Physics 195a
Problem set number 6 – Solutions to Problems 33 and 34
Due 2 PM, Thursday, November 14, 2002

READING: Read the "The Simple Harmonic Oscillator: Creation and Destruction Operators" course note.

PROBLEMS:

30. K^0 system in density matrix formalism: Exercise 2 of the K^0 course note.

31. [Worth two problems] "Regeneration": Exercise 3 of the K^0 course note.

32. Qualitative features of wave functions: Exercise 1 of the Harmonic Oscillator course note.

33. One of the failings of classical mechanics is that matter should be "unstable". Let us investigate this in the following system: Consider a system consisting of N particles with masses m_k and charges q_k, $k = 1, 2, \ldots, N$, where we suppose some of the charges are positive and some negative. The Hamiltonian of this multiparticle system is:

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + \sum_{N \geq j > k \geq 1} \frac{q_k q_j}{|\mathbf{x}_k - \mathbf{x}_j|},$$

where $p_k = |\mathbf{p}_k|$ is the magnitude of the momentum of the particle labelled "k".

(a) Assume we have solved the equations of the motion, with solutions $\mathbf{x}_k = \mathbf{s}_k(t)$. Show that for any $\omega > 0$ we can select a number $c > 0$ such that $\mathbf{x}_k = c\mathbf{s}_k(\omega t)$ is also a solution of the equations of motion. Remember, we are dealing with the classical equations of motion here.

Solution: The solutions $\mathbf{s}_k(t)$ must satisfy "$\mathbf{F} = m\mathbf{a}$", that is:

$$\sum_{j \neq i} \frac{q_i q_j}{|\mathbf{s}_i - \mathbf{s}_j|^3} (\mathbf{s}_i - \mathbf{s}_j) = m_i \frac{d^2}{dt^2} \mathbf{s}_i(t). \qquad (10)$$

Let $\mathbf{x}_i(t) = c\mathbf{s}_i(\omega t)$. Then,

$$\frac{d^2}{dt^2}\mathbf{x}_i(t) = \omega^2 c \frac{d^2}{dt^2}\mathbf{s}_i(t). \tag{11}$$

Also,

$$\sum_{j\neq i} \frac{q_i q_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}(\mathbf{x}_i - \mathbf{x}_j) = \frac{1}{c^2}\sum_{j\neq i} \frac{q_i q_j}{|\mathbf{s}_i - \mathbf{s}_j|^3}(\mathbf{s}_i - \mathbf{s}_j). \tag{12}$$

Thus, if $\omega^2 c = 1/c^2$, then cfx_i is also a solution.

(b) Find scaling laws relating the total energy, total momentum, total angular momentum, position of an individual particle, and momentum of an individual particle for the original $\mathbf{s}_k(t)$ solution and the scaled $c\mathbf{s}_k(\omega t)$ solution. The only parameter in your scaling laws should be ω. Make sure that any time dependence is clearly stated.

Solution: With $c = \omega^{-2/3}$ the position of a particle scales as:

$$\mathbf{x}_k(t) = \omega^{-2/3}\mathbf{s}_k(\omega t). \tag{13}$$

The momentum of a particle scales as:

$$\mathbf{p}(t) \to \mathbf{p}'(t) = m_i \frac{d}{dt}\mathbf{x}_k(t) = m_i \omega^{-2/3}\frac{d}{dt}\mathbf{s}_k(\omega t) = \omega^{1/3}\mathbf{p}(\omega t). \tag{14}$$

The total momentum is a constant of the motion, and scales as:

$$\mathbf{P} \to \mathbf{P}' = \sum_k \mathbf{p}'_k(t) = \omega^{1/3}\mathbf{P}. \tag{15}$$

The total energy is a constant of the motion, and scales as:

$$E \to E' = \sum_k \frac{[\mathbf{p}'_k(t)]^2}{m_k} + \frac{1}{2}\sum_{j,k;j\neq k} \frac{g_j q_k}{|\mathbf{x}_k - \mathbf{x}_j|} = \omega^{2/3}\mathbf{E}. \tag{16}$$

The total angular momentum is a constant of the motion, scaling like $\mathbf{r}\times\mathbf{p}$:

$$\mathbf{L} \to \mathbf{L}' = \omega^{-1/3}\mathbf{L}. \tag{17}$$

(c) Hence, draw the final conclusion that there does not exist any stable "ground state" of lowest energy. As an aside, what Kepler's law follows from your analysis?

Solution: If we have any bound state with $E < 0$, such as for two particles when $q_j = -q_k$, then we have another solution with energy $\omega^{2/3}E$. Since ω can be taken arbitrarily large, there is no lowest energy solution.

