StudentID:

PHYS 451: Quantum Mechanics I – Spring 2016 Instructor: Sergiy Bubin Final Exam

Instructions:

- All problems are worth the same number of points (although some might be more difficult than the others). The problem for which you get the lowest score will be dropped. Hence, even if you do not solve one of the problems you can still get the maximum score for the exam.
- This is a closed book exam. No notes, books, phones, tablets, calculators, etc. are allowed. Some information and formulae that might be useful are provided in the appendix. Please look through this appendix *before* you begin working on the problems.
- No communication with classmates is allowed during the exam.
- Show all your work, explain your reasoning. Answers without explanations will receive no credit (not even partial one).
- Write legibly. If I cannot read and understand it then I will not be able to grade it.
- Make sure pages are stapled together before submitting your work.

Problem 1. A particle of mass m moves in the symmetric potential

$$V(x) = -\alpha \Big[\delta(x-b) + \delta(x+b) \Big],$$

where α and b are positive constants and $\delta(x)$ is the Dirac delta function. Find the ground state wave function and the transcendental equation that relates the corresponding energy to the values of α and b. What is the energy in the limit $b \to 0$?

Problem 2. Consider the potential in the form of a step function:

$$V(x) = \begin{cases} 0, & x \le 0, \\ V_0 & x > 0. \end{cases}$$

Given that the incident particles come from the left calculate the reflection coefficient for the case when $E > V_0$.

Problem 3. Using the formalism of the creation and annihilation operators, find the explicit matrix form of operators \hat{x} , \hat{p} , and \hat{H} in the basis of eigenstates of the harmonic oscillator.

Problem 4. Consider a 1D quantum harmonic oscillator with the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2}$$

and a set of two operators

$$\hat{X} = \hat{x}\cos\omega t - \frac{\hat{p}}{m\omega}\sin\omega t$$
$$\hat{P} = \hat{x}m\omega\sin\omega t + \hat{p}\cos\omega t.$$

- (a) Do these operators commute with \hat{H} ?
- (b) How do their expectation values evolve with time?
- (c) Do you find the results in parts (a) and (b) contradicting each other? Explain.

Problem 5. The electron in a hydrogen atom is in the following state

$$\psi = R_{21}(r) \left[\sqrt{\frac{1}{3}} Y_1^0(\theta, \phi) \chi_+ - i \sqrt{\frac{2}{3}} Y_1^1(\theta, \phi) \chi_- \right],$$

where the traditional notations are used: R_{nl} are the radial components of the hydrogen wave functions, Y_l^m are spherical harmonics, and χ_{\pm} is the spin part of the wave function. Assuming that $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is the total angular momentum of the electron, give answers to the following questions:

- (a) If you measured L^2 , what values you might get and with what probability?
- (b) Same for L_z
- (c) Same for \mathbf{S}^2
- (d) Same for S_z
- (e) Same for \mathbf{J}^2
- (f) Same for J_z

- (g) If you measured the position of the particle, what would be the probability density for finding it at r, θ, ϕ ?
- (h) If you measured simultaneously both the z component of the spin and the distance from the origin (note that these two observables are compatible), what would be the probability density for finding the particle with spin up and at radius r?

Problem 6. An electron moves along the *y*-axis through a uniform magnetic field that is also directed along the *y*-axis, $\mathbf{B} = B\mathbf{e}_y$. At time t = 0 its spin state is $\chi(0) = \chi_-$ (notations χ_+ and χ_- stand for the states with a positive or negative projection of the spin on the *z*-axis).

- (a) What is $\chi(t)$ for t > 0?
- (b) What would be the expectation values for measurements of the observables S_x , S_y , and S_z ?

The Schrödinger equation

Time-dependent: $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$ Stationary: $\hat{H}\psi_n = E_n\psi_n$

De Broglie relations

 $\lambda = h/p, \ \nu = E/h$ or $\mathbf{p} = \hbar \mathbf{k}, \ E = \hbar \omega$

Heisenberg uncertainty principle

Position-momentum: $\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$ Energy-time: $\Delta E \, \Delta t \geq \frac{\hbar}{2}$ General: $\Delta A \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|$

Probability current

1D: $j(x,t) = \frac{i\hbar}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right)$ 3D: $j(\mathbf{r},t) = \frac{i\hbar}{2m} \left(\psi \nabla \psi^* - \psi^* \nabla \psi \right)$

