APPENDIX E

PARABOLIC POTENTIAL WELL

An example of an extremely important class of one-dimensional bound state in quantum mechanics is the simple harmonic oscillator whose potential can be written as

$$V(x) = \frac{1}{2}Kx^2, \tag{E.1}$$

where K is the force constant of the oscillator.

The Hamiltonian operator is given by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}Kx^2. \tag{E.2}$$

The Schrödinger equation that gives the possible energies of the oscillator is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2} + \frac{1}{2}Kx^2\varphi(x) = E_n\varphi(x). \tag{E.3}$$

This equation can be simplified by choosing a new measure length and a new measure of energy, each of which is dimensionless. $\zeta \equiv (\frac{mK}{\hbar^2})^{1/4}x$ and $\eta = \frac{2E_n}{\hbar\omega}$, where $\omega = \sqrt{\frac{K}{m}}$. With these substitutions, Equation E.3 becomes

$$\frac{d^2\varphi(\zeta)}{d\zeta^2} + (\eta - \zeta^2)\varphi(\zeta) = 0. \tag{E.4}$$

Introduction to Nanomaterials and Devices, First Edition. Omar Manasreh.

In looking for bounded solutions, one can notice that as η approaches infinity and becomes too small compared to ζ^2, the resulting differential equation can be easily solved to yield

$$\varphi(\zeta) \sim e^{\pm\frac{1}{2}\zeta^2}. \tag{E.5}$$

This expression for the asymptotic dependence is suitable only for the negative sign in the exponent. It is clear that because of the very rapid decay of the resulting Gaussian function as ζ goes to infinity, the function will still have the same asymptotic dependence; it is multiplied by any finite polynomial in ζ (Dicke and Wittke)

$$\varphi(\zeta) = H(\zeta)e^{-\frac{1}{2}\zeta^2}. \tag{E.6}$$

where $H(\zeta$ is a finite polynomial. By substituting Equation E.5 into Equation E.4, one can obtain

$$\frac{d^2H(\zeta)}{d\zeta^2} - 2\zeta\frac{dH(\zeta)}{d\zeta} + (\eta - 1)H(\zeta) = 0. \tag{E.7}$$

If we assume a solution to this equation in the form of a finite polynomial

$$H(\zeta) = A_0 + A_1\zeta + A_2\zeta^2 + \cdots + A_n\zeta^n, \tag{E.8}$$

a recursion formula connecting the coefficients can be obtained in the following form:

$$A_{n+2} = \frac{(2n + 1 - \eta)}{(n + 2)(n + 1)}A_n, \quad \text{for } n \geq 0. \tag{E.9}$$

For an upper cutoff to the coefficients such that the polynomial $H(\eta)$ remains finite, the condition

$$\eta = 2n + 1 \tag{E.10}$$

must be satisfied. Substituting $\eta = \frac{2E_n}{\hbar\omega}$ into Equation E.10, we obtain

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{E.11}$$

The energy levels and the parabolic potential are shown in Fig. E1.

The polynomial solutions lead to wave functions that approach zero at $x = \pm\infty$ and allow normalization. These polynomials are called *Hermite polynomials*, and they are the acceptable solutions as wave functions. The Hermite polynomial is defined as follows:

$$H_n(\zeta) = (-1)^n e^{\zeta^2}\frac{d^n}{dx^n}(e^{-\zeta^2}). \tag{E.12}$$

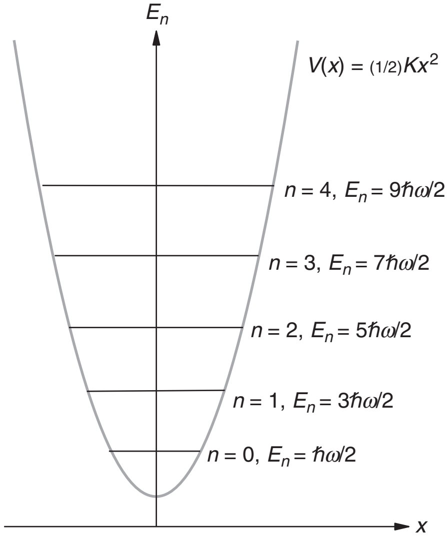

FIGURE E1 A parabolic one-dimensional potential well with a few of the allowed energy levels are shown.

Finally, the wave function can be written as

$$\varphi(\zeta) = N_n H_n(\zeta) e^{-\frac{1}{2}\zeta^2} = N_n (-1)^n e^{\frac{1}{2}\zeta^2} \frac{d^n}{dx^n}(e^{-\zeta^2}). \tag{E.13}$$

The normalization factor N_n can be found to be

$$N_n = \frac{1}{2^n!}\sqrt{\frac{\alpha}{\pi}}, \text{ where } \alpha = \left(\frac{mK}{\hbar^2}\right)^{1/2}. \tag{E.14}$$

The first lowest four wave functions are illustrated in Fig. E2a. The probability amplitude for the $n = 5$ eigenstate is shown in Fig. E2b along with the classical probability density. The first few Hermite polynomial functions are shown below.

