1. (a) The value of k_F for the "boundary sphere" is ½ the shortest reciprocal lattice vector:

$$\frac{2\pi}{a}(1,1,1) = \vec{G}, \quad \frac{1}{2}|\vec{G}| = \frac{2\pi}{a}\cdot\frac{1}{2}\sqrt{3} = \sqrt{3}\,\frac{\pi}{a}$$

$$n = \frac{k_F^3}{3\pi^2} \text{ in 3D} \; ; \; n = \frac{1}{3\pi^2}\cdot\frac{\pi^3}{a^3}\,3\sqrt{3} = \frac{\sqrt{3}\,\pi}{a^3}$$

$$= \frac{\sqrt{3}\,\pi}{4}\cdot\frac{1}{(a^3/4)}$$ primitive cell volume

$$= 1.36 \; e^-\text{s} \,/\, \text{primitive cell}$$

Make sense; the full BZ holds 2 e^-s / primitive cell

(b) Square lattice, solution by observation

Area of BZ $= \left(\frac{2\pi}{a}\right)^2 \longleftrightarrow 2 \; e^-$s/cell
spin

Area of Fermi circle $= \pi\left(\frac{\pi}{a}\right)^2 = \frac{\pi^3}{a^2}$

Density of states in k-space $\Rightarrow$

$$n = \#\text{ electrons / cell} = 2 \text{ in BZ} \times \frac{(\text{circle area})}{(\text{BZ area})}\;\frac{\pi^3/a^2}{4\pi^2/a^2}$$

$$n = 2\times\frac{\pi}{4} = \frac{\pi}{2} = 1.57 \; e^-\text{s/cell}$$

$$= 1.57/a^2 \; e^-\text{s / unit volume}$$

2. $V(r) = -4V_0 \cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)$, $\vec{G} = l\frac{2\pi}{a}\hat{x} + k\frac{2\pi}{a}\hat{y}$

$$V_G = \frac{1}{a^2}\int_0^a dx \int_0^a dy (-4V_0)\cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right) e^{-i[l\frac{2\pi}{a}x]} e^{-i[k\frac{2\pi}{a}y]}$$

$$= \frac{-4V_0}{a^2}\left(\int_0^a \cos\left(\frac{2\pi x}{a}\right) e^{-il\frac{2\pi}{a}x} dx\right)\left(\int_0^a \cos\left(\frac{2\pi y}{a}\right) e^{-ik\frac{2\pi}{a}y} dy\right).$$

$$\cos\left(\frac{2\pi x}{a}\right) = \frac{1}{2}\left(e^{i\frac{2\pi x}{a}} + e^{-i\frac{2\pi x}{a}}\right)$$

$$\cos\left(\frac{2\pi y}{a}\right) = \frac{1}{2}\left(e^{i\frac{2\pi y}{a}} + e^{-i\frac{2\pi y}{a}}\right)$$

$$\Rightarrow V_G = -\frac{4V_0}{a^2}\left(\int_0^a \frac{1}{2}\left(e^{i\frac{2\pi x}{a}(1-l)} + e^{i\frac{2\pi x}{a}(-1-l)}\right)dx\right)$$
$$\left(\int_0^a \frac{1}{2}\left(e^{i\frac{2\pi y}{a}(1-k)} + e^{i\frac{2\pi y}{a}(-1-k)}\right)dy\right)$$

$$= -\frac{V_0}{a^2}\left(a\,\delta_{l,1} + a\,\delta_{l,-1}\right)\left(a\,\delta_{k,1} + a\,\delta_{k,-1}\right)$$

$$= -V_0\left(\delta_{l,1} + \delta_{l,-1}\right)\left(\delta_{k,1} + \delta_{k,-1}\right)$$

$\Rightarrow$ $V_G = -V_0$ for $\vec{G} = \frac{2\pi}{a}\hat{x} + \frac{2\pi}{a}\hat{y}$

or $\frac{2\pi}{a}\hat{x} - \frac{2\pi}{a}\hat{y}$.

