Ph135 - Problem Set 5

November 19, 2019

Problem 1

(a) The reciprocal lattice vectors $\vec{k}_j$ satisfy

$$\vec{a}_i \cdot \vec{k}_j = 2\pi\delta_{ij}, \tag{1}$$

from which we get

$$\begin{aligned} \vec{k}_1 &= \frac{2\pi}{a}\hat{x}, \\ \vec{k}_2 &= \frac{2\pi}{a}\hat{y}. \end{aligned} \tag{2}$$

(b) See Figure 1 below.

(c) V_{nm} are just the Fourier coefficients of $V(x,y)$. We use the Villain form of the potential $V(x,y)$ and get

$$\begin{aligned} V_{nm} &= \left(\frac{1}{a}\right)^2 \int_{-a/2}^{a/2}\int_{-a/2}^{a/2} e^{-i(nkx+mky)}V(x,y)\ dxdy \\ &= -V_0\left(\frac{1}{a}\int_{-a/2}^{a/2} e^{-inkx}e^{-\frac{1}{2}\lambda k^2x^2}\ dx\right)\left(\frac{1}{a}\int_{-a/2}^{a/2} e^{-imky}e^{-\frac{1}{2}\lambda k^2y^2}\ dy\right) \\ &\approx -V_0\left(\frac{1}{a}\int_{-\infty}^{\infty} e^{-inkx}e^{-\frac{1}{2}\lambda k^2x^2}\ dx\right)\left(\frac{1}{a}\int_{-\infty}^{\infty} e^{-imky}e^{-\frac{1}{2}\lambda k^2y^2}\ dy\right) \\ &= -\frac{V_0}{2\pi\lambda}e^{-\frac{n^2+m^2}{2\lambda}} \end{aligned} \tag{3}$$

We made use of the fact that $\lambda \gg 1$, and thus ignored the contribution of $e^{-\frac{1}{2}\lambda k^2(x-n'a)^2}e^{-\frac{1}{2}\lambda k^2(y-m'a)^2}$ for all $|n'| > 0$ and $|m'| > 0$.

(d) The Hamiltonian is given by

$$H = H_0 + V, \tag{4}$$

where

$$H_0 = \frac{p^2}{2m}, \quad \text{and } V = \sum_{nm} V_{nm}e^{i(nkx+mky)}. \tag{5}$$

Ignoring V, the eigenstates of H are

$$|p\rangle = \frac{1}{\sqrt{L_1L_2}}e^{i(p_1x+p_2y)}, \tag{6}$$

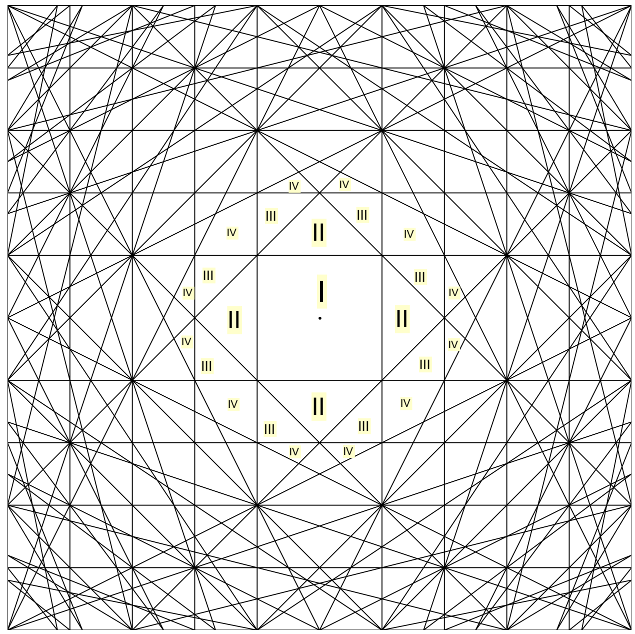


Figure 1: Illustration of the Brillouin zones.

