Final Exam: Tuesday Apr 9, 2024 Name:_

Allowed: Formula sheet (given), calculator, 2.5 hours

PART 1 – answer questions 1 – 7 using your exam booklet and **then** use your scratch card: <u>One</u> scratch = 100%; <u>two</u> scratches 50%; <u>three</u> scratches 25% (part 1 total is <u>40%</u>) PART 2 – answer questions 8 – 10 in the exam booklet provided (each question here is worth <u>20%</u>)

1) The one-dimensional *time-independent Schrödinger equation* for a particle of mass $2m_e$ (note the mass) is:

$$\mathbf{A.} \quad -\frac{\hbar^2}{2m_e} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \qquad \qquad \mathbf{B.} \quad -\frac{\hbar^2}{2m_e} \frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x,t)\Psi(x,t) = \frac{\partial\Psi}{\partial t}(x,t) \\ \mathbf{C.} \quad -\frac{\hbar^2}{2m_e} \frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x,t)\Psi(x,t) = 0 \qquad \qquad \qquad \mathbf{D.} \quad -\frac{\hbar^2}{4m_e} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \\ \mathbf{E.} \quad -\frac{\hbar^2}{2m_e} \frac{\partial^2\Psi(x,t)}{\partial x^2} + \Psi(x,t) = i\hbar \frac{\partial\Psi}{\partial t}(x,t) \end{aligned}$$

2) A particle moving along the *x*-axis experiences a potential energy $U(x) = 3x^3$ J, where *x* is in metres. Sketch the potential energy from x = 0 to x = 2 m. What is the force at the three positions $x = \{-1, 0, 1\}$ m?

A.
$$F_x = \{0, -3, -6\}$$
 N
B. $F_x = \{-9, 0, -9\}$ N
C. $F_x = \{0, 12, 24\}$ N
D. $F_x = \{0, -12, -48\}$ N
E. $F_x = \{0, -9, -18\}$ N

3) The ground state wavefunction of the simple harmonic oscillator for mass *m* and force constant *k* is:

$$\psi_0(x) = \left(\frac{b}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}b^2x^2}$$
 where $b = \left(\frac{mk}{\hbar^2}\right)^{1/4}$

Which of the following integrals provides the *expectation value* of the potential energy in the ground state? [Hint: check each option carefully.]

A.
$$k \int_{0}^{\infty} \left(\frac{b}{\sqrt{\pi}}\right) x^2 e^{-b^2 x^2} dx$$
 B. $\int_{-\infty}^{\infty} \left(\frac{b}{\sqrt{\pi}}\right) \frac{1}{2} k x^2 e^{-\frac{1}{2}b^2 x^2} dx$ **C.** $\int_{0}^{\infty} \left(\frac{b}{\sqrt{\pi}}\right)^{1/2} \frac{1}{2} k x^2 e^{-\frac{1}{2}b^2 x^2} dx$
D. $\int_{0}^{\infty} \left(\frac{b}{\sqrt{\pi}}\right) \frac{1}{2} k x^2 e^{-b^2 x^2} dx$ **E.** $\int_{-\infty}^{\infty} \left(\frac{b}{\pi}\right) \frac{1}{2} k x^2 e^{-b^2 x^2} dx$

Trent: PHYS 2610H – Introductory Quantum Physics: 2023-2024

4) If the *orbital angular momentum quantum number* of an electron takes the value 4, then within a vector model picture what is the smallest possible angle between the vector \vec{L} and the *z*-axis?

Qu's 5 – 7: Consider a state of atomic hydrogen (neglecting spin) with quantum numbers given by $(n, \ell, m_{\ell}) = (3, 1, 0)$.

5) With the help of the formula sheet, which of the following is the correct mathematical form of the wave function, $\psi(r, \theta, \phi)$ for this state, neglecting any normalization constant?

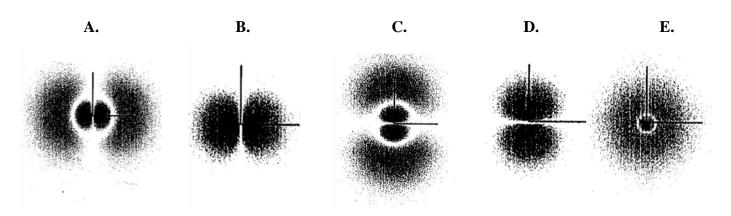
A.
$$\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$$
 B. $re^{-r/2a_0}\cos\theta$ **C.** $\left(6-\frac{r}{a_0}\right)re^{-r/3a_0}\cos\theta$ **D.** $\left(6-\frac{r}{a_0}\right)re^{-r/3a_0}\sin\theta e^{i\phi}$ **E.** $re^{-r/2a_0}\sin\theta e^{i\phi}$

6) What is the energy of this state? (You may either substitute the wave function into the time independent Schrodinger equation for hydrogen and do a long algebraic calculation, or instead a quicker calculation using your formula sheet).

A.
$$\sqrt{3\hbar}$$
 B. -5.42×10^{-19} J C. -2.17×10^{-18} J D. -2.41×10^{-19} J E. $1\hbar$

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7) Which of the following probability density plots (i.e. density plots of $|\psi(r,\theta,\phi)|^2$) best resembles this state? Note that the *z*-axis points vertically up the page.



PART II – answer all <u>three</u> questions in exam booklet provided

8. Based on its absorption spectrum, the hydrogen chloride molecule (HCl) behaves to a good approximation as a quantum harmonic oscillator of spring constant 480 N/m, and a mass given by that of the hydrogen atom. Assume that this system is in its ground state:

a) Sketch on the same plot the potential energy function, and the ground state wave function of this system. Find the location of the classical turning points in the ground state and denote them on the plot.b) What wavelength of light would excite this molecule to its next-highest vibrational energy state, and in which region of the electromagnetic spectrum does it lie?

9. Consider the 3s electron in a hydrogen atom.

a) Sketch, showing the rough shape, with labelled axes with units, the radial probability density, P(r),

for this electron. Note that the largest, and outermost, maximum occurs at $r \approx 13 a_0$. Locate the zeros, or *nodes*, of this function.

b) Estimate the probability that the electron may be found within the small range of distance $\Delta r = 0.02 a_0$ from the nucleus, at a distance of $r = 9a_0$.

10. Two spinless particles, assumed initially to be *distinguishable* from each other, occupy two different states (n=3 and n=4) in a 1-D infinite well of length L.

a) Write down the <u>single-particle</u> wavefunction $\psi(x)$, with normalization constant *A*, for one particle being in state n = 3 in an infinite well, and find *A*.

b) Write down a <u>two-particle</u> product wave function, $\psi(x_1, x_2)$, with normalization constant *B*, and find *B*.

c) If the two particles are now *identical* how should this product wave function (use now normalization constant *C*) be adapted to form two realistic wave functions? Write down for each case the integrals you would compute to find the probability of one particle being in the **left third** of the well (i.e. between L/3 and 2L/3) and the other particle in the **right third** of the well (i.e. between 2L/3 and L).