StudentID: ____________________

PHYS 452 Quantum Mechanics II (Fall 2019)
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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 the $5S_{1/2}$ state ($n = 5$, $l = 0$) of the ^{87}Rb atom. The nucleus in this alkali atom has spin 3/2. The interaction of the valence electron spin and the nuclear spin is described by the hyperfine Hamiltonian $H_{hf} = A\,\mathbf{S}\cdot\mathbf{I}$, where A is some constant.

(a) What are the possible values of the total angular momentum of the electron $\mathbf{J}$?

(b) What are the possible values of the total atomic angular momentum $\mathbf{F}$?

(c) Which basis is most convenient for the calculations of the hyperfine structure of the given state? Explain.

(d) How many levels the $5S_{1/2}$ splits into? What are their degeneracy? What are their shifts from the unperturbed position?

Problem 2. Consider a particle of mass m in the fourth excited state of the 3D infinite potential well that has a rectangular shape ($0 \leq x \leq a$, $0 \leq y \leq a$, $0 \leq z \leq 2a$). The particle is subject to a perturbing potential in the form $V(x, y, z) = \beta xyz$, where β is a constant. Find the first order-correction to the energy.

Problem 3. A particle of mass m moves in a spherically symmetric potential $V(r) = \frac{\alpha}{\sqrt{r}}$, where α is a constant. Are there any restrictions/conditions on α in order to ensure that the system has discrete energy levels? Assuming that there are such levels, estimate the ground state energy using the variational method. Pick the most appropriate simple trial wave function that will allow you to do all necessary calculations analytically and with relative ease. Give a reason for your choice, i.e. explain why it should be better than alternatives.

Problem 4. Consider a 1D quantum harmonic oscillator of mass m and frequency ω. It is subjected to a momentum-dependent perturbation in the form γp^2, where γ is a small positive constant. Find the correction to the ground state energy of this particle up to the second order in γ.

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: $\int_0^a \phi_n^*(x)x\,\phi_k(x)dx = \begin{cases} a/2, & n = k \\ 0, & n \neq k;\; n \pm k \text{ is even} \\ -\frac{8nka}{\pi^2(n^2-k^2)^2}, & n \neq k;\; n \pm k \text{ is odd} \end{cases}$

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: $\langle\phi_n|\hat{x}|\phi_k\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{k}\,\delta_{n,k-1} + \sqrt{k+1}\,\delta_{n,k+1}\right)$

$$\langle\phi_n|\hat{x}^2|\phi_k\rangle = \frac{\hbar}{2m\omega}\left(\sqrt{k(k-1)}\,\delta_{n,k-2} + (2k+1)\,\delta_{nk} + \sqrt{(k+1)(k+2)}\,\delta_{n,k+2}\right)$$

Matrix elements of the momentum: $\langle\phi_n|\hat{p}|\phi_k\rangle = -i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{k}\,\delta_{n,k-1} - \sqrt{k+1}\,\delta_{n,k+1}\right)$

$$\langle\phi_n|\hat{p}^2|\phi_k\rangle = -\frac{m\hbar\omega}{2}\left(\sqrt{k(k-1)}\,\delta_{n,k-2} - (2k+1)\,\delta_{nk} + \sqrt{(k+1)(k+2)}\,\delta_{n,k+2}\right)$$

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

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

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

$Y_0^0 = \frac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\,\frac{z}{r} \qquad Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi} = \mp\sqrt{\frac{3}{8\pi}}\,\frac{x\pm iy}{r}$

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: $\hat{J}_\pm|j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}\,|j,m\pm1\rangle$

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

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

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

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

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

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

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

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

$$\int x\sin^2 x\,dx = \frac{x^2}{4} - \frac{\cos 2x}{8} - \frac{x\sin 2x}{4}$$

$$\int\limits_0^{\infty} x^{2k}e^{-\beta x^2}dx = \sqrt{\pi}\frac{(2k)!}{k!\,2^{2k+1}\beta^{k+1/2}} \quad (\mathrm{Re}\,\beta > 0,\ k = 0, 1, 2, ...)$$

$$\int\limits_0^{\infty} x^{2k+1}e^{-\beta x^2}dx = \frac{1}{2}\frac{k!}{\beta^{k+1}} \quad (\mathrm{Re}\,\beta > 0,\ k = 0, 1, 2, ...)$$

$$\int\limits_0^{\infty} x^k e^{-\gamma x}dx = \frac{k!}{\gamma^{k+1}} \quad (\mathrm{Re}\,\gamma > 0,\ k = 0, 1, 2, ...)$$

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

$$\int\limits_0^{\pi} \sin^{2k} x\,dx = \pi\frac{(2k-1)!!}{2^k\,k!} \quad (k = 0, 1, 2, ...)$$

$$\int\limits_0^{\pi} \sin^{2k+1} x\,dx = \frac{2^{k+1}\,k!}{(2k+1)!!} \quad (k = 0, 1, 2, ...)$$

$$\int\limits_0^{2\pi} \cos m\phi\, e^{in\phi}\,dx = \pi(\delta_{m,n} + \delta_{m,-n}) \quad (m, n = 0, \pm 1, \pm 2, ...)$$

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

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