where L_1 (L_2) is the size of the system in the x (y) direction. If we include V, according to first order perturbation theory, the first order corrected wave function is given by

$$|\tilde{p}\rangle = |p\rangle + \frac{1}{E_p - \hat{H}_0}\hat{V}|p\rangle. \tag{7}$$

To calculate the band gaps that emerge at the Brillouin zones linked by $n\vec{k}_1 + m\vec{k}_2$, we focus on the momentum $\vec{p}$ near $\pm(n\vec{k}_1 + m\vec{k}_2)/2$ where the energy is degenerate. Let

$$\begin{aligned} |+\rangle &= \left|\frac{n}{2}\vec{k}_1 + \frac{m}{2}\vec{k}_2 + \delta_1\hat{k}_1 + \delta_2\hat{k}_2\right\rangle, \\ |-\rangle &= \left|-\frac{n}{2}\vec{k}_1 - \frac{m}{2}\vec{k}_2 + \delta_1\hat{k}_1 + \delta_2\hat{k}_2\right\rangle. \end{aligned} \tag{8}$$

In the subspace spanned by $|+\rangle$ and $|-\rangle$, the Hamiltonian is of the form

$$\begin{aligned} H_{\text{eff}} &= \begin{pmatrix} \frac{1}{2m}\left[(\frac{nk}{2} + \delta_1)^2 + (\frac{mk}{2} + \delta_2)^2\right] & V_{nm} \\ V_{nm} & \frac{1}{2m}\left[(-\frac{nk}{2} + \delta_1)^2 + (-\frac{mk}{2} + \delta_2)^2\right] \end{pmatrix} \\ &= \left[\frac{(n^2 + m^2)k^2}{8m} + \frac{\delta_1^2 + \delta_2^2}{2m}\right]\mathbb{1} + \frac{k(n\delta_1 + m\delta_2)}{2m}\sigma_z + V_{nm}\sigma_x, \end{aligned} \tag{9}$$

and the eigenvalues are given by

$$E_\pm = \frac{(n^2 + m^2)k^2}{8m} + \frac{\delta_1^2 + \delta_2^2}{2m} \pm \sqrt{\left[\frac{k(n\delta_1 + m\delta_2)}{2m}\right]^2 + V_{nm}^2}. \tag{10}$$

As $\delta_1, \delta_2 \to 0$,

$$\Delta E = E_+ - E_- = 2|V_{nm}| = \frac{V_0}{\pi\lambda}e^{-\frac{n^2+m^2}{2\lambda}}. \tag{11}$$

(e) To calculate m_{eff} at the bottom of the lowest band, let $\vec{p} = \delta_1\hat{k}_1 + \delta_2\hat{k}_2$. By perturbation theory,

$$E = \frac{p^2}{2m} + \langle p|V|p\rangle + \sum_{\vec{p}' \neq \vec{p}} \frac{|\langle p'|V|p\rangle|^2}{p^2/(2m) - p'^2/(2m)} + O(V^3). \tag{12}$$

Now

$$
\begin{aligned}
E^{(1)} = \langle p|V|p\rangle &= \sum_{nm} V_{nm}\langle \delta_1\hat{k}_1 + \delta_2\hat{k}_2|(\delta_1+nk)\hat{k}_1 + (\delta_2+mk)\hat{k}_2\rangle \\
&= V_{00} = -\frac{V_0}{2\pi\lambda},
\end{aligned} \tag{13}
$$

