2663

SECOND PUBLIC EXAMINATION

Honour School of Physics Part A: 3 and 4 Year Courses

Honour School of Physics and Philosophy Part A

A3: QUANTUM PHYSICS

TRINITY TERM 2012

Friday, 15 June, 9.30 am – 12.30 pm

Answer **all** *of Section A and* **three** *questions from Section B.*

For Section A start the answer to each question on a **fresh page.**
For Section B start the answer to each question in a **fresh book.**

A list of physical constants and conversion factors accompanies this paper.

The numbers in the margin indicate the weight that the Examiners expect to assign to each part of the question.

Do NOT turn over until told that you may do so.

Section A

1. A particle of mass m moves in a 1-dimensional potential well with $V = 0$ for $0 < x < a$ and $V = \infty$ elsewhere. A normalised solution of the time-dependent Schrödinger equation for the particle is

$$\Psi(x,t) = \Psi_0(x,t)\sin\gamma + \Psi_1(x,t)\cos\gamma,$$

where

$$\Psi_0(x,t) = A\sin\frac{\pi x}{a}\exp\left(-\mathrm{i}\frac{E_0}{\hbar}t\right), \quad \Psi_1(x,t) = A\sin\frac{2\pi x}{a}\exp\left(-\mathrm{i}\frac{E_1}{\hbar}t\right).$$

What are the values of A, E_0 and E_1? What are the possible outcomes of measurement of the energy of the particle in the state $\Psi(x,t)$ and the probability of each outcome? [5]

2. A particle of mass m is confined in a cubical box which has corners at $(0,0,0)$ and (a,a,a). The particle has infinite potential energy in the walls and zero potential energy in the box. Determine the normalised time-independent wave function of the ground state and an expression for the energy levels. [5]

3. Particles of a particular energy E moving in the direction of the positive x-axis encounter a double potential step defined by

$$\begin{aligned} V(x) &= 0\,, & x &< 0 \\ &= V_1\,, & 0 \le x &< a \\ &= V_2\,, & x &\ge a, \end{aligned}$$

where $V_{1,2}$ are constants satisfying $E > V_2 > V_1 > 0$. Write down the form of the wave function in the three regions and the boundary conditions which apply at $x = 0$. [5]

4. The wave function $\psi(x,t)$ satisfies the time-dependent Schrödinger equation for a free particle of mass m, moving in one dimension. Consider a second wave function:

$$\phi(x,t) = \mathrm{e}^{\mathrm{i}(ax-bt)}\psi(x-vt,t)\,.$$

$e^{i(kx-\omega t)}$.

Show that $\phi(x,t)$ obeys the same time-dependent Schrödinger equation, provided the constants a, b and v are related by:

$$b = \frac{\hbar a^2}{2m} \quad \text{and} \quad v = \frac{\hbar a}{m}\,.$$

$e^{i(kx-2\omega t)}$ $(ck-b$

C

$e^{i((k+a)x-(2\omega+b)t)}$

What is their physical relevance? [8]

$b = \frac{av}{2}$

$= \frac{a\omega}{2k}$

5. The ground state wavefunction for a hydrogen-like atom with nuclear charge Z is given by $\psi_a = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\mathrm{e}^{-Zr/a_0}$. Evaluate the expectation value of $\frac{Ze^2}{4\pi\epsilon_0 r}$ in this state. Express the Bohr radius a_0 and the electron charge e in terms of the fine structure constant α and hence express your result in terms of Z, α, the mass of the electron m and the speed of light c. Comment on the physical significance of your expression. [8]

$\psi = (x-vt)^2 + t$

$\frac{\partial \psi}{\partial x} = 2(x-vt)^2 \quad \frac{\partial \psi}{\partial (x-vt)}$

$\frac{64}{100}$

6. The Pauli spin matrices

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

satisfy anti-commutation relations

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 0 \quad (i \neq j) .$$

Verify this relation for the case $i = x$, $j = y$. What is the value of the anti-commutator when $i = j$?

Show that the matrices $s_i = \frac{1}{2}\hbar\sigma_i$ satisfy the commutation relations for angular momentum. The matrix s^2 is defined by

$$s^2 = \left(\frac{\hbar}{2}\right)^2 (\sigma_x^2 + \sigma_y^2 + \sigma_z^2).$$

Show that $s^2 = \frac{3}{4}\hbar^2 I$, where I is the unit matrix. [9]

Section B

$C_1 = \frac{a+b}{2}$

$C_2 = \frac{a-b}{2}$

7. A system of two spin-$\frac{1}{2}$ particles 1 and 2 has the Hamiltonian

$$H = a\sigma_z(1) + b\sigma_z(2) + c\vec{\sigma}(1) \cdot \vec{\sigma}(2) .$$

$= C_1(\sigma_z(1) + \sigma_z(2)) + C_2(\sigma_z(1) - \sigma_z(2)) + c\,\vec{\sigma}(1)\cdot\vec{\sigma}(2)$

Show that $[\Sigma_z, \mathbf{\Sigma}^2] = 0$, where $\mathbf{\Sigma} \equiv \vec{\sigma}(1) + \vec{\sigma}(2)$, and $\vec{\sigma}(1)$, $\vec{\sigma}(2)$ are the vectors of Pauli operators. [5]

Show that

$$\vec{\sigma}(1) \cdot \vec{\sigma}(2) = 2[\sigma^+(1)\sigma^-(2) + \sigma^-(1)\sigma^+(2)] + \sigma_z(1)\sigma_z(2),$$

$\frac{1}{2}(\Sigma^2 - \sigma^2(1) - \sigma^2(2))$

where

$$\sigma^{\pm}(j) = \frac{1}{2}(\sigma_x(j) \pm \mathrm{i}\sigma_y(j)), \quad j = 1, 2 .$$

[3]

For the case $a = b$, relate the eigenvalues of H to the eigenvalues of $(\Sigma_z, \mathbf{\Sigma}^2)$, which are $(2m, 4\ell(\ell + 1))$ with $(\ell, m) = (1, 1), (1, 0), (1, -1), (0, 0)$. [6]

For the general case $a \neq b$ write down the results of applying H to the simultaneous eigenstates of $\sigma_z(1)$, $\sigma_z(2)$. [6]

[The action of $\sigma^{\pm}(j)$ on the eigenstates of $\sigma_z(j)$ is:

$$\sigma^+(j)|m_j> = \begin{cases} 0 & m_j = 1 \\ |1\rangle & m_j = -1 \end{cases}, \quad \sigma^-(j)|m_j\rangle = \begin{cases} |-1\rangle & m_j = 1 \\ 0 & m_j = -1 \end{cases} . \ ]$$

$+\int e^{-\frac{v^2}{v_{th}^2}} \cos(4\pi\nu_0(\tau - \frac{v}{c}))\, dv$

8. (a) A system has two stationary states i, j separated in energy by $\hbar\omega$. It is subject to a small perturbation V which is constant from time $t = 0$ to $t = T$ and has matrix elements $V_{ji} = V_{ij}^*$ between these states. Show that if the system is initially in state i, the probability of a transition to state j is approximately

$$P_{ij} = 4|V_{ij}|^2 \frac{\sin^2(\omega T/2)}{(\hbar\omega)^2} \, .$$ [8]