The Kepler's law that follows from this analysis is the third: The size of a trajectory scales as $\omega^{-2/3}$. The period of the trajectory scales as $1/\omega$. Thus, if a is the semi-major axis of the orbit, and τ is the period,

$$a \propto \omega^{-2/3} \tag{18}$$

$$\tau \propto \omega^{-1} \tag{19}$$

$$\propto a^{3/2}. \tag{20}$$

(d) We assert that quantum mechanics does not suffer from this disease, but this must be proven. You have seen (or, if not, see the following problem) the analysis for the hydrogen atom in quantum mechanics, and know that it has a ground state of finite energy. However, it might happen for larger systems that stability is lost in quantum mechanics – there are typically several negative terms in the potential function which could win over the postive kinetic energy terms. We wish to prove that this is, in fact, not the case. The Hamiltonian is as above, but now $\mathbf{p}_k = -i\partial_{\mathbf{k}}$ ($\partial_{\mathbf{k}} = (\frac{\partial}{\partial x_k}, \frac{\partial}{\partial y_k}, \frac{\partial}{\partial z_k})$).

Find a rigorous lower bound on the expectation value of H. It doesn't have to be very "good"– any lower bound will settle this question of principle. You may take it as given that the lower bound exists for the hydrogen atom, since we have already demonstrated this. You may also find it convenient to consider center-of-mass and relative coordinates between particle pairs.

Solution: We know that the energy spectrum of the one-electron atom is bounded below. Thus, the Hamiltonian

$$H_1 = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{|\mathbf{x}|}, \tag{21}$$

has a lower bound on the energy. For any acceptable wave function $|f_1\rangle$, we have

$$\langle f_1|H_1|f_1\rangle \geq -Z^2\alpha^2 m/2. \tag{22}$$

We will make use of this in analyzing our more complicated system.

We must consider the Hamiltonian

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + \sum_{N\geq j>k\geq 1} \frac{q_k q_j}{|\mathbf{x}_k - \mathbf{x}_j|}. \tag{23}$$

Let $f(x)$ be any wave function in the allowed Hilbert space, normalized so that $\langle f|f\rangle = 1$. We wish to show that $\langle f|H|f\rangle > -\infty$. We already know that some of the individual terms are bounded below by zero:

$$\begin{aligned} \langle f|\sum_{k=1}^{N} \frac{p_k^2}{2m_k}|f\rangle &\geq 0 & (24)\\ \langle f|\sum_{N\geq j>k\geq 1} \frac{q_k q_j}{|\mathbf{x}_k - \mathbf{x}_j|}|f\rangle &\geq 0, \quad \text{for } q_k q_j \geq 0. & (25) \end{aligned}$$

We must concentrate our energy on those terms in the potential energy with opposite charge particles.

The total energy is the sum of the individual expectation values. If we can show that no term goes to $-\infty$, then the sum will also be bounded below (since the number of terms is finite). Consider particle j. Suppose there are n_j particles with sign opposite to particle j. Suppose that particle k is one such particle. We can thus write each the the potentially troublesome terms in the Hamiltonian in the form of a two-particle problem with Hamiltonian:

$$H_{jk} = \frac{1}{n_j}\frac{\mathbf{p}_j^2}{2m_j} + \frac{1}{n_k}\frac{\mathbf{p}_k^2}{2m_k} - \frac{|q_j q_k|}{|\mathbf{x}_j - \mathbf{x}_k|}. \tag{26}$$

We have arranged it such that the total Hamiltonian includes a term of this form for each pair of oppositely charged particles, and all of the potentially troublesome terms are included as terms of this form. Note that this piece of the total Hamiltonian is the Hamiltonian for two particles of masses $n_j m_j$ and $n_k m_k$, and charges q_j and q_k.

We may rewrite H_{jk} in terms of the relative and center-of-mass motion of the two-particle subsystem: $H_{jk} = H_{jk;\text{CM}} + H_{jk;\text{rel}}$, where

$$H_{jk;\text{CM}} = \frac{(\mathbf{p}_j + \mathbf{p}_k)^2}{2(n_j m_j + n_k m_k)} \tag{27}$$

$$H_{jk;\text{rel}} = \frac{\mathbf{p}^2}{2m} - \frac{|q_j q_k|}{|\mathbf{x}|}, \tag{28}$$

where $\mathbf{x} \equiv \mathbf{x}_j - \mathbf{x}_k$, $m = n_j n_k m_j m_k/(n_j m_j + n_k m_k)$, and $\mathbf{p} = (n_k m_k \mathbf{p}_j - n_j m_j \mathbf{p}_k)/(n_j m_j + n_k m_k)$.
Since $H_{jk;\text{CM}}$ involves the square of a Hermitian operator, its spectrum is non-negative. If we can show that the spectrum of $H_{jk;\text{rel}}$ is bounded below, then we will have completed our task. We achieve this by noting the similarity with the Hamiltonian for the one-electron atom:

