

1. Near the boundary of the first Brillouin zone, for a one-dimensional chain of atoms, at  $k = \pi/a$ , the nearly free electron theory predicts that the most important term in the lattice potential is  $V(x) \approx V_1 \cos[2\pi x/a]$ . The wavefunction is then approximately

$$\psi(x) \approx \alpha e^{ikx} + \beta e^{i(k-2\pi/a)x}.$$

Substitute this wavefunction into Schrödinger's equation:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = \epsilon \psi(x).$$

To find equations for  $\alpha$  and  $\beta$  we can use that  $e^{ikx}$  and  $e^{i(k-2\pi/a)x}$  are *orthogonal*. Let us do this explicitly. Multiply the result of your substitution of the  $\psi(x)$  into Schrödinger's equation by

- (a)  $e^{ikx}$ , and
- (b)  $e^{i(k-2\pi/a)x}$ .

Then integrate over all space to find two equations for  $\alpha$  and  $\beta$ . Solve these equations and show that

$$\epsilon = \frac{\hbar^2 k^2}{2m} + \frac{\pi \hbar^2}{ma} \left[ \frac{\pi}{a} - k \pm \sqrt{\left(\frac{\pi}{a} - k\right)^2 + \left(\frac{amV_1}{2\pi \hbar^2}\right)^2} \right]$$

is the energy. Show that this agrees with our solution near  $k = \pi/a$  and  $k = 0$ .

2. Consider a monovalent metal with a simple cubic lattice of spacing  $a$ . Calculate the radius of the Fermi sphere using the free electron theory. Is this sphere contained completely within the first Brillouin zone?