(b) A neutral particle with spin $\frac{1}{2}$ and magnetic moment μ is travelling at speed v in a region of uniform magnetic field with flux density B. Over a small length ℓ of its path an additional flux density b ($\ll B$) is applied at right angles to B. The spin eigenket of the particle satisfies a Schrödinger equation with a time-dependent Hamiltonian $H(t)$ given by:

$$\begin{aligned} H(t) &= -\mu(B\sigma_z + b\sigma_x), \quad \text{for} \quad 0 < t < \ell/v, \\ &= -\mu B\sigma_z, \quad \text{otherwise.} \end{aligned}$$

The system originally has spin $+\frac{1}{2}$ with respect to the direction of B. Find the probability that it makes a transition to the state with opposite spin:

(i) by using the result of (a) [4]

(ii) by finding the exact evolution of the state. [8]

9. The Hamiltonian of a one-dimensional harmonic oscillator can be written as $H = \hbar\omega(P^2 + X^2)$ where

$$X = x\sqrt{\frac{m\omega}{2\hbar}}\,, \quad P = \frac{p}{\sqrt{2m\hbar\omega}}\,,$$

are scaled versions of x, p, the original position and momentum operators.

Defining $a^+ = X - \mathrm{i}P, \;\; a^- = X + \mathrm{i}P,$ show that

$$a^+a^- = \frac{H}{\hbar\omega} - \frac{1}{2}\,, \quad a^-a^+ = \frac{H}{\hbar\omega} + \frac{1}{2}\,, \quad [a^-, a^+] = 1\,,$$ [4]

and that a^+ (or a^-) transforms the eigenstate $|n\rangle$ of H into new eigenstates of H which differ in their eigenvalues by $\hbar\omega$ (or $-\hbar\omega$). (You may do just one of these cases.) [4]

Energy eigenvalues cannot be negative so there must be a minimum energy eigenstate $|0\rangle$. What happens when the operator a^- is applied to this state? What is the minimum energy? Give a general expression for the energy corresponding to $|n\rangle$. [3]

Generalise the 1-D result to obtain the eigenvalues of a 3-D harmonic oscillator. What is the degeneracy of the lowest 3 energy levels? [5]

The 3-D oscillator can also be solved in polar coordinates. The spherical harmonics $Y_{\ell,m}(\theta, \phi)$ can be used to describe the angular dependence of the eigenkets. Using your knowledge of the degeneracies of these functions, suggest suitable ℓ values for the lowest 3 energy levels of the 3-D oscillator. [4]

10. Under certain assumptions the time-independent Schrödinger equation for atomic helium can be written as

$$\left\{-\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0 r_{12}}\right\}\psi = E\psi$$

where r_1 and r_2 are the radial coordinates of the two electrons and r_{12} is their separation. What is the physical origin of each term in this expression? [3]

A solution of the form $\psi_{a,b} = \psi_a(r_1)\psi_b(r_2)$ can be found when the term $e^2/4\pi\epsilon_0 r_{12}$ is ignored, where a and b label the states occupied by electrons 1 and 2. By considering the exchange principle explain why a wave function of the form $\psi_{a,b}$ is *not* acceptable for two identical particles. [4]

For the ground state, use a trial solution of the form $\psi_{a,a}$, and assume ψ_a takes the form of the single particle wave function $\frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0}$. Evaluate the expectation value of the helium Hamiltonian in this state. You may assume that the ground state energy of a hydrogen-like atom is $-\alpha^2 Z^2 mc^2/2$ and the expectation value of $e^2/4\pi\epsilon_0 r_{12}$ in the state $\psi_{a,a}$ is $\frac{5}{4}Z(\alpha^2 mc^2/2)$. [4]

Now assume that the value of Z in the trial wave function takes an effective value Z^*. Evaluate the ground state energy of helium by using the variational method to minimise the expectation value of the Hamiltonian with respect to Z^*. [7]

Comment on the value of Z^* obtained in your minimisation. [2]

$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137}$

$a_0 = \frac{\hbar}{\alpha mc}.$

$a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}.$

$\mu \approx m$

A3 2012

First Attempt

1.

$$\Psi(x,t) = \Psi_0(x,t)\sin\gamma + \Psi_1(x,t)\cos\gamma$$

$$\underline{A = \sqrt{\frac{2}{a}}} \qquad \underline{E_0 = \frac{\pi^2\hbar^2}{2ma^2}} \qquad \underline{E_1 = \frac{4\pi^2\hbar^2}{2ma^2}}$$

possible outcomes	E_0	E_1
probabilities	$\sin^2\gamma$	$\cos^2\gamma$

2. the solution of 3-D box is separable

$$\psi(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

ψ_x, ψ_y, ψ_z are ~~one-D~~ wavefunctions of 1-D box

$\psi_i = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi i}{a}\right)$

$$\Rightarrow \psi_{n_x n_y n_z}(x,y,z) = \left(\frac{2}{a}\right)^3 \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n\pi y}{a}\right)\sin\left(\frac{n\pi z}{a}\right)$$

Ground state:

$$\underline{\psi_{(1,1,1)}(x,y,z) = \left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)\sin\left(\frac{\pi z}{a}\right)}$$