$$\langle f|H_{jk;\text{rel}}|f\rangle \geq -\frac{(q_j q_k)^2 m}{2}. \tag{29}$$

There are finite many terms of this form, all other contributions are non-negative. Therefore,

$$\langle f|H|f\rangle > -\infty. \tag{30}$$

34. The one-electron atom (review?): Continuing from problem 29, now consider the case of the one-electron atom, with an electron under the influence of a Coulomb field due to the nucleus of charge Ze:

$$V(r) = -\frac{Ze^2}{r}, \tag{31}$$

 (a) Without knowing the details of the potential, we may evaluate the form of the radial wave function ($R_{n\ell}(r) = u_{n\ell}(r)/r$, where $\psi_{n\ell m}(\mathbf{x}) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi)$) for small r, as long as the potential depends on r more slowly than $1/r^2$. Here, n is a quantum number for the radial motion. Likewise, we find the asymptotic form of the wave function for large r, as long as the potential approaches zero as r becomes large. Find the allowable forms for the radial wave functions in these two limits.

Solution: In problem 29, we showed that we could write the Schrödinger equation for the relative motion in the form:

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\ell(\ell+1)}{2mr^2}\right] u_{n\ell}(r) = E u_{n\ell}(r). \qquad (32)$$

We wish to find the solution for small r. If we multiply the equation through by r^2, and assume that $r^2 V(r) \to 0$ as $r \to 0$, then we have the approximate equation for small r:

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2mr^2}\right] u_{n\ell}(r) = 0 \qquad (33)$$

The solutions are $u_{n\ell}(r) \propto r^{\ell+1}$, and $u_{n\ell}(r) \propto r^{-\ell}$. The normalization condition is:

$$\int_{(\infty)} |\psi(\mathbf{x})|^2 = 1. \qquad (34)$$

Since the $Y_{\ell m}$ functions are normalized to one themselves, the radial portion of the wave function is normalized as:

$$1 = \int_0^\infty r^2 |R_{n\ell}|^2 dr = \int_0^\infty |u_{n\ell}(r)|^2 \, dr. \qquad (35)$$

For $\ell > 0$, the $r^{-\ell}$ solution diverges too rapidly near $r = 0$ for this normalization condition.

The situation for $\ell = 0$ is more subtle. Often, this is glossed over, and people just lump it in with the $\ell > 0$ case, but the same argument for excluding the r^0 solution really doesn't work. For this case, $u_{n0}(r) =$ constant, and hence, $\psi_{n0}(\mathbf{x}) \propto 1/r$ at small r. But

$$\nabla^2 \left(\frac{1}{r}\right) = -4\pi\delta(r), \qquad (36)$$

so this solution doesn't satisfy the Schödinger equation at $r = 0$.

Thus, the physical solution is $u_{n\ell}(r) \propto r^{\ell+1}$ as $r \to 0$. Or, $\psi_{n\ell}(\mathbf{x}) \propto r^\ell$ as $r \to 0$. For $\ell > 0$, $\psi_{n\ell} \to 0$, and for $\ell = 0$, $\psi_{n\ell} \to$ constant, as $r \to 0$.

Now consider large r, and assume $V(r) \to 0$ as $r \to \infty$. Then the asymptotic Schrödinger equation is:

$$-\frac{1}{2m}\frac{d^2}{dr^2} u_{n\ell}(r) = E u_{n\ell}(r). \qquad (37)$$

The solutions to this equation are:

$$u_{n\ell}(r) \propto e^{\pm ikr}, \quad E = \frac{k^2}{2m}, \quad \text{for } E > 0; \tag{38}$$

$$u_{n\ell}(r) \propto e^{-\kappa r}, \quad E = -\frac{\kappa^2}{2m}, \quad \text{for } E < 0. \tag{39}$$

The $E < 0$ solutions are the bound states ($\kappa > 0$). Note that the $e^{+\kappa r}$ solutions are unnormalizable. The asymptotic wave functions are thus of the form $e^{\pm ikr}/r$ (spherical waves outgoing or incoming) for the unbound states, and of the form $e^{-\kappa r}/r$ for the bound states.

One final remark: in the asymptotic limit, we can multiply these solutions by r^a, correct to leading order in r.

