HW8 Solutions

3. (a) At k = 0 the determinantal equation is (P/Ka) sin Ka + cos Ka = 1. In the limit of small positive P this equation will have a solution only when Ka $\ll 1$. Expand the sine and cosine to obtain in lowest order $P \simeq \frac{1}{2}(Ka)^2$. The energy is $\varepsilon = \hbar^2 K^2/2m \simeq \hbar^2 P/ma^2$. (b) At k = π/a the determinantal equation is (P/Ka) sin Ka + cos Ka = –1. In the same limit this equation has solutions Ka = π + δ, where $\delta \ll 1$. We expand to obtain $(P/\pi)(-\delta) + \left(-1 + \frac{1}{2}\delta^2\right) = -1$, which has the solution δ = 0 and δ = 2P/π. The energy gap is $E_g = (\hbar^2/2ma^2)(2\pi\delta) \simeq (\hbar^2/2ma^2)(4P)$.

4. (a) There are two atoms in the basis, and we label them a and b. Then the crystal potential may be written as $U = U_1 + U_2 = U_1(\underset{\sim}{r}) + U_1\left(x + \frac{1}{4}a,\ y + \frac{1}{4}a,\ z + \frac{1}{4}a\right)$ and the Fourier transform has components $U_{\underset{\sim}{G}} = U_{1\underset{\sim}{G}} + U_{2\underset{\sim}{G}} = U_{1\underset{\sim}{G}}\left(1 + e^{i(G_x + G_y + G_z)\frac{1}{4}a}\right)$. If $\underset{\sim}{G} = 2A\underset{\sim}{\hat{x}}$, then the exponential is $e^{i\frac{1}{2}Aa} = e^{i\pi} = -1$, and $U_{\underset{\sim}{G}=2A} = 0$, so that this Fourier component vanishes. Note that the quantity in parentheses above is just the structure factor of the basis. (b) This follows directly from (44) with U set equal to zero. In a higher order approximation we would go back to Eq. (31) where any non-vanishing $U_{\underset{\sim}{G}}$ enters.

6. U(x,y) = – U[$e^{i(2\pi/a)(x+y)}$ + other sign combinations of ± x ± y]. The potential energy contains the four reciprocal lattice vectors (2 π/a) (±1; ±1). At the zone corner the wave function $e^{i(\pi/a)(x+y)}$ is mixed with $e^{-i(\pi/a)(x+y)}$. The central equations are

$$(\lambda - \varepsilon)C\left[\frac{\pi}{a}; \frac{\pi}{a}\right] - UC\left[-\frac{\pi}{a}; -\frac{\pi}{a}\right] = 0\ ;$$

$$(\lambda - \varepsilon)C\left[-\frac{\pi}{a}; -\frac{\pi}{a}\right] - UC\left[\frac{\pi}{a}; \frac{\pi}{a}\right] = 0\ ,$$

where $\lambda = 2(\hbar^2/2m)(\pi/a)^2$. The gap is 2U.