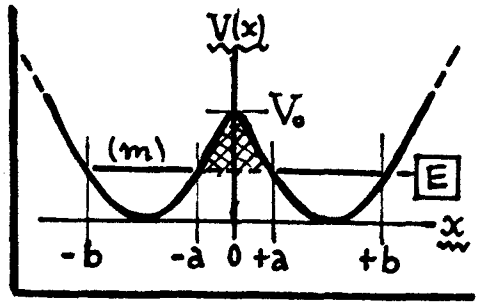
ϕ506 Problems



(43) [30 pts]. A symmetric potential $V(x)$ consists of two wells separated by a barrier of height V_0 as shown. A particle of mass m and energy $E < V_0$ is initially placed in one well. m can tunnel thru the barrier ($-a \leqslant x \leqslant a$), coupling the wells.

(A) Use the WKB method to show that the condition determining the system eigenenergies is:

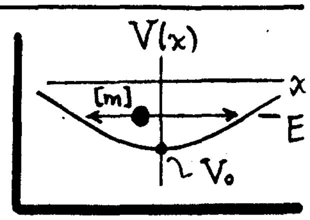
$$\boxed{\operatorname{ctn} \phi = \pm \tfrac{1}{2} e^{-\theta}} \int^{w/} \begin{array}{l} \phi = \int_a^b k(x)\,dx,\ k(x) = \sqrt{(2m/\hbar^2)[E - V(x)]}\ ; \\ \theta = \int_{-a}^{+a} \kappa(x)\,dx,\ \kappa(x) = \sqrt{(2m/\hbar^2)[V(x) - E]}\ . \end{array}$$

‖ Please use this notation.

HINT: establish this condition by starting out with $\psi_1 = (A/\sqrt{\kappa})\, e^{-\int_x^{-b} \kappa dx'}$ in the region $x < -b$, and connecting $\psi_1 \to \psi_2 \to \psi_3 \to \psi_4 \to \psi_5$ in $x > b$. Make sure ψ_5 doesn't diverge.

(B) For $V_0 \gg E$, $\theta \to$ "large", and the condition of part (A) is: $\phi \simeq (n + \frac{1}{2})\pi \pm \frac{1}{2} e^{-\theta}$. Let $E_n^{(0)}$ be the n^{th} energy level of either well alone (w/o barrier). Show that the presence of a penetrable barrier perturbs $E_n^{(0)}$ by an amount which is approximated to lowest order by: $\Delta E_n = \pm (\hbar \omega_n / 2\pi) \exp\left\{-\int_{-a}^{+a} \sqrt{(2m/\hbar^2)[V(x) - E_n^{(0)}]}\, dx\right\}$. Here ω is the classical natural frequency of motion in the well, defined by: natural period $= \frac{2\pi}{\omega} = 2 \int_a^b dx / [p(x)/m]$.

(C) Suppose the well is: $V(x) = \frac{1}{2} m \omega^2 (|x| - x_0)^2$ [double SHO well]. Calculate the splitting ΔE_0 (in the $n=0$ ground state) explicitly in terms of ω & $V_0 = \frac{1}{2} m \omega^2 x_0^2$.

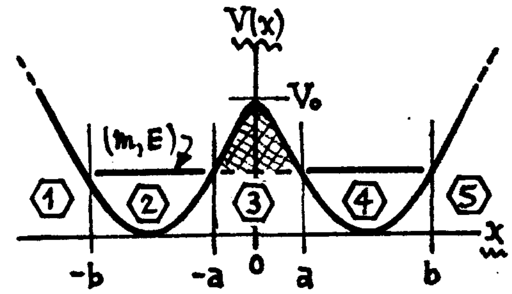


(44) Use the Bohr-Sommerfeld quantization rule to find the allowed energies for a particle of mass m in a potential well $V(x) = -V_0 \operatorname{sech}^2(x/a)$, w/ V_0 & a are (+)ve consts. Then, find the number of energy levels in this well. Finally, state the condition on V_0 & a under which your WKB estimates are expected to be reliable.