(b) Find the bound state eigenvalues and eigenfunctions of the one-electron atom. [Hint: it is convenient to express the wave function, or rather $u_{n\ell}$, with its asymptotic dependence explicit, so that may be "divided out" in solving the rest of the problem.] You may express your answer in terms of the **Associated Laguerre Polynomials**:

$$L_{n+\ell}^{2\ell+1}(x) = \sum_{k=0}^{n-\ell-1} \frac{(-)^{k+1}(n+\ell)!}{(n-\ell-1-k)!(2\ell+1+k)!k!} x^k. \tag{40}$$

Solution: We look for solutions of the form

$$\psi_{n\ell m}(r,\theta,\phi) = \frac{u_{n\ell}(r)}{r} Y_{\ell m}(\theta,\phi), \tag{41}$$

where $u_{n\ell}(r)$ satisfies the equaivalent one-dimensional Schrödinger equation:

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2} - \frac{Ze^2}{r} + \frac{\ell(\ell+1)}{2mr^2}\right] u_{n\ell}(r) = E_{n\ell} u_{n\ell}(r). \tag{42}$$

It is generally convenient to put such problems into dimensionless form. Here, define

$$\kappa = \sqrt{-8mE} \tag{43}$$

$$\rho = \kappa r \tag{44}$$

$$v(\rho) = u_{n\ell}(\rho/\kappa). \tag{45}$$

With these substitutions (the "8" is chosen for later convenience...), we have the differential equation:

$$\left[\frac{d^2}{d\rho^2} - \frac{\lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2} - \frac{1}{4}\right] v(\rho) = 0, \tag{46}$$

where we have defined the dimensionless constant:

$$\lambda \equiv \frac{2mZe^2}{\kappa}. \tag{47}$$

We take the hint, and put in explicit asymptotic dependence. The asymptotic equation is:

$$\left(\frac{d^2}{d\rho^2} - \frac{1}{4}\right) v(\rho) = 0. \tag{48}$$

The asymptotic solution is thus:

$$v(\rho) = \rho^n e^{-\rho/2}, \tag{49}$$

where ρ is any number. We'll therefore look for solutions of the form:

$$v(\rho) = F(\rho)e^{-\rho/2}, \tag{50}$$

where f is a power series in ρ of finite order:

$$F(\rho) = \rho^{\ell+1}(c_0 + c_1\rho + c_2\rho^2 + \ldots + c_n\rho^M) \tag{51}$$

$$= \rho^{\ell+1} f(\rho), \tag{52}$$

where the second relation defines $f(\rho)$. The lowest power $\rho^{\ell+1}$ is required to to give the right dependence at $r = 0$, as we determined in part (a).
The differential equation for F is:

$$F'' - F' + \left[\frac{\lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right] F = 0. \tag{53}$$

This gives the following differential equation satisfied by $f(\rho)$:

$$\rho f'' + [2(\ell+1) - \rho]\, f' + (\lambda - \ell - 1)f = 0. \tag{54}$$

If we plug our series form for $f(\rho)$ into this equation, we find the recurrence relation for the coeeficients:

$$c_{k+1} = \frac{k - \lambda + \ell + 1}{(k+1)(k+2\ell+2)} a_k. \tag{55}$$

At this point, it may be demonstrated that the series must indeed terminate, or else we would obtain an unacceptable asymptotic form of $e^{\rho/2}$ instead of $e^{-\rho/2}$.

Assuming $k = m$ is the highest term, we must have, from our recurrence relation:

$$a_{M+1} = 0 = \frac{M - \lambda + \ell + 1}{(M+1)(M+2\ell+2)} a_M. \tag{56}$$

Thus, $n = \lambda - \ell - 1$. Since ℓ and n are non-negative integers, λ must also be an integer, with $\lambda \geq 1$. Lambda is known as the **principal quantum number** (n_p), and M is known as the **radial quantum number** (n_r). Since λ can only take on discrete values, we have the quantization of the energy levels:

$$E_\lambda = -\frac{Z^2 e^4}{2} \frac{m}{\lambda^2}, \quad \lambda = 1, 2, \ldots. \tag{57}$$

For $Z = 1$ and $\lambda = 1$ this gives the familiar $E_1 = -13.6$ eV ground state energy of hydrogen.

The differential equation for f is known as the **Associated Laguerre Equation**. It may readily be verified that the coefficients in the associated Laguerre polynomials given in the problem statement satisfy the desired recurrence relation, hence the radial wave function is given by (after properly normalizing):

$$R_{n_p \ell}(r) = \left(\frac{2Z}{n_p a_0}\right)^{3/2} \sqrt{\frac{(n_p - \ell - 1)!}{2n_p \left[(n_p + \ell)!\right]^3}} \rho^\ell e^{-\rho/2} L^{2\ell+1}_{n_p+\ell}(\rho), \tag{58}$$

where

$$\rho = \frac{2Z}{na_0} r, \tag{59}$$

$$a_0 = \frac{1}{me^2} = \frac{1}{m\alpha}, \quad \text{is the } \textbf{Bohr radius}. \tag{60}$$