> Time-evolution of the expectation value of an observable Q(generalized Ehrenfest theorem)

$$\frac{d}{dt}\langle \hat{Q}\rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}]\rangle + \langle \frac{\partial \hat{Q}}{\partial t}\rangle$$

Infinite square well $(0 \le x \le a)$

Energy levels: $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$, $n = 1, 2, ..., \infty$ Eigenfunctions: $\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$ $(0 \le x \le a)$ Matrix elements of the position: $\int_{0}^{a} \phi_{n}^{*}(x) x \phi_{k}(x) dx = \begin{cases} a/2, & n = k \\ 0, & n \neq k; \ n \pm k \text{ is even} \\ -\frac{8nka}{\pi^{2}(n^{2}-k^{2})^{2}}, & n \neq k; \ n \pm k \text{ is odd} \end{cases}$

Quantum harmonic oscillator

The few first wave functions $(\alpha = \frac{m\omega}{\hbar})$: $\phi_0(x) = \frac{\alpha^{1/4}}{\pi^{1/4}} e^{-\alpha x^2/2}, \ \phi_1(x) = \sqrt{2} \frac{\alpha^{3/4}}{\pi^{1/4}} x e^{-\alpha x^2/2}, \ \phi_2(x) = \frac{1}{\sqrt{2}} \frac{\alpha^{1/4}}{\pi^{1/4}} \left(2\alpha x^2 - 1\right) e^{-\alpha x^2/2}$ Matrix elements of the position: $\langle \phi_n | \hat{x} | \phi_k \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{k} \, \delta_{n,k-1} + \sqrt{n} \, \delta_{k,n-1} \right)$ $\langle \phi_n | \hat{x}^2 | \phi_k \rangle = \frac{\hbar}{2m\omega} \left(\sqrt{k(k-1)} \,\delta_{n,k-2} + \sqrt{(k+1)(k+2)} \,\delta_{n,k+2} + (2k+1) \,\delta_{nk} \right)$ Matrix elements of the momentum: $\langle \phi_n | \hat{p} | \phi_k \rangle = i \sqrt{\frac{m\hbar\omega}{2}} \left(\sqrt{k} \, \delta_{n,k-1} - \sqrt{n} \, \delta_{k,n-1} \right)$

Creation and annihilation operators for harmonic oscillator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + \frac{i}{\sqrt{2m\hbar\omega}} \hat{p} \qquad \qquad \hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right) \qquad \qquad \hat{N} = \hat{a}^{\dagger} \hat{a} \qquad \qquad [\hat{a}, \hat{a}^{\dagger}] = 1 \\ \hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - \frac{i}{\sqrt{2m\hbar\omega}} \hat{p} \qquad \qquad \hat{a} \left| n \right\rangle = \sqrt{n} \left| n - 1 \right\rangle \qquad \qquad \hat{a}^{\dagger} \left| n \right\rangle = \sqrt{n+1} \left| n + 1 \right\rangle$$

Equation for the radial component of the wave function of a particle moving in a spherically symmetric potential V(r)

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]R_{nl} = E_{nl}R_{nl}$$

Energy levels of the hydrogen atom

$$E_n = -\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{n^2},$$

The few first radial wave functions R_{nl} for the hydrogen atom $(a = \frac{4\pi\epsilon_0\hbar^2}{mZe^2})$

$$R_{10} = 2a^{-3/2} e^{-\frac{r}{a}} \qquad R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2}\frac{r}{a}\right) e^{-\frac{r}{2a}} \qquad R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-\frac{r}{2a}}$$

The few first spherical harmonics

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{4\pi}} \frac{z}{r} \qquad Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta \, e^{\pm i\phi} = \mp \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$$

Operators of the square of the orbital angular momentum and its projection on the z-axis in spherical coordinates

$$\hat{\mathbf{L}}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \qquad \hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}$$

Fundamental commutation relations for the components of angular momentum

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \qquad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x \qquad [\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$$

Raising and lowering operators for the z-projection of the angular momentum

$$\hat{J}_{\pm} = \hat{J}_x \pm i \hat{J}_y$$
 Action: $\hat{J}_{\pm} | j, m \rangle = \hbar \sqrt{j(j+1) - m(m\pm 1)} | j, m \pm 1 \rangle$

Relation between coupled and uncoupled representations of states formed by two subsystems with angular momenta j_1 and j_2

$$|J M j_1 j_2\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle j_1 m_1 j_2 m_2 | J M j_1 j_2 \rangle | j_1 m_1 \rangle | j_2 m_2 \rangle \qquad m_1 + m_2 = M$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Electron in a magnetic field