---

(45) Write a letter home, telling your friends and relatives what an enjoyable time you have had in ϕ506. Be sure to mention how much you have learned, the extreme charm and erudition of your instructor, and how reverential you feel about $\hbar$. Don't forget to ask for a nice holiday gift (for instructor, too!)

(43) [30 pts]. Double-well analysis via WKB method.



$k(x) = \sqrt{\frac{2m}{\hbar^2}[E - V(x)]}$, in ② & ④;

$\kappa(x) = \sqrt{\frac{2m}{\hbar^2}[V(x) - E]}$, in ①, ③, ⑤.

(A) 1) Per hint, start with WKB form in region ① $(x < (-)b)$:

$$\rightarrow \psi_1 = \frac{A}{\sqrt{\kappa}} e^{-\int_x^{-b} \kappa(x')dx'}, \text{ for } x < -b. \qquad (1)$$

By the connection formulas [Eqs. (53) & (54), p. 18 of WKB Notes], $\psi_1 \rightarrow \psi_2 = \frac{2A}{\sqrt{k}} \sin\left(\int_{-b}^{x} k(x')dx' + \frac{\pi}{4}\right)$ in region ②. Refer the integral in ψ_2 to the RH edge $x = -a$ (via $\int_{-b}^{x} = \int_{-b}^{-a} - \int_{x}^{-a}$; this picks up a phase: $\underline{\phi = \int_{-b}^{-a} k(x)dx = \int_a^b k(x)dx}$). So:

$$\rightarrow \psi_2 = \frac{2A}{\sqrt{k}} \left\{ (\cos\phi) \cos\left(\int_x^{-a} k\,dx' + \frac{\pi}{4}\right) + (\sin\phi) \sin\left(\int_x^{-a} k\,dx' + \frac{\pi}{4}\right) \right\}. \qquad (2)$$

2) When $\psi_2 \rightarrow \psi_3$ in region ③, the $\cos(\;) \rightarrow e^{+\int_{-a}^{x} \kappa\,dx'}$ by the connection formulas, while $\sin(\;) \rightarrow \frac{1}{2} e^{-\int_{-a}^{x} \kappa\,dx'}$. Refer the new integrals to the RH edge of ③; this generates another "phase": $\underline{\theta = \int_{-a}^{+a} \kappa(x)dx}$. Result is:

$$\rightarrow \psi_3 = \frac{2A}{\sqrt{\kappa}} (e^{\theta} \cos\phi)\, e^{-\int_x^a \kappa\,dx'} + \frac{A}{\sqrt{\kappa}} (e^{-\theta} \sin\phi)\, e^{+\int_x^a \kappa\,dx'}. \qquad (3)$$

Continuing (literally), the $e^{-} \rightarrow 2\sin\left(\int_a^x k\,dx' + \frac{\pi}{4}\right)$ in going from ③ to ④, while the $e^{+} \rightarrow \cos\left(\int_a^x k\,dx' + \frac{\pi}{4}\right)$. Again, shift reference points in the integrals, via $\int_a^x k\,dx' = \int_a^b k\,dx' - \int_x^b k\,dx'$. We again pick up: $\phi = \int_a^b k\,dx$, as phase. Then:

$$\psi_4 = \frac{4A}{\sqrt{k}} (e^{\theta} \cos\phi) \cos\left[\phi - \left(\int_x^b k\,dx' + \frac{\pi}{4}\right)\right] - \frac{A}{\sqrt{k}} (e^{-\theta} \sin\phi) \sin\left[\phi - \left(\int_x^b k\,dx' + \frac{\pi}{4}\right)\right]$$

$$\xrightarrow{\text{or}} \psi_4 = \frac{A}{\sqrt{k}} \left\{ \left[4e^{\theta} \cos^2\phi - e^{-\theta} \sin^2\phi\right] \cos\left(\int_x^b k\,dx' + \frac{\pi}{4}\right) + \right.$$

$$\left. + \left[(4e^{\theta} + e^{-\theta}) \sin\phi \cos\phi\right] \sin\left(\int_x^b k\,dx' + \frac{\pi}{4}\right) \right\}. \qquad (4)$$

