QM II
phys 652

Solutions of HW #4

Problem #1 $\Rightarrow$ find $\langle \frac{1}{r} \rangle$

Use the virial theorem (phys 651):

if $V = C r^k \Rightarrow \underbrace{\langle T \rangle}_{\text{kinetic}} = \frac{k}{2} \underbrace{\langle V \rangle}_{\text{potential}}$

energy

For the H-atom:

$$V = -\frac{e^2}{r} \Rightarrow k = -1 \Rightarrow \langle T \rangle = -\frac{1}{2}\langle V \rangle$$

Then,

$$\langle H \rangle = E_n = \langle T \rangle + \langle V \rangle = \frac{1}{2}\langle V \rangle =$$

$$= -\frac{e^2}{2}\langle \frac{1}{r} \rangle \Rightarrow \langle \frac{1}{r} \rangle = -\frac{2E_n}{e^2} =$$

$$= \frac{\mu e^4}{\hbar^2 n^2 e^2} = \underbrace{\frac{\mu e^2}{\hbar^2}}_{= \frac{1}{a_0}} \cdot \frac{1}{n^2} = \frac{1}{n^2 a_0}$$

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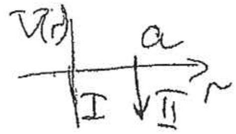
Problem #2 ~~[scribbled out]~~

(But with $V(r)$ instead of $\frac{-e}{r}$)

From Eq. (5.3) of Lecture #4 $\Rightarrow$ at $\ell = 0 \Rightarrow$



$$\frac{d^2 u(r)}{dr^2} + \left[\frac{2mV_0}{\hbar^2}\delta(r-a) - \underbrace{\kappa^2}_{= -\frac{2mE}{\hbar^2}}\right] u(r) = 0$$

$(E<0)$ $\uparrow$ bound states

$\Downarrow$

$$u(r) = C_1 e^{\kappa r} + C_2 e^{-\kappa r}$$

$u_I = C_1 e^{\kappa r} + C_2 e^{-\kappa r}$ $\quad (0 < r < a)$

$u_{II} = C_3 e^{-\kappa r}$ $\quad (r > a)$

Since at $r=0 \Rightarrow u(0) = 0 \Rightarrow C_1 = -C_2 \Rightarrow$

$u_I = A \sinh \kappa r$

Continuity of the wave function at $r = a$:

$$\frac{A \sinh \kappa a}{a} = \frac{C e^{-\kappa a}}{a} \Rightarrow A \sinh \kappa a = C e^{-\kappa a}$$

Discontinuity of the derivative:

$$\underbrace{\left.\frac{du}{dr}\right|_{a+\varepsilon}}_{= -\kappa \underbrace{C e^{-\kappa a}}_{= A\sinh \kappa a}} - \underbrace{\left.\frac{du}{dr}\right|_{a-\varepsilon}}_{= \kappa A \cosh \kappa a} + \frac{2mV_0}{\hbar^2}\underbrace{u(a)}_{C e^{-\kappa a} = A \sinh \kappa a} = 0 \Rightarrow$$

$$-\kappa A \sinh \kappa a - \kappa A \cosh \kappa a + \frac{2mV_0}{\hbar^2} A \sinh \kappa a = 0$$

