

2.12 Since $E_n = n^2 h^2 / 8mL^2$ [eqn 2.31],

$$F = -(dE_n/dL) = \underline{n^2 h^2 / 4mL^3}$$

For an electron ($m = m_e$) with $n=1$, $F = h^2 / 4m_e L^3$, hence

$$L = (h^2 / 4m_e F)^{1/3} = 0.4939 \text{ pm} / (F/N)^{1/3}$$

hence, when $F = 1.0 \text{ N}$, $L = 0.49 \text{ pm}$.

Exercise: Consider the case of N particles in a cubic box. Find an expression for the product pV (p : pressure, V : volume). Discuss the relation of this result with the perfect gas equation of state.

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2.29 $\langle x \rangle = 0$ by symmetry, $\langle p_x \rangle = 0$ by reality [Problem 2.15]. Alternatively

$$\langle p_x \rangle \propto \int_{-\infty}^{\infty} e^{-y^2/2} (d/dy) e^{-y^2/2} dy \propto \int_{-\infty}^{\infty} y e^{-y^2} dy = 0 \text{ by symmetry.}$$

$$\langle x^2 \rangle = N_0^2 \int_{-\infty}^{\infty} x^2 e^{-y^2} dx$$

[The wavefunctions are normalized in the sense that $\int_{-\infty}^{\infty} \psi^2 dy = 1$]

$$\langle x^2 \rangle = (1/\pi^{1/2})(\hbar/m\omega) \int_{-\infty}^{\infty} y^2 e^{-y^2} dy = \frac{1}{2}(\hbar/m\omega) = \frac{1}{2}(\hbar\omega/k)$$

$$\begin{aligned} \langle p_x^2 \rangle &= \int \psi_0^* (\hbar/i)^2 (d^2/dx^2) \psi_0 d\tau = -\hbar^2 N_0^2 \int_{-\infty}^{\infty} e^{-y^2/2} (d/dx)^2 e^{-y^2/2} dx \\ &= -\hbar^2 N_0^2 (m\omega/\hbar)^{1/2} \int_{-\infty}^{\infty} e^{-y^2/2} (d/dy)^2 e^{-y^2/2} dy \\ &= -\hbar^2 N_0^2 (m\omega/\hbar)^{1/2} \int_{-\infty}^{\infty} (y^2 - 1) e^{-y^2} dy \\ &= -\hbar^2 N_0^2 (m\omega/\hbar)^{1/2} \left\{ \frac{1}{2}\sqrt{\pi} - \sqrt{\pi} \right\} = \frac{1}{2}\hbar m\omega = \frac{1}{2}\hbar k/\omega \end{aligned}$$

(Note that these results can be obtained more simply by using the virial theorem: $\langle p_x^2 \rangle/2m = \frac{1}{2}k\langle x^2 \rangle = \frac{1}{2}E = \frac{1}{4}\hbar\omega$.) It follows that

$$\left. \begin{aligned} \Delta x &= \{ \langle x^2 \rangle - \langle x \rangle^2 \}^{1/2} = \langle x^2 \rangle^{1/2} = (\hbar\omega/k)^{1/2}/\sqrt{2} \\ \Delta p_x &= \{ \langle p_x^2 \rangle - \langle p_x \rangle^2 \}^{1/2} = \langle p_x^2 \rangle^{1/2} = (\hbar k/\omega)^{1/2}/\sqrt{2} \end{aligned} \right\} \Delta x \Delta p_x = \frac{1}{2}\hbar$$

which is in accord with $\Delta x \Delta p_x \geq \frac{1}{2}\hbar$. A Gaussian function is a *minimum uncertainty* function.

Exercise: Deduce that $\Delta x \Delta p_x = (v + \frac{1}{2})\hbar$ for a general value of v .