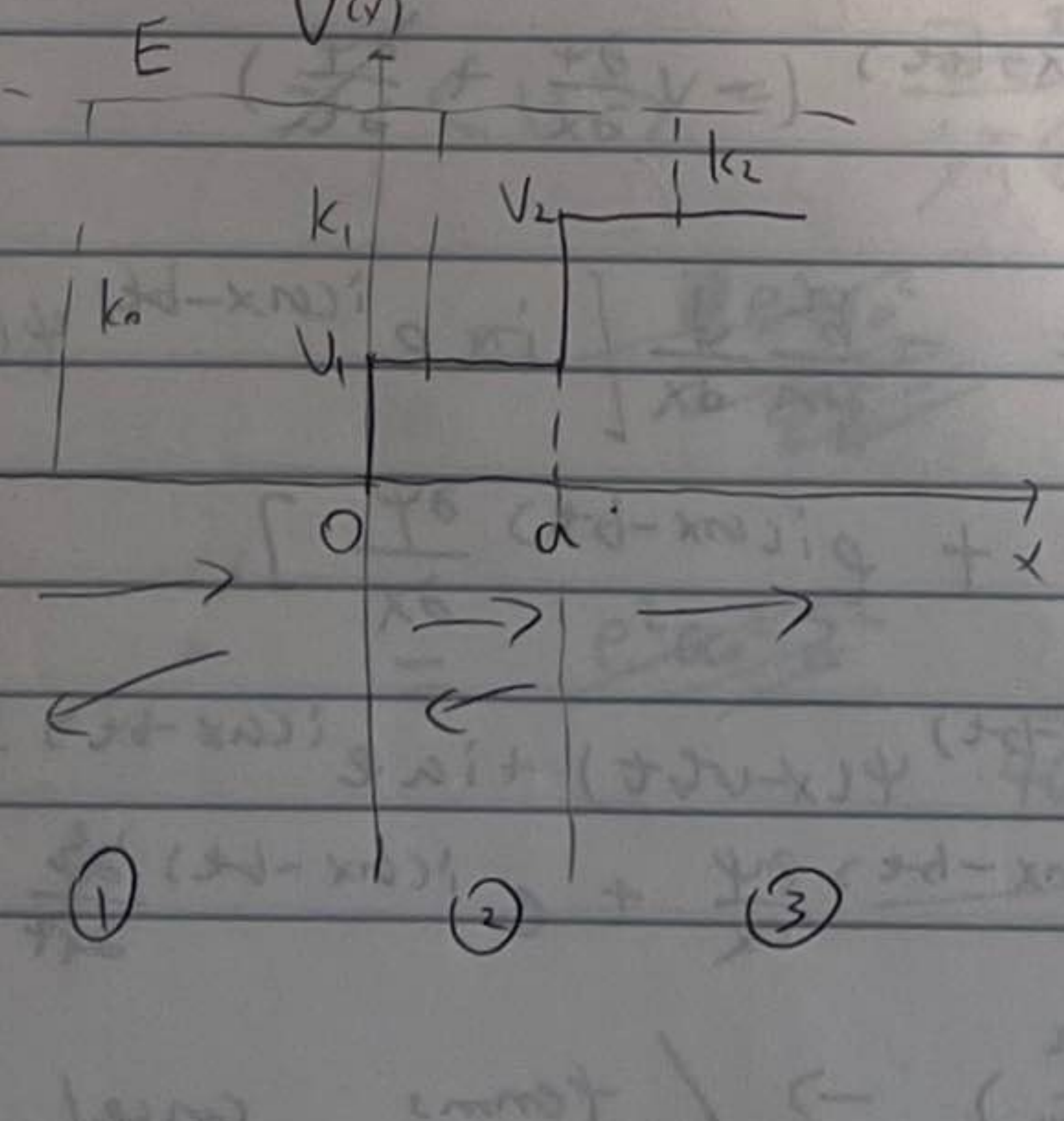
Energy $E_1 = E_{x_1} + E_{y_1} + E_{z_1} = \cancel{3 \times \frac{\pi^2\hbar^2}{}}\ \underline{\frac{3\pi^2\hbar^2}{2ma^2}}$

Energy levels $E_{n_x n_y n_z} = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2)$

misread

-2

3.



① $\psi_1 = e^{ik_0 x} + re^{-ik_0 x}$

② $\psi_2 = be^{ik_1 x} + ce^{-ik_1 x}$

③ $\psi_3 = te^{ik_2 x}$

$$k_0 = \sqrt{\frac{2mE}{\hbar^2}},\quad k_1 = \sqrt{\frac{2m(E-V_1)}{\hbar^2}}$$

$$k_2 = \sqrt{\frac{2m(E-V_2)}{\hbar^2}}$$

Boundary condition at $x=0$

1> $\psi_1(x=0) = \psi_2(x=0)$

2> $\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}$

free particle.

4. TDSE : $i\hbar\frac{\partial\psi}{\partial t} = H\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$

$\phi(x,t) = e^{i(ax-bt)}\psi(x-vt,t)$

let $x-vt=u$

$\frac{\partial u}{\partial t} = -v$

$\frac{\partial u}{\partial x} = 1$

$\frac{\partial\psi}{\partial u} = \frac{\partial\psi}{\partial x}$

$i\hbar\frac{\partial\phi}{\partial t} = -ibe^{i(ax-bt)}\psi(x-vt,t)(i\hbar)$

$+e^{i(ax-bt)}\left(\frac{\partial\psi}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial\psi}{\partial t}\right)i\hbar$

$\cancel{\frac{\partial\psi}{\partial x}\ (-v)}$

$\cancel{H\phi = -\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2}} = -\frac{\hbar^2}{2m}\left[-a^2e^{i(ax-bt)}\psi(x-vt,t)\right.$

$\cancel{+e^{i(ax-bt)}\frac{\partial^2\psi}{\partial u^2}}\Big]$.

$\cancel{\frac{\partial^2\psi}{\partial x^2}}$

$\frac{\partial\psi}{\partial u}\frac{\partial u}{\partial x}$

$\frac{\partial}{\partial x}\frac{\partial\psi}{\partial u}$

$\frac{\partial}{\partial u}\left(\frac{\partial\psi}{\partial u}\right)\frac{\partial u}{\partial x}$

$=\frac{\partial^2\psi}{\partial u^2}$

$= b\hbar e^{i(ax-bt)}\psi(x-vt,t)$

$+i\hbar e^{i(ax-bt)}\left(-v\frac{\partial\psi}{\partial x} + \cancel{\frac{\partial\psi}{\partial t}}\right)$

$H\phi = -\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = -\frac{\hbar^2}{2m}\frac{d}{dx}\left[iae^{i(ax-bt)}\psi(x-vt,t)\right.$

$\left.+e^{i(ax-bt)}\frac{\partial\psi}{\partial x}\right]$.

$= -\frac{\hbar^2}{2m}\left[-a^2e^{i(ax-bt)}\psi(x-vt,t) + iae^{i(ax-bt)}\frac{\partial\psi}{\partial x}\right.$

$\left.+iae^{i(ax-bt)}\frac{\partial\psi}{\partial x} + e^{i(ax-bt)}\frac{\partial^2\psi}{\partial x^2}\right]$

$i\hbar\frac{\partial\psi}{\partial t} = \frac{\partial^2\psi}{\partial x^2}\left(-\frac{\hbar^2}{2m}\right) \rightarrow$ / terms cancel

→ for $i\hbar \frac{\partial \phi}{\partial t} = H\phi$

need $\left(-\frac{\hbar^2}{2m}\right)(-a^2) = b\hbar \rightarrow b = \frac{\hbar a^2}{2m}$

and $\left(-\frac{\hbar^2}{2m}\right)(2ia) = i\hbar(-v) \rightarrow v = \frac{\hbar a}{m}$

pause time -3

$\phi(x,t)$ describes the Galilean transformation of wavefunction $\psi(x,t)$, the $e^{i(ax-bt)}$ is simply a gauge factor

$|\phi(x,t)|^2 = |\psi(x-vt,t)|^2 \rightarrow$ probability distribution invariant under Galilean transformation.