3) Finally, continue $\psi_4 \rightarrow \psi_5$. In Eq. (4), the $\cos(\;) \rightarrow e^{+\int_x^b \kappa\,dx'}$, and the $\sin(\;) \rightarrow 2\,e^{-\int_x^b \kappa\,dx'}$. This specifies the WKB wavefcn in region ⑤ as...

$$\rightarrow \psi_5 = \frac{A}{\sqrt{\kappa}} \underbrace{[4e^{\theta}\cos^2\phi - e^{-\theta}\sin^2\phi]}_{C} e^{+\int_b^x \kappa dx'} + \\ + \frac{2A}{\sqrt{\kappa}}[(4e^{\theta}+e^{-\theta})\sin\phi\cos\phi]\, e^{-\int_b^x \kappa dx'}. \quad (5)$$

Now ψ_5 is in the classically inaccessible region ⑤, so it must <u>decrease</u> exponentially for $x > b$. This requires that the coefficient $C \equiv 0$, so -- as required...

$$\left[\!\!\left[\begin{array}{l} C \equiv 0 \Rightarrow 4e^{\theta}\cos^2\phi = e^{-\theta}\sin^2\phi, \text{ or } \boxed{\operatorname{ctn}\phi = \pm\tfrac{1}{2}e^{-\theta}}, \\ \text{where: } \underline{\phi = \int_a^b k(x)\,dx}, \ \underline{\theta = \int_{-a}^{+a}\kappa(x)\,dx}. \end{array} \right] \right\} (6)$$

---

4) For $\theta \to$ "large", $e^{-\theta} \to$ small, and the quantum condition of Eq. (6) is (approx'ly):

(B) $$\left[\!\!\left[\phi = \int_a^b k(x)\,dx \simeq (n+\tfrac{1}{2})\pi \pm \tfrac{1}{2}e^{-\theta} \right]\!\!\right]. \quad (7)$$

Now if $E_n^{(0)}$ are the energy levels of either well separately, then

$$\rightarrow \int_a^b k_n^{(0)}(x)\,dx = (n+\tfrac{1}{2})\pi, \text{ w/ } k_n^{(0)}(x) = \sqrt{(2m/\hbar^2)[E_n^{(0)} - V(x)]}, \quad (8)$$

by the Bohr-Sommerfeld rule. The term in $e^{-\theta}$ in Eq. (7) perturbs the energies: $E_n^{(0)} \to E_n = E_n^{(0)} + \Delta E_n$; so also $k_n^{(0)}(x) \to k_n(x) = \sqrt{(2m/\hbar^2)[E_n - V(x)]}$. Then for small ΔE_n, $k_n(x)$ can be expanded as

$$\rightarrow k_n(x) = \left(\frac{2m}{\hbar^2}[E_n^{(0)} + \Delta E_n - V(x)]\right)^{\frac{1}{2}} \simeq k_n^{(0)}(x) + \frac{m}{\hbar}\Delta E_n \Big/ \sqrt{2m[E_n^{(0)} - V(x)]}. \quad (9)$$

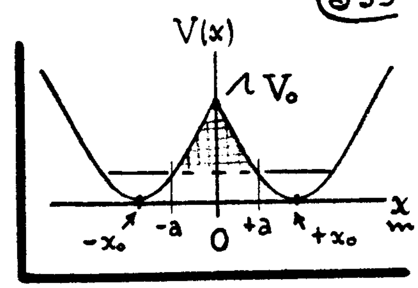
Identify: $\int_a^b k_n(x)\,dx = (n+\tfrac{1}{2})\pi \pm \tfrac{1}{2}e^{-\theta}$, by Eq. (7). Then, with (8), (9) yields

$$\rightarrow \frac{m}{\hbar}\Delta E_n \int_a^b dx/p_n^{(0)}(x) \simeq \pm\tfrac{1}{2}e^{-\theta}, \text{ w/ } p_n^{(0)}(x) = \sqrt{2m[E_n^{(0)} - V(x)]}. \quad (10)$$