Figure E2 shows several oscillations in the $\varphi^*(\zeta)\varphi(\zeta))$ curve, with their amplitudes fairly small near the origin and considerably larger near the end of the curve. As n is increased, the probability density becomes larger and larger near the end of the curves and smaller and smaller near the center of the curve, approaching the classical limit. According to classical mechanics (McKelvey), the probability of finding a particle in an interval dx is proportional to the time dt it spends in that interval. This is directly related to the velocity by $dx = \upsilon_x dt$. More precisely, if $T/2$ is the half period of oscillation, the fraction of time spent in dx is $dt/(T/2)$ or $2dx/(T\upsilon_x)$. This fraction is the classical analog of the probability density $\varphi^*(\zeta)\varphi(\zeta)$ For a classical harmonic oscillator, conservation of energy

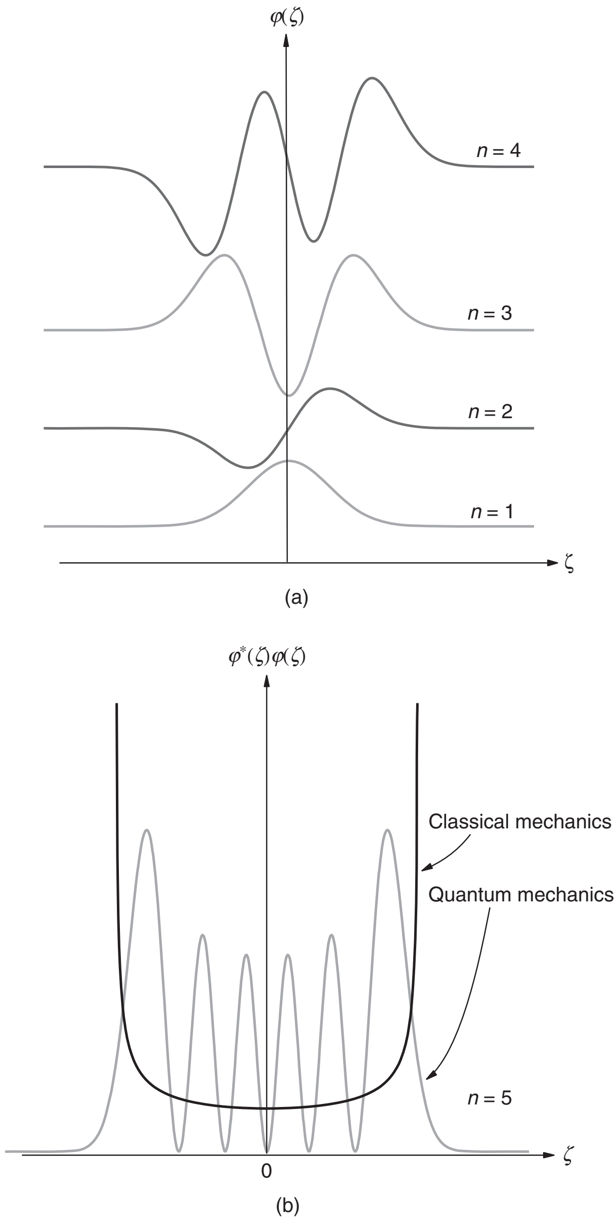

FIGURE E2 (a) Wave functions plotted for the lowest eigenstates. (b) The probability amplitude for $n = 5$ is shown along the classical probability density.

requires that the total energy E be

$$E = \frac{1}{2}m\upsilon_x^2 + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 A^2. \tag{E.15}$$

Solving for υ_x, we have $\upsilon_x = \omega(A^2 - x^2)^{1/2}$. The classical analog to $\varphi^*(\zeta)\varphi(\zeta)$ can then be written as $p(x)\mathrm{d}x$, where

$$p(x)\mathrm{d}x = \frac{2\mathrm{d}x}{T\upsilon_x} = \frac{\mathrm{d}x}{\pi\sqrt{A^2 - x^2}}. \tag{E.16}$$

If the quantum energy is given by Equation E.11, with the help of Equation E.15, one can write the classical probability as

$$p(x) = \frac{2\mathrm{d}x}{T\upsilon_x} = \frac{\mathrm{d}x}{\pi\sqrt{\frac{2n+1}{\alpha} - x^2}}, \tag{E.17}$$

where α is defined in Equation E.14.

N	$H_a(\zeta)$
0	1
1	2ζ
2	$4\zeta^2 - 2$
3	$8\zeta^3 - 12\zeta$
4	$16\zeta^4 - 48\zeta^2 - 12$
5	$32\zeta^5 - 160\zeta^3 + 120\zeta$

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