5. expectation value $= \int d^3r\, \psi_a^* \left(\frac{Ze^2}{4\pi\varepsilon_0 r}\right)\psi_a = \langle V\rangle$

$4\pi\int_0^\infty dr \cdot r^2 \cdot \frac{1}{r} e^{-2Zr/a_0} = 4\pi\left(\frac{a_0}{2Z}\right)^2 \int_0^\infty du\, \underbrace{u e^{-u}}_{1!=1}$

$u = \frac{2Zr}{a_0}$

$r = \frac{a_0}{2Z}u$

$dr = \frac{a_0}{2Z}du$

$= 4\pi\left(\frac{a_0}{2Z}\right)^2$

$\therefore \langle V\rangle = \frac{Ze^2}{\cancel{4\pi}\varepsilon_0} \cdot \cancel{4\pi} \cdot \left(\frac{a_0}{2Z}\right)^2 \frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3$

$= \cancel{\frac{Ze^2 a_0^2}{4Z}} \frac{Ze^2 a_0^2 Z^2}{\varepsilon_0 \cdot 4Z^2 \cdot a_0^3 \pi}$

$= \cancel{\frac{e^2 a_0^2 Z^2}{}} \frac{e^2 Z^2}{4 a_0 \varepsilon_0 \pi}$

checked

-3

→ looked up α -3

$$\boxed{\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}} \qquad \therefore \frac{e^2}{4\pi\varepsilon_0} = \alpha\hbar c$$

$$\boxed{a_0 = \frac{\hbar}{\alpha m c}}$$

$\therefore$ ~~$\langle v \rangle =$~~

$$\rightarrow \langle v \rangle = Z^2 \left(\frac{e^2}{4\pi\varepsilon_0}\right)\left(\frac{1}{a_0}\right)$$

$$= Z^2 (\alpha \hbar c)\left(\frac{\alpha m c}{\hbar}\right)$$

$$= \underline{m\alpha^2 m^2 Z^2}$$

higher nuclear charge → higher absolute value of ~~Coulo~~ Coulomb potential energy

6. $$\sigma_x \sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

$$\sigma_y \sigma_x = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$

$$\rightarrow \sigma_x\sigma_y + \sigma_y\sigma_x = 0$$

when $i = j$ $\quad \sigma_i \sigma_i = I$

$$\therefore \{\sigma_i, \sigma_i\} = 2I = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

$$[S_i, S_j] = S_i S_j - S_j S_i = S_i S_j - (-S_i S_j)$$

$$= 2 S_i S_j$$

$[S_x\ S_y] = 2S_xS_y = \cancel{\frac{\hbar}{2}}\ \hbar(\frac{\hbar}{2}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \cancel{i\hbar}$

$= \hbar(\frac{\hbar}{2}) \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\hbar \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \underline{i\hbar S_z}$

$[S_y, S_z] = 2S_yS_z = \hbar(\frac{\hbar}{2}) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 0$

$= i\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \underline{i\hbar S_x}$

$[S_z\ S_x] = 2S_xS_z = \hbar(\frac{\hbar}{2}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$= i\hbar \begin{pmatrix} 0 & -1 \\ i & 0 \end{pmatrix} = \underline{i\hbar S_y}$

~~was~~ expecting -1

$\rightarrow \quad [S_i, S_j] = i\hbar \varepsilon_{ijk} S_k \rightarrow$ angular momentum

$S^2 = (\frac{\hbar}{2})^2 (\sigma_x^2 + \sigma_y^2 + \sigma_z^2) \rightarrow \because \underline{\sigma_i\sigma_i = I}$

$= (\frac{\hbar}{2})^2 \cdot 3I = \frac{3}{4}\hbar^2 I$

end of part A. ~~2:07:02~~ 2:07'22" 90

31/40

7.

$H = a\sigma_z(1) + b\sigma_z(2) + c\, \vec{\sigma}(1) \cdot \vec{\sigma}(2)$

$\Sigma = \vec{\sigma}(1) + \vec{\sigma}(2) \qquad \Sigma_z = \sigma_z(1) + \sigma_z(2)$

$\Sigma^2 = \sigma^2(1) + \sigma^2(2) + 2\vec{\sigma}(1) \cdot \vec{\sigma}(2)$

$$\therefore \; [\Sigma_z, \Sigma^2] = [\sigma_z(1) + \sigma_z(2),\ \sigma^2(1) + \sigma^2(2) + 2\vec{\sigma}(1)\cdots$$

$$= \underbrace{[\sigma_z(1),\ \sigma^2(1)]}_{=0} + \underbrace{[\sigma_z(2),\ \sigma^2(2)]}_{=0}$$

$$+\, 2[\sigma_z(1),\ \vec{\sigma}(1)\cdot\vec{\sigma}(2)] + 2[\sigma_z(2),\ \vec{\sigma}(1)\cdot\vec{\sigma}(2)]$$

$$[\sigma_z(1),\ \vec{\sigma}(1)\cdot\vec{\sigma}(2)] = [\sigma_z(1),\ \sigma_x(1)\sigma_x(2) + \sigma_y(1)\sigma_y(2) + \sigma_z(1)\sigma_z(2)]$$

$$= \cancel{i\hbar(\sigma_x(1)\sigma_y(1) - \sigma_y(1)\sigma_x(2))}$$
$$i\hbar(\sigma_y(1)\sigma_x(2) - \sigma_x(1)\sigma_y(2))$$

Similary, $[\sigma_z(2),\ \vec{\sigma}(1)\cdot\vec{\sigma}(2)] = i\hbar(\sigma_x(1)\sigma_y(2) - \sigma_y(1)\sigma_x(2))$

they cancel $\rightarrow [\Sigma_z, \Sigma^2] = 0$ QED

$$\rightarrow 2[\sigma^+(1)\sigma^-(2) + \sigma^-(1)\sigma^+(2)] + \sigma_z(1)\sigma_z(2)$$

$$= \frac{1}{2}(\sigma_x(1) + i\sigma_y(1))(\sigma_x(2) - i\sigma_y(2)) + \frac{1}{2}(\sigma_x(1) - i\sigma_y(1)) \times (\sigma_x(2) + i\sigma_y(2)) + \sigma_z(1)\sigma_z(2)$$

$$= \frac{1}{2}[\sigma_x(1)\sigma_x(2) + i(\sigma_y(1)\sigma_x(2) - \sigma_x(1)\sigma_y(2)) + \sigma_y(1)\sigma_y(2) + \sigma_x(1)\sigma_x(2) + i(\sigma_x(1)\sigma_y(2) - \sigma_y(1)\sigma_x(2)) + \sigma_y(1)\sigma_y(2)] + \sigma_z(1)\sigma_z(2)$$

$$= \sigma_x(1)\sigma_x(2) + \sigma_y(1)\sigma_y(2) + \sigma_z(1)\sigma_z(2)$$

$$= \vec{\sigma}(1)\cdot\vec{\sigma}(2)$$

QED

pause time 8/2?

