PHYS 451: Quantum Mechanics I – Spring 2018
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Midterm Exam 2

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 two particles with spins $s_1 = 1$ and $s_2 = 1/2$. For the case of $S = 3/2$ ($\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2$ is the operator of the total spin) we have the following four eigenstates of $\hat{\mathbf{S}}^2$ and $\hat{S}_z$:

$$|S\,M\,s_1\,s_2\rangle \;=\; \left|\frac{3}{2}\,\frac{3}{2}\,1\,\frac{1}{2}\right\rangle, \quad \left|\frac{3}{2}\,\frac{1}{2}\,1\,\frac{1}{2}\right\rangle, \quad \left|\frac{3}{2}\,-\frac{1}{2}\,1\,\frac{1}{2}\right\rangle, \quad \left|\frac{3}{2}\,-\frac{3}{2}\,1\,\frac{1}{2}\right\rangle.$$

Express theese four states in terms of the eigenstates of $\hat{S}_1^2$, $\hat{S}_{1z}$, and $\hat{S}_2^2$, $\hat{S}_{2z}$

Problem 2. A particle of spin 1 is placed in a uniform magnetic field $\mathbf{B} = (0, B, 0)$. The gyromagnetic ratio that relates the particle's spin to its magnetic moment is g. Initially, at time $t = 0$, the particle is in the state with zero projection of its spin on the z-axis. What is the probability that the particle remains in that state at $t > 0$?

Problem 3. Two non-interacting particles, each of mass m, are placed in an infinite square well ($0 < x < a$). One particle is in the state ϕ_n, while the other one is in the state ϕ_l ($n \neq l$). Calculate the average square of the interparticle distance if

(a) the particles are distinguishable

(b) they are bosons

(c) they are fermions

Problem 4.

(a) Consider the helium atom, which has two electrons (recall that electrons are spin $1/2$ fermions). If there were no Coulomb repulsion between the electrons, what would be the total wave function for the ground state of this atom? Write it explicitly and explain each term. What is the total energy that corresponds to that wave function? Give a number either in atomic units (hartrees).

(b) Now consider the boron atom, which has five electrons. Again, if you ignore the inter-electron repulsion completely, what is the total energy of the ground state? In this case you do not need to write any wave functions, just give the energy (but explain how you got it!).

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

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

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

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 $\left(a = \frac{a_0}{Z} = \frac{4\pi\epsilon_0\hbar^2}{mZe^2}\right)$

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

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

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

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

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \qquad \text{Action:}\quad \hat{J}_\pm|j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\,|j, m\pm 1\rangle$$

Pauli matrices

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

Matrix form of angular momentum operators for $l = 1$

$$L_x = \frac{1}{\sqrt{2}}\hbar\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad L_y = \frac{1}{\sqrt{2}}\hbar\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad L_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

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

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

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

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

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

Dirac delta function

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

Fourier transform conventions

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

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

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

Useful integrals

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

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

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

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

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

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