PC 2232 : Assignment 2

1) a) Given :- $V(x) = -\frac{\hbar^2 a}{m} \operatorname{sech}^2(ax)$

i) Show that $\psi(x) = A \operatorname{sech}(ax)$ is a bound state

1D. SE.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - \frac{\hbar^2 a^2}{m}\operatorname{sech}^2(ax)\,\psi(x) = E\,\psi(x).$$

$\therefore$ consider LHS,

$$\frac{d}{dx} A\operatorname{sech}(ax) = \frac{d}{dx} A\frac{1}{\cosh(ax)} = \left[\frac{\sinh(ax)}{\cosh^2(ax)}\right][-aA] = -aA\tanh(ax)\operatorname{sech}(ax).$$

$$\therefore \frac{d^2}{dx^2} A\operatorname{sech}(ax) = \frac{d}{dx}\left[-aA\tanh(ax)\operatorname{sech}(ax)\right]$$

$$= -aA\left[\frac{d}{dx}(\tanh(ax))\operatorname{sech}(ax) + \tanh(ax)\frac{d}{dx}\frac{1}{\cosh(ax)}\right]$$

$$\text{But } \frac{d}{dx}[\tanh(ax)] = \frac{d}{dx}\left[\frac{\sinh(ax)}{\cosh(ax)}\right]$$

$$= a - \frac{a\sinh^2(ax)}{\cosh^2(ax)}$$

$$= a - a\tan^2(ax)$$

$$= a\operatorname{sech}^2(ax).$$

$$\therefore \frac{d^2}{dx^2} A\operatorname{sech}(ax) = -a^2 A\left[\operatorname{sech}^3(ax) - \tanh^2(ax)\operatorname{sech}(ax)\right]$$

$$= -a^2 A\operatorname{sech}^3(ax)\left[1 - \sinh^2(ax)\right].$$

$$\therefore -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - \frac{\hbar^2 a}{m}A\operatorname{sech}^3(ax) = \frac{\hbar^2 a^2}{2m}A\operatorname{sech}^3(ax)\left[1 - \sinh^2(ax) - 2\right].$$

$$= -\frac{\hbar^2 a^2}{2m}A\operatorname{sech}^3(ax)\left[1 + \sinh^2(ax)\right]$$

$$= -\frac{\hbar^2 a^2}{2m}A\operatorname{sech}^3(ax)\cosh^2(ax)]$$

$$= -\frac{\hbar^2 a^2}{2m}A\operatorname{sech}(ax)$$

$$= -\frac{\hbar^2 a^2}{2m}\psi_1(x).$$

$$\therefore E = -\frac{\hbar^2 a^2}{2m} \quad \alpha \quad \Rightarrow \text{proven}$$

Give them : $\tanh(x) = \dfrac{\sinh(x)}{\cosh(x)}$ | $\operatorname{sech}(x) = \dfrac{1}{\cosh(x)}$

$\frac{d}{dx}\sinh(x) = \cosh(x)$ | $\cosh^2(x) = 1 + \sinh^2(x).$

$\frac{d}{dx}\cosh(x) = \sinh(x)$

ii) Show that $\psi_k(x) = B\left(\frac{ik - a\tanh[ax]}{ik+a}\right)e^{ikx}$ is a free particle solution.

↳ is it called free particle sol?

To simplify the math, consider the terms seperately

$$\frac{d}{dx}[ike^{ikx}] = -k^2 e^{ikx} \Rightarrow \frac{d^2}{dx^2}[ike^{ikx}] = -ik^3 e^{ikx}.$$

$$\frac{d}{dx}\left[a\tanh[ax]\, e^{ikx}\right] = a^2\operatorname{sech}^2(ax)\,e^{ikx} + ika\tanh(ax)\,e^{ikx}.$$

$$\frac{d^2}{dx^2}[-a\tanh(ax)\, e^{ikx}] = -ika^2\operatorname{sech}^2(ax)e^{ikx} + k^2 a\tanh(ax)e^{ikx}$$

$$+2a^3\operatorname{sech}^2(ax)\tan(ax)e^{ikx} - ika^2\operatorname{sech}^2(ax)e^{ikx}.$$

$$\therefore -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_k(x) = \frac{-\hbar^2}{2m}\frac{B}{ik+a}\left[-ik^3 - 2ika^2\operatorname{sech}^2(ax) + k^2 a\tanh(ax) + 2a^3\operatorname{sech}^2(ax)\tanh(ax)\right]e^{ikx}$$

∴ the other term of the LHS :-

$$V(x)\psi_k(x) = \frac{-\hbar^2}{2m}\frac{B}{ik+a}\left[2a^2\operatorname{sech}^2(ax)[ik - a\tanh[ax]]\right]e^{ikx}$$

∴ LHS reduce to :
$$\frac{-\hbar^2}{2m}\frac{B}{ik+a}[-ik^3 + k^2 a\tanh(ax)]$$
$$= \frac{\hbar^2 k^2}{2m}\frac{B}{ik+a}[ik - a\tanh(ax)]$$
$$= \frac{\hbar^2 k^2}{2m}\psi_k(x).$$

iii) Given that: $\tanh x = \frac{1+e^{-2x}}{1-e^{-2x}}$.