and

$$
\begin{aligned}
E^{(2)} &= \sum_{\vec{p}'\neq\vec{p}} \frac{|\langle p'|V|p\rangle|^2}{p^2/(2m) - p'^2/(2m)} \\
&= \sum_{(n,m)\neq(0,0)} \frac{\left|\left\langle (\delta_1+nk)\hat{k}_1 + (\delta_2+mk)\hat{k}_2\right| V \left|\delta_1\hat{k}_1 + \delta_2\hat{k}_2\right\rangle\right|^2}{\frac{\delta_1^2+\delta_2^2}{2m} - \frac{(\delta_1+nk)^2+(\delta_2+mk)^2}{2m}} \\
&= \sum_{(n,m)\neq(0,0)} \frac{V_{nm}^2}{\frac{\delta_1^2+\delta_2^2}{2m} - \frac{(\delta_1+nk)^2+(\delta_2+mk)^2}{2m}} \\
&= -\frac{mV_0^2}{2\pi^2\lambda^2} \sum_{(n,m)\neq(0,0)} \frac{e^{-\frac{n^2+m^2}{\lambda}}}{2(n\delta_1+m\delta_2)k + (n^2+m^2)k^2} \\
&= -\frac{mV_0^2}{2\pi^2\lambda^2} \sum_{(n,m)\neq(0,0)} \frac{e^{-\frac{n^2+m^2}{\lambda}}}{2(n\vec{k}_1+m\vec{k}_2)\cdot\vec{p} + (n^2+m^2)k^2}
\end{aligned} \tag{14}
$$

Since p is small, we can expand the RHS of the above equation in powers of p. We get

$$
E^{(2)} = -\frac{mV_0^2}{2\pi^2\lambda^2} \sum_{(n,m)\neq(0,0)} \frac{e^{-\frac{n^2+m^2}{\lambda}}}{(n^2+m^2)k^2} \left(1 - 2\frac{(n\vec{k}_1+m\vec{k}_2)\cdot\vec{p}}{(n^2+m^2)k^2} + 4\frac{\left((n\vec{k}_1+m\vec{k}_2)\cdot\vec{p}\right)^2}{(n^2+m^2)^2k^4} + O(p^3)\right). \tag{15}
$$

In the above summation, terms linear in p vanishes. Therefore,

$$
E = \frac{p^2}{2m} - \frac{V_0}{2\pi\lambda} - \frac{mV_0^2}{2\pi^2\lambda^2} \sum_{(n,m)\neq(0,0)} \frac{e^{-\frac{n^2+m^2}{\lambda}}}{(n^2+m^2)k^2} \left(1 + 4\frac{\left((n\vec{k}_1+m\vec{k}_2)\cdot\vec{p}\right)^2}{(n^2+m^2)^2k^4}\right). \tag{16}
$$

The coefficient in front of the p^2 term in the above equation is $1/(2m_{\text{eff}})$. Since $\lambda \gg 1$, we can approximate the summation above by an integral, and

$$
\begin{aligned}
E &\approx \frac{p^2}{2m} - \frac{V_0}{2\pi\lambda} - \frac{mV_0^2}{2\pi^2\lambda^2} \int_1^\infty \int_0^{2\pi} \frac{re^{-r^2/\lambda}}{r^2k^2} \left(1 + 4\frac{r^2p^2\cos^2\theta}{r^4k^2}\right) d\theta dr \\
&= \frac{p^2}{2m} - \frac{V_0}{2\pi\lambda} - \frac{mV_0^2}{2\pi^2\lambda^2} \left(\frac{\pi}{k^2}\Gamma(0,\frac{1}{\lambda}) + \frac{2\pi}{k^4}\left(e^{-1/\lambda} - \frac{1}{\lambda}\Gamma(0,\frac{1}{\lambda})\right)p^2\right),
\end{aligned} \tag{17}
$$

where

$$
\Gamma(0,\frac{1}{\lambda}) \approx -\gamma - \log\left(\frac{1}{\lambda}\right) + \frac{1}{\lambda} + \ldots, \tag{18}
$$

is the incomplete Gamma function, and $\gamma \approx 0.5772$ is the Euler constant. Therefore,

$$
\begin{aligned}
\frac{1}{2m_{\text{eff}}} &\approx \frac{1}{2m} - \frac{mV_0^2}{\pi\lambda^2k^4}\left(1 + \frac{1}{\lambda}(\gamma-1) - \frac{1}{\lambda}\log\left(\frac{1}{\lambda}\right)\right) \\
&\approx \frac{1}{2m} - \frac{mV_0^2}{\pi\lambda^2k^4},
\end{aligned} \tag{19}
$$

and so

$$m_{\text{eff}} = m + \frac{2V_0^2 m^3}{\pi \lambda^2 k^4} + O(V_0^3). \tag{20}$$

