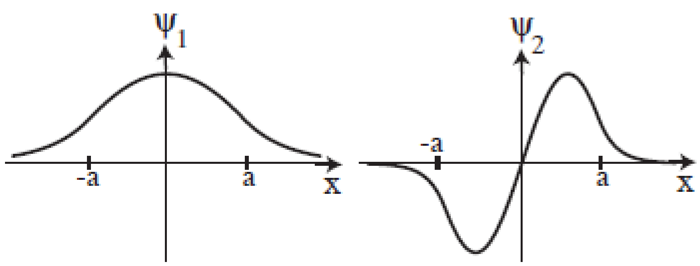
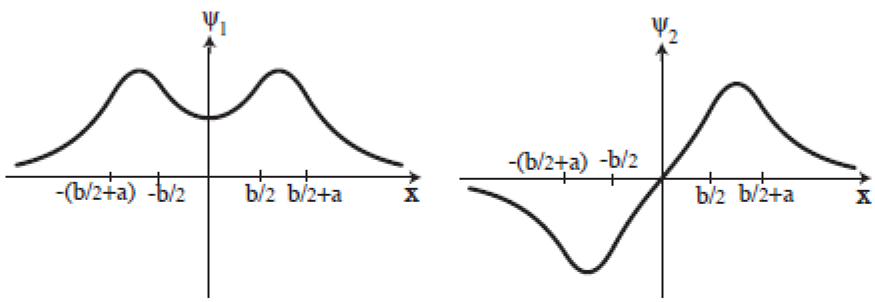
یک.

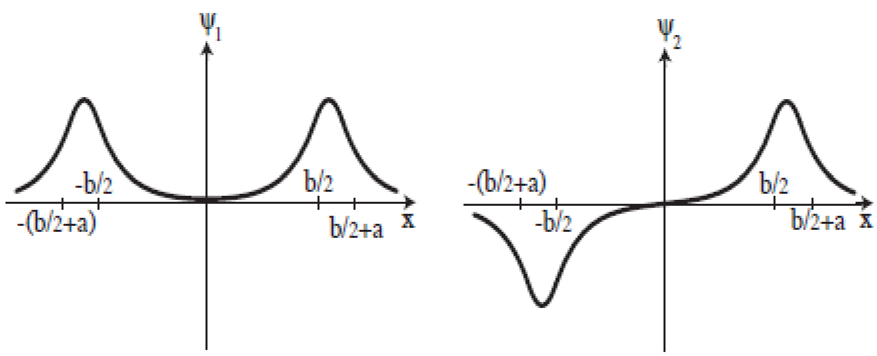
b = distance between wells, a= width of the wells.
(i) As b goes to 0, we get an single finite square well which has exponential decay outside of the well and sinusoidal behavior inside of it. (Cosine for ψ_1 and Sine for ψ_2). ψ_1 *has no nodes and* ψ_2 *has two*.
(b) The ground state is an even one, which has exponential decay outside of the well and hyperbolic cosine behavior inside of it. The first excited state is odd with a hyperbolic sine in the barrier.
ψ_1 *has no nodes and* ψ_2 *has one*.

Diagrams: (copied out of Griffiths' book, I ran out of time before I could draw it with matlab. :D)





(iii) For b >> a, it is the same as (ii), but the wave function is very small in the barrier region. Essentially two *isolated* finite square wells; ψ_1 *and* ψ_2 are degenerate (in energy). They are even and odd linear combinations of the ground states of the two separate wells.



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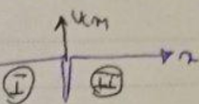
For simplicity, we assume that the delta potential is placed at $x=0$, — (2) الف

i.e. $V(x) = \delta(x)$, So our environment will be: 

1. Since both (I) and (II) go to infinity at some point and we don't want them to blow up, the wavefunction will be:
$$\psi(x) = \begin{cases} Ae^{Kx} & -\infty < x < 0 \quad \text{(I)} \\ Be^{-Kx} & 0 < x < \infty \quad \text{(II)} \end{cases}$$

Now, given the continuity condition of $\psi(x)$, $\lim_{x\to 0^+} \psi(x) = \lim_{x \to 0^-} \psi(x)$. Therefore,
$$Ae^{Kx_0} = Be^{-Kx_0} \Rightarrow A = B$$