On the LHS here: $m\int_a^b dx/p_n^{(0)}(x) = \tfrac{1}{2}(2\pi/\omega_n)$, w/ ω_n the natural frequency in the (unperturbed) state. So Eq. (10) gives the energy splitting due to tunneling:

$$\boxed{\Delta E_n \simeq \pm(\hbar\omega_n/2\pi)\exp\left[(-)\int_{-a}^{a}\kappa(x)\,dx\right]}, \ \kappa(x) = \sqrt{(2m/\hbar^2)[V(x) - E_n^{(0)}]}. \quad (11)$$

φ506 Solutions



(C)

5) We calculate the total splitting in the $n=0$ ground state, where the (unperturbed) energy is $E_0^{(0)} = \frac{1}{2}\hbar\omega$, and the natural frequency is ω. According to Eq. (11), this is:

$$\rightarrow \Delta E_0 = (\hbar\omega/\pi)\exp[-J], \text{ w/ } J = \int_{-a}^{a}\sqrt{(2m/\hbar^2)[V(x)-E_0^{(0)}]}\,dx. \tag{12}$$

Put in: $V(x) = \frac{1}{2}m\omega^2(|x|-x_0)^2$, which is symmetric about $x=0$. Then...

$$\rightarrow J = 2\int_0^a \left\{\frac{2m}{\hbar^2}\left[\frac{1}{2}m\omega^2(x-x_0)^2 - E_0^{(0)}\right]\right\}^{1/2} dx$$

$$= 2\sqrt{2mE_0^{(0)}/\hbar^2}\int_0^a \left\{\frac{1}{2}\frac{m\omega^2}{E_0^{(0)}}(x-x_0)^2 - 1\right\}^{1/2} dx. \tag{13}$$

Let $\xi^2 = (m\omega^2/2E_0^{(0)})(x_0-x)^2$, so: $dx = (-)\sqrt{2E_0^{(0)}/m\omega^2}\,d\xi$. The integral is...

$$\rightarrow J = 2\sqrt{\frac{2mE_0^{(0)}}{\hbar^2}\cdot\frac{2E_0^{(0)}}{m\omega^2}}\int_{x=a}^{x=0}\{\xi^2-1\}^{1/2}d\xi. \tag{14}$$

Out in front here, the $\sqrt{\ } = 2E_0^{(0)}/\hbar\omega = 1$. The integral limit $x=0 \Rightarrow \xi = \xi_0 = \sqrt{m\omega^2/2E_0^{(0)}}\,x_0 = \sqrt{V_0/E_0^{(0)}}$, where $V_0 = V(0)$ is the barrier height. At the other limit $x=a$ (such that $V(a) = E_0^{(0)}$ is a turning point), we have $\xi = 1$. Thus...

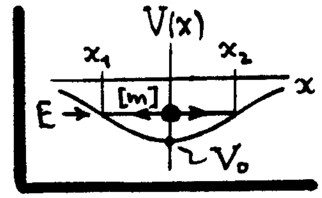
$$J = 2\int_1^{\xi_0}\sqrt{\xi^2-1}\,d\xi, \text{ w/ } \underline{\underline{\xi_0}} = \sqrt{V_0/E_0^{(0)}} = \sqrt{m\omega/\hbar}\,x_0 \gg 1;$$

$$\xrightarrow{\text{or}} J = \xi_0\sqrt{\xi_0^2-1} - \ln\left(\xi_0 + \sqrt{\xi_0^2-1}\right) \simeq \xi_0^2 - \ln 2\xi_0, \text{ for } \xi_0 \gg 1. \tag{15}$$

$\xi_0 \gg 1$ because by WKB conditions, the particle energy $E_0^{(0)}$ must lie well below the barrier height. Put J of (15) into Eq. (12) to obtain the total splitting...

$$\boxed{\Delta E_0 = (\hbar\omega/\pi)\cdot 2\xi_0 e^{-\xi_0^2} = \frac{2\hbar\omega}{\pi}\sqrt{2V_0/\hbar\omega}\,e^{-(2V_0/\hbar\omega)}}, \tag{16}$$

good for $V_0 \gg \frac{1}{2}\hbar\omega$. Considered as a fcn of $(2V_0/\hbar\omega)$, ΔE_0 actually goes thru a maxm @ $(2V_0/\hbar\omega) = \frac{1}{2}$. This is too small to qualify for the present approxn.



