## KEELE UNIVERSITY

DEGREE EXAMINATIONS, 2009
Level 2 (PRINCIPAL COURSE)
DAYDAY DATEDATE, 14:30-16:30
PHYSICS/ASTROPHYSICS
PHY-20006
QUANTUM MECHANICS

Candidates should attempt to answer FOUR questions.
Tables of physical and mathematical data may be obtained from the invigilator.

1. (a) What is a wavefunction?
(b) For each of the three functions given below, state why the function is not allowable as part of a wavefunction and state all values of $x$ at which the function is not allowable.
i. $\quad f_{1}(x)=\left\{\begin{array}{l}1 /(1-x) \\ 1 /(1+x)\end{array}\right.$
$(x<0)$
$(x \geq 0)$

ii. $\quad f_{2}(x)=\left\{\begin{array}{l}\exp \left(-x^{2}\right) \\ 1+\cos (x) \\ 0\end{array}\right.$

$$
\begin{aligned}
& (x \leq 0) \\
& (0<x<\pi) \\
& (x \geq \pi)
\end{aligned}
$$


iii.

$$
f_{3}(x)= \begin{cases}e^{x} & (x<0) \\ 1+\log _{e}(1+x) & (x \geq 0)\end{cases}
$$


$[3 \times 10$ ]
(c) The wavefunction for a particle has the following dependance on position, $x$.

$$
\psi(x)= \begin{cases}\psi_{A}=A(1+\sin x) & -\pi / 2<x<\pi \\ \psi_{B}=B x^{\beta} & x \geq \pi\end{cases}
$$

Show that the mathematical properties for an allowable wavefunction at $x=\pi$ require that $\beta=-\pi$.
(d) Explain why a wavefunction $\Psi(x, t)$ must also be a continuous function of time, $t$.
2. Consider a particle with mass $m$ and energy $E$ incident on a barrier with height $V_{B}$ and width $a$ such that $E<V_{B}$.

(a) Show that the energy eigenfunction

$$
\psi_{1}=A_{I} e^{i k x}+A_{R} e^{-i k x},
$$

is a solution of the time independent Schrödinger equation for the region $x<0$ if $k^{2}=2 m E / \hbar^{2}$.
(b) What is the physical interpretation of the quantity $R=\frac{\left|A_{R}\right|^{2}}{\left|A_{I}\right|^{2}}$ ?
(c) Give an expression for the energy eigenfunction in the region $x>a$ in terms of the amplitude $A_{T}$. Explain your answer.
(d) Give one example of a physical process that demonstrates or exploits the fact that $T=\frac{\left|A_{T}\right|^{2}}{\left|A_{I}\right|^{2}}>0$. State the physical origin and approximate height of the barrier, $V_{B}$, for your example.
(e) What would be the energy eigenfunction in the region $0<x<a$ in the case of a more energetic particle with $E>V_{B}$ ? Explain your answer.

The time-independent Schrödinger equation in 1-dimension is:

$$
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi}{d x^{2}}+V(x) \psi=E \psi
$$

3. A particle of mass $m$ is located in a 'square well' of width $a$, where the potential $V$ inside the well is zero and is infinite otherwise.

$$
V(x)= \begin{cases}\infty & x<0 \\ 0 & 0 \leq x \leq a \\ \infty & x>a\end{cases}
$$

The energy eigenfunctions for the particle in the region $0 \leq x \leq a$ is

$$
\psi_{n}(x)=\sqrt{\frac{2}{a}} \sin (n \pi x / a)
$$

where $n=1,2,3, \ldots$.
The energy of the particle in the state $\psi_{n}$ is

$$
E_{n}=\frac{n^{2} \pi^{2} \hbar^{2}}{2 m a^{2}}
$$

(a) What are the main differences between the predictions of classic physics and the predictions of quantum mechanics regarding the energy of the particle? [10]
(b) Show that the probability of observing the particle in the region $x<a / 3$ approaches the value predicted by classical physics if $n$ is large.
(c) Give an expression for the energy eigenfunctions of a particle trapped in a cube of side $a$ together with an expression for the energy of these states.
(d) What is the largest number of electrons that can be contained in a cube of side $a$ with energy less than or equal to $3 \pi^{2} \hbar^{2} /\left(m_{e} a^{2}\right)$ ? Explain your answer. (Ignore any interactions between the electrons for the purposes of answering this question).