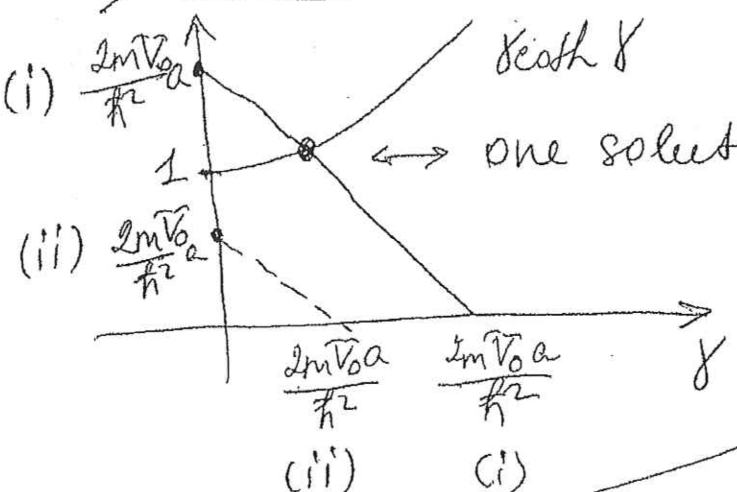
$$\Downarrow$$

$$-\kappa - \kappa \coth(\kappa a) + \frac{2mV_0}{\hbar^2} = 0 \; ; \quad \kappa a \coth(\kappa a) = \frac{2mV_0}{\hbar^2} a - \kappa a$$

$$\kappa a \equiv \gamma \qquad \Leftarrow$$

$$\Downarrow$$

$$\gamma \coth \gamma = \frac{2mV_0}{\hbar^2} a - \gamma \Rightarrow$$ from this find allowed energy levels



$\longleftrightarrow$ one solution $\longleftrightarrow$ (i) $\frac{2mV_0}{\hbar^2} a > 1$

(ii) $\frac{2mV_0}{\hbar^2} a < 1$

no solution

So, for $a < \frac{\hbar^2}{2mV_0} \Rightarrow$ no bound states

$a > \frac{\hbar^2}{2mV_0} \Rightarrow$ one bound state

The radial part of the wave function is

$$R = \frac{u(r)}{r} = \begin{cases} A \frac{\sinh \kappa r}{r}, & 0 < r < a \\ C \frac{e^{-\kappa r}}{r}, & r > a \end{cases}$$

$$\int_0^\infty |R|^2 r^2 dr = 1 = A^2 \int_0^a \sinh^2 \kappa r \, dr + C^2 \int_a^\infty e^{-2\kappa r} dr =$$

$$= A^2\left[\frac{1}{4\kappa}\sinh 2\kappa a - \frac{a}{2}\right] + C^2\,\frac{e^{-2\kappa a}}{2\kappa} \underset{\uparrow}{=}$$

$$= A^2\left[\frac{1}{4\kappa}\sinh 2\kappa a - \frac{a}{2} + \frac{\sinh^2 \kappa a}{2\kappa}\right] = 1 \qquad Ce^{-\kappa a} = A\sinh \kappa a$$

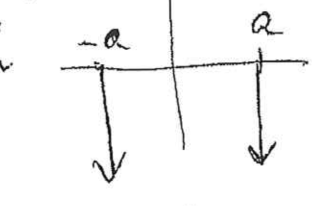
$$\Downarrow$$

$$A = \frac{2\sqrt{\kappa}}{\sqrt{\sinh 2\kappa a + 2\sinh^2 \kappa a - 2\kappa a}}$$

Then, $\psi_{n00}(\vec{r}) = \frac{1}{\sqrt{4\pi}} R_{n0}(r) =$

$$= \sqrt{\frac{\kappa}{\pi}}\,\frac{1}{\sqrt{\sinh 2\kappa a + 2\sinh^2 \kappa a - 2\kappa a}} \begin{cases} \dfrac{\sinh \kappa r}{r}, & 0<r<a \\ \dfrac{e^{-\kappa r}}{r}, & r>a \end{cases}$$

Note that $u(r)$ for $0<r<a$ and $r>a$ has the same form as $\psi_{odd}(x)$ in a 1D problem with



symmetric double-delta potential (see HW#13 of Phys 651). The condition for bound states is also the same as that for ψ_{odd} case in 1D. This is not surprising, taking into account that the 3D problem for s-states is essentially the same as 1D symmetric δ-potential for odd parity.

