Physics 221A
Fall 2005
Homework 4
Due Thursday, September 29, 2005

Reading Assignment: Sakurai, pp. 89–109, Notes 5. Sakurai's discussion of WKB theory is pretty poor, but the notes will make up for it.

1. Consider the Hamiltonian for a particle of charge q in an electromagnetic field:

$$H = \frac{1}{2m}\Big[\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{x},t)\Big]^2 + q\Phi(\mathbf{x},t), \tag{1}$$

where we allow all fields to be space- and time-dependent.

(a) Define the kinetic momentum operator $\boldsymbol{\pi}$ by

$$\boldsymbol{\pi} = \mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{x},t). \tag{2}$$

Notice that $\boldsymbol{\pi}$ has an explicit time dependence, due to the $\mathbf{A}$ term. Work out the commutation relations, $[x_i, \pi_j]$ and $[\pi_i, \pi_j]$. Use these to work out the Heisenberg equations of motion for the operators $\mathbf{x}$, $\boldsymbol{\pi}$. Then eliminate $\boldsymbol{\pi}$, and find an expression for $\ddot{\mathbf{x}}$ (the Heisenberg analog of the Newton-Lorentz equations).

(b) By taking expectation values, show that if $\mathbf{B}$ is uniform in space and $\mathbf{E}$ has the form,

$$E_i(\mathbf{x}) = a_i + \sum_j b_{ij}\, x_j, \tag{3}$$

where a_i and b_{ij} are constants, then the expectation value of $\mathbf{x}$ follows the classical orbit.

2. The Bohr-Sommerfeld quantization condition for an oscillator will be derived in class on Friday, September 23. It is

$$\frac{1}{2\pi\hbar}\oint p\,dx = n + \frac{1}{2}, \tag{4}$$

where the integral is taken around a bound orbit. The value of the integral is the x-p area of the orbit; this area is a function of the energy, so certain orbits, of energy E_n, are "quantized." The Bohr-Sommerfeld rule is not exact; rather it is the leading term in the expansion of the energy eigenvalues in powers of $\hbar$.

(a) In classical mechanics, the *action* of a periodic orbit is defined by

$$J = \frac{1}{2\pi} \oint p\, dx. \tag{5}$$

The action is a function of the energy of the orbit, $J = J(E)$, which can be inverted to give $E = E(J)$. Show that

$$\frac{dE}{dJ} = \omega, \tag{6}$$

where ω is the frequency of the orbit. The frequency is in general a function of E or J (but not for the harmonic oscillator, where ω is a constant).

(b) In the days of the old quantum theory, people tried to understand spectral lines in terms of a model of a classically radiating charge. A classical charged particle in a periodic orbit of frequency ω will radiate at frequency ω as well as at all higher harmonics (say, $m\omega$, where m is an integer). Consider the highly excited states of a quantum mechanical oscillator (large quantum number n), and suppose the system makes a transition to a nearby state $n \to n + \Delta n$, where Δn is not too large. By using the Bohr-Sommerfeld rule (4) and by treating n as a continuous variable, show that the frequencies of the emitted radiation do indeed obey the predictions for a classically radiating charge when $n \gg 1$.

3. Consider the Bohr-Sommerfeld quantization of a 1-dimensional oscillator in a potential $V(x)$.

(a) Integrate the square of the WKB wave function ψ between the two turning points to obtain the normalization constant. The wave function blows up at the turning points, but you can do the integral anyway. Write out the normalized wave function. (The damped waves in the classically forbidden regions can be ignored.) Replace $\cos^2$ by the average value $1/2$ in the integrand before doing the integral. Express the normalization constant both in terms of the classical period T and the quantity $\partial E_n/\partial n$, where n is treated as a continuous quantity.

(b) Now assume the potential well is symmetric, $V(-x) = V(x)$, with $V(0) = 0$. Show that

$$|\psi(0)|^2 = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}\frac{\partial E_n}{\partial n}\cos^2\left(\frac{n\pi}{2}\right), \tag{7}$$

and

$$|\psi'(0)|^2 = \frac{\sqrt{8m^3E}}{\pi\hbar^3}\frac{\partial E_n}{\partial n}\sin^2\left(\frac{n\pi}{2}\right). \tag{8}$$

Carry your calculations only out to leading order in $\hbar$.

