# Computational Quantum Physics
# Exercise 10

PHYS-463
Prof. G. Carleo

---

**Problem 10.1 Reptation Quantum Monte Carlo**

The goal of this first exercise is to implement the Reptation Quantum Monte Carlo algorithm for particles in $d = 1$ spatial dimension. Using this algorithm we ultimately want to find the ground-state and its energy for the anharmonic oscillator $V = \frac{1}{2}x^2 + \lambda x^4$ ($\hbar = m = 1$).

a) For the Reptation Quanutum Monte Carlo algorithm we need an Ansatz wave-function for $|\Psi(\tau = 0)\rangle$ as well as a way to compute its energy. As an Ansatz we choose $\Psi = \exp[-\theta x^2]$ for $\theta > 0$. From the lecture (Chapter 8.1.1.1) we know that the estimator for the energy (local energy) can be written as

$$E_{\text{loc}} = \int dx' \langle x| \hat{H} |x'\rangle \frac{\langle x'|\psi\rangle}{\langle x|\psi\rangle} = \frac{\langle x| \hat{H} |\psi\rangle}{\langle x|\psi\rangle} \tag{1}$$

From the real-space representation of the potential energy operator $\hat{V}|x\rangle = V(x)|x\rangle$ and momentum operator $\hat{p}|x\rangle = i\frac{\partial}{\partial x}|x\rangle$ and using the Anstaz $\Psi$ derive an explicit expression for the local energy!
(*HINT*: To verify your results it holds that for an Ansatz of the form $\Psi = \exp[J(x)]$ the local energy is given by: $E_{\text{loc}} = -\frac{1}{2}[J''(x) + (J'(x))^2] + V(x)$.)

b) Using the above, implement the Reptation Quantum Monte Carlo algorithm as described in Chapter 11.4.2.2. You can use the template provided on Moodle.

c) **Imaginary-Time evolution**
In a first step, compute the imaginary-time evolution for a harmonic oscillator in 1D i.e. $V(x) = \frac{1}{2}x^2$ with the gaussian initial state $\Psi$ defined above.

Take $\theta = 0.1$, and a time step $\Delta_\tau = 0.1$. Do simulations at different imaginary times $\tau = 0.1, 0.2, \ldots 2$, and on each measure the expectation value (and its error) of the Hamiltonian, using the estimator derived above. Does it converge to the exact value?

d) **Potential energy**
For the same simulations, compute also the expectation value of the potential energy and its statistical error.

e) **Wave-Function evolution**
Determine the wave-function sampled by the Reptation QMC at each imaginary time $\tau$.

Do simulations at different imaginary times $\tau = 0.1, 0.5, 2, 5$ and for each simulation compute the histogram of configurations in the middle of the path. How are they distributed? What distribution should they approach in the limit of large $\tau$?

f) **Time step**
Now change the time step, for example take $\Delta_\tau = 0.1, 0.2, 0.5, 0.7$ and for each of those do an imaginary-time evolution for $\tau = 5$. Plot the expectation value of the energy as a function of the time step. Why does it change?

g) **Exact evolution**
How would you compute analytically or numerically (with exact diagonalization techniques) the exact imaginary-time evolution? Compute it and compare the expectation value of the energy with the one obtained with the QMC.

h) **Anharmonic oscillator**
Finally consider the anharmonic oscillator $V_1 = \frac{1}{2}x^2 + \lambda x^4$ and use the Reptation QMC to find the exact ground-state energy and wave-function for $\lambda = 0.2$ using the same variational Ansatz as for the harmonic case.

**Problem 10.2 Helium atom [Only for the brave]**

a) **3 dimensions**
Adapt the QMC code to work in 3 dimensions and for $N$ particles.

b) **Importance-Sampled propagator**
Change transition probability to implement the propagator with importance sampling. Change also, according to the prescriptions in the lecture notes, the acceptance probabilities.

c) **Local Energy**
Now consider the Helium atom Hamiltonian in the approximation of infinitely heavy nucleus:

$$H(\vec{r_1}, \vec{r_2}) = -\frac{1}{2}\nabla^2_{r_1} - \frac{1}{2}\nabla^2_{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \tag{2}$$

where $r_{12} = |\vec{r_1} - \vec{r_2}|$ is the distance between the two electrons, and $r_1$ is the distance of atom 1 from the nucleus (assumed to be fixed at the coordinate center) and equally for $r_2$, the distance of the other electron from the nucleus. Take as a variational state the two-body Jastrow wave-function:

$$\Psi(\vec{r_1}, \vec{r_2}) = \exp\left[-2r_1 - 2r_2 + \frac{r_{12}}{2(1+\theta\, r_{12})}\right] \tag{3}$$

, where $\theta$ is a variational parameter. Show that the local energy in this case is:

$$E_{\rm loc}(\vec{r_1}, \vec{r_2}) = -4 + \frac{\theta}{(1+\theta\, r_{12})} + \frac{\theta}{(1+\theta\, r_{12})^2} + \frac{\theta}{(1+\theta\, r_{12})^3} - \frac{1}{4(1+\theta\, r_{12})^4} + \frac{\hat{r}_{12}\cdot(\hat{r}_1 - \hat{r}_2)}{(1+\theta\, r_{12})^2}, \tag{4}$$

where $\hat{r} = \vec{r}/|r|$.

Start with a reasonable value of $\theta$ and compute the exact ground-state energy with the Reptation QMC.