1.00344
	0.1	0.92021	0.92356	0.92253	0.92256	?
	0.25	0.80053	0.80388	0.79652	0.79671	?
	0.5	0.60106	0.60440	0.57197	0.57272	?
	1.0	0.20212	0.20546	0.06063	0.06293	?
2.0	0.0	1.0	1.05960	1.08899	1.09494	1.09692
	0.1	0.92021	0.97981	1.0096	1.0160	?
	0.25	0.80053	0.86013	0.88527	0.89257	?
	0.5	0.60106	0.66066	0.66111	0.67068	?
	1.0	0.20212	0.26172	0.13703	0.15504	?

- Check dependence on M

[4] Truncation at non-interacting excitation of $2\hbar\omega$ would for instance mean that we consider Hilbert space spanned on these 2-particle states: $\frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle)$, $\frac{1}{\sqrt{2}}(|2,0\rangle - |0,2\rangle)$, $\frac{1}{\sqrt{2}}(|3,0\rangle - |0,3\rangle)$, $\frac{1}{\sqrt{2}}(|2,1\rangle - |1,2\rangle)$.

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Supplements

Download and installation of the ALPS library:
`<http://alps.comp-phys.org/mediawiki/index.php/Download_and_install_ALPS_2>`

Usage of the statistical tools from ALPS library in your `c++` program:
`<http://alps.comp-phys.org/mediawiki/index.php/Tutorials:AleaHOWTO>`

Usage of the statistical tools from ALPS library in your `Python` program:
`<http://alps.comp-phys.org/mediawiki/index.php/Tutorials:Code-01_Python>`