~~*~~ If $a=b$, then

$$H = a(\sigma_z(1) + \sigma_z(2)) + c\,\vec{\sigma}(1)\cdot\vec{\sigma}(2)$$

$$\cancel{= a\Sigma_z + 2c[\sigma^+(1)\sigma^-(2) + \sigma^-(1)\sigma^+(2)] + c\,\sigma_z(1)\sigma_z(2)}$$

$$= a\Sigma_z + c\left[\tfrac{1}{2}\right]\left[\Sigma^2 - \sigma^2(1) - \sigma^2(2)\right]$$

$$= a\Sigma_z + \frac{c}{2}\left[\Sigma^2 - \sigma^2(1) - \sigma^2(2)\right]$$

$\because$ two particles both have spin 1/2

$\therefore$ $\sigma^2(1)$ and $\sigma^2(2)$ will both give eigenvalues of 3 ~~(3I)~~ (matrix $= 3I$)

$$\therefore H|l,m\rangle = a\Sigma_z|l,m\rangle + \frac{c}{2}\Sigma^2|l,m\rangle - \sigma^2(1)|l,m\rangle - \sigma_2^2|l,m\rangle$$

$$= \boxed{2am + 2c\,l(l+1) - \cancel{3}c}\,|l,m\rangle$$

mutual eigenstates of $\sigma_z(1)$ $\sigma_z(2)$ $\Rightarrow$ $|\sigma_z(1), \sigma_z(2)\rangle$
$= |m_1, m_2\rangle$
~~$= |m_1\rangle|m_2\rangle$~~
$= |m_1\rangle|m_2\rangle$

when $a \neq b$, ~~$H = \sigma\sigma$~~

$$H = a\sigma_z(1) + b\sigma_z(2) + c\,\vec{\sigma}(1)\cdot\vec{\sigma}(2)$$

$$= a\sigma_z(1) + b\sigma_z(2) + 2c\sigma^+(1)\sigma^-(2) + 2c\sigma^-(1)\sigma^+(2) + c\sigma_z(1)\sigma_z(2)$$

$$\therefore H|m_1, m_2\rangle = am_1|m_1,m_2\rangle + bm_2|m_1,m_2\rangle$$
$$\cancel{+2c}\ c\,m_1m_2|m_1,m_2\rangle + 2c[\sigma^+(1)\sigma^-(2) + \sigma^-(1)\sigma^+(2)]|m_1 m_2\rangle$$

$\sigma^+(1)\,\sigma^-(2)\,|m_1, m_2\rangle \neq 0$ only if $|m_1\rangle|m_2\rangle = |-1\rangle|1\rangle$

in this case $\sigma^+(1)\,\sigma^-(2)\,|-1, 1\rangle = |1, -1\rangle$

$\sigma^-(1)\,\sigma^+(2)\,|m_1, m_2\rangle \neq 0$ only if $|m_1\rangle|m_2\rangle = |1\rangle|-1\rangle$

in this case $\sigma^-(1)\,\sigma^+(2)\,|1, -1\rangle = |-1, 1\rangle$

$\therefore$ ~~$H\,|m_1, m_2\rangle$~~

$$H\,|1\rangle_1|1\rangle_2 = (am_1 + bm_2 + c\,m_1 m_2)\,|1\rangle_1|1\rangle_2 = \underline{(a+b+c)\,|1\rangle_1|1\rangle_2}$$

$$H\,|-1\rangle_1|-1\rangle_2 = (am_1 + bm_2 + c\,m_1 m_2)\,|-1\rangle_1|-1\rangle_2 = \underline{(-a-b+c)\,|-1\rangle_1|-1\rangle_2}$$

$$H\,|1\rangle_1|-1\rangle_2 = \underline{(a-b-c)\,|1\rangle_1|-1\rangle_2 + 2c\,|-1\rangle_1|1\rangle_2}$$

$$H\,|-1\rangle_1|1\rangle_2 = \underline{(-a+b-c)\,|-1\rangle_1|1\rangle_2 + 2c\,|1\rangle_1|-1\rangle_2}$$

not choosing this one

8. (a)

$H = H_0 + V$ $\qquad$ $H_0 |E_n\rangle = \cancel{i\hbar \frac{\partial |E_n\rangle}{\partial t}}\; E_n |E_n\rangle$

stationary states.

let $|\psi\rangle = a_i e^{-iE_it/\hbar} |E_i\rangle + a_2 e^{-iE_jt/\hbar} |E_j\rangle$

and $H|\psi\rangle = i\hbar \frac{\partial |\psi\rangle}{\partial t}$

$\rightarrow$ $\cancel{a_i E_i e^{-iE_it/\hbar} |E_i\rangle} + \cancel{a_j E_j e^{-iE_jt/\hbar} |E_j\rangle}$

$+ a_i V |E_i\rangle e^{-iE_it/\hbar} + a_j V |E_j\rangle e^{-iE_jt/\hbar}$

$= i\hbar \dot{a}_i e^{-iE_it/\hbar} |E_i\rangle + \cancel{E_i a_i e^{-iE_it/\hbar} |E_i\rangle}$

$+ i\hbar \dot{a}_j e^{-iE_jt/\hbar} |E_j\rangle + \cancel{E_j a_j e^{-iE_jt/\hbar} |E_j\rangle}$

$a_i \approx 1$ $\qquad a_i(0) = 1 \qquad a_j(0) = 0$

$\langle E_j| \cdot$

$\Rightarrow$ $\cancel{i\hbar \dot{a}_j e^{-iE_j}}$ $\; i\hbar \dot{a}_j e^{-iE_jt/\hbar} =$

$= a_i \langle E_j|V|E_i\rangle e^{-iE_it/\hbar} + a_j \langle E_j|V|E_j\rangle e^{-iE_jt/\hbar}$

$\because a_i(0) = 1 \quad a_j(0) = 0$ for T not too large

$i\hbar \dot{a}_j e^{-iE_jt/\hbar} = \underbrace{\langle E_j|V|E_i\rangle}_{V_{ij}^*} e^{-iE_it/\hbar}$

$\therefore \dot{a}_j = -\frac{i}{\hbar} V_{ij}^* \exp(i(\underbrace{E_j - E_i}_{\hbar\omega})t/\hbar)$

$\rightarrow a_j = \int_0^T \dot{a}_j \, dt$ $\qquad (\because a_j(0) = 0)$

$\because$ V independent of time

$$\rightarrow \quad a_j = -\frac{i}{\hbar} V_{ji}^* \int_0^T dt\, e^{i\omega t}$$

$$= -\frac{i}{\hbar} V_{ji}^* \frac{-1}{i\omega}\left(1 - e^{i\omega T}\right)$$

$$= V_{ji}^* \frac{(1 - e^{i\omega T})}{\hbar\omega}$$

$$P_{ij} = |a_j|^2 = |V_{ij}|^2 \left(\frac{1}{\hbar\omega}\right)^2 \left|1 - e^{i\omega T}\right|^2$$

$$\left|1 - e^{i\omega T}\right|^2 = \left|\cancel{(1-\cos\theta)}\,(1 - \cos\omega T) - i\sin\omega T\right|^2$$

$$= (1 - \cos\omega T)^2 + \sin^2\omega T = 2 - 2\cos\omega T$$

$$= 4\sin^2\left(\frac{\omega T}{2}\right)$$

$$\therefore \quad P_{ij} = 4|V_{ij}|^2 \frac{\sin^2\left(\frac{\omega T}{2}\right)}{(\hbar\omega)^2}$$

QED

(b) (i) system originally has spin $+\frac{1}{2}$ w.r.t direction of B $\rightarrow$ $|E_i\rangle = |+\rangle$