2. Since our wavefunction should be normalized, $\int_{\text{I}} \psi\psi^* dx + \int_{\text{II}} \psi\psi^* dx = 1$ should be true. $\rightarrow$
$$A^2\int_{-\infty}^{0} e^{2Kx} dx + A^2\int_{0}^{+\infty} e^{-2Kx} dx = 1 = A^2\left(\left[\frac{e^{2Kx}}{2K}\right]_{-\infty}^{0} + \left[\frac{e^{-2Kx}}{-2K}\right]_{0}^{+\infty}\right)$$
$$= A^2\left(\frac{1}{2K} + \frac{1}{2K}\right) = \frac{A^2}{K} = 1 \Rightarrow A = \sqrt{K}$$

3. Since ψ' should also be continuous, the TIS says $\psi''(x) = \frac{-2m}{\hbar^2}(E + \underset{\text{well depth}}{w_0}\delta(x))\psi(x)$

Assuming the well's width to be 2ϵ, we integrate both sides of the equation around zero
$$\int_{-\epsilon}^{+\epsilon} \psi''(x) dx = \frac{-2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon}(E + w_0\delta(x))\psi(x) dx = \psi'(\epsilon) - \psi'(-\epsilon) = \frac{-2m}{\hbar^2}\left(2\epsilon E \psi(x)\Big]_{-\epsilon}^{\epsilon} + w_0\psi(0)\right)$$
$$\Rightarrow -KAe^{-K\epsilon} - KAe^{-K\epsilon} = \frac{-2m}{\hbar^2}w_0\psi(0) \xrightarrow{\lim\limits_{\epsilon \to 0}} -2KA = \frac{-2m}{\hbar^2}w_0 A$$
$$\Rightarrow K = \frac{mw_0}{\hbar^2}$$. As we know, K also equals $\sqrt{\frac{-2mE}{\hbar^2}}$, therefore
$$\left(\frac{mw_0}{\hbar^2}\right)^2 = \frac{-2mE}{\hbar^2} \Rightarrow E = -\frac{w_0^2 m}{2\hbar^2}$$

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Knowing that $\psi'' = -K^2\psi$, the odd solutions are of form $A_2 \sin Kx$ ③ ولی

(A_2 is for normalization). So the general solution will be : $\psi_{odd}(x) = \begin{cases} -A_1 e^{Rx} & -\infty < x < -a \\ A_2 \sin(Kx) & -a < x < a \\ A_1 e^{-Rx} & a < x < \infty \end{cases}$

Since ψ' and ψ should be continuous at $x = a$, we write :

$A_2 \sin Ka = A_1 e^{-Ra} \Rightarrow \sin Ka = A' e^{-Rx}$ $\left(A' = \frac{A_1}{A_2}\right)$ for ψ and

for ψ': $K a \cos Ka = -A' R e^{-Ra}$. Dividing the two equations, $\frac{\text{for } \psi'}{\text{for } \psi} = -K \cot Ka = R$

to make both sides dimensionless and having defined $\zeta = Ka$ and $\eta = Ra$,

we multiply by a to get $\Rightarrow$ $\eta = -\zeta \cot \zeta$ where $\eta^2 + \zeta^2 = \frac{2m}{\hbar^2} a^2 V$

الف) اولین eigenstate یک تابع زوج است، جواب بین eigenstate های زوج و فرد جابجا می‌شوند. از E_2 به بعد جواب‌های فرد وجود دارند؛ به علت شکل $\cot$، همیشه نقطه تلاقی که η هم مثبت باشد احتمالا نداریم پس همیشه bound state نداریم.

