Homework #6 — Phys622 — Fall 1998 Victor Yakovenko, Assistant Professor
Deadline: Wednesday, October 14, 1998. Office: Physics 2314
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Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of Schwabl.
Equation numbers without period, like (5), refer to the equations of this homework.

Angular Momentum (Chapter 5)

1. **(a)** [**3 points**] Find the energy eigenvalues E and eigenfunctions $\psi_E(\varphi)$ of a plane rotor, an object that can rotate around a single axis z with the moment of inertia I. This system has one degree of freedom: the angle of rotation φ, and its Hamiltonian is:

$$\hat{H} = \frac{\hat{L}_z^2}{2I} = -\frac{\hbar^2}{2I}\frac{d^2}{d\varphi^2}. \tag{1}$$

(b) [**2 points**] Find the energy eigenvalues of a spherical rotor, an object that can rotate around the x, y, and z axes with the equal moments of inertia I. An example of such a system is the methane molecule CH_4. The Hamiltonian of the system is:

$$\hat{H} = \frac{\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2}{2I} = \frac{\hat{\mathbf{L}}^2}{2I}. \tag{2}$$

2. [**3 points**] Using the $-$ and $+$ signs, indicate which of the following physical quantities change sign and which remain the same under the parity operation ($\mathbf{r} \to -\mathbf{r}$) and the time-reversal operation ($t \to -t$).

	Parity	Time reversal
Mass m		
Coordinate $\mathbf{r}$		
Velocity $\mathbf{v} = d\mathbf{r}/dt$		
Momentum $\mathbf{p} = m\mathbf{v} = -i\hbar\partial/\partial\mathbf{r}$		
Angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$		
Electric charge e		
Electric current $\mathbf{J}$		
Scalar potential ϕ		
Vector potential $\mathbf{A}$		
Electric field $\mathbf{E} = -\partial\mathbf{A}/c\partial t - \partial\phi/\partial\mathbf{r}$		
Magnetic field $\mathbf{B} = \partial/\partial\mathbf{r} \times \mathbf{A}$		

3. Under the parity operation, a vector may change sign (as $\mathbf{r}$), or remain the same (as $\mathbf{L}$). The first type of a vector is called a *polar vector*; the second an *axial vector*. Typically, axial vectors involve vector product, which behaves "abnormally" under the parity transformation.

Similarly a scalar may remain the same (as mass m) or change sign (as, for example, $\mathbf{E}\cdot\mathbf{L}$) under the parity operation. The first type of a scalar is called a *true scalar*, the second a *pseudoscalar*.

(a) [**3 points**] Suppose, a wave function ψ_g is even and a wave function ψ_u is odd under the parity transformation:

$$\psi_g(-\mathbf{r}) = \psi_g(\mathbf{r}), \qquad \psi_u(-\mathbf{r}) = -\psi_u(\mathbf{r}) \tag{3}$$

Formulate selection rules for the matrix elements of

i. a true scalar,
ii. a pseudoscalar,
iii. a polar vector,

iv. an axial vector

between the two states, each state being either ψ_g or ψ_u. In other words, specify which of these matrix elements must vanish by symmetry, and which are not.
Hint: The matrix elements are given by some integrals $\int d^3r$. Change the variable of integration $\mathbf{r} \to -\mathbf{r}$ and see what happens to the integrals.

(b) [**3 points**] Formulate the parity selection rules for the four types of scalars and vectors between the states of different angular momentum l.
Directions: Use Eq. (5.35b), which relates parity and angular momentum of a wave function. Check that the wave functions considered in Problems 5 and 6 of Homework 5 satisfy Eq. (5.35b).

The Central Potential (Chapter 6)

4. Let us discuss the two-dimensional (2D) Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\psi(x,y)=E\psi(x,y). \tag{4}$$

Such an equation describes, for example, an electron trapped at the surface of a semiconductor or at an interface between two semiconductors.