Problem 2

(a) We need to solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi''(x) - V_0\delta(x)\psi(x) = E\psi(x). \tag{21}$$

For $x > 0$ and $x < 0$, the particle is free, and

$$\psi(x) = \begin{cases} \psi_L(x) = A_r e^{ikx} + A_l e^{-ikx}, & x < 0 \\ \psi_R(x) = B_r e^{ikx} + B_l e^{-ikx}, & x > 0, \end{cases} \tag{22}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}. \tag{23}$$

Continuity of ψ at $x = 0$ yields

$$A_r + A_l = B_r + B_l, \tag{24}$$

Integrating the Schrödinger equation around $x = 0$, over an interval $[-\epsilon, \epsilon]$ yields

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon} \psi''(x)\, dx + \int_{-\epsilon}^{\epsilon} V(x)\psi(x)\, dx = E\int_{-\epsilon}^{\epsilon} \psi(x)\, dx. \tag{25}$$

In the limit $\epsilon \to 0$, the above equation reduces to

$$-\frac{\hbar^2}{2m}\Big(\psi_R'(0) - \psi_L'(0)\Big) - V_0\psi(0) = 0, \tag{26}$$

which implies that

$$-\frac{\hbar^2}{2m} ik(-A_r + A_l + B_r - B_l) - V_0(A_r + A_l) = 0. \tag{27}$$

For bound states $E < 0$, and k is imaginary. We let $k = i\sqrt{2m|E|}/\hbar = i\kappa$. In order for the wave function to be finite at infinity, we need $A_r = B_l = 0$. Then

$$\psi(x) = \begin{cases} \psi_L(x) = A_l e^{\kappa x}, & x < 0 \\ \psi_R(x) = B_r e^{-\kappa x}, & x > 0, \end{cases} \tag{28}$$

and (24) and (27) implies that

$$\begin{cases} A_l = B_r = \sqrt{\kappa}, \\ \kappa = mV_0/\hbar^2. \end{cases} \tag{29}$$

The energy of the bound state is given by

$$E = -\frac{mV_0^2}{2\hbar^2}, \tag{30}$$

and the wave function

$$\psi(x) = \begin{cases} \psi_L(x) = \sqrt{\kappa} e^{\kappa x}, & x < 0 \\ \psi_R(x) = \sqrt{\kappa} e^{-\kappa x}, & x > 0, \end{cases} \tag{31}$$

where $\kappa = mV_0/\hbar^2$.

(b)

$$|p\rangle = \psi_p(x) = \sum_n \psi(x-na)e^{inap}, \tag{32}$$

hence

$$\begin{aligned}\psi_p(x+a) &= \sum_n \psi(x-(n-1)a)e^{i(n-1)ap}e^{iap} \\ &= e^{iap}\sum_m \psi(x-ma)e^{imap} \\ &= e^{iap}\psi_p(x), \end{aligned}\tag{33}$$

where in the second equality we let $m = n-1$. Therefore, $|p\rangle$ satisfies the Bloch theorem.

