Physics 221A
Fall 2007
Homework 12
Due Monday, November 26, 2007 at 5pm

Reading Assignment: Sakurai, pp. 248–275; rest of Notes 16, Notes 17, pp. 1–12 of Notes 18.

Note: This homework is due the Monday after Thanksgiving, but there will be another due as usual on the following Friday.

1. Consider a one-dimensional periodic potential $V(x)$, as in the figure. The potential is periodic with period a, while the x variable is periodic with period Na, as in lecture. In this problem we use WKB theory to understand the band structure of the energy levels in this potential.

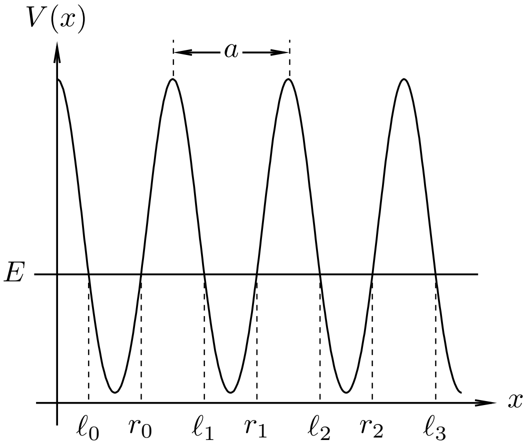

Figure for Problem 1. A periodic potential with lattice spacing a. The left and right turning points in the j-th region are ℓ_j and r_j, respectively.

(a) Consider an energy E as in the figure. Notice the left and right turning points ℓ_j and r_j in each well, where $j = 0, \ldots, N-1$. The energy is assumed to be not too close to the top of the potential wells. "Not too close" means that the tunnelling action κ, defined by

$$\kappa = \frac{1}{\hbar}\int_{r_j}^{\ell_{j+1}} dx\,|p(x)|dx, \tag{1}$$

is large enough that e^{κ} can be considered large and $e^{-\kappa}$ small. Here

$$p(x) = \sqrt{2m[E - V(x)]}, \tag{2}$$

as usual in one-dimensional WKB theory. Thus we will be studying the energy levels (and energy bands) that are close to the ground state.

Let us define the phase Φ as a function of energy E by

$$\Phi = \Phi(E) = \frac{1}{\hbar} \oint p\,dx = \frac{2}{\hbar} S(r_j, \ell_j), \tag{3}$$

where

$$S(x, \ell_j) = \int_{\ell_j}^{x} p(x')\,dx'. \tag{4}$$

If the tunneling between wells could be neglected, for example, if the barriers between wells were raised infinitely high, then the Bohr-Sommerfeld rules would say that the m-th energy eigenvalue E_m in each well would be given by

$$\Phi(E_m) = \Phi_m = (m + \tfrac{1}{2})2\pi. \tag{5}$$

Call E_m the "nominal" Bohr-Sommerfeld energy eigenvalue. Also, the eigenfunction inside the j-th classically allowed region would be,

$$\psi(x) = \frac{1}{\sqrt{p(x)}} \cos\Big[\frac{S(x, \ell_j)}{\hbar} - \frac{\pi}{4}\Big], \tag{6}$$

apart from normalization.

Because of tunneling, however, the wave functions in the different wells do communicate with each other. Let the wave function in the classically allowed region of the j-th well be

$$\psi_j(x) = \frac{1}{\sqrt{p(x)}} \Big[A_j \cos\Big(\frac{S(x, \ell_j)}{\hbar} - \frac{\pi}{4}\Big) + B_j \sin\Big(\frac{S(x, \ell_j)}{\hbar} - \frac{\pi}{4}\Big)\Big], \tag{7}$$

where A_j and B_j are coefficients to be determined. Use WKB theory to obtain the 2×2 matrix M such that

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = M \begin{pmatrix} A_j \\ B_j \end{pmatrix}. \tag{8}$$

Show that $\det M = 1$.

(b) Now let M be any real, 2×2 matrix with unit determinant,

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{9}$$

with $ad - bc = 1$, and let $q = (1/2)\,\mathrm{tr}\, M = (a + d)/2$. Show that if $|q| > 1$, then the eigenvalues of M are real and reciprocals of one another, so that one is > 1 in absolute value and one is < 1 in absolute value. Show that if $|q| < 1$, then the eigenvalues are phase factors that are complex conjugate pairs. In that case, write $\lambda = e^{\pm i\theta}$.