or $-\frac{2\pi}{a}\hat{x} + \frac{2\pi}{a}\hat{y}$

or $-\frac{2\pi}{a}\hat{x} - \frac{2\pi}{a}\hat{y}$

$V_G = 0$ otherwise

3. (a)

$$\psi(x) = C(k)e^{ikx} + C(k-G)e^{i(k-G)x}$$

$$\Rightarrow \begin{cases} (\varepsilon_k - \varepsilon)C(k) + V_G\, C(k-G) = 0 \\ V_G\, C(k) + (\varepsilon_{k-G} - \varepsilon)C(k-G) = 0 \end{cases}$$

Solve $\begin{vmatrix} \varepsilon_k - \varepsilon & V_G \\ V_G & \varepsilon_{k-G} - \varepsilon \end{vmatrix} = 0$

$$\boxed{\begin{aligned} \varepsilon_k &= \frac{\hbar^2 k^2}{2m} \\ \varepsilon_{k-G} &= \frac{\hbar^2}{2m}(k-G)^2 \end{aligned}}$$

$$\Rightarrow (\varepsilon - \varepsilon_k)(\varepsilon - \varepsilon_{k-G}) - V_G^2 = 0$$

$$\varepsilon^2 - (\varepsilon_k + \varepsilon_{k-G})\varepsilon + \varepsilon_k \varepsilon_{k-G} - V_G^2 = 0$$

$$\therefore \varepsilon = \frac{1}{2}\left[(\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{(\varepsilon_k + \varepsilon_{k-G})^2 - 4(\varepsilon_k \varepsilon_{k-G} - V_G^2)}\right]$$

$$= \frac{1}{2}(\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{\frac{1}{4}(\varepsilon_k - \varepsilon_{k-G})^2 + V_G^2}$$

✓ Let $\delta \equiv \frac{1}{2}G - k$, $k = \frac{1}{2}G - \delta$, $\lambda_1 = \dfrac{\hbar^2(\frac{1}{2}G)^2}{2m}$

$$\Rightarrow \varepsilon = \left(\frac{\hbar^2}{2m}\right)\left(\frac{1}{4}G^2 + \delta^2\right) \pm \left[4\lambda_1(\hbar^2\delta^2/2m) + V_G\right]^{1/2}$$

$$\simeq \left(\frac{\hbar^2}{2m}\right)\left(\frac{1}{4}G^2 + \delta^2\right) \pm V_G\left[1 + 2\left(\frac{\lambda_1}{V_G^2}\right)\left(\frac{\hbar^2\delta^2}{2m}\right)\right]$$

$$\Rightarrow \begin{cases} \varepsilon_k(+) = \varepsilon_1(+) + \dfrac{\hbar^2\delta^2}{2m}\left(1 + \dfrac{2\lambda_1}{V_G}\right) \\ \varepsilon_k(-) = \varepsilon_1(-) + \dfrac{\hbar^2\delta^2}{2m}\left(1 - \dfrac{2\lambda_1}{V_G}\right) \end{cases},$$

where $\varepsilon_1(\pm) = \dfrac{\hbar^2}{2m}\left(\frac{1}{2}G_1\right)^2 \pm V_G$

(b) At $k = \frac{\pi}{a}$ $\quad (\varepsilon_k \equiv \varepsilon_{k-G})$

$$u_0(k) = \frac{1}{V_G}\left[\pm\sqrt{0 + V_G^2}\right] = \pm 1$$

So normalized eigenvectors are $\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}, \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} = \begin{bmatrix}u_0\\u_G\end{bmatrix}$

Now, write these for $k - \frac{\pi}{a} = -\delta$ in simples form, to lowest order (δ^1):

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \rightarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1 + \frac{\hbar^2 G\delta}{2mV_G}\\1 + \frac{\hbar^2 G\delta}{2mV_G}\end{bmatrix}$$

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} \rightarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1 + \frac{\hbar^2 G\delta}{2mV_G}\\-1 + \frac{\hbar^2 G\delta}{2mV_G}\end{bmatrix}$$

Higher order correction (δ^2): $2\left(\frac{\lambda_1}{V_G^2}\right)\left(\frac{\hbar^2\delta^2}{2m}\right)$

(c) To lowest order, $\Delta E = \varepsilon_k(+) - \varepsilon_k(-) \sim 2V_G$

$$\Delta E = 1\mathrm{eV} \longrightarrow V_G = \frac{1}{2}\mathrm{eV}$$