Computational Science 2

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Seminar
Exercises

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Exercise 8 (25.06.2013):

Variational estimate of ground states

from ***An Introduction to Computer Simulation Methods***,
Chapter 16, Problems 16.24,25

a) It is useful to test the variational method on an exactly solvable problem. Consider the one-dimensional harmonic oscillator with $V(x) = x^2/2$. Choose the trial wave function to be $\Psi(x) \propto e^{-\lambda x^2}$, with λ the variational parameter. Generate values of x using the Metropolis method. Remember that it is necessary to wait for equilibrium (convergence to the distribution Ψ^2) before computing the average value of the local energy E_L. Look for a systematic trend in $\langle E_L \rangle$ over the course of the random walk. Choose a step size δ that gives a reasonable value for the acceptance ratio. How many trials are necessary to obtain $\langle E_L \rangle$ to within 1% accuracy compared to the exact analytic result?

b) Instead of finding the minimum of $\langle E_L \rangle$ as a function of the various variational parameters, minimize the quantity $\sigma_L^2 = \langle E_L^2 \rangle - \langle E_L \rangle^2$. Verify that the exact minimum value of $\sigma_L^2[\Psi]$ is zero, whereas the exact minimum value of $E_L[\Psi]$ is unknown in general.

c) Consider the anharmonic potential $V(x) = \frac{1}{2}x^2 + bx^4$. Plot $V(x)$ as a function of x for $b = 1/8$. Use first-order perturbation theory to calculate the lowest order change in the ground state energy due to the x^4 term. Then choose a reasonable form for your trial wave function and use your Monte Carlo program to estimate the ground state energy. How does your result compare with first-order perturbation theory?

d) Consider the anharmonic potential of part (c) with $b = -1/8$. Plot $V(x)$. Use first-order perturbation theory to calculate the lowest order change in the ground state energy due to the x^4 term, and then use your program to estimate E_0. Do your Monte Carlo estimates for the ground state energy have a lower bound? Why or why not?

e) Modify your program so that it can be applied to the ground state of the hydrogen atom. In this case we have $V(r) = -e^2/r$, where e is the magnitude of the charge on the electron. The element of integration dx is replaced by $4r^2dr$. Choose $\Psi \propto e^{-r/a}$, where a is the variational parameter. Measure lengths in terms of the Bohr radius $\hbar^2/me^2$ and energy in terms of the Rydberg $me^4/2\hbar^2$. In these units $\mu = e^2 = \hbar = 1$. Find the optimal value of a. What is the corresponding energy?

f) Consider the Yukawa or screened Coulomb potential for which $V(r) = -e^2e^{-\alpha r}/r$, where $\alpha > 0$. In this case the ground state and wave function can only be obtained numerically. For $\alpha = 0.5$ and $\alpha = 1.0$ the most accurate numerical estimates of E_0 are -0.14808 and -0.01016, respectively. What is a good choice for the form of the trial wave function? How close can you come to these estimates?

g) Helium has long served as a testing ground for atomic trial wave functions. Consider the ground state of the helium atom with the interaction

$$V(r_1, r_2) = -2e^2 \left(\frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{e^2}{r_{12}} \tag{1}$$

where r_{12} is the separation between the two electrons. Assume that the nucleus is fixed and ignore relativistic effects. Choose $\Psi(r_1, r_2) = Ae^{-Z_{\text{eff}}(r_1+r_2)/a_0}$, where Z_{eff} is a variational parameter. Estimate the upper bound to the ground state energy based on this functional form of Ψ.