Problem Set 8

Due Tuesday December 3 at 9:30 AM.
Submit in class or in TA's mailbox in the Physics office.

1. Shankar 11.4.1

2. Shankar 11.4.2

3. Shankar 11.4.3

4. Consider a system of five atomic sites arranged in a square, with site 5 at the center of the square. Let

$$\langle\varphi_i|H|\varphi_{i+1}\rangle = -\Delta,\ i = 1,2,3 \tag{1}$$
$$\langle\varphi_4|H|\varphi_1\rangle = -\Delta \tag{2}$$
$$\langle\varphi_i|H|\varphi_5\rangle = -\Delta,\ i = 1,2,3,4 \tag{3}$$
$$\langle\varphi_i|H|\varphi_i\rangle = \varepsilon,\ i = 1,2,3,4,5 \tag{4}$$
$$\tag{5}$$

   where Δ is real. All other matrix elements, apart from those constrained by the fact that H is Hermitian, are 0. We will use symmetries of H to find the energy eigenvectors and eigenvalues. For concreteness, let's say that site 1 is in the upper left, and that the site numbering goes clockwise from there.

   (a) First, find the eigenvectors and eigenvalues of the Hamiltonian using the Π_x symmetry, where Π_x is the operator which reflects the system across a vertical line through site 5.

   (b) Next, find the eigenvectors and eigenvalues of the Hamiltonian using the symmetry of a rotation through an appropriate angle.

   (c) Verify that the two approaches yield consistent results, both in terms of eigenvalues and eigenvectors of the Hamiltonian.

5. This problem deals with the anharmonic oscillator:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + \lambda x^4 \tag{6}$$

   (a) Rescale the variables so that the problem for $\lambda = 0$ is given in dimensionless variables. (Hint: express the dimensionless operator $h = H/(\hbar\omega)$ in terms of the dimensionless position operator $z = \beta x$ which we have used in class.) Show that the eigenvalues of H take the form

$$E = \hbar\omega f(\Lambda), \tag{7}$$

   with $\Lambda = \hbar\lambda/m^2\omega^3$ (a dimensionless quantity). From here on, you can set $m = k = \hbar = \omega = 1,\ \lambda = \Lambda$.

(b) Estimate the ground state energy of the anharmonic oscillator by computing

$$E_{\text{try}} = \langle 0|H|0\rangle, \tag{8}$$

where $|0\rangle$ is the ground state of the oscillator with $\Lambda = 0$. This calculation is quite straightforward if you use ladder operators.

(c) Compute the 'exact' ground state energy of the anharmonic oscillator for the cases $\Lambda = 0.2$ and $\Lambda = 1$ by numerically integrating the Schrödinger equation, and compare to the result of part (b). The answer in part (b) should be an upper bound to the numerical result. Explain this inequality.

(d) To get a better estimate of the ground state energy of the anharmonic oscillator, form a trial state from a larger basis set. To begin, try to form the ground state as a linear combination of the states $|0\rangle$ and $|2\rangle$. (Why not $|1\rangle$?). This leads to a 2×2 matrix problem, for which the lowest eigenvalue estimates the ground state energy. Again, it is easiest to compute the matrix elements of this matrix by using ladder operators.

(e) Actually, it is not much harder to consider a larger basis set. Using the ladder operator calculations in part (d), write down the matrix elements of the Hamiltonian between the states of the set $|0\rangle$, $|2\rangle$, $|4\rangle$, $|6\rangle$. Use Mathematica or equivalent to compute the eigenvalues of this 4×4 matrix numerically for the cases $\Lambda = 0.2$ and $\Lambda = 1$. Compare to the results of part (b).