StudentID: ________________________

PHYS 451: Quantum Mechanics I – Spring 2018
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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. Consider a 1D quantum harmonic oscillator. At time $t = 0$, it is in the state

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{3}}\big(|1\rangle + |2\rangle + |3\rangle\big),$$

where $|n\rangle$ is the n-th energy eigenstate. Find the expectation value of the position and energy at time t.

Problem 2. In the questions below $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ are basis kets that span some Hilbert space $\mathcal{H}$, while a and b are some complex constants. Are the following operators Hermitian in $\mathcal{H}$?

(a) $|1\rangle\langle 2| + i|2\rangle\langle 1|$

(b) $|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 4| + |4\rangle\langle 3|$

(c) $\big(a|1\rangle + b^*|2\rangle\big)^\dagger \big(b|1\rangle - a^*|2\rangle\big)|3\rangle\langle 2| + |4\rangle\langle 4|$

(d) $|1\rangle\langle 1| + i|2\rangle\langle 1| - i|1\rangle\langle 2| + |2\rangle\langle 2|$

Let $|\psi\rangle$ be some normalized ket in $\mathcal{H}$ and $\hat{1}$ is the identity operator. Is the following operator a projection operator?

(e) $\hat{A} = \frac{1}{\sqrt{2}}\left(\hat{1} + |\psi\rangle\langle\psi|\right)$

Let $\hat{I}$ be the inversion operator, whose action on an arbitrary function $f(x)$ is defined as $\hat{I}f(x) = f(-x)$. Find the explicit form (i.e. simplify) the following operator

(f) $\exp(i\pi\hat{I})$

Find the Hermitian conjugate of the following operator

(g) $\frac{d^5}{dx^5}$

Assuming the case of a spin 1/2 particle, find the explicit matrix form of the following operator in the basis of eigenstates of $\hat{S}_z$

(h) Projection operator on the state with the positive projection of spin on the y-axis

Problem 3. Consider a particle of mass m in 3D that is constrained to move freely between two concentric impermeable spheres of radii a and b ($a < b$). Find the ground state energy and normalized wave function. You can use any knowledge about the properties of ground state wave functions to simplify your work, but make sure to clearly explain what it is.

Problem 4. The Hamiltonian for a spin 1 system is given by

$$\hat{H} = \alpha\hat{S}_z^2 + \beta(\hat{S}_x^2 - \hat{S}_y^2),$$

where α and β are real constants. Find the allowed energies and the corresponding eigenstates for this system.

Problem 5. Consider a finite 1D well that can support only a single bound state $|g(x)\rangle$ that is well separated in energy from the continuum states. The energy of this bound state is ε. Now two more such wells are added – one on the right and one on the left, both at distanse a from the center. Use the method of linear combination of atomic orbitals (LCAO) to estimate the energy levels of a particle in this potential created by the three wells. For simplicity, assume that the overlap between two neighbouring "atomic" states $g(x)$ and $g(x \pm a)$ is is small yet finite. At the same time the overlap between states $g(x-a)$ and $g(x+a)$ is negligibly small. You can also introduce some notations to simplify your calculations, e.g.

$$\varepsilon \equiv \langle g(x)|\hat{H}|g(x)\rangle, \qquad \beta \equiv \langle g(x-a)|\hat{H}|g(x)\rangle,$$

where $\hat{H}$ is the Hamiltonian of a single well located in the center.

Appendix: formula sheet

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 $(0 \leq x \leq a)$

Energy levels: $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},\ \ n = 1, 2, ..., \infty$

Eigenfunctions: $\phi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad (0 \leq x \leq a)$

Matrix elements of the position: $\int\limits_0^a \phi_n^*(x)x\,\phi_k(x)dx = \begin{cases} a/2, & n = k \\ 0, & n \neq k;\ n \pm k \text{ is even} \\ -\frac{8nka}{\pi^2(n^2-k^2)^2}, & n \neq k;\ n \pm k \text{ is odd} \end{cases}$

Quantum harmonic oscillator

The few first wave functions ($\alpha = \frac{m\omega}{\hbar}$):

$\phi_0(x) = \frac{\alpha^{1/4}}{\pi^{1/4}}\,e^{-\alpha x^2/2},\ \ \phi_1(x) = \sqrt{2}\frac{\alpha^{3/4}}{\pi^{1/4}}\,x\,e^{-\alpha x^2/2},\ \ \phi_2(x) = \frac{1}{\sqrt{2}}\frac{\alpha^{1/4}}{\pi^{1/4}}\,(2\alpha x^2 - 1)\,e^{-\alpha x^2/2}$

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

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

$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}$ $\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$ $\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$

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

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

Energy levels of the hydrogen atom ($a = \frac{a_0}{Z} = \frac{4\pi\epsilon_0\hbar^2}{mZe^2}$)

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

The few first radial wave functions R_{nl} for the hydrogen atom

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

The few first spherical harmonics

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

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

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

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

Pauli matrices

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

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

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

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

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 $V(x+a) = V(x)$

$\psi(x) = e^{ikx} u(x)$, where $u(x+a) = u(x)$ Equivalent form: $\psi(x+a) = e^{ika}\psi(x)$

Dirac delta function

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

Fourier transform conventions

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

or, in terms of $p = \hbar k$

$$\tilde{f}(p) = \tfrac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} f(x) e^{-ipx/\hbar} dx \qquad f(x) = \tfrac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{f}(p) e^{ipx/\hbar} dp$$

Useful integrals

$$\int_0^\infty x^{2k} e^{-\beta x^2} dx = \sqrt{\pi} \frac{(2k)!}{k!\, 2^{2k+1} \beta^{k+1/2}} \quad (\mathrm{Re}\,\beta > 0,\ k = 0, 1, 2, ...)$$

$$\int_0^\infty x^{2k+1} e^{-\beta x^2} dx = \frac{1}{2} \frac{k!}{\beta^{k+1}} \quad (\mathrm{Re}\,\beta > 0,\ k = 0, 1, 2, ...)$$

$$\int_0^\infty x^k e^{-\gamma x} dx = \frac{k!}{\gamma^{k+1}} \quad (\mathrm{Re}\,\gamma > 0,\ k = 0, 1, 2, ...)$$

$$\int_{-\infty}^\infty e^{-\beta x^2} e^{iqx} dx = \sqrt{\frac{\pi}{\beta}} e^{-\frac{q^2}{4\beta}} \quad (\mathrm{Re}\,\beta > 0)$$

$$\int_0^\pi \sin^{2k} x\, dx = \pi \frac{(2k-1)!!}{2^k\, k!} \quad (k = 0, 1, 2, ...)$$

$$\int_0^\pi \sin^{2k+1} x\, dx = \frac{2^{k+1}\, k!}{(2k+1)!!} \quad (k = 0, 1, 2, ...)$$