Answer THREE questions.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

[Part marks]

1. The time-independent Hamiltonian operator H describing a one-dimensional quantum mechanical system has a lowest energy eigenvalue E_0. Show that the expectation value of H, for any normalizable function ϕ that satisfies the boundary conditions, obeys

$$\frac{\int \phi^*(x)\, H\phi(x)\, \mathrm{d}x}{\int \phi^*(x)\, \phi(x)\, \mathrm{d}x} \geq E_0,$$

where the integration is over the allowed region in x. [4]

Explain how this expression may be used to obtain a limit on the ground state energy of the system.

Discuss briefly and qualitatively the conditions and problems associated with extending this method to obtaining estimates of the energies of excited states. [4]

A particle of mass m moves in the one-dimensional potential

$$V(x) = \Lambda x^4 \qquad -\infty < x < \infty, \qquad \Lambda > 0.$$

Explain why

$$\phi_0(x) = \mathrm{e}^{-\lambda x^2}$$

is a suitable trial function, with λ a parameter, with which to estimate the ground state energy.

Show that the best estimate of the ground state energy, E, provided by this function is

$$E = \left(\frac{3}{4}\right)^{4/3} \left(\frac{\Lambda \hbar^4}{m^2}\right)^{1/3}.$$ [10]

Suggest, giving reasons for your choice, a suitable trial function $\phi_1(x)$ to be used for a variational calculation of the energy of the first excited state. [2]

$$\int_{-\infty}^{\infty} x^{2n} \mathrm{e}^{-\beta x^2}\, \mathrm{d}x = \frac{(2n)!}{2^{2n} n! \beta^n} \sqrt{\frac{\pi}{\beta}} \quad \text{for } n = 0, 1, 2, \ldots, \ \beta > 0.$$

2. The ladder operators $S_\pm$ are defined in terms of the Cartesian components of the spin operator $\mathbf{S}$ by $S_\pm = S_x \pm iS_y$. The actions of $S_\pm$ on the spin states $|S, M\rangle$ are

$$S_\pm |S, M\rangle = [S(S+1) - M(M \pm 1)]^{1/2} \hbar |S, M \pm 1\rangle .$$

By expressing S_x and S_y in terms of S_+ and S_-, show that

(a) if $\hat{\mathbf{n}}$ is the unit vector $(\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta)$ then

$$\mathbf{S} \cdot \hat{\mathbf{n}} = \tfrac{1}{2} \left(S_+ \mathrm{e}^{-i\phi} + S_- \mathrm{e}^{i\phi} \right) \sin\theta + S_z \cos\theta.$$ **[2]**

(b) for a spin-$\frac{1}{2}$ particle, the spin components s_x, s_y and s_z satisfy

$$s_x^2 = s_y^2 = s_z^2 = \frac{\hbar^2}{4}, \qquad \text{and} \qquad s_x s_y + s_y s_x = 0,$$

and

$$(\mathbf{s} \cdot \hat{\mathbf{n}})^2 = \frac{\hbar^2}{4}.$$ **[6]**

The two protons in a crystallization water molecule in a gypsum monocrystal occupy fixed positions in the crystal and interact via a magnetic dipole-dipole interaction

$$V(\hat{\mathbf{n}}) = \Lambda \{3(\mathbf{s}_1 \cdot \hat{\mathbf{n}})(\mathbf{s}_2 \cdot \hat{\mathbf{n}}) - \mathbf{s}_1 \cdot \mathbf{s}_2\}$$

where $\hat{\mathbf{n}}$ is the unit vector of the line joining the two protons, $\mathbf{s}_1$ and $\mathbf{s}_2$ are their spin operators and Λ is a constant. Show that $V(\hat{\mathbf{n}})$ can be expressed in terms of the total spin operator $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$ as

$$V(\hat{\mathbf{n}}) = \frac{\Lambda}{2} \left\{ 3(\mathbf{S} \cdot \hat{\mathbf{n}})^2 - \mathbf{S}^2 \right\}.$$ **[4]**

