THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION

**JUNE 2014**

**PHYS 3210 Quantum Mechanics**

**PHYS 3011 Quantum Mechanics + Electrodynamics (Paper 2)**

Time Allowed – 2 hours

Total number of questions – 3

ALL questions need to be addressed

Question marks range from 30 to 35.

This paper may be retained by the candidate.

Students may provide their own UNSW approved calculators.

Answers must be written in ink. Except where they are expressly required, pencils may only be used for drawing, sketching or graphical work.

**For calculations** one can use either the absolute units, or the special units $\hbar = m = 1$; moreover in a problem at hand one can make an additional simplification, for example setting $\omega = 1$ in Eq.(1.7), or put $|e| = 1$ in Eq.(2.4) and similar ones.
However, the **final answers** should be presented in absolute units.

**Question 1.** Basic properties of Schrödinger equation (Marks 35).

a. Write down the non-stationary Schrödinger equation for the wave function $\psi(\boldsymbol{r}, t)$, which describes the propagation of a particle of mass $m$ and charge $e$ in an external, time dependent electromagnetic field represented by the potentials $V(r,t)$ and $\boldsymbol{A}(\boldsymbol{r},t)$.
b. Consider a particle of mass $m$ and charge $e$, which propagates in an external, static electric field described by the potential $V(r)$.
   - Prove that wave functions, which describe stationary states, can be chosen to be real.
   - Prove that if $|\psi_n\rangle = \psi_n(\boldsymbol{r})$ and $|\psi_m\rangle = \psi_m(\boldsymbol{r})$ are two wave functions for two different energy levels, $E_n \neq E_m$, then these functions are necessarily orthogonal

$$\langle\psi_n|\psi_m\rangle = 0. \qquad (1.1)$$

Hint: remember conventional notation for the matrix elements

$$\langle\psi_n|\psi_m\rangle = \int \psi_n^*(\boldsymbol{r})\psi_m(\boldsymbol{r})\, d^3r, \qquad (1.2)$$

and

$$\langle\psi_n|\hat{A}|\psi_m\rangle = \int \psi_n^*(\boldsymbol{r})\ \hat{A}\, \psi_m(\boldsymbol{r})\, d^3r, \qquad (1.3)$$

which is used below,

c. Consider a particle of mass $m$, which propagation is governed by the Hamiltonian

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + U(\boldsymbol{r}, t), \quad \hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla} \qquad (1.4)$$

Let the two wave functions $|\psi_i\rangle = \psi_i(\boldsymbol{r}, t),\ i = 1,2$ , satisfy the non-stationary Schrödinger equation.

- Prove that the matrix elements of the momentum and coordinates sandwiched in between these functions obeys the following attractive relation

$$\frac{\partial}{\partial t}\langle\psi_2|m\boldsymbol{r}|\psi_1\rangle = \langle\psi_2|\hat{\boldsymbol{p}}|\psi_1\rangle \qquad (1.5)$$

- Prove that the matrix elements of the coordinate and force satisfy another appealing identity

$$\frac{\partial}{\partial t}\langle\psi_2|\,\hat{\boldsymbol{p}}\,|\psi_1\rangle = \langle\psi_2|\,\boldsymbol{F}\,|\psi_1\rangle \qquad (1.6)$$

Here

$$\boldsymbol{F} = -\boldsymbol{\nabla} U \qquad (1.7)$$

is the force.

Hint: it is convenient firstly to prove the following commutation relations

$$[\boldsymbol{r}, \hat{H}] = m[\boldsymbol{r}, \frac{\hat{p}^2}{2m}] = i\hbar\, \hat{\boldsymbol{p}} \qquad (1.8)$$

$$[\hat{\boldsymbol{p}}, \hat{H}] = [\hat{\boldsymbol{p}}, U(\boldsymbol{r}, t)] = -i\hbar \boldsymbol{\nabla} U(\boldsymbol{r}, t)\,, \qquad (1.9)$$

which follow directly from an obvious $[\mathrm{r}_a, \hat{p}_b] = i\hbar\, \delta_{a,b}$, where indexes $a,b$ indicate the coordinates, $a, b = x, y, z$, while $\delta_{a,b}$ is a conventional Kronecker symbol.
After that one needs to use the Schrödinger equation for $\psi_1$ and $\psi_2^*$ in the left-hand sides of Eqs.(1.5),(1.6).

Comment: clearly, Eqs.(1.5) and (1.6) can be considered as quantum generalizations of a conventional relation between the velocity and momentum as well as the second Newton law, respectively.

- Consider particular example of the potential in Eq.(1.4), the 3D quantum oscillator

$$U(\boldsymbol{r}, t) = \frac{m\,\omega^2}{2} \boldsymbol{r}^2 \qquad (1.10)$$

where $\omega$ is a constant. Introduce the "averaged" trajectory as the following matrix element

$$\boldsymbol{R}(t) = \langle \psi_2 |\, \boldsymbol{r}\, | \psi_1 \rangle \qquad (1.11)$$

and derive the second order differential equation on the function $\boldsymbol{R}(t)$.
Hint: it is convenient to rely on Eqs.(1.5)-(1.6).