$\Rightarrow$ the opposite spin $\rightarrow$ $|E_j\rangle = |-\rangle$

$$H_0 = -\mu B \sigma_z \quad , \quad V = -\mu b\, \sigma_x$$

$$H_0|E_i\rangle = H_0|+\rangle = -\mu B|+\rangle \qquad H_0|E_j\rangle = H_0|-\rangle = \mu B|-\rangle$$

$$\therefore \rightarrow E_i = -\mu B \qquad E_j = \mu B \qquad \Delta E = E_j - E_i = 2\mu B$$

$$\rightarrow \quad \hbar\omega = 2\mu B \quad \rightarrow \quad \omega = \frac{2\mu B}{\hbar}$$

$$\therefore\ P_{+\to -} = 4|\langle -|V|+\rangle|^2 \frac{\sin^2(\frac{\mu B T}{\hbar})}{4\mu^2 B^2}$$

$$-\frac{1}{\mu b}\langle +|V|-\rangle = (1\ 0)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = (1\ 0)\begin{pmatrix}1\\0\end{pmatrix} = 1$$

$\rightarrow$ ~~$P_{+\to -} = \frac{\sin^2(\frac{\mu B T}{\hbar})}{}$~~ $\quad V_{ij} = -\mu b \rightarrow |V_{ij}|^2 = \mu^2 b^2$

$\rightarrow$ ~~$V_{ij} = \frac{1}{\mu b} \rightarrow |V_{ij}|^2 = \frac{1}{\mu^2 b^2}$~~

$$\rightarrow\ \underline{P_{+\to -} = \left(\frac{b}{B}\right)^2 \sin^2\left(\frac{\mu B T}{\hbar}\right) = \left(\frac{b}{B}\right)^2 \sin^2\left(\frac{\mu B l}{\hbar v}\right)}$$

(ii) $\quad 0 < t < l/v$

$$H = -\mu(B\sigma_z + b\sigma_x) = -\mu\begin{pmatrix}B & b\\ b & -B\end{pmatrix}$$

eigenvalues $-\mu\lambda = \Lambda$, eigenstates $|\phi\rangle$, then. $(|\phi\rangle = \begin{pmatrix}c_1\\c_2\end{pmatrix}$

$$\det\begin{pmatrix}B-\lambda & b\\ b & -B-\lambda\end{pmatrix} = 0$$

$$\rightarrow\ (-B-\lambda)(B-\lambda) - b^2 = 0$$

$$\therefore\ \lambda^2 - B^2 - b^2 = 0 \ \rightarrow\ \lambda = \pm\sqrt{B^2+b^2}$$

$$\therefore\ \Lambda = \mp\mu\sqrt{B^2+b^2}$$

$$\Lambda = +\mu\sqrt{B^2+b^2} \rightarrow \begin{pmatrix}B+\sqrt{B^2+b^2} & b\\ b & -B+\sqrt{B^2+b^2}\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$$

$= E_+$

$$\rightarrow\ -b c_1 = (\sqrt{B^2+b^2} - B)c_2$$

$$b^2 + \left(\sqrt{B^2+b^2} - B\right)^2 = b^2 + B^2 + b^2 - 2B\sqrt{B^2+b^2} + B^2$$
$$= 2\left(B^2+b^2 - B\sqrt{B^2+b^2}\right)$$

$$\therefore |\phi_1\rangle = \frac{1}{\sqrt{2(B^2+b^2-B\sqrt{B^2+b^2})}} \begin{pmatrix} \sqrt{B^2+b^2} - B \\ -b \end{pmatrix}$$

Similarly if $\Lambda = -\mu\sqrt{B^2+b^2}$, then
$= E_-$

$$\begin{pmatrix} B - \sqrt{B^2+b^2} & b \\ b & \cancel{-B-B\sqrt{B}} \; -B-\sqrt{B^2+b^2} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\therefore \quad c_1 b = \left(B + \sqrt{B^2+b^2}\right) c_2$$

$$\therefore |\phi_2\rangle = \frac{1}{\sqrt{2(B^2+b^2+B\sqrt{B^2+b^2})}} \begin{pmatrix} B + \sqrt{B^2+b^2} \\ b \end{pmatrix}$$

in the basis of $|+\rangle$, $|-\rangle$

$\therefore$ At time $t=0$, state of system is

$$|\psi(0)\rangle = |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \langle\phi_1|+\rangle|\phi_1\rangle + \langle\phi_2|+\rangle|\phi_2\rangle$$

$$\langle\phi_1|+\rangle = \frac{\sqrt{B^2+b^2} - B}{\sqrt{2(B^2+b^2-B\sqrt{B^2+b^2})}} \qquad \langle\phi_2|+\rangle = \frac{B + \sqrt{B^2+b^2}}{\sqrt{2(B^2+b^2+B\sqrt{B^2+b^2})}}$$

At time $t = T$

$$\cancel{|+,t\rangle} = |\psi(t)\rangle = \langle\phi_1|+\rangle e^{-iE_+T/\hbar} + \langle\phi_2|+\rangle e^{iE_-T/\hbar}$$

$|\psi(T)\rangle = \langle\phi_1|+\rangle e^{-iE_+T/\hbar}|\phi_1\rangle + \langle\phi_2|+\rangle e^{-iE_-T/\hbar}|\phi_2\rangle$

→ probability amplitude for finding the ~~system~~ particle in state $|-\rangle$ is

$$a_j = \langle -|\psi(T)\rangle = \langle\phi_1|+\rangle\langle -|\phi_1\rangle e^{-iE_+T/\hbar} + \langle\phi_2|+\rangle\langle -|\phi_2\rangle \times e^{-iE_-T/\hbar}$$

$|-\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ $\quad \langle -|\phi_1\rangle = \dfrac{-b}{\sqrt{2(B^2+b^2-B\sqrt{B^2+b^2})}}$ $\quad \langle -|\phi_2\rangle = \dfrac{b}{\sqrt{2(B^2+b^2+B\sqrt{B^2+b^2})}}$

$$\therefore\ a_j = \frac{-1}{2}\frac{(\sqrt{B^2+b^2}-B)b}{(B^2+b^2-B\sqrt{B^2+b^2})}e^{-iE_+T/\hbar} + \frac{1}{2}\frac{(\sqrt{B^2+b^2}+B)b}{B^2+b^2+B\sqrt{B^2+b^2}} \times e^{-iE_-T/\hbar}$$

$B^2+b^2-B\sqrt{B^2+b^2} = \sqrt{B^2+b^2}(\sqrt{B^2+b^2}-B)$

$B^2+b^2+B\sqrt{B^2+b^2} = \sqrt{B^2+b^2}(\sqrt{B^2+b^2}+B)$

$$\rightarrow\ a_j = \frac{b}{\sqrt{B^2+b^2}}\left(\frac{1}{2}(e^{-iE_-T/\hbar} - e^{-iE_+T/\hbar})\right)$$

$$= \frac{b}{\sqrt{B^2+b^2}}\ \cancel{\sin}\left(\frac{1}{2}(e^{\frac{iT}{2\hbar}(E_+-E_-)} - e^{-\frac{iT}{2\hbar}(E_+-E_-)}\right) \times e^{i\frac{E_++E_-}{2}\frac{T}{\hbar}}$$

$$= \frac{-bi}{\sqrt{B^2+b^2}}e^{i\left(\frac{E_++E_-}{2}\right)T/\hbar}\sin\left(\frac{\overbrace{(E_+-E_-)}^{\hbar\omega}T}{2\hbar}\right) \quad \left(\omega = \frac{2\mu B}{\hbar},\ T = \frac{l}{v}\right)$$

$$\therefore\ P_{ij} = |a_j|^2 = \frac{b^2}{B^2+b^2}\sin^2\left(\frac{\mu B l}{\hbar v}\right)$$

for $b \ll B$. $\dfrac{b^2}{B^2+b^2} \approx \dfrac{b^2}{B^2}$ → consistent

(2) $i\hbar \dot{a}_+ e^{-iE_+t/\hbar} = a_+ e^{-iE_+t/\hbar} \langle E_+|V|E_+\rangle$

