StudentID: ________________________

PHYS 452 Quantum Mechanics II (Fall 2018)
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Midterm Exam 1

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 particle of mass m moving inside a hollow spherically symmetric shell (in 3D):

$$V(r) = \begin{cases} 0, & a < r < b \\ \infty, & \text{otherwise} \end{cases}$$

(a) Devise a simple (as simple as possible) yet *meaningful* trial wave function to approximate the ground state wave function.

(b) Using the above trial wave function estimate the ground state energy.

Problem 2. A three-level quantum system is described by the following Hamiltonian (in some units)

$$H_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}.$$

It is subject to a weak additional interaction in the form

$$V = \begin{pmatrix} 0 & \beta & 0 \\ \beta & 0 & 0 \\ 0 & 0 & \beta \end{pmatrix},$$

where $\beta \ll 1$. Use the formalism of the perturbation theory to find corrections to both the energy levels and eigenstates up to the first order in β.

Problem 3. Consider a particle of mass m in a 2D square box ($0 < x < a$, $0 < y < a$). The system is perturbed by a weak additional constant potential that has nonzero value only in the first quadrant of the box, i.e.

$$H'(x, y) = \begin{cases} \gamma, & 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{a}{2}, \\ 0, & \text{otherwise.} \end{cases}$$

Find the first-order energy corrections and proper zero-order wave functions for the ground and first excited states.

Problem 4. Consider an electron in the hydrogen atom. The electron is in the state with the principal quantum number n. Answer the questions below. Be specific, show things clearly, give your reasoning, and use formulae when necessary.

(a) What is the degeneracy of this state?

(b) Is any of that degeneracy lifted by a uniform external electric field?

(c) Is any of that degeneracy lifted by a uniform external magnetic field?

(d) Is any of that degeneracy lifted by the spin-orbit interaction?

(e) Using the relativistic formula for the total energy of the electron and assuming that the electon's velocity is small compared to the speed of light, derive the leading correction to the nonrelativistic kinetic energy (known as the mass-velocity term). Is any of the above mentioned degeneracy lifted by the mass-velocity term?

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

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

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

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

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

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

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

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

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

$$|j_1\, m_1\rangle\, |j_2\, m_2\rangle = \sum_{J=|j_1-j_2|}^{j_1+j_2} \langle JMj_1j_2 | j_1m_1j_2m_2\rangle\, |J\, M\, j_1\, j_2\rangle \qquad M = m_1 + m_2$$

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

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

Density matrix $\hat{\rho}$

$\hat{\rho} = \sum_i p_i|\psi_i\rangle\langle\psi_i|$, where $\sum_i p_i = 1$

Expectation value of some observable A: $\langle\hat{A}\rangle = \sum_i p_i\langle\psi_i|\hat{A}|\psi_i\rangle = \mathrm{tr}(\hat{\rho}\hat{A})$, where $\mathrm{tr}(\hat{\rho}) = 1$

Time evolution operator

$$\hat{U}(t_f, t_i) = \hat{\mathcal{T}}\exp\left[-\frac{i}{\hbar}\int_{t_i}^{t_f}\hat{H}(t)dt\right] = 1 + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 \ldots \int_{t_i}^{t_{n-1}} dt_n \hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)$$

In particular, $\hat{U}(t_f, t_i) = \exp\left[-\frac{i}{\hbar}\hat{H}(t_f - t_i)\right]$ when $\hat{H} \neq \hat{H}(t)$

Schrödinger, Heisenberg and interaction pictures

$\psi_H = \hat{U}^{-1}\psi_S,\ \ \psi_H = \psi_S(t{=}0),\ \ \hat{A}_H = \hat{U}^{-1}\hat{A}_S\hat{U},\ \ i\hbar\frac{\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}] + i\hbar\frac{\partial \hat{A}_H}{\partial t},\ \ \frac{\partial \hat{A}_H}{\partial t} \equiv \hat{U}^{-1}\frac{\partial \hat{A}_S}{\partial t}\hat{U}$

If $\hat{H} = \hat{H}_0 + \hat{V}(t)$, then

$\psi_I = \hat{U}_0^{-1}\psi_S,\ \ \hat{U}_0 = \exp\left[-\frac{i}{\hbar}\hat{H}_0 t\right],\ \ \hat{A}_I = \hat{U}_0^{-1}\hat{A}_S\hat{U}_0,\ \ i\hbar\frac{\partial\hat{\psi}_I}{\partial t} = \hat{V}_I\psi_I$

$\psi_I(t) = \psi_I(0) + \frac{1}{i\hbar}\int\limits_0^t \hat{V}_I(t')\psi_I(t')dt'$

Rayleigh-Ritz variational method

$$\psi_{\text{trial}} = \sum_{i=1}^{n} c_i\phi_i \qquad Hc = \epsilon Sc, \qquad \text{where } c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \qquad \text{and} \quad \begin{array}{l} H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle \\ S_{ij} = \langle\phi_i|\phi_j\rangle \end{array}$$

Stationary perturbation theory formulae

$$H = H^0 + \lambda H', \qquad E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots, \qquad \psi_n = \psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots$$

$$E_n^{(1)} = H'_{nn}$$

$$\psi_n^{(1)} = \sum_m c_{nm}\psi_m^{(0)}, \quad c_{nm} = \begin{cases} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}, & n \neq m \\ 0, & n = m \end{cases}$$

$$E_n^{(2)} = \sum_{m\neq n} \frac{|H'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$\psi_n^{(2)} = \sum_m d_{nm}\psi_m^{(0)}, \quad d_{nm} = \begin{cases} \frac{1}{E_n^{(0)} - E_m^{(0)}}\left(\sum\limits_{k\neq n}\frac{H'_{mk}H'_{kn}}{E_n^{(0)} - E_k^{(0)}}\right) - \frac{H'_{nn}H'_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}, & n \neq m \\ 0, & n = m \end{cases}$$

Dirac delta function

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

Fourier transform conventions

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

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

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

Useful integrals

$$\int \sqrt{a^2-x^2}\,dx = \frac{1}{2}\left(x\sqrt{a^2-x^2} + a^2 \arctan\left[\frac{x}{\sqrt{a^2-x^2}}\right]\right)$$

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

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

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

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

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

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

$$\int\limits_{0}^{2\pi} \cos m\phi\, e^{in\phi}\,dx = \pi(\delta_{m,n} + \delta_{m,-n}) \quad (m,n = 0,\pm1,\pm2,...)$$

Useful trigonometric identities

$$\sin(\alpha\pm\beta) = \sin\alpha\cos\beta \pm \cos\alpha\sin\beta \qquad \cos(\alpha\pm\beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta$$

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

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

Useful identities for hyperbolic functions

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