In a particular magnetic resonance experiment the $|1, 0\rangle$ and $|0, 0\rangle$ states would be degenerate in the absence of the dipole-dipole interaction. By calculating the expectation values of $V(\hat{\mathbf{n}})$ for these states, demonstrate that the dipole-dipole interaction removes this degeneracy by a level splitting given by

$$\langle 1, 0| V(\hat{\mathbf{n}}) |1, 0\rangle - \langle 0, 0| V(\hat{\mathbf{n}}) |0, 0\rangle = -\frac{\Lambda \hbar^2}{2} \left(3\cos^2\theta - 1 \right).$$ **[8]**

3. Show, by direct substitution, that the wave function

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2}\int G(\mathbf{r},\mathbf{r}')\, V(\mathbf{r}')\, \psi(\mathbf{r}')\, d^3\mathbf{r}'$$

is a solution of the time-independent Schrödinger equation

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r})\, \psi(\mathbf{r})$$

for a potential $V(\mathbf{r})$, energy E and $k^2 = 2mE/\hbar^2$, provided $G(\mathbf{r},\mathbf{r}')$ satisfies

$$\left(\nabla^2 + k^2\right) G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}').$$ **[3]**

Given that a suitable form for $G(\mathbf{r},\mathbf{r}')$ for a particle of incident momentum $\hbar\mathbf{k}_i$ that scatters elastically from a short-range central potential is

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{e^{ik_f|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|},$$

show how this expression leads to the integral representation

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{k}_f\cdot\mathbf{r}'} V(\mathbf{r}')\, \psi(\mathbf{r}')\, d^3\mathbf{r}'$$

for the scattering amplitude $f(\theta)$, where $\hbar\mathbf{k}_f$ is the particle's final momentum. Hence deduce the first Born approximation for the scattering amplitude

$$f_{\mathrm{B}}(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{i\mathbf{q}\cdot\mathbf{r}'} V(\mathbf{r}')\; d^3\mathbf{r}',$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$. **[7]**

Show that within the first Born approximation the differential cross section, $\dfrac{d\sigma}{d\Omega}$, for the scattering from the Gaussian central potential

$$V(\mathbf{r}) = V_0 \exp\left(-r^2/a^2\right)$$

is given by

$$\frac{d\sigma}{d\Omega} = \frac{\pi m^2 V_0^2 a^6}{4\hbar^4} e^{-q^2a^2/2}.$$ **[7]**

Verify that as $E \to \infty$ the total cross section $\sigma \sim \Lambda/E$ with Λ a constant. **[3]**

$$\int_0^\infty x e^{-\alpha x^2} \sin\beta x\, dx = \left(\frac{\beta}{4}\right)\left(\frac{\pi}{\alpha^3}\right)^{1/2} e^{-\beta^2/4\alpha} \quad \text{for } \alpha > 0.$$

4. A general solution of the time-dependent Schrödinger equation for a system described by a time-independent Hamiltonian H_0 can be written as

$$\psi(\mathbf{r},t) = \sum_n c_n(t)\,\phi_n(\mathbf{r})\,\mathrm{e}^{-iE_n t/\hbar},$$

where $\phi_n(\mathbf{r})$ is an eigenfunction of H_0 with eigenvalue E_n. State the physical interpretation that can be placed on the coefficients $c_n(t)$.
If the system is acted on by a weak time-dependent perturbation $\lambda H'(t)$ show that the coefficients satisfy the coupled differential equations

$$\frac{\mathrm{d}c_k(t)}{\mathrm{d}t} = \frac{\lambda}{i\hbar}\sum_n H'_{kn}(t)\,\mathrm{e}^{i\omega_{kn}t}c_n(t)\,,$$

where $H'_{kn}(t) = \langle\phi_k(\mathbf{r})|H'(t)|\phi_n(\mathbf{r})\rangle$ and $\omega_{kn} = (E_k - E_n)/\hbar$. **[4]**

If at time t_0, the system is in a definite eigenstate $\phi_i(\mathbf{r})$ with energy E_i, show that the probability, $P_k(t)$, that at a later time t the system has made a transition to a state $\phi_k(\mathbf{r})$ of energy E_k is given to lowest order in λ by

$$P_k(t) = \frac{1}{\hbar^2}\left|\int_{t_0}^{t}\langle\phi_k(\mathbf{r})|\lambda H'(t')|\phi_i(\mathbf{r})\rangle \mathrm{e}^{i\omega_{ki}t'}\,\mathrm{d}t'\right|^2.$$

