Quantum Physics 2011/12

Tutorial Sheet 5: Variational Method

An asterisk denotes a harder problem, which you are nevertheless encouraged to try!

1. Estimate the ground-state energy of a 1-dimensional simple harmonic oscillator using as trial function

   (a) $\psi_a(x) = \cos \alpha x$ for $|\alpha x| < \pi/2$, zero elsewhere,

   (b) $\psi_b(x) = \alpha^2 - x^2$ for $|x| < \alpha$, zero elsewhere,

   (c) $\psi_c(x) = C \exp(-\alpha x^2)$

   (d) * $\psi_d(x) = C(\alpha - |x|)$ (for $|x| < \alpha$, zero elsewhere)

   (e) $\psi_e(x) = C \sin \alpha x$ (for $|\alpha x| < \pi$, zero elsewhere)

   In each case, α is the variational parameter. Don't forget the normalisation. Sketch the wavefunctions and compare them with the actual ground-state wavefunction.

   Numerical answers for checking (a) $0.568\hbar\omega$ (b) $0.598\hbar\omega$ (c) $0.5\hbar\omega$ (d) $0.5477\hbar\omega$ (e) $1.67\hbar\omega$

   Where does the kinetic energy come from in (d)? You will have to consider carefully how to calculate it.

   Write down the overlap integral $\langle \psi_i(x) | \psi_j(x) \rangle$ between the wavefunction in (e) and each of the other four: Why does (e) represent an estimate of the first excited state?

   You may use the results

   $$\int_{-\infty}^{\infty} \exp(-\alpha x^2) \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} \qquad \text{and} \qquad \int_{-\infty}^{\infty} x^2 \exp -\alpha x^2 dx = \frac{\sqrt{\pi}}{2\alpha^{3/2}}$$

   $$\int_{-\pi/2\alpha}^{\pi/2\alpha} x^2 \cos^2 \alpha x \, \mathrm{d}x = \pi(\pi^2 - 6)/24\alpha^3$$

2. * A particle moves in one dimension in the potential

   $$V(x) = \infty, \quad |x| > a, \qquad V(x) = 0, \quad |x| \le a$$

   Use a trial function of the form

   $$\psi_T(x) = \begin{cases} (a^2 - x^2)(1 + cx^2), & |x| \le a \\ 0, & |x| > a \end{cases}$$

   and show that the energy is

   $$E(c) = \left(\frac{3\hbar^2}{4ma^2} \right) \frac{11a^4c^2 + 14a^2c + 35}{a^4c^2 + 6a^2c + 21}$$

   Now, treating c as a variational parameter, obtain an upper bound on the ground-state energy. (You may wish to use maple).

$$E(c^{(1)}) = 1.23372\frac{\hbar^2}{ma^2}, \qquad E(c^{(2)})$$

How does your bound compare with the exact ground-state energy?

3. * Repeat the previous problem taking

$$\psi_T(x) = \begin{cases} (a^2 - x^2)(x + cx^3), & |x| \leq a \\ 0, & |x| > a \end{cases}$$

as the trial function. Why does this give an upper bound for the first excited energy level? Compare your variational result with the exact eigenvalue of the $n = 2$ level.

4. A "1d atom" has ground state wavefunction $u_1(x) = \exp -\alpha|x|$.

   Consider a ring of N such atoms, one centred on $x = 0$ separated by a distance d. Using the single site wavefunctions $u_{1j}(x + jd)$ as LCAO basis functions, what are the eigenfunctions according to Bloch's theorum in 1D.

   write down the single-particle ground state wavefunction which is an eigenstate of the displacement operator assuming that

$$\langle u_1(x)|u_1(x + d)\rangle << 1$$

   What is the normalisation for this wavefunction?

   A computational physicist solves for this wavefunction using the variational method, with a trial wavefunction $\psi_T(r)$ and a set of variational parameters c_k, $k = 2\pi/Nd$

$$\psi_T(x) = \sum_k c_k \cos kx$$

   Using your knowledge of the symmetry of the exact atomic solution u_1, what can you say without calculation about the coefficients c_k, and allowed values of k?

   What would you get from a trial wavefunction of the form

$$\psi_T(r) = \sum_k c_k \sin kx$$

5. Obtain a variational estimate of the ground-state energy of the hydrogen atom by taking as trial function

$$\psi_T(r) = \exp(-\alpha r^2)$$

   How does your result compare with the exact result? Sketch the trial wavefunction and the actual wavefunction on the same graph.

   You may use the integrals in Question 1 and

$$\int_0^\infty r^4 exp(-2ar)dr = \frac{3\sqrt{2\pi}}{64a^{5/2}}$$

$$\int e^{-\alpha r^2}(4\alpha^2 r^2 - 6\alpha)e^{-\alpha r^2}4\pi r^2 dr = \frac{-3}{16}\sqrt{\frac{2\pi}{a}}$$