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2.32 The wavefunction $\psi(x)$ is given as a sum of normalized particle-in-a-box eigenfunctions $\psi_n(x)$. Therefore, according to quantum mechanical postulate 3', a single measurement of the energy yields a single outcome which is one of the eigenvalues E_n (associated with the eigenfunction ψ_n appearing in the expansion of ψ). The probability of obtaining E_n is $|c_n|^2$ where c_n is the coefficient of ψ_n in the expansion.

(a) When the energy of the particle is measured, possible outcomes are

$$E_1 = \frac{h^2}{8mL^2} \quad E_3 = \frac{9h^2}{8mL^2} \quad E_5 = \frac{25h^2}{8mL^2}$$

(b) The probability of obtaining each result is

$$\begin{aligned} |c_1|^2 &= (1/3)^2 = 1/9 && \text{for } E_1 \\ |c_3|^2 &= |(i/3)|^2 = 1/9 && \text{for } E_3 \\ |c_5|^2 &= [-(7/9)^{1/2}]^2 = 7/9 && \text{for } E_5 \end{aligned}$$

(c) The expectation value is the weighted sum of the possible eigenvalues:

$$\frac{1}{9}E_1 + \frac{1}{9}E_3 + \frac{7}{9}E_5 = \frac{185h^2}{72mL^2}$$

Exercise: If the linear momentum of the particle described above were measured, what would we expect to find?

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4. We have 2π bonds and hence 4 p electrons, which fill up the first two energy levels, so the ground state has 2 electrons in each of the $n=1$ and $n=2$ energy levels, the first excited state moves an electron from the $n=2$ energy level to the $n=3$ energy level. So starting with:

$$E_n = \frac{n^2 h^2}{8mL^2}$$

We calculate the total energy as:

$$E_{total} = 2(E_1 + E_2) = 2 \left[(1^2 + 2^2) \frac{h^2}{8mL^2} \right] = \frac{5h^2}{4mL^2} = 3.35 \times 10^{-18} \text{ J}$$

Where $L = 44 \times 10^{-10} \text{ m}$, and $m = m_e = 9.109 \times 10^{-31} \text{ kg}$.

To calculate the energy difference between the adjacent energy levels we use:

$$E_{n \rightarrow n+1} = \frac{(2n+1)h^2}{8mL^2}$$

For the 2nd and 3rd levels this gives:

$$E_{2 \rightarrow 3} = \frac{(5)h^2}{8mL^2} = 1.68 \times 10^{-18} \text{ J}$$

Now $\lambda = hc/E$, so $\lambda = 118 \text{ nm}$.

5 A & B.

Description	Mass (m_e)	V (h_e)	L (a_0)	Probability for $E/V=.66$
1.2 nm	1	0.1	22.7	2.6×10^{-5}
0.6nm	1	0.1	11.35	9.6×10^{-3}
0.24nm	1	0.1	4.54	0.29
0.12nm	1	0.1	2.27	0.69

5 C.

Description	Mass (m_e)	V (h_e)	L (a_0)	Probability for $E/V=.66$
.09 nm	1	0.1	1.7	0.81
.10nm	1	0.1	1.9	0.77
.11nm	1	0.1	2.1	0.73

Relative change is about 5 % which means that if we can measure these currents with a resolution of at least 5% that we can measure the tunneling distance to at least 0.1 angstroms.

5 D.

Description	Mass (m_e)	V (h_e)	L (a_0)	Probability for $E/V=.66$
.09 nm	1833	0.1	1.7	1.17×10^{-16}
.10nm	1833	0.1	1.9	1.35×10^{-18}
.11nm	1833	0.1	2.1	1.55×10^{-20}

If electron tunneling gave us a current with a magnitude that we could comfortably work with, then proton tunneling probably won't because we would need to detect and quantify and distinguish between currents nearly twenty orders of magnitude smaller than with electron tunneling. Therefore proton tunneling for STM is not very promising. However, as some students pointed out, the relative difference in probability is huge, so if we did have a way to measure changes in current that small, we could get extremely good resolution