StudentID: ____________________

PHYS 451 Quantum Mechanics II (Fall 2017)
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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 in the potential

$$V(x) = g|x|, \quad -\infty < x < \infty,$$

where g is a positive constant. In the framework of the variational method estimate the energy of the first excited state using a trial wave function that has an exponential asymptotics, namely

$$\psi(x) = Af(x)e^{-b|x|}.$$

Here A is a normalization constant, b is an adjustable parameter, and $f(x)$ is some function. You need to choose $f(x)$ in such a way that your estimate is meaningful. Keep it simple and do not introduce any additional adjustable parameters in $f(x)$.

Problem 2. Consider a particle of mass m in a 2D box, $0 \le x \le a$, $0 \le y \le a$. A small perturbation in the form $V(x, y) = Cxy$ is applied. Find the energy change for the ground and first excited state up to the lowest nonvanishing order in V.

Problem 3. Consider a particle with spin 1. The Hamiltonian of the particle is given by $H = \alpha S_z^2$, where α is a constant and S_z is the z-component of the particle's spin. The particle is now subjected to an additional (and weak) interaction. The matrix elements of that interaction in the basis of the eigenstates of H are such that all diagonal elements vanish, while all off-diagonal ones are equal to $\hbar^2\beta$, where β is a constant such that $\beta \ll \alpha$. Using the perturbation theory, find corrections to the energy levels of the particle up to the second order in the small parameter $\gamma = \frac{\beta}{\alpha}$.

Problem 4. Consider a particle of mass m moving in the Gaussian well potential

$$V(x) = -V_0 e^{-\beta x^2},$$

where V_0 and β are positive constants. The exact analytic solution to the Schrödinger equation with this potential is not known. However, under certain condition the ground state energy level is located deep at the bottom of the well and the problem can be treated perturbatively.

(a) What is this condition?

(b) Find the expansion of the ground state energy in powers of the relevant small parameter up to the lowest nontrivial order.

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

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

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

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

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

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

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

Fourier transform conventions

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

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

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

Useful integrals

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

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

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

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

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

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

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

$$\int_0^{2\pi} \cos m\phi\, e^{in\phi}\,dx = \pi(\delta_{m,n} + \delta_{m,-n}) \quad (m,n = 0,\pm 1,\pm 2,...)$$

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

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