If for states k and i, $\langle\phi_k(\mathbf{r})|H'(t)|\phi_i(\mathbf{r})\rangle = 0$, show that the transition probability, to the next order, is given by

$$P_k(t) = \frac{1}{\hbar^4}\left|\sum_n\int_{t_0}^{t}\mathrm{d}t'\lambda H'_{kn}(t')\,\mathrm{e}^{i\omega_{kn}t'}\int_{t_0}^{t'}\mathrm{d}t''\,\lambda H'_{ni}(t'')\,\mathrm{e}^{i\omega_{ni}t''}\right|^2.$$ **[7]**

The Hamiltonian for a particle of mass m moving freely in a circle of radius a has acceptable eigenfunctions $\phi_n(\theta) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{in\theta}$ with energies $E_n = \frac{n^2\hbar^2}{2ma^2}$ and $n = 0, \pm 1, \pm 2, \ldots$. The particle is acted on by a weak time-dependent potential

$$V(\theta,t) = \Lambda\sin\theta\,\mathrm{e}^{-\mu t}, \quad \Lambda \ll \frac{\hbar^2}{2ma^2}, \quad \mu > 0, \quad \text{for } t \geq 0.$$

Between which states can transitions be induced to lowest order in Λ? **[2]**

If initially, at $t_0 = 0$, the system is in its ground state,

(a) calculate the transition probability to the first excited state after a time $t \gg 1/\mu$. **[5]**

(b) discuss qualitatively how transitions to the second excited state can occur. What is the dependence on Λ of their transition probability? **[2]**

5. Write down the asymptotic form of the wave function representing the elastic scattering of a monoenergetic beam of spinless particles of mass m and momentum $\hbar\mathbf{k}$ by a finite-range, central potential. Give a physical interpretation for the terms in the expression. **[2]**

A plane wave may be expressed as an asymptotic superposition of incoming and outgoing spherical waves as

$$\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \underset{r\to\infty}{=} \frac{1}{2k}\sum_{\ell=0}^{\infty}(2\ell+1)\,i^{\ell+1}\left[\frac{\mathrm{e}^{-i(kr-\ell\pi/2)}}{r}-\frac{\mathrm{e}^{i(kr-\ell\pi/2)}}{r}\right]P_\ell(\cos\theta),$$

with $P_\ell(\cos\theta)$ a Legendre polynomial. Use this expansion to show how the scattering effect of a short-range central potential, centred on the origin of coordinates, may be described by the phase changes introduced into the spherical waves. In particular show that in the partial wave analysis the scattering amplitude is given by

$$f(\theta,k)=\frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\,\mathrm{e}^{i\delta_\ell(k)}\sin\delta_\ell(k)\,P_\ell(\cos\theta),$$

where $\delta_\ell(k)$ is the phase shift of the ℓ-th partial wave. **[5]**

Show, by physical arguments, that the phase shift is positive if the scattering potential is weakly attractive. **[4]**

A particle of mass m and energy E scatters from an attractive square-well potential

$$V(r)=\begin{cases}-V_0 & 0<r<a, \quad V_0>0\\ 0 & r\geq a.\end{cases}$$

The s-wave reduced radial wave function, $u_0(r)$, satisfies the differential equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u_0(r)}{\mathrm{d}r^2}-V_0u_0(r)=Eu_0(r).$$

Show that the s-wave phase shift, $\delta_0(k)$, is given by

$$\delta_0(k)=\tan^{-1}\left[\frac{k}{K}\tan(Ka)\right]-ka$$

where $K^2=2m(E+V_0)/\hbar^2$ and $k^2=2mE/\hbar^2$. **[4]**

Establish a relationship that must exist between the quantities V_0, a and m such that the s-wave cross section vanishes at zero energy ($E=0$).

By first performing a power series expansion in k of K and $\tan(Ka)$ to order k^2, show that the s-wave phase shift $\delta_0\simeq k^3a^3/6$. Hence show that the s-wave total cross section, σ, as $E\to 0$ behaves as

$$\sigma \underset{E\to 0}{=} \frac{4\pi a^6m^2}{9\hbar^4}E^2.$$ **[5]**

Note: The Taylor series expansion $\tan(a+x)=\tan a+x\sec^2 a+O(x^2)$ for $x\ll a$,
Also $\tan^{-1}x=x-\frac{1}{3}x^3+O(x^5)$ for small x.

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