4. Consider the potential energy illustrated in Fig. 1.

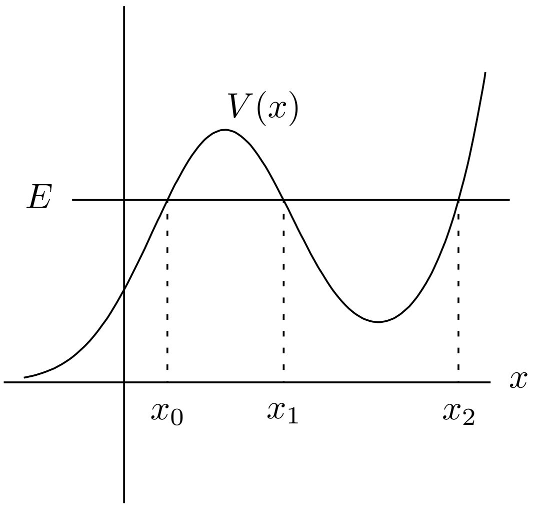

Fig. 1. Potential for problem 4.

For the energy shown, there are three turning points. In the region to the left of x_0 let ψ have the form,

$$\psi(x) = \frac{1}{p(x)^{1/2}} \left(e^{iS(x,x_0)/\hbar} + r e^{-iS(x,x_0)/\hbar} \right), \tag{9}$$

where r is the reflection amplitude. Find r as a function of the energy E. Please use the following notation:

$$\Phi = \frac{2}{\hbar} S(x_2, x_1), \tag{10}$$

and

$$\kappa = \frac{1}{\hbar} K(x_1, x_0). \tag{11}$$

Hint: work from right to left.

Show that $|r|^2 = 1$, which means that all particles sent in from the left come back (ingoing and outgoing fluxes are equal). Show that when the energy is not close to a nominal Bohr-Sommerfeld energy level of the well, then $r \approx -i$ (the value r would have if there were no well to the right of x_0), but that when E increases through such an energy level, then the phase of r rapidly increases by 2π. This is a resonance. Estimate the range

ΔE over which this change takes place. Assume that the energy is not too close to the top of the well, i.e., the quantity $e^{-\kappa}$ is small.

Estimate the ratio $\psi_{\rm in}/\psi_{\rm out}$ of the wave function inside and outside the well, in the case where E is far from a Bohr-Sommerfeld energy level of the well, and in the case where E is equal to one of these energy levels.

5. As you know, the radial wave equation in 3-dimensional problems with central force potentials looks like a 1-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2 f}{dr^2} + U(r)f(r) = Ef(r), \tag{12}$$

except that r ranges from 0 to ∞, and the potential $U(r)$ is the sum of the centrifugal potential and the true potential $V(r)$,

$$U(r) = \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r). \tag{13}$$

Therefore one-dimensional WKB theory can be applied to the radial wave equation. It can be shown that more accurate results are obtained in the WKB treatment if the quantity $\ell(\ell+1)$ in the centrifugal potential is replaced by $(\ell+\frac{1}{2})^2$. This is called the *Langer modification.* Just accept this fact for the purposes of this problem; the justification has to do with the singularity of the centrifugal potential as $r \to 0$.

(a) Take the case of a free particle, $V(r) = 0$. Find the WKB solution in the classically allowed region. For boundary conditions in the classically forbidden region near $r = 0$, just assume that there is only a growing wave (as r increases). Evaluate all functions explicitly; use the abbreviation $k = \sqrt{2mE}/\hbar$. Take the limit $r \to \infty$, and reconcile the result with the asymptotic forms of the spherical Bessel function $j_\ell(\rho)$, quoted by Sakurai in his Eq. (A.5.15). (Sakurai's $\rho = kr$.)

(b) Consider a potential $V(r)$ which is not zero, but which approaches 0 as $r \to \infty$. Since the particle approaches a free particle as $r \to \infty$, we might expect the solution at large r to look like a free particle solution, but with a phase shift. Explicitly, if the free particle solution has the form $f(r) = \cos(kr + \alpha_f)$ as $r \to \infty$, where α_f is the phase shift for the free particle, and the solution in the presence of the potential has the form $f(r) = \cos(kr + \alpha_p)$ as $r \to \infty$, where α_p is the phase shift in the presence of the potential, then we define $\delta = \alpha_p - \alpha_f$ as the phase shift in the potential scattering, measured relative to the phase shift of a free particle. Use WKB theory to write down an expression for δ, which will involve the limit of a certain quantity as $r \to \infty$.

(c) Does this limit exist? It can be shown that it does if $V(r)$ falls off more rapidly as $r \to \infty$ than the centrifugal potential, i.e., more rapidly than $1/r^2$; the limit also exists when the true potential falls off exactly as fast as the centrifugal potential, i.e., as $1/r^2$. Therefore consider the case that $V(r)$ approaches 0 as $1/r^\alpha$, where $0 < \alpha < 2$. Show that the phase shift exists only if $1 < \alpha < 2$. In particular, in the important case of the Coulomb potential ($\alpha = 1$), the phase shift does not exist (the asymptotic form of the radial wave function f is more complicated than a phase-shifted free particle solution).