Name: ____________________, ____________________

PHYSICS 401 : SPRING SEMESTER 2018

Project #10: Variational Monte Carlo

Reference Reading: Sections 11.5, 11.7, 16.7.

Downloads: None.

1) Consider the harmonic oscillator Hamiltonian operator

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2.$$

If we take a trial wave function (not normalized) as

$$\psi(x) = \mathrm{e}^{-\alpha x^2},$$

what is the local energy function

$$E_L(x) = \frac{\hat{H}\psi(x)}{\psi(x)}?$$

2) Now generate $\{x_i\}$ according to $p(x) \propto \psi^2(x) \propto \mathrm{e}^{-2\alpha x^2}$ using the Box-Mueller method. (Note that here, $\Delta t = 1/(4\alpha)$) and compute the expectation value via

$$\langle E_L \rangle = \frac{1}{n}\sum_{i=1}^{n} E_L(x_i)$$

for $\alpha = 0.2 - 0.8$ in steps of $\Delta\alpha = 0.05$ with $n = 10^6$. Plot $\langle E_L \rangle$ vs. α and hand in this graph. What is the minimum value of $\langle E_L \rangle$, corresponding to what values of α?

3) Now generate 3 Gaussian random variables $\{x_i, y_i, z_i\}$ at the same time to sample the 3D wave function

$$\psi(r) = \psi(x, y, z) = \exp[-\alpha(x^2 + y^2 + z^2)]$$

as a trial wave function for the *Hydrogen* Hamiltonian:

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}$$

where $r = \sqrt{x^2 + y^2 + z^2}$. What is your the local energy function (it is a function of x, y, z via r)

$$E_L(x, y, z) = \frac{H\psi(x, y, x)}{\psi(x, y, z)}$$

in this case ? Now again compute the expectation values

$$\langle E_L \rangle = \frac{1}{n}\sum_{i=1}^{n} E_L(x_i, y_i, z_i)$$

for $\alpha = 0.05 - 0.5$ in steps of $\Delta\alpha = 0.05$ with $n = 10^6$. Plot $\langle E_L \rangle$ vs. α and hand in this graph. What is the minimum value of $\langle E_L \rangle$, corresponding to what values of α?

4. Use the Metropolis algorithm to sample a set of 3-dimensional vectors $\{\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N\}$ (take $N = 10^6$) according to

$$\Psi_T^2(r) = \mathrm{e}^{-2\alpha r},$$

where $r = \sqrt{x^2 + y^2 + z^2}$. You do this by starting at some initial position

$$\mathbf{r} = (x, y, z),$$

change it by adding to it a uniform random displacement vector

$$\Delta\mathbf{r} = (r_{max} * [ran(iseed) - .5], r_{max} * [ran(iseed) - .5], r_{max} * [ran(iseed) - .5]),$$

getting

$$\mathbf{r}' = \mathbf{r} + \Delta\mathbf{r},$$

then accept or reject this new position according to the ratio

$$R = \frac{\Psi_T^2(\mathbf{r}')}{\Psi_T^2(\mathbf{r})}$$

as prescribed by the Metropolist algorithm. Adjust r_{max} so that the new position $\mathbf{r}'$ is accepted about 50% to 30% of the time. After you have updated 50-100 times, (allowing the system to equilibrate to its equilibrium distribution), evaluate the variational energy as

$$\langle E_L \rangle = \frac{1}{n} \sum_{i=1}^{n} E_L(x_i, y_i, z_i)$$

where now

$$E_L(x_i, y_i, z_i) = \frac{H\Psi_T(x, y, x)}{\Psi_T(x, y, z)}$$

and

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}.$$

Plot $\langle E_L \rangle$ vs α (take α=0.5 to 1.5 in increments of 0.05). Plot also the curve corresponding to the expected theoretical result

$$E_V = \frac{1}{2}\alpha^2 - \alpha.$$

Hand in this plot and comment on the comparison.

5. (10 pt bonus) Plot your results using the standard error σ_{E_L} as your error bar. (Don't forget to divide by $\sqrt{n}$ where n is the number of uncorrelated data points you averaged over.)