You may find the following standard integral to be useful.

$$
\int \sin ^{2} x d x=\frac{1}{2}(x-\sin x \cos x)+C
$$

4. The harmonic oscillator potential for a particle of mass $m$ is

$$
V(x)=\frac{1}{2} k x^{2} .
$$

The solutions of the time-independent Schrödinger equation for this potential have energies given by the expression

$$
E_{n}=\left(n+\frac{1}{2}\right) \hbar \omega, \quad n=0,1,2, \ldots
$$

where $\omega=\sqrt{k / m}$.
Consider a particle in the state described by the eigenfunction

$$
\psi_{1}(x)=A_{1}\left(\frac{x}{a}\right) e^{-x^{2} / 2 a^{2}}
$$

where $a=\sqrt{\hbar / m \omega}$.
(a) Explain how the value of the constant $A_{1}$ is calculated. (You do not need to calculate $A_{1}$, but you should show the first step in the calculation.)
(b) Show that the most probable value for the observed position of the particle with the eigenfunction $\psi_{1}(x)$ is $x= \pm a$.
(c) Sketch the probability distribution for the observed position of the particle with the eigenfunction $\psi_{1}(x)$. Include an indication of the scale on the x -axis of your sketch.
(d) Show that the eigenfunction $\psi_{1}$ has well defined parity and state the value of the parity.
(e) The bond strength in a ${ }^{13} \mathrm{C}^{16} \mathrm{O}$ molecule is $k=1908 \mathrm{Nm}^{-1}$. Calculate the wavelength of the photon emitted due to the transition between the vibrational states $n=3 \rightarrow 1$.
(f) Discuss briefly whether the following two statements are consistent with each other.

- The momentum of a particle with kinetic energy $E_{1}$ is given by $p=\sqrt{2 m E_{1}}$.
- The expectation value of the momentum for the particle described by $\psi_{1}(x)$ is $\langle p\rangle=0$.

5. The eigenfunctions for a particle in a central potential have the form

$$
\psi_{n, \ell, m_{\ell}}(r, \theta, \phi)=R_{n, \ell}(r) Y_{\ell, m_{\ell}}(\theta, \phi) .
$$

(a) Explain the significance of the commutator relation $\left[\hat{L^{2}}, \hat{L_{z}}\right]=0$.
(b) What is the relation between the function $Y_{\ell, m_{\ell}}(\theta, \phi)$, the operators $\hat{L^{2}}$ and $\hat{L_{z}}$ and the quantum numbers $\ell$ and $m_{\ell}$.
(c) The dependence of the eigenfunctions on the azimuthal coordinate $\phi$ is given by

$$
\psi_{n, l, m_{l}} \propto e^{i m_{l} \phi}
$$

By considering the values of $\psi_{n, l, m_{l}}$ at angles $\phi$ and $\phi+2 \pi$, show that $m_{l}$ must be an integer.
(d) Explain why the polar diagram for states with $\ell=0$ is a circle.
(e) Outline the main features of the Stern-Gerlach experiment. Explain how this experiment shows that the eigenfunctions $\psi_{n, \ell, m_{\ell}}$ do not give a complete description for the properties of an electron in a hydrogen atom.
6. Consider a particle in the ground state with energy $E_{1}^{\prime}$ for the potential shown below. The value of the potential for $x<-b$ and $x>b$ is $V(x)=\infty$.


The step of height $V_{B}$ can be considered as a perturbation to the infinite square well potential. The energy eigenfunction of the ground state for the unperturbed potential $\left(V_{B}=0\right)$ is

$$
\psi_{1}=\sqrt{\frac{1}{b}} \cos \left(\frac{\pi x}{2 b}\right)
$$

(a) What is the value of the wavefunction for the particle for $x>b$ ? Explain your answer.
(b) With the aid of a sketch, describe the main differences between the unperturbed energy eigenfunctions of the ground state, $\psi_{1}$, and the perturbed energy eigenfunctions, $\psi_{1}^{\prime}$ for the perturbed potential $\left(V_{B}>0\right)$.
(c) Estimate the ground state energy, $E_{1}^{\prime}$, for the perturbed potential in terms of $E_{1}$ and $V_{B}$.
(d) Discuss whether your expression for $E_{1}^{\prime}$ in part (c) can be applied to the case $V_{B}<0$.

You may find the following standard integral to be useful.

$$
\int \cos ^{2} x d x=\frac{1}{2}(x+\sin x \cos x)+C
$$

