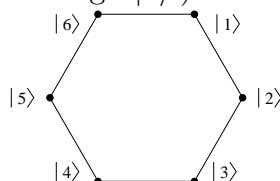


Homework Set #4 – Due Friday, February 7

1. A molecule is composed of six identical atoms which form a regular hexagon. Consider a single electron which can be localized on any one of the atoms. Let $|n\rangle$ denote the state in which it is localized on the n -th atom. (This is a six-dimensional Hilbert space, spanned by the states $|1\rangle$ through $|6\rangle$.)



Let R be the discrete rotation operator, $R|i\rangle = |i + 1\rangle$ (where we let $|7\rangle \equiv |1\rangle$ and $|0\rangle \equiv |6\rangle$). We assume that the Hamiltonian has the form

$$H = \sum_{i=1}^6 \left(E_0 |i\rangle\langle i| - \lambda (|i\rangle\langle i+1| + |i\rangle\langle i-1|) \right)$$

(λ represents a nearest-neighbor electron hopping interaction).

- a) Find the eigenvalues and eigenstates of R , and show that they are non-degenerate.
 - b) Show that R commutes with the Hamiltonian, and find the eigenvalues and eigenstates of H .
2. Show that, to next order in the semi-classical expansion, the WKB wavefunction may be written as

$$\psi(x) = \frac{1}{\sqrt{k(x)}} e^{\pm i \int k(x) dx} \left[1 \mp \frac{i\hbar}{4} \left(m \frac{F(x)}{p^3(x)} + \frac{1}{2} m^2 \int \frac{F^2(x)}{p^5(x)} dx \right) + \dots \right]$$

where $p(x) = \hbar k(x)$, and $F(x) = p'(x)p(x)/m$ is the classical force. Explain why the second order term may often be neglected, while the first order term (the $1/\sqrt{k(x)}$ factor) should be retained in the WKB approximation.

3. A neutron falling in a gravitational field and bouncing off a horizontal mirror exhibits quantized energy levels [see Nesvizhevsky *et al.*, Nature **415** (2002) 297]. The potential felt by the neutron is essentially

$$V(z) = \begin{cases} mgz & z > 0 \\ \infty & z < 0 \end{cases}$$

- a) Use the WKB bound state condition for turning points at $z = 0$ and $z = E/mg$ to find the quantized energy levels of the bouncing neutron. Write down the first three energy levels in units of $(mg^2\hbar^2)^{1/3}$.

- b) Note that this potential is essentially half of the absolute value potential $V(z) = mg|z|$ [see *Merzbacher* pp. 123–125]. However, for the neutron, because of the mirror at $z = 0$, we must impose a boundary condition $\psi(0) = 0$. This is equivalent to finding odd-parity solutions of the $V(z) = mg|z|$ problem.

Find a WKB expression for the odd-parity energy levels of the $V(z) = mg|z|$ problem. Again, write down the first three energy levels in units of $(mg^2\hbar^2)^{1/3}$.

- c) Compare your energies from parts a) and b) with the exact values (in units of $(mg^2\hbar^2)^{1/3}$)

$$E_0 = 1.8558, \quad E_1 = 3.2446, \quad E_2 = 4.3817$$

(for the neutron, $E_0 \approx 1.41 \times 10^{-12}$ eV). Which approximation is the better one, and why?

4. For a spherically symmetric potential, the radial equation for $u(r)$, where $\psi(r, \theta, \varphi) = r^{-1}u(r)Y_\ell^m(\theta, \varphi)$, is effectively one-dimensional

$$-\frac{\hbar^2}{2m} \frac{d^2u}{dr^2} + V_{\text{eff}}(r)u = Eu, \quad V_{\text{eff}}(r) = V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}$$

As a result, we may apply WKB to $u(r)$, however with a slight refinement of using

$$V_{\text{WKB}}(r) = V(r) + \frac{\hbar^2(\ell + \frac{1}{2})^2}{2mr^2}$$

instead of V_{eff} . Show that the WKB bound state condition gives the exact energy levels for both the hydrogen atom ($V(r) = -e^2/r$) and the three-dimensional harmonic oscillator ($V(r) = \frac{1}{2}m\omega^2r^2$). You may want to use the integral

$$\int_a^b \frac{dr}{r} \sqrt{-(r-a)(r-b)} = \frac{\pi}{2}(a+b-2\sqrt{ab}), \quad 0 < a < b$$