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ب)

$$1 = 2\int_0^{\infty} |\psi|^2 dx = 2\left(A_2^2 \int_0^a \sin^2 kx\, dx + A_1^2 \int_a^{\infty} e^{-2Rx} dx\right)$$

$$= 2\left(\frac{A_2^2}{2}\left(x - \frac{1}{2k}\sin(2kx)\right)\Big|_0^a + A_1^2\left(\frac{-1}{2R} e^{-2Rx}\right)\Big|_a^{\infty}\right) = 2\Big(\frac{A_2^2}{2}\left(a - \frac{\sin 2ka}{2k}\right)$$

$$+ A_1^2 \frac{e^{-2Ra}}{2a}\Big)$$, Knowing $A_1 = A_2 \sin ka\, e^{+Ra}$, we get,

$$1 = A_2^2\left(a - \frac{\sin 2ka}{2k} + \frac{\sin^2 ka}{R}\right)$$, also, $R = -K\cot ka \implies$

$$1 = A_2^2\left(a - \frac{\sin 2ka}{2k} + \frac{\sin^3 ka}{-K\cos ka}\right) = A_2^2\left(a - \frac{2\sin ka\cos ka}{2k} + \frac{\sin^3 ka}{-K\cos ka}\right)$$

$$= A_2^2\left(a - \frac{\sin ka}{K\cos ka}\left(\cos^2 ka + \sin^2 ka\right)\right) = A_2^2\left(a - \frac{\tan ka}{K}\right) = A_2^2\left(a - \frac{1}{K\cot ka}\right)$$

$$\implies A_2^2\left(a - \frac{1}{R}\right) = 1 \implies A_2 = \sqrt{\frac{1}{a - \frac{1}{R}}}\ ,\ A_1 = \sqrt{\frac{1}{a - \frac{1}{R}}} \times \sin ka\, e^{+Ra}$$

پ)

For scattering states ($E > 0$), where $V(x) = 0$, we have,

$\psi(x) = Ae^{iRx} + Be^{-iRx}$ (for $x < -a$) with $R = \frac{\sqrt{2mE}}{\hbar}$, Inside the well, we have,

$V(x) = -V_0$ and $\psi(x) = C\sin(Kx) + D\cos(Kx)$ (General Solution)

with $K = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ $(-a < x < a)$ and $\psi(x) = Fe^{iRx}$ (Arriving or leaving wave)

Continuity for ψ for $x = -a$, we have, $Ae^{-iRa} + Be^{iRa} = -C\sin(Ka) + D\cos(Ka)$

For ψ', we have, (at $-a$) $iK\left[Ae^{-iRa} - Be^{iRa}\right] = K\left(C\cos(Ka) + D\sin(Ka)\right)$

For ψ at $x = a \rightarrow C\sin(Ka) + D\cos(Ka) = Fe^{iRa}$

For ψ' at $x = a \rightarrow K\left[C\cos(Ka) - D\sin(Ka)\right] = iKFe^{iRa}$

$$\implies B = i\frac{\sin(2Ka)}{2KR}\left(K^2 - R^2\right)F\ ,\ F = \frac{e^{-2iRa} A}{\cos(2Ka) - i\frac{(K^2+R^2)}{2KR}\sin(2Ka)}$$

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T (Transmission Coefficient) = $\frac{F^2}{A^2}$, $T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$

with the sine = 0, which is when $\frac{2a}{\hbar}\sqrt{2m(E_n+V_0)} = n\pi$

$T = 1$. (n is any integer)

Perfect Transmission $\Longrightarrow$ $E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$ $\Longrightarrow$ Exactly infinite square well energies.

ت) با فرض z_0 کوچک، تعداد bound state ها کم می‌شود تا جایی که برای $z_0 \ll \pi/2$ فقط یکی باقی می‌ماند! اما همیشه این یکی هست، چرا که به صورت delta well درمی‌آید که آن نیز همیشه یک حالت مقید دارد.

چهار.

سوال ④

الف) مولکول‌های حلقوی مانند نفتالین، چرا که اصولاً ترکیبات ما به ساخت اوربیتال‌های π مولکولی علاقه دارند که این اوربیتال‌ها گذرگاه خوبی برای الکترون‌ها هستند.

ب) زیرا هر PO_3 جای عبور الکترون را می‌گیرد.

پ) صفحه‌ی اول ایجاد برهم‌کنش‌ها فاصله‌ی پتانسیل بیرونی و درونی B.V را زیاد می‌کند (عبور الکترون سخت است)، و صفحه‌ی دوم لایه‌های آلی احتمال رد شدن الکترون‌ها را زیاد می‌کند، پس فاصله‌ی ترازهای انرژی کاهش می‌یابد. (همچنین آنتروپی بیشتری خواهیم داشت)، الکترون‌ها راحت‌تر جابجا می‌شوند.