(44) Approximate energy levels in $V(x) = -V_0 \operatorname{sech}^2(x/a)$.

1. The Bohr-Sommerfeld rule [WKB Notes, p. 18, Eq. (52)] is:

$$\rightarrow \int_{x_1}^{x_2} \sqrt{2m\left[E + V_0 \operatorname{sech}^2(x/a)\right]}\, dx = (n+\tfrac{1}{2})\pi\hbar;\quad n = 0, 1, 2, \ldots; \tag{1}$$

w/ $E = -E_n$ is negative for bound states, and x_1 & x_2 are the turning points, found by: $V_0 \operatorname{sech}^2(x/a) = E_n \Rightarrow \cosh(x_2/a) = \sqrt{V_0/E_n}$, and $x_1 = -x_2$ (by symmetry). This condition can be written as...

$$\rightarrow \underline{\underline{J(E)}} = \int_{x_1}^{x_2} \sqrt{E + V_0 \operatorname{sech}^2(x/a)}\, dx = (n+\tfrac{1}{2})\pi\hbar/\sqrt{2m}. \tag{2}$$

2. A way to evaluate the integral $J(E)$ in (2) is first to differentiate w.r.t. E...

$$\rightarrow \frac{\partial J}{\partial E} = \frac{1}{2}\int_{x_1}^{x_2}\left(1/\sqrt{E + V_0 \operatorname{sech}^2(x/a)}\right)dx = \frac{1}{2}\int_{x_1}^{x_2} \frac{\cosh(x/a)\,dx}{\sqrt{E\cosh^2(x/a) + V_0}}. \tag{3}$$

The contributions from $\partial x_2/\partial E$ & $\partial x_1/\partial E$ are zero, since the integrand of $J(E)$ vanishes at those points. Now change variables to $y = \sinh(x/a)$ in (3), to get:

$$\rightarrow \frac{\partial J}{\partial E} = \frac{a}{2}\int_{y_1}^{y_2} dy\Big/\sqrt{(1+y^2)E + V_0},\quad \text{w/ } y_2 = \sqrt{(V_0/E_n) - 1} = -y_1$$

$$\text{so/ } \frac{\partial J}{\partial E} = \frac{a}{\sqrt{-E}}\int_0^{y_2} \frac{dy}{\sqrt{y_2^2 - y^2}} = \frac{a}{\sqrt{-E}}\cdot\frac{\pi}{2},\quad \text{and/ } \underline{\underline{J(E)}} = -\pi a\sqrt{-E} + \text{const}. \tag{4}$$

The integration const is fixed by noting that when $E = (-)V_0$, the integration range $x_1 \rightarrow x_2$ shrinks to zero. So $J(-V_0) = 0$, and the const is $\pi a\sqrt{V_0}$.

$$\text{Thus/ } \underline{\underline{J(E_n) = \pi a\left(\sqrt{V_0} - \sqrt{E_n}\right)}},\quad \text{w/ } E = -E_n \text{ for bound states}. \tag{5}$$

3. Use (5) in (2) to write: $\pi a(\sqrt{V_0} - \sqrt{E_n}) = (n+\frac{1}{2})\pi\hbar/\sqrt{2m}$. Solve for E_n to get...

$$\boxed{E_n = (\hbar^2/2ma^2)\left[\sqrt{2mV_0a^2/\hbar^2} - (n+\tfrac{1}{2})\right]^2};\ n = 0, 1, 2, \ldots. \tag{6}$$

There is a <u>finite</u> # energy levels in the well, viz $\underline{N = \sqrt{2mV_0a^2/\hbar^2}}$ (with p_n real). The approxn implicit in (6) is ~ good when $N \rightarrow$ large, i.e. when $\underline{V_0 \gg \hbar^2/2ma^2}$.