2.3 periodic boundary condition

$L = 18.2$ atomic units $\quad a = 2.89$ a.u

$$E_n = \frac{\hbar^2}{2m}\left(\frac{2n\pi}{L}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{2n\pi}{2\pi a}\right)^2 = \frac{\hbar^2}{2ma^2}\, n^2$$

$$= \frac{1}{2\times 2.89^2}\, n^2 \, (\times 27.21\,\mathrm{eV}) = (1.62\,\mathrm{eV}) \times n^2$$

$n = 0, \pm 1,$

Total $E = 1.62\ (\times 1) \times 4 = 6.52$ eV

Excitation energy $= 1.62\,\mathrm{eV}\,(2^2 - 1) = 4.86$ eV

2.4 infinite square well

$$E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2\pi a}\right)^2 = \frac{\hbar^2}{8ma^2} \times n^2$$

$$= \frac{1.62}{4} \times n^2 = 0.40 \times n^2 \ (\mathrm{eV})$$

$n = 1, 2, 3 \ldots$

Total energy $= 0.40 \times 2 \times (1^2 + 2^2 + 3^2) = 0.8 \times 14 = 11.2$ eV

To break up benzene $= (11.2 - 6.52)\ \mathrm{eV} = \boxed{4.68\ \mathrm{eV}}$

4.3

$$H = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_2} = \frac{L^2 - L_z^2}{2I_1} + \frac{L_z^2}{2I_2}$$

$$H\, Y_{lm} = \lambda_{lm} Y_{lm}$$

$$\lambda_{lm} = \frac{l(l+1)\hbar^2}{2I_1} + m^2\hbar^2\left(\frac{1}{I_2} - \frac{1}{I_1}\right)$$

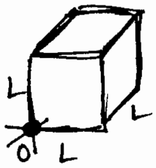
4.5 Remember in spherical symmetry, the degeneracy is $2(2l+1)$.

Applied Quantum

Assignment #2

Mat Leonard

2-1




So, for the boundary conditions

$\psi(0) = \psi(L) = 0 \quad \psi'(0) = \psi'(L) = 0$

$k_i L = n_i \pi$

The unit volume in k space is $(k_x L)(k_y L)(k_z L) = \pi^3$ so $k^3 = \frac{\pi^3}{V}$ V is $L^3$

The total k space up to $k_F$ is $\frac{1}{8}(4/3 \pi k_F^3)$ since $n\pi$ is only positive values.

So $N = 2 \frac{\frac{1}{8} \frac{4}{3} \pi k_F^3}{\pi^3/V} = 2\left[\left(\frac{V}{8\pi^3}\right)\left(\frac{4}{3}\pi k_F^3\right)\right]$

This is the same result as with periodic boundary conditions.

$k_F = \sqrt[3]{\frac{3\pi^2 N}{V}} \quad E_F = \frac{\hbar^2 \left(\frac{3\pi^2 N}{V}\right)^{2/3}}{2m}$

2-5

$N = 2\left(\frac{A}{4\pi^2}\right)\left(\pi k_F^2\right)$ $\quad E_F = \frac{\hbar^2 k_F^2}{2m}$ $\quad k_F^2 = \frac{2mE}{\hbar^2}$

$N = 2\left(\frac{A}{4\pi^2}\right)\pi\left(\frac{2mE}{\hbar^2}\right)$

$\frac{dN}{dE} = \frac{A}{\pi}\frac{m}{\hbar^2}$ $\quad \frac{dN}{A\,dE} = \frac{m}{\pi\hbar^2} = n(E)$

$$\boxed{n(E) = \frac{m}{\pi\hbar^2}}$$

OK.

4-6




• **Figure 9–4** $|Y_{\ell m}|^2$ represents the probability of finding the electron in a solid angle $\sin\theta\, d\theta\, d\varphi$. We plot the distributions for **(a)** $\ell = 0, m = 0$; **(b)** $\ell = 1, m = \pm 1$, $\ell = 1, m = 0$; and **(c)** $\ell = 2, m = \pm 2$, $m = \pm 1$, and $m = 0$. We also include $\ell = 5, m = 0$, to show the growing complexity of the distribution.

from Bernstein, Fishbane, and Gasiorowicz Modern Physics, 2000.