Hamiltonian: $H = -\boldsymbol{\mu} \cdot \mathbf{B} = -\gamma \mathbf{B} \cdot \mathbf{S} = \frac{e}{m} \mathbf{B} \cdot \mathbf{S} = \mu_{\mathrm{B}} \mathbf{B} \cdot \boldsymbol{\sigma}$ here e > 0 is the magnitude of the electron electric charge and $\mu_{\mathrm{B}} = \frac{e\hbar}{2m}$

Bloch theorem for periodic potentials V(x+a) = V(x)

 $\psi(x+a) = e^{iKa}\psi(x)$

Dirac delta function

$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)dx = f(x_0) \qquad \delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx}dk \qquad \delta(-x) = \delta(x) \qquad \delta(cx) = \frac{1}{|c|}\delta(x)$$

Fourier transform conventions

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)e^{-ikx}dx \qquad \qquad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{f}(k)e^{ikx}dk$$

or, in terms of $p = \hbar k$ $\tilde{f}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} f(x)e^{-ipx/\hbar} dx$ $f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{f}(p)e^{ipx/\hbar} dp$

Useful integrals

$$\begin{split} \int x \sin(\alpha x) \, dx &= \frac{\sin(\alpha x)}{\alpha^2} - \frac{x \cos(\alpha x)}{\alpha} \\ \int x^2 \sin(\alpha x) \, dx &= \frac{2x \sin(\alpha x)}{\alpha^2} - \frac{(\alpha^2 x^2 - 2) \cos(\alpha x)}{\alpha^3} \\ \int x^3 \sin(\alpha x) \, dx &= \frac{3(\alpha^2 x^2 - 2) \sin(\alpha x)}{\alpha^4} - \frac{x(\alpha^2 x^2 - 6) \cos(\alpha x)}{\alpha^3} \\ \int x^4 \sin(\alpha x) \, dx &= \frac{4x(\alpha^2 x^2 - 6) \sin(\alpha x)}{\alpha^4} - \frac{(\alpha^4 x^4 - 12\alpha^2 x^2 + 24) \cos(\alpha x)}{\alpha^5} \\ \int_0^\infty x^{2k} e^{-\beta x^2} \, dx &= \sqrt{\pi} \frac{(2k)!}{k! 2^{2k+1} \beta^{k+1/2}} \quad (\text{Re } \beta > 0, \, k = 0, 1, 2, ...) \\ \int_0^\infty x^{2k+1} e^{-\beta x^2} \, dx &= \frac{1}{2} \frac{k!}{\beta^{k+1}} \quad (\text{Re } \beta > 0, \, k = 0, 1, 2, ...) \\ \int_0^\infty x^k e^{-\gamma x} \, dx &= \frac{k!}{\gamma^{k+1}} \quad (\text{Re } \gamma > 0, \, k = 0, 1, 2, ...) \\ \int_{-\infty}^\infty e^{-\beta x^2} e^{iqx} \, dx &= \sqrt{\frac{\pi}{\beta}} e^{-\frac{q^2}{4\beta}} \quad (\text{Re } \beta > 0) \\ \int_{-\infty}^\pi \sin^{2k} x \, dx &= \pi \frac{(2k-1)!!}{2^k k!} \quad (k = 0, 1, 2, ...) \end{split}$$

Useful trigonometric identities

$\sin(\alpha \pm \beta) = \sin \alpha \cos \beta \pm \cos \alpha \sin \beta$	$\cos(\alpha \pm \beta) = \cos\alpha \cos\beta \mp \sin\alpha \sin\beta$
$\sin \alpha \sin \beta = \frac{1}{2} [\cos(\alpha - \beta) - \cos(\alpha + \beta)]$	$\cos \alpha \cos \beta = \frac{1}{2} [\cos(\alpha - \beta) + \cos(\alpha + \beta)]$
$\sin \alpha \cos \beta = \frac{1}{2} [\sin(\alpha + \beta) + \sin(\alpha - \beta)]$	$\cos \alpha \sin \beta = \frac{1}{2} [\sin(\alpha + \beta) - \sin(\alpha - \beta)]$

Useful identities for hyperbolic functions

 $\cosh^2 x - \sinh^2 x = 1$ $\tanh^2 x + \operatorname{sech}^2 x = 1$ $\operatorname{coth}^2 x - \operatorname{csch}^2 x = 1$