(a) [**5 points**] The analog of a spherically-symmetrical potential in the 2D case is a cylindrically-symmetrical potential $V(\rho)$ that depends only on $\rho=\sqrt{x^2+y^2}$.
Show that

$$\hat{L}_z^2=\mathbf{r}^2\hat{\mathbf{p}}^2-(\mathbf{r}\cdot\hat{\mathbf{p}})^2, \tag{5}$$

where $\mathbf{r}$ and $\hat{\mathbf{p}}$ are the 2D vectors of coordinate and momentum. Hint: Going from 3D to 2D changes the coefficient in Schwabl's remark after Eq. (6.2) from 3 to 2.
Using Eq. (5), show that the kinetic energy in 2D case can be written as

$$\frac{\hat{\mathbf{p}}^2}{2\mu}=-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}\right)+\frac{\hat{L}_z^2}{2\mu\rho^2}. \tag{6}$$

Here we use the letter μ for the mass of a particle in order to distinguish it from the eigenvalue of $\hat{L}_z$ which is denoted by m.

(b) [**5 points**] Show that the eigenfunction of Eq. (4) for a cylindrically-symmetrical potential $V(\rho)$ can be written in the form

$$\psi_{Em}(\rho,\varphi)=R_{Em}(\rho)\Phi_m(\varphi), \tag{7}$$

where we use the cylindrical coordinates ρ and φ instead of the Cartesian coordinates x and y,

$$\Phi_m(\varphi)=\frac{e^{im\varphi}}{\sqrt{2\pi}} \tag{8}$$

is the eigenfunction of the angular momentum $\hat{L}_z$ with the eigenvalue $\hbar m$, and the radial function $R_{Em}(\rho)$ satisfies the equation

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{m^2}{\rho^2}\right)+V(\rho)\right]R_{Em}(\rho)=ER_{Em}(\rho). \tag{9}$$

Show that the change of variables

$$R_{Em}(\rho)=\frac{u_{Em}(\rho)}{\sqrt{\rho}} \tag{10}$$

converts Eq. (9) into the following equation:

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2}-\frac{m^2-1/4}{\rho^2}\right)+V(\rho)\right]u_{Em}(\rho)=Eu_{Em}(\rho), \tag{11}$$

with the boundary condition $u(0)=0$.

(c) [**5 points**] Find discrete energy spectrum of the Coulomb potential in 2D:

$$V(\rho) = -\frac{\alpha}{\rho}, \qquad \alpha > 0. \tag{12}$$

Describe degeneracy of the energy levels and compare it with the case of the 3D Coulomb potential. (You don't need to repeat Schwabl's solution of Eq. (11) with (12); just use the known answer for the 3D hydrogen atom.)

5. [**8 points total**] Let us discuss asymptotic behavior of an energy eigenfunction at $r \to \infty$ for a generic spherically-symmetrical potential $V(r)$ that decays at infinity slower than $1/r$:

$$V(r) \to 0, \qquad \text{but} \quad rV(r) \not\to 0 \qquad \text{at} \quad r \to \infty \tag{13}$$

For such long-range potentials, Eq. (6.13b) need to be corrected.

(a) Substitute a wave function in the form $u(r) = f(r)\exp(-\kappa r)$ for a bound state and $u(r) = f(r)\exp(\pm ikr)$ for an unbound state into Eq. (6.11).

(b) Neglect the centrifugal term and the second derivative of $f(r)$. Solve the resulting first-order differential equation for $f(r)$.

(c) Show that, at $r \to \infty$, $f(r) \to$ const for short-range potentials such that $rV(r) \to 0$, but $f(r)$ is a significant function of r for long-range potentials such that $rV(r) \not\to 0$.

(d) Given your solution for $f(r)$, show that the approximations made in part 5b are justified at $r \to \infty$.

(e) Find explicit form of $f(r)$ for the Coulomb potential $V(r) = -Ze^2/r$.

(f) Substituting the explicit expression (6.24') for the energies of the bound states of the Coulomb potential into the result of Problem 5e, show that

$$R_{nl}(r) = \frac{u(r)}{r} \propto r^{n-1}\, e^{-Zr/na} \quad \text{at} \quad r \to \infty \quad \text{independent of } l, \tag{14}$$

Compare this result with the explicit form of the Laguerre polynomials given in Problem 6.2(a). (In the special case $l = n - 1$, Eq. (14) is valid for all r.)