$+ a_- e^{-iE_-t/\hbar} \langle E_+|V|E_-\rangle$

$|E_+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$|E_-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$i\hbar \dot{a}_- e^{-iE_-t/\hbar} = a_+ e^{-iE_+t/\hbar} \langle E_-|V|E_+\rangle$

$+ a_- e^{-iE_-t/\hbar} \langle E_-|V|E_-\rangle$

$V = -\mu b \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rightarrow \langle E_+|V|E_-\rangle = \langle E_-|V|E_+\rangle = 1$

$\langle E_+|V|E_+\rangle = \langle E_-|V|E_-\rangle = 0$

$\because E_- - E_+ = \Delta E = \hbar\omega = 2\mu B$

$\therefore \dot{a}_+ = -\frac{i}{\hbar}$

9.

$a^+ = x - iP \quad a^- = x + iP \quad . \quad H = \hbar\omega(x^2+P^2)$

$\therefore a^+a^- = (x-iP)(x+iP) = x^2 - iPx + i\,xP + P^2$

$= \underbrace{x^2+P^2}_{\frac{H}{\hbar\omega}} + i\underbrace{[x,P]}$

$[x,P] = \sqrt{\frac{m\omega}{2\hbar}\cdot\frac{1}{2m\hbar\omega}}\,[\underbrace{\hat{x},\hat{P}}_{i\hbar}]$

$= \frac{i}{2}\frac{\hbar}{\hbar} = \frac{i}{2}$

$\therefore a^+a^- = \frac{H}{\omega\hbar} + i\left(\frac{i}{2}\right) = \underline{\frac{H}{\hbar\omega} - \frac{1}{2}}$

Similarly $a^-a^+ = x^2+P^2 - i\underbrace{[x,P]}_{\frac{i}{2}} = \underline{\frac{H}{\hbar\omega} + \frac{1}{2}}$

$[a^-, a^+] = a^-a^+ - a^+a^- = \underline{1}$

$Ha^+|n\rangle = \hbar\omega(a^+a^- + \frac{1}{2})a^+|n\rangle$ (If $H|n\rangle = E_n|n\rangle$)

$= \omega\hbar\, a^+a^-a^+|n\rangle + \frac{1}{2}\hbar\omega\, a^+|n\rangle$

$= \omega\hbar\, a^+a^+a^-|n\rangle + \omega\hbar\, a^+\underbrace{[a^-,a^+]}_{1}|n\rangle + \frac{1}{2}\hbar\omega\, a^+|n\rangle$

$= a^+\hbar\omega(a^+a^- + \frac{1}{2})|n\rangle + a^+\hbar\omega|n\rangle$

$= \cancel{H|n\rangle}\ \cancel{H|n\rangle}\ H(a^+|n\rangle + \hbar\omega|a^+|n\rangle)$

$= \underline{(E_n + \hbar\omega)\, a^+|n\rangle}$

$\therefore$ a^+ transforms $|n\rangle$ to new state with energy higher by $\hbar\omega$

$$a^-|0\rangle = 0$$

minimum energy ~~E_0~~ $H|0\rangle = E_0|0\rangle$

$$H|0\rangle = \hbar\omega(a^+a^- + \tfrac{1}{2})\underbrace{|0\rangle}_{a^-|0\rangle=0} = \underbrace{\tfrac{1}{2}\hbar\omega}_{E_0}|0\rangle$$

$$\rightarrow \quad E_0 = \tfrac{1}{2}\hbar\omega$$

above E_0 each energy level is higher than the previous one by $\hbar\omega$

$$\therefore \quad E_n = (n + \tfrac{1}{2})\hbar\omega$$

For 3-D harmonic oscillator

$$H = \hbar\omega(P_x^2 + P_y^2 + P_z^2 + X^2 + Y^2 + Z^2)$$

$\because$ No interaction term between x, y, z coordinates. $\therefore$ wavefunctions multiply and energy levels simply add. ~~$E_{nx,ny,nz} = \hbar\omega(n_x + n_y$~~

$$\boxed{E_{nx,ny,nz} = \hbar\omega(n_x + n_y + n_z + \tfrac{3}{2})}$$

lowest 3 levels of energy are.

Ground : $(n_x, n_y, n_z) = (0,0,0)$ $\quad E = \frac{3}{2}\hbar\omega$

1st excited : $(n_x, n_y, n_z) = (1,0,0), (0,1,0), (0,0,1)$

$$E = \frac{5}{2}\hbar\omega$$

2nd excited : $(n_x, n_y, n_z) = (2,0,0), (0,2,0), (0,0,2)$
$(1,1,0), (0,1,1), (1,0,1)$

$\rightarrow$ $E = \frac{7}{2}\hbar\omega$

~~$Y_{0,0}$ degeneracy = 1, $Y_{1,1}$ degeneracy = 3~~
~~Ground state~~ Y.

Spherical harmonics

l	wavefunction	degeneracy
0	Y_{00}	1
1	Y_{11}, Y_{10}, Y_{1-1}	3
2	$Y_{22}, Y_{21}, Y_{20}, Y_{2-1}, Y_{2-2}$	5

For 3-D oscillator :

Ground state : degeneracy $= 1 \rightarrow Y_{0,0} \rightarrow l = 0$

1st excited : degeneracy $= 3 \rightarrow l = 1$

2nd excited : degeneracy $= 6 = 5 + 1$

$\therefore l = 2$ or 0

5 degenerate | 1 degenerate

15/20

10.

$$H\psi = \left(-\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_1} - \frac{Ze^2}{4\pi\varepsilon_0 r_2} + \frac{e^2}{4\pi\varepsilon_0 r_{12}}\right)\psi = E\psi$$

kinetic energy of 1st electron

K.E. of 2nd electron

Coulumb potential energy of 1st electron due to nucleus

Coulumb potential of 2nd electron due to nucleus

Coulumb ~~tract~~ interaction between 2 electrons.

identical particles are described by either symmetric or antisymmetric wavefunctions because of exchange principle, but $\psi_{a,b} = \psi_a(r_1)\psi_b(r_2)$ is not symmetric or antisymmetric, → not acceptable.

