QM 15-Phys-710-001(/002/003) Fall 2000
Final
Wednesday, December 6

1. (20) Find the condition for the transmission coefficient through a rectangular potential well

$$V(x) = \begin{array}{ll} -V_0 < 0, & 0 < x < a \\ 0, & 0 < x,\ x > a \end{array}$$

to be 1.

Solution

Wave function ($k = \sqrt{2mE/\hbar^2}$, $\varkappa = \sqrt{2m(E+V_0)/\hbar^2}$)

$$\psi(x) = \begin{array}{l} e^{ikx} + Ae^{-ikx},\ x < 0 \\ Be^{i\varkappa x} + Ce^{-i\varkappa x},\ 0 < x < a \\ Ge^{ik(x-a)},\ a < x \end{array}$$

whereof

$$\begin{aligned} 1 + A &= B + C \\ k(1-A) &= \varkappa(B-C) \\ G &= Be^{i\varkappa a} + Ce^{-i\varkappa a} \\ kG &= \varkappa\left(Be^{i\varkappa a} - Ce^{-i\varkappa a}\right) \end{aligned}$$

for $A = 0$

$$\begin{aligned} \frac{B-C}{B+C} &= \frac{k}{\varkappa} \\ \frac{Be^{i\varkappa a} - Ce^{-i\varkappa a}}{Be^{i\varkappa a} + Ce^{-i\varkappa a}} &= \frac{k}{\varkappa} \end{aligned}$$

so $e^{i\varkappa a} = 1$ that is $\cos\varkappa a = 1$ and $\sin\varkappa a = 0$.

2. (30) For a one-dimensional harmonic oscillator,

a) Derive the wave function and the energy of the first excited state.

b) Using the trial wave function $\psi(x) = Ax\exp(-\alpha|x|)$, where α is the variational parameter, find the energy of the first excited state and compare it with the exact energy (from a) above), explaining the difference. Sketch the exact wave function versus the variational one, explaining the behavior at 0 and ∞.

Note: No answers, even correct ones, will be accepted without a first-principles derivation.

Solution

a) Schrödinger equation

$$\psi'' + \left(\frac{2E}{\hbar\omega} - \xi^2\right)\psi = 0,\ \xi = \sqrt{\frac{m\omega}{\hbar}}x \qquad (0.1)$$

For large ξ,

$$\psi'' - \xi^2\psi = 0$$

and

$$\psi \propto \exp\left(-\frac{\xi^2}{2}\right)$$

Substitute

$$\psi = \chi\exp\left(-\frac{\xi^2}{2}\right)$$

into eq. (0.1)

$$\chi'' - 2\xi\chi' + 2n\chi = 0,\ n = \frac{E}{\hbar\omega} - \frac{1}{2}$$

For the first excited state[1],

$$\begin{aligned}
\chi_1 &= a_0 + a_1\xi \Rightarrow -2a_1\xi + 2n\left(a_0 + a_1\xi\right) = 0 \Rightarrow a_0 = 0 \text{ and } n = 1 \Rightarrow E_1 = \frac{3}{2}\hbar\omega \\
\psi_1 &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} 2^{1/2}\sqrt{\frac{m\omega}{\hbar}}\, x \exp\left(-\frac{m\omega x^2}{2\hbar}\right)
\end{aligned}$$

b) Normalization gives

$$A^2 = 2\alpha^3$$

whereof the expectation values of kinetic and potential energies are

$$\begin{aligned}
\overline{T} &= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{\partial\psi}{\partial x}\right)^2 dx = \frac{\hbar^2\alpha^2}{2m} \\
\overline{U} &= \frac{3k}{2\alpha^2}
\end{aligned}$$

Minimizing $\overline{E} = \overline{T} + \overline{U}$ with respect to α,

$$\overline{E}\left(\alpha_{\min}\right) = \sqrt{3}\hbar\omega,\ \omega = \sqrt{\frac{k}{m}}$$

[1] Since the solution ought to be odd, the a_0 term nee not, inprinciple, be written.