**Question 2.** Spherical symmetry, Coulomb problem etc (Marks 35).

Consider the spherically symmetric potential energy *U(r)*.

a. Write down the Schrödinger equation for the s-wave radial wave function $P_0(r)$, which describes the radial motion of a particle with zero orbital momentum, *l=0,* in this potential. Remember that the wave function in this case can be presented as follows

$$\psi(\boldsymbol{r}) = \frac{1}{r} P_0(r)\,. \qquad (2.1)$$

Hint: keep in mind that in spherical coordinates the Laplacian reads

$$\Delta = \Delta_r + \frac{\Lambda}{r^2}, \tag{2.2}$$

where the angular part of the Laplacian $\Lambda$ includes derivatives over the spherical angles $\theta, \phi$, while the radial part satisfies

$$\Delta_r\left(\frac{P_0(r)}{r}\right) = \frac{1}{r} P_0''(r) . \tag{2.3}$$

b. Assume that the potential energy equals the Coulomb energy

$$U(r) = -\frac{e^2}{r} \tag{2.4}$$

Verify that in this case the 1s wave function

$$\psi_{1s}^{(0)}(r) = \frac{1}{\sqrt{\pi a_B^3}} e^{-r/a_B} \tag{2.5}$$

where $a_B = \frac{\hbar^2}{me^2}$, satisfies the Schrödinger equation and prove that the corresponding energy level equals

$$E_{1s}^{(0)} = -\frac{1}{2}\frac{me^2}{\hbar^2} = -Ry \tag{2.6}$$

c. Assume now that the potential energy has a more sophisticated form

$$U(r) = -\frac{e^2}{r} + \frac{\hbar^2}{2m}\frac{\lambda(\lambda+1)}{r^2} \tag{2.7}$$

where $\lambda > 0$ is a constant. Find an explicit simple formula, which describes the s-wave discrete energy levels

$$E_n = ?, \quad n = 1, 2, \ldots \tag{2.8}$$

Hint: remember the known fact, the Whittaker boundary problem

$$y''(x) + \left(-\frac{1}{4} + \frac{\kappa^2}{x} - \frac{\nu(\nu+1)}{x^2}\right) y(x) = 0 \tag{2.9}$$
$$y(0) = y(\infty) = 0$$

implies that the parameters in the Whittaker equation (2.9) have to satisfy

$$\kappa = \nu + n, \quad n = 1, 2, \ldots \tag{2.10}$$

**Question 3.** Perturbation theory (Marks 30).

Consider conventional formulation of the stationary perturbation theory assuming that

$$\hat{H} = \hat{H}^{(0)} + \hat{U} \tag{3.1}$$

where $\hat{H}^{(0)}$ is the initial Hamiltonian and $\hat{U}$ is a small perturbation. Assume that $\psi_n^{(0)}$ is a set of the wave function, which satisfy the initial Schrödinger equation

$$E_n^{(0)}\psi_n^{(0)} = \hat{H}^{(0)}\psi_n^{(0)} \tag{3.2}$$

while $E_n^{(0)}$ are the corresponding energy levels

a. Present (not derive) in general terms the first and second order corrections, $\delta E_n^{(1)}, \delta E_n^{(2)}$, to the n-th energy level.
b. Prove that the second order correction to the ground state level is always negative.
c. Let us choose $\hat{H}^{(0)}$ and $\hat{U}$ as follows

$$\hat{H}^{(0)} = \frac{\hat{p}^2}{2m} - \frac{e^2}{r}, \quad \hat{U} = U(r) = \frac{\hbar^2}{2m}\frac{\zeta}{r^2}, \tag{3.3}$$

where $\zeta$ is presumed small, $\zeta \ll 1$.

- Using the perturbation theory find the lowest, first order in powers of $\zeta$ correction to the 1s energy level $\delta E_{1s}$, which is produced by $U(r)$ from (3.3).

Hint. The only necessary in these calculations integral reads

$$\int_0^\infty e^{-\alpha x} x^n \, dx = \frac{n!}{\alpha^{n+1}} \tag{3.4}$$

Remember also that for a spherically symmetric case

$$d^3r = 4\pi r^2 \, dr \tag{3.5}$$

To verify dimensions keep in mind that

$$\mathrm{Ry} = \frac{1}{2}\frac{me^4}{\hbar^2} = \frac{1}{2}\frac{\hbar^2}{ma_B^2} \tag{3.6}$$

- Compare the found here correction $\delta E_{1s}$ with the one, which follows from an accurate (without perturbation theory) treatment of the problem suggested in Q2, see Eqs.(2.7)-(2.8). Remember that here we consider the 1s-state, while in Q2 the quantum number $n$ was presumed arbitrary; so that making comparison one needs to set $n=1$. Also keep in mind that parameters $\lambda, \zeta$ in Eqs.(2.7) and (3.3) need to be related as follows, $\zeta = \lambda(\lambda+1) \approx \lambda$, where the last equality comes from the fact that both these parameters need to be small to make the perturbation theory applicable.