$$\psi_{a,a} = \frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3 e^{-Zr_1/a_0} e^{-Zr_2/a_0} = \psi_a(r_1)\psi_a(r_2)$$

$$\langle H\rangle = \int d^3r_1\, \psi_a^*(r_1)\psi_a^*(r_2)\, H\, \psi_a(r_1)\psi_a(r_2)\, d^3r_2$$

$$= \int d^3r_1 \cancel{d^3r_2} \cancel{|\psi_a(r_1)|^2}\, \psi_a(r_1) \underbrace{\left(-\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_1}\right)\psi_a(r_1)}_{-\frac{\alpha Z^2 mc^2}{2}\psi_a(r_1)}$$

$$+ \int d^3r_2\, \psi_a(r_2) \underbrace{\left(-\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_1}\right)\psi_a(r_2)}_{= -\frac{\alpha Z^2 mc^2}{2}\psi_a(r_2)}$$

$$+ \int d^3r_1 d^3r_2\, \psi_a(r_1)\psi_a(r_2)\left(\frac{e^2}{4\pi\varepsilon_0 r_{12}}\right)\psi_a(r_1)\psi_a(r_2)$$

$$= -\alpha^2 Z^2 mc^2 \int d^3r_1 \underbrace{\psi_a^2(r_1)}_{1}$$

$$+ \frac{5}{4} Z \left(\frac{\alpha^2 mc^2}{2}\right) = \underline{-\alpha^2 Z^2 mc^2 + \frac{5}{8} Z \alpha^2 mc^2}$$

$$\int d^3r_1\, \psi_a^2(r_1) = 4\pi \int dr\, r^2 \frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3 e^{-2Zr/a_0}$$

$$= \frac{4Z^3}{a_0^3} \int dr\, e^{-2Zr/a_0} r^2$$

$$= \left(\frac{4Z^3}{a_0^3}\right)\left(\frac{a_0}{2Z}\right)^3 \int du\, \underbrace{u^2 e^{-u}}_{2!} = 1 \quad \underline{確認!}$$

→ Z in the Hamiltonian remains to be Z

Z in the trail wavefunction is replaced by Z^*

No more true (15/20)

$$\therefore \psi_a(r_1) = \frac{1}{\sqrt{\pi}}\left(\frac{Z^*}{a_0}\right)^{\frac{3}{2}} e^{-Z^* r/a_0}$$

Virial theorem $\quad |PE| = 2|KE|$

$PE + 2KE = 0.$

$\downarrow \qquad \downarrow$

$-ve \qquad +ve$

$\therefore$ Consider $H_Z \psi_a(Z, r_1) = E_Z \psi_a(Z, r_1)$ for single electron

$$E_Z = -\frac{1}{2}\alpha^2 mc^2 Z^2$$

$$\therefore PE_Z = -\alpha^2 mc^2 Z^2 \qquad KE_Z = \frac{1}{2}\alpha^2 mc^2 Z^2$$

$\because$ $\hat{KE} = -\frac{\hbar^2}{2m}\nabla_1^2$ independent of Z

$\therefore$ replace all Z in KE_Z with Z^*

$\rightarrow$ $KE_{Z^*} = \frac{1}{2}\alpha^2 mc^2 Z^{*2}$

$\because$ $\hat{PE} = -\frac{Ze^2}{4\pi\varepsilon_0 r_1}$ $\propto Z$ $\therefore$ replace Z^2 by ZZ^*

$\therefore$ $PE_Z^* = -\alpha^2 mc^2 ZZ^*$

$\because$ $\frac{e^2}{4\pi\varepsilon_0 r_{12}}$ independent of Z

$\therefore$ $\cancel{\frac{5}{8}}$ replace all Z by Z^*.

$E_{int} = \frac{5}{8} Z^* \alpha^2 mc^2$

$\therefore$ Total energy

$$\langle H\rangle = 2\left(-\alpha^2 mc^2 ZZ^* + \frac{1}{2}\alpha^2 mc^2 Z^{*2}\right) + \frac{5}{8}Z^*\alpha^2 mc^2$$

$$= \alpha^2 mc^2\left(-2ZZ^* + Z^{*2} + \frac{5}{8}Z^*\right)$$

set $0 = \frac{d\langle H\rangle}{dZ^*}$ $\rightarrow$ $0 = -2Z + 2Z^* + \frac{5}{8}$.

$\frac{32-5}{16}$

错了!

没有!

$2Z^* = 2Z - \frac{5}{8}$

$Z^* = Z - \frac{5}{16} =$

$\psi_{a_{Z^*}}(r_1) = \frac{1}{\sqrt{\pi}}\left(\frac{Z^*}{a_0}\right)^{\frac{3}{2}} e^{-Z^* r/a}$

$\because$ $\psi_{a_Z}(r_1)$ is the eigenfunction of hamitonian

$H_{1Z} = -\frac{\hbar^2}{2m}\nabla_1^2 + \frac{Ze^2}{4\pi\varepsilon_0 r_1}$ with eigenvalue

(eigen energy) $E_Z = -\frac{1}{2}\alpha^2 mc^2 Z^2$.

$\therefore$ By Viral theorem

$PE_Z = -\alpha^2 mc^2 Z^2$ $\quad$ $KE_Z = \frac{1}{2}\alpha^2 mc^2 Z^2$

if wavefunction changes to $\psi_{aZ^*}(r_1)$ instead of $\psi_{aZ}(r_1)$, then $\psi_{aZ^*}(r_1)$ is no longer eigenstate of H_{1Z}. Viral theorem does not hold.

~~PEz~~ $\because$ $\hat{KE} = -\frac{\hbar^2}{2m}\nabla^2$ independent of Z

$\therefore$ replace all Z in KE_Z with Z^*

$\rightarrow$ $KE_Z^* = \frac{1}{2}\alpha^2 mc^2 Z^{*2}$

$\because$ $\hat{PE}_Z = -\frac{Ze^2}{4\pi\varepsilon_0 r_1}$

$\therefore$ replace Z^2 in PE_Z by ZZ^*

$\rightarrow$ $PE_{Z^*} = -\alpha mc^2 ZZ^*$

$\because$ $\frac{e^2}{4\pi\varepsilon_0 r_{12}}$ independent of Z

$\therefore$ In interaction energy replace all Z by Z^*

$\therefore \quad E_{int} = \frac{5}{8} Z^* \alpha^2 mc^2$

Total energy

$\cancel{E} \quad \langle H \rangle = 2(-\alpha^2 mc^2 Z Z^* + \frac{1}{2}\alpha^2 mc^2 Z^{*2})$

$+ \frac{5}{8} Z^* \alpha^2 mc^2$

$= \alpha^2 mc^2 (-2ZZ^* + Z^{*2} + \frac{5}{8} Z^*)$

set $\quad 0 = \frac{d\langle H \rangle}{dZ^*} \rightarrow 0 = -2Z + 2Z^* + \frac{5}{8}$

$\therefore \quad Z^* = Z - \frac{5}{16}$

the effective nuclear charge is descreased because ~~of~~ the electron close to the nucleas ~~shaild~~ shields a part of the ~~nuclear~~ Coulumb ~~interaction~~ ~~to~~ force experienced by the electron ~~from~~ far from the nucleas.