Quantum Mechanics II PHYS-4601
Second In-Class Test

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Instructions:

- Do not turn over until instructed.
- You will have 75 minutes to complete this test.
- No electronic devices or hardcopy notes are allowed.
- INSTRUCTIONS REGARDING THE QUESTIONS WILL GO HERE.
- **Answer all questions briefly and completely.**
- **Only the lined pages of your exam book will be graded. Use the blank pages for scratch work only.**

Useful Formulae:

- Schrödinger Equation
  - time-dependent and position-basis time-independent

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \ , \quad \langle\vec{x}|H|\psi\rangle = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{x})\psi(\vec{x}) = E\psi(\vec{x})$$

  - Radial equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = Eu \ , \quad u(r) = rR(r)$$

- Angular momentum
  - Commutation relations (ϵ_{ijk} is the antisymmetric tensor):

$$[L_i, L_j] = i\hbar\sum_k \epsilon_{ijk}L_k \ , \quad [L_z, L_\pm] = \pm\hbar L_\pm \text{ for } L_\pm = L_x \pm iL_y \quad (\text{and for } \vec{L}\to\vec{S})$$

  - Raising and Lowering

$$L_\pm|\ell, m\rangle = \hbar\sqrt{(\ell\mp m)(\ell\pm m+1)}\,|\ell, m\pm 1\rangle$$

  - $s = 1/2$ spin operators in the S_z eigenbasis are $\vec{S} = (\hbar/2)\vec{\sigma}$, with Pauli matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \ , \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \ , \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \ .$$

  - The "total" quantum number j for two added angular momenta of quantum numbers j_1 and j_2 is $j = j_1 + j_2, j_1 + j_2 - 1, \cdots |j_1 - j_2|$ (one multiplet of each value)

- Hydrogen
  - States are denoted $|n, \ell, m, m_s\rangle$ or $|n, j, \ell, m_j\rangle$ (recall that $s = 1/2$ always for electrons).
  - Bohr radius $a = 4\pi\epsilon_0\hbar^2/me^2$ and energy $E_n = -(\hbar^2/2ma^2)(1/n^2) = -13.6\text{ eV}/n^2$
  - Spatial wavefunction

$$\psi_{n\ell m}(\vec{x}) \equiv \langle\vec{x}|n, \ell, m\rangle = R_{n\ell}(r)Y_\ell^m(\theta, \phi) \quad (R_{n\ell}\text{ normalized})$$

  - Spherical harmonics and associated Legendre functions

$$Y_\ell^m = (-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}e^{im\phi}P_\ell^m(\cos\theta)\ (m \geq 0)\ ,\quad Y_\ell^{-m} = (-1)^m(Y_\ell^m)^*$$

$$P_\ell^m(x) = (1-x^2)^{m/2}\left(\frac{d}{dx}\right)^m P_\ell(x)\ ,\quad P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

TABLE 4.3: The first few spherical harmonics, $Y_l^m(\theta, \phi)$.

$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$	$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta e^{\pm 2i\phi}$
$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$	$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta - 3\cos\theta)$
$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi}$	$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2}\sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$	$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2}\sin^2\theta\cos\theta e^{\pm 2i\phi}$
$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$	$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2}\sin^3\theta e^{\pm 3i\phi}$

TABLE 4.7: The first few radial wave functions for hydrogen, $R_{nl}(r)$.

$R_{10} = 2a^{-3/2}\exp(-r/a)$
$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$
$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$
$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$
$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1 - \frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$
$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$

- Quantum Computing
  - 1-bit gates $I : (|0\rangle \to |0\rangle, |1\rangle \to |1\rangle)$; $NOT : (|0\rangle \to |1\rangle, |1\rangle \to |0\rangle)$;
    $R(\phi) : (|0\rangle \to |0\rangle, |1\rangle \to e^{i\phi}|1\rangle)$; $\mathbb{H} : (|0\rangle \to (|0\rangle + |1\rangle)/\sqrt{2}, |1\rangle \to (|0\rangle - |1\rangle)/\sqrt{2}$
  - 2-bit controlled NOT gate $CNOT(|x\rangle|y\rangle) = |x\rangle|x \oplus y\rangle$
- Possibly useful integrals
  - Gaussian integral

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}}e^{b^2/4a}$$

    where a, b can be complex as long as $\mathrm{Re}\, a > 0$
  - Exponential integrals

$$\int_0^\infty dx\, x^p e^{-x/b} = p!b^{p+1}$$