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~~Solutions of HW #8~~

Problem #1

Consider $(\hat{\vec{\sigma}}\cdot\vec{a})(\hat{\vec{\sigma}}\cdot\vec{b}) = (\hat{\sigma}_x a_x + \hat{\sigma}_y a_y + \hat{\sigma}_z a_z)\cdot$

$\cdot(\hat{\sigma}_x b_x + \hat{\sigma}_y b_y + \hat{\sigma}_z b_z) = \hat{\sigma}_x^2 a_x b_x + \hat{\sigma}_y^2 a_y b_y +$

$+\hat{\sigma}_z^2 a_z b_z + \hat{\sigma}_x\hat{\sigma}_y a_x b_y + \hat{\sigma}_y \sigma_x a_y b_x + \hat{\sigma}_x\hat{\sigma}_z a_x b_z +$

$+\hat{\sigma}_z \sigma_x a_z b_x + \hat{\sigma}_y\hat{\sigma}_z a_y b_z + \hat{\sigma}_z\hat{\sigma}_y a_z b_y \underset{\uparrow}{=} (\vec{a}\cdot\vec{b}) +$

Properties of the Pauli matrices $\Rightarrow$
- $\sigma_i^2 = I$, $i = x, y, z$; $\sum_i a_i b_i = \vec{a}\cdot\vec{b}$
- $\sigma_i\sigma_j + \sigma_j\sigma_i = 0$ for $i \neq j$

$+\hat{\sigma}_x\hat{\sigma}_y (a_x b_y - a_y b_x) +$

$+\hat{\sigma}_x\hat{\sigma}_z (a_x b_z - a_z b_x) + \hat{\sigma}_y\hat{\sigma}_z (a_y b_z - a_z b_y) =$

$\underset{\uparrow}{=} (\vec{a}\cdot\vec{b}) + i\hat{\sigma}_z(a_x b_y - a_y b_x) + i\hat{\sigma}_y(a_z b_x - a_x b_z) +$

$[\sigma_i, \sigma_j] = 2i\sigma_k \Rightarrow \sigma_i\sigma_j - \sigma_j\sigma_i = 2\sigma_i\sigma_j = 2i\sigma_k \Rightarrow$
(ijk - cyclic)
$\underline{\sigma_i\sigma_j = i\sigma_k}$

$+ i\hat{\sigma}_x(a_y b_z - a_z b_y) = \underline{(\vec{a}\cdot\vec{b}) + i\hat{\vec{\sigma}}\cdot(\vec{a}\times\vec{b})}$

Problem #2

(a) $e^{-i\alpha \sigma_x} \underset{\uparrow}{=} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \alpha^n (\sigma_x)^n =$

$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

$= \sum_{n=0}^{\infty} \frac{(-i)^{2n}}{(2n)!} \alpha^{2n} (\sigma_x)^{2n} + \sum_{n=0}^{\infty} \frac{(-i)^{2n+1}}{(2n+1)!} \alpha^{2n+1} (\sigma_x)^{2n+1} =$

$\underset{\uparrow}{=} I \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \alpha^{2n} - i\sigma_x \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} \alpha^{2n+1} =$

$(\sigma_x)^2 = 1 \Rightarrow (\sigma_x)^{2n} = \underset{\uparrow}{1} \equiv I$

$(\sigma_x)^{2n+1} = \sigma_x$ unit matrix

$= \underline{I \cos\alpha - i\sigma_x \sin\alpha}$

(b) $e^{i\alpha\sigma_x} \sigma_z e^{-i\alpha\sigma_x} \underset{\text{use (a)}}{=} (\cos\alpha + i\sigma_x \sin\alpha)\sigma_z \cdot$

$\cdot (\cos\alpha - i\sigma_x \sin\alpha) = \sigma_z \cos^2\alpha + \sigma_x \overbrace{\sigma_z \sigma_x}^{= -\sigma_x\sigma_z} \sin^2\alpha +$

$+ i \underbrace{[\sigma_x, \sigma_z]}_{= -2i\sigma_y} \sin\alpha\cos\alpha = \sigma_z \cos^2\alpha - \underbrace{\sigma_x^2}_{=1} \sigma_z \sin^2\alpha +$

$+ 2\sigma_y \sin\alpha\cos\alpha = \underline{\sigma_z \cos 2\alpha + \sigma_y \sin 2\alpha}$