Use the boundary conditions on the wave function to find the allowed values of q and hence θ. Show that the allowed values of θ correspond to the eigenfunctions of the translation operator, as discussed in class. Call these θ_n, $n = 0, \ldots, N-1$.

(c) Now return to the specific matrix M found in part (a). Using the approximation $e^{-\kappa} \ll 1$, set $\Phi = \Phi_m + \delta$, where δ is small, and solve for δ in terms of n and m. Now use the classical relation

$$\frac{dJ}{dE} = \frac{2\pi}{\omega}, \tag{10}$$

where $J = \Phi\hbar$ is the action of the orbit and ω is the classical frequency of oscillation, to obtain the energy levels E_{mn} in the periodic potential in terms of the nominal Bohr-Sommerfeld level E_m plus a small correction that depends on n. Show that as n goes from 0 to $N-1$, the levels cycle up and down in a small band centered on E_m.

(d) For the eigenvalue $\lambda = e^{i\theta}$ of M, find the eigenvector of M in the approximation $e^{-\kappa} \ll 1$. Call the eigenvector (A_0, B_0). Normalize by setting $A_0 = 1$, and show that the coefficient B_0 is small. Show that the energy eigenfunctions are real and nondegenerate when $\theta = 0$ or $\theta = \pi$, at the top or the bottom of the bands, but in between, they are complex and 2-fold degenerate (the two degenerate eigenfunctions are complex conjugates of each other).

2. This is essentially Sakurai's problem 4.4, p. 282, but I've rewritten it to make it more clear.

We did not discuss the spin angular functions in class, but these are spinor functions on the unit sphere that arise when we combine orbital and spin angular momentum for a central force problem for a spinning particle. Here we will take the case $s = \frac{1}{2}$ (for example, in hydrogen). Let $|n\ell m_\ell\rangle$ be ket language for the wave function $R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)$, the solution of the Schrödinger equation for a spinless particle in a central force field, and let $|sm_s\rangle$ be the usual spin states (here $s = \frac{1}{2}$ and $m_s = \pm\frac{1}{2}$). We distinguish between m_ℓ and m_s, the two types of magnetic quantum numbers. We multiply the wave functions times the spin functions and form linear combinations with the Clebsch-Gordan coefficients to get eigenstates of J^2 and J_z, where $\mathbf{J} = \mathbf{L} + \mathbf{S}$. These are

$$|n\ell jm_j\rangle = \sum_{m_\ell, m_s} |n\ell m_\ell\rangle |sm_s\rangle \langle \ell s m_\ell m_s | jm_j\rangle. \tag{11}$$

The spatial wave functions $\psi_{n\ell m_\ell}(\mathbf{r}) = R_{n\ell}(r) Y_{\ell m_\ell}(\theta, \phi)$ factor into a radial part times an angular part. Let us write this in ket language as $|n\ell m_\ell\rangle = |n\ell\rangle|\ell m_\ell\rangle$. The factor $R_{n\ell}(r)$ or $|n\ell\rangle$ is the same for all terms in the sum above, so it can be taken out and what is left is a two-component spinor that depends only on the angles. This is what in wave function language Sakurai calls $\mathcal{Y}_\ell^{jm_j}$; in ket language we will write

$$|\ell j m_j\rangle = \sum_{m_\ell m_s} |\ell m_\ell\rangle|s m_s\rangle\langle \ell s m_\ell m_s | j m_j\rangle. \tag{12}$$

(a) For the case $\ell = 0$, $j = \frac{1}{2}$, $m_j = \frac{1}{2}$, write out the two-component spinor $\mathcal{Y}_\ell^{jm_j}$ as functions of (θ, ϕ).

(b) Multiply this by $\sigma \cdot \mathbf{r}$ ($\mathbf{r}$ = Sakurai's $\mathbf{x}$), and express the result as a linear combination of other spin angular functions $\mathcal{Y}_\ell^{jm_j}$.

(c) Certain values of j, m_j and ℓ occur in the sum, and certain others do not. Use symmetry principles to explain why the values that occur are allowed and the others are not.
Hint: It may help to think of three kinds of rotations: spin rotations, orbital rotations, and total (spin plus orbital) rotations.

3. Sakurai, problem 4.5, p. 282. The effects of parity violation in atomic physics. When he says further restrictions on the quantum numbers, he means restrictions that go beyond those due to symmetry considerations.