Quantum Mechanics II PHYS-4601 Second In-Class Test

Dr. Andrew Frey

14 Feb 2019

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

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

– Radial equation

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

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

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

– 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

$$
\sigma_x = \left[\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right] , \quad \sigma_y = \left[\begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right] , \quad \sigma_z = \left[\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right]
$$

.

– The "total" quantum number j for two added angular momenta of quantum numbers j_1 and j_2 is $j = j_1 + j_2, j_1 + j_2 - 1, \dots |j_1 - j_2|$ (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 $a = 4\pi\epsilon_0\hbar^2/m e^2$ and energy $E_n = -(\hbar^2/2ma^2)(1/n^2) = -13.6 \text{ eV}/n^2$
	- Spatial wavefunction

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

– Spherical harmonics and associated Legendre functions

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

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

 $R_{nl}(r)$.

TABLE 4.7: The first few radial wave functions for hydrogen,

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

 $R_{10} = 2a^{-3/2} \exp(-r/a)$ $Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$ $Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2 \theta e^{\pm 2i\phi}$ $R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a} \right) \exp(-r/2a)$ $Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5 \cos^3 \theta - 3 \cos \theta)$ $Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$ $R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} \exp(-r/2a)$ $Y_1^{\pm 1} = \pm \left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{\pm i\phi}$ $Y_3^{\pm 1} = \pm \left(\frac{21}{64\pi}\right)^{1/2} \sin \theta (5 \cos^2 \theta - 1) e^{\pm i\phi}$ $R_{30} = \frac{2}{\sqrt{27}} a^{-3/2} \left(1 - \frac{2}{3} \frac{r}{a} + \frac{2}{27} \left(\frac{r}{a} \right)^2 \right) \exp(-r/3a)$ $Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$ $Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2 \theta \cos \theta e^{\pm 2i\phi}$ $R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2} \left(1 - \frac{1}{6} \frac{r}{a}\right) \left(\frac{r}{a}\right) \exp(-r/3a)$ $Y_2^{\pm 1} = \pm \left(\frac{15}{8\pi}\right)^{1/2} \sin \theta \cos \theta e^{\pm i\phi}$ $Y_3^{\pm 3} = \pm \left(\frac{35}{64\pi}\right)^{1/2} \sin^3 \theta e^{\pm 3i\phi}$ $R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2} \left(\frac{r}{a}\right)^2 \exp(-r/3a)$

• Quantum Computing

- 1-bit gates
$$
I : (|0\rangle \rightarrow |0\rangle, |1\rangle \rightarrow |1\rangle)
$$
; $NOT : (|0\rangle \rightarrow |1\rangle, |1\rangle \rightarrow |0\rangle)$;
\n $R(\phi) : (|0\rangle \rightarrow |0\rangle, |1\rangle \rightarrow e^{i\phi} |1\rangle)$; $\mathbb{H} : (|0\rangle \rightarrow (|0\rangle + |1\rangle)/\sqrt{2}, |1\rangle \rightarrow (|0\rangle - |1\rangle)/\sqrt{2}$
\n- 2-bit controlled NOT gate $CNOT(|x\rangle |y\rangle) = |x\rangle |x \oplus y\rangle$, \oplus = addition mod 2

• 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 $\text{Re } a > 0$

– Exponential integrals

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