Phys 535 **Exercises**

Deadline: Friday 4 November 2005

Question 1 *Quantum Monte Carlo*

Consider a particle in the potential well

$$U(x) = \begin{cases} \infty \ , & x < 0 \ , \\ \alpha x \ , & x \geq 0 \ . \end{cases}$$

The Schrödinger equation is

$$\hat{H}\psi \equiv -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi \ ,$$

where $\hat{H}$ is the Hamiltonian, $\hbar$ is Planck's constant, m is the particle mass, and E is the energy for the eigenstate ψ.

(a) Non-dimensionalize the equation: Introduce new dimensionless variables ξ and $\tilde{E}$ via

$$x = L\xi \ , \qquad E = \varepsilon\tilde{E} \ ,$$

where L and ε are characteristic length and energy, respectively. Choose L and ε such that the Schrödinger equation takes the form

$$-\frac{d^2\psi}{d\xi^2} + \xi\psi = \tilde{E}\psi \ . \tag{1}$$

(b) The variational principle for Eq. (1) states that

$$E_0 \ \leq \ \frac{\int\limits_{-\infty}^{\infty} \Phi(x)\hat{H}\Phi(x)\,dx}{\int\limits_{-\infty}^{\infty} \Phi(x)^2\,dx}$$

(for a real wave function $\Phi(x)$). Using the trial wave function

$$\Phi(x) = Axe^{-kx} \ ,$$

find a Monte Carlo approximation E to the energy E_0 of the ground state for a particle in the potential well:

(i) Monitor the acceptance ratio and try to ensure that it is always ≈ 0.5.

(ii) Find $E(k)$ for a set of values of the parameter k, at least $\{0.5, 1, 1.5, 2\}$.

(iii) Obtain an estimate of the statistical error.

(iv) Compare your result (lowest energy and corresponding trial wave function) to the analytic solution

$$\tilde{E} = -a_1 \qquad \psi(x) \propto \mathrm{Ai}(\xi - \tilde{E}) \;, \tag{2}$$

where $\mathrm{Ai}\,x$ is the *Airy function* of the first kind, and $a_1 \approx -2.33811$ is its first negative zero.

[Hint: You can find an IDL import of the Airy function under `gsl_airy.pro` — see the documentation in that file.] and discuss.

(c) For $k = 1.$ (and the step length that gave you an acceptance ratio ≈ 0.5), plot the autocorrelation coefficient

$$a(n) = \varrho(x_i, x_{i+n})$$

and give an estimate of the correlation "time".

Hints:

- For time lags n larger than the correlation time, the autocorrelation coefficient fluctuates around zero, while for shorter time lags ϱ is considerably larger than 0.
- IDL has a routine `correlate` that calculates $\varrho()$.

(d) If you choose a normal distribution for the displacement instead of a uniform one, do the energies change? Can you explain?