StudentID: ____________________

PHYS 452: Quantum Mechanics II – Fall 2016
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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. Use a linear trial wave function (i.e. $ar + b$) to estimate the ground state energy of a particle of mass m in an infinite spherical well of radius R. Make sure the linear function satisfies the boundary conditions properly.

Problem 2. 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 potential that has the following form:

$$V(x) = \begin{cases} \beta, & \frac{a}{4} < x < \frac{3a}{4} \text{ and } \frac{a}{4} < y < \frac{3a}{4}, \\ 0, & \text{otherwise.} \end{cases}$$

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

Problem 3. Consider a quantum rotor constrained to rotate in a plane (let us suppose in xy-plane). Thus, its position is defined by a single angle, ϕ. The Hamiltonian of the rotor is

$$\hat{H} = \frac{\hat{L}_z^2}{2I},$$

where I is its moment of inertia (a constant). Obviously, the wave function of the rotor must be periodic, i.e. $\psi(\phi + 2\pi) = \psi(\phi)$.

(a) Determine the eigenvalues and normalized eigenfunctions of $\hat{H}$. Are any of the energy levels degenerate?

(b) Now add a small perturbation in the form $\hat{H}' = -\lambda \cos 2\phi$ and compute the lowest non-vanishing correction to the ground state energy due to that perturbation.

(c) Calculate the ground state wave function to the first order in λ.

(d) Calculate the lowest non-vanishing energy correction for the first excited energy level.

Problem 4. Use the semiclassical approach to estimate the energy levels of a particle of mass m moving in the potential $V(x) = \alpha|x|$. As a sanity check, compare the dependence of E_n on n in the limit of large n for this potential with the two cases for which exact analytic expressions are known: the harmonic oscillator and particle in a box.

Appendix: formula sheet

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 ($0 \leq x \leq a$)

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 ($\alpha = \frac{m\omega}{\hbar}$):

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

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

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

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

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

$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \qquad$ 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 $V(x+a) = V(x)$

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

Rayleigh-Ritz variational method

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

Stationary perturbation theory formulae

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

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

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

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

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

WKB wave function

$$\psi(x) = \frac{A}{\sqrt{p(x)}} \exp\left[+\frac{i}{\hbar}\int p(x)dx\right] + \frac{B}{\sqrt{p(x)}} \exp\left[-\frac{i}{\hbar}\int p(x)dx\right], \text{ where } p(x) = \sqrt{2m(E - V(x))}$$

Bohr-Sommerfeld quantization rules

$\int\limits_a^b p(x)dx = (n - \frac{1}{2})\pi\hbar$ – the potential has no vertical walls at a or b

$\int\limits_a^b p(x)dx = (n - \frac{1}{4})\pi\hbar$ – only one wall of the potential is vertical

$\int\limits_a^b p(x)dx = n\pi\hbar$ – both walls of the potential are vertical

Here a and b are classical turning points and $n = 1, 2, 3, \ldots$

Semiclassical barrier tunneling

$$T \sim \exp\left[-2\int\limits_a^b \kappa(x)dx\right] \qquad \kappa(x) = \frac{1}{\hbar}\sqrt{2m(V(x) - E)}$$

Dirac delta function

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

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

$$\int x\sin(\alpha x)\,dx = \frac{\sin(\alpha x)}{\alpha^2} - \frac{x\cos(\alpha x)}{\alpha}$$

$$\int x^2\sin(\alpha x)\,dx = \frac{2x\sin(\alpha x)}{\alpha^2} - \frac{\left(\alpha^2x^2-2\right)\cos(\alpha x)}{\alpha^3}$$

$$\int x^3\sin(\alpha x)\,dx = \frac{3\left(\alpha^2x^2-2\right)\sin(\alpha x)}{\alpha^4} - \frac{x\left(\alpha^2x^2-6\right)\cos(\alpha x)}{\alpha^3}$$

$$\int x^4\sin(\alpha x)\,dx = \frac{4x\left(\alpha^2x^2-6\right)\sin(\alpha x)}{\alpha^4} - \frac{\left(\alpha^4x^4-12\alpha^2x^2+24\right)\cos(\alpha x)}{\alpha^5}$$

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

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

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

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

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

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

$$\int\limits_0^{2\pi} \cos m\phi\, e^{in\phi}\,dx = \pi(\delta_{m,n}+\delta_{m,-n}) \quad (m,n=0,\pm1,\pm2,...)$$

Useful trigonometric identities

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

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

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

Useful identities for hyperbolic functions

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