Show that for a free particle incident on this potential, there is no reflected wave cond. $\psi(x)$.

$$\psi(x) = B\left(\frac{ik + a\tanh[ax]}{ik+a}\right).e^{ikx}$$

∴ when $x \to \infty$,

$$\lim_{x\to\infty}\tanh[ax] = \frac{1+e^{-2\infty}}{1-e^{-2\infty}} = 1.$$

$$\therefore \psi(x\to\infty) = \frac{B(ik-1)}{ik+a}.e^{ikx}$$

when $x \to -\infty$,

$$\lim_{x\to\infty}\tanh[ax] = \frac{e^{2x}+1}{e^{2x}-1} = -1$$

$$\therefore \psi(x\to\infty) = \frac{B(ik+1)}{ik+a}e^{ikx}$$

Note that $x\to\infty$ does not really affect e^{ikx}

e^{-ikx}

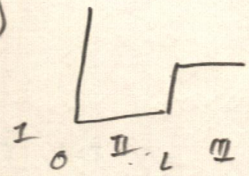
∴ throughout all of x, if the incident particle is travelling right, it will continue travelling right

∴ there is no reflection.

b) $U(x) = \infty \quad x \le 0$

$-\frac{32\hbar^2\pi^2}{mL^2} \quad 0 \le x \le a$

$0 \quad x > a$.

① 

i) How many bound state are there?

=> Bound states -> $E < 0$.

$\because$ the minimum E possible is $-\frac{32\hbar^2\pi^2}{mL^2}$ (no E can exist below this potential,

$\therefore$ The highest E for bound state will have a magnitude of $\frac{32\hbar^2\pi^2}{mL^2}$

Recall for ∞-sq well, $E = \frac{n^2h^2}{8mL^2}$.

$\therefore$ if this was an infinite sq well, $E' = 32\frac{\hbar^2\pi^2}{mL^2} = 32\frac{h^2}{4mL^2} = 64\frac{h^2}{8mL^2}$

$\therefore n = 4$.

$\because$ E of finite sq well < E of ∞ sq well, (but only by a little),

highest bound state here would be $n = 8$

ii) Solving for this potential for both cases.

Region I : 0

Region II : $\psi(x) = A\sin kx + \cancel{B\cos kx}$ -> Bound. cond. @ 0

Region III : $\psi(x) = \cancel{Ce^{\alpha x}} + De^{-\alpha x}$.

because it does not blow up

$\therefore A\sin kL = De^{-\alpha L}$

$kA\cos kL = \alpha Ce^{\alpha L}$.

} $E < 0$.

Region I : 0

Region II : $\psi(x) = A\sin kx + \cancel{B\cos kx}$

Region III : $\psi(x) = Fe^{ikx} + Ge^{-ikx}$

$A\sin kL = Fe^{ikL}$

$kA\cos kL = ikFe^{ikL}$

} $E > 0$.

we cannot throw away Ge^{-ikx} term $\because$ since region I has $U \to \infty$, particle must be incident from region III.

iii) Briefly discuss how to find energies of the bound states.

- Bound states only occur for $E < 0$.
- W/ the boundary cond. eq. obtain an eq. that relates k to α.
- $\because$ both these are related to E we can reexpress tt eq in terms of E
- Plot a graph of LHS w.r.t E & R.H.S w.r.t E. & find intersections.

2 a) $F(E) = \frac{N_n}{d_n} = \frac{1}{e^{\frac{E_n - E_F}{k_B T}} + 1}$

i) when $T = 0$, $E_n < E_F$

$$f(E) = \frac{1}{e^{-\infty} + 1} = 1$$

$T = 0$, $E_n > E_F$

$$f(E) = \frac{1}{e^{+\infty} + 1} = 0$$

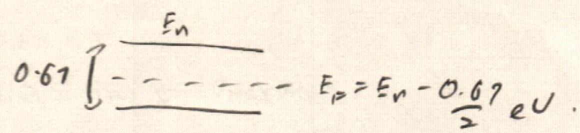
ii) • Fermi E is the energy value that, at 0 T, the highest E particle has.

Better phrased version: At 0 K, the highest E particle has the energy value : E_F.

• Fermi dirac distribution is basically the probability that a certain energy level E_n is filled at a certain temperature T.

b) Band gap = 0.67 eV.

i) $T_1 = 250k$, $T_2 = 300k$ and $T_3 = 350k$



Probability that state at the bottom of conduction band is occupied?

$$\therefore f(E_n) = \frac{1}{e^{0.385}}$$