(c) Suppose $m > n$,

$$\begin{aligned} M_{nm} &= \int_{-\infty}^{\infty} \psi^*(x-na)\psi(x-ma)\ dx \\ =&\kappa\left(\int_{-\infty}^{na} e^{-\kappa((n+m)a-2x)}\ dx + \int_{na}^{ma} e^{-\kappa(m-n)a}\ dx + \int_{ma}^{\infty} e^{-\kappa(2x-(n+m)a)}\ dx\right) \\ =&\kappa\left(\frac{1}{2\kappa}e^{\kappa(n-m)a} + (m-n)ae^{-\kappa(m-n)a} + \frac{1}{2\kappa}e^{\kappa(n-m)a}\right) \\ =&\Big(1+\kappa(m-n)a\Big)e^{-\kappa(m-n)a}. \end{aligned}\tag{34}$$

Similarly, when $n > m$,

$$M_{nm} = \Big(1+\kappa(n-m)a\Big)e^{-\kappa(n-m)a}. \tag{35}$$

Hence,

$$M_{nm} = \Big(1+\kappa|n-m|a\Big)e^{-\kappa|n-m|a}. \tag{36}$$

(d) We first diagonalize M using plane wave ansatz. Let

$$\vec{v}(p) = (\ldots, e^{2ipa}, e^{ipa}, 1, e^{-ipa}, e^{-2ipa}, \ldots)^T, \tag{37}$$

then

$$\begin{aligned}\sum_{n=-\infty}^{\infty} M_{mn}v_n(p) &= \sum_{n=-\infty}^{\infty}\Big(1+\kappa|n-m|a\Big)e^{-\kappa|n-m|a}e^{-inpa} \\ &= \sum_{l=-\infty}^{\infty}\Big(1+\kappa|l|a\Big)e^{-\kappa|l|a}e^{i(l-m)pa} \\ &= \left(\sum_{l=-\infty}^{\infty}\Big(1+\kappa|l|a\Big)e^{-\kappa|l|a}e^{ilpa}\right)e^{-impa} \\ &= \lambda(p)v_m(p). \end{aligned}\tag{38}$$

Hence, $\vec{v}(p)$ is an eigenvector of M with eigenvalue

$$\begin{aligned}\lambda(p) &= \left(\sum_{l=-\infty}^{\infty}\Big(1+\kappa|l|a\Big)e^{-\kappa|l|a}e^{ilpa}\right) \\ &= \sum_{l=-\infty}^{\infty} e^{ilpa-\kappa|l|a} - (\kappa a)\frac{\partial}{\partial(\kappa a)}\left(\sum_{l=-\infty}^{\infty} e^{ilpa-\kappa|l|a}\right). \end{aligned}\tag{39}$$

Now

$$\begin{aligned}
\sum_{l=-\infty}^{\infty} e^{ilpa-\kappa|l|a} &= 1 + \sum_{l=-\infty}^{-1} e^{ilpa+\kappa la} + \sum_{l=1}^{\infty} e^{ilpa-\kappa la} \\
&= 1 + \sum_{l=1}^{\infty} e^{-ilpa} e^{-\kappa la} + \sum_{l=1}^{\infty} e^{ilpa-\kappa la} \\
&= 1 + \frac{e^{-\kappa a} e^{-ipa}}{1 - e^{-\kappa a} e^{-ipa}} + \frac{e^{-\kappa a} e^{ipa}}{1 - e^{-\kappa a} e^{ipa}} \\
&= \frac{1 - e^{-2\kappa a}}{1 + e^{-2\kappa a} - 2\cos(pa) e^{-\kappa a}} \\
&= \frac{\sinh(\kappa a)}{\cosh(\kappa a) - \cos(pa)}. \qquad (40)
\end{aligned}$$

Therefore,

$$\begin{aligned}
\lambda(p) &= \frac{\sinh(\kappa a)}{\cosh(\kappa a) - \cos(pa)} - (\kappa a) \frac{\partial}{\partial(\kappa a)} \left(\frac{\sinh(\kappa a)}{\cosh(\kappa a) - \cos(pa)} \right) \\
&= \frac{\sinh(\kappa a)}{\cosh(\kappa a) - \cos(pa)} - \frac{1 - \cos(pa)\cosh(\kappa a)}{(\cosh(\kappa a) - \cos(pa))^2} \\
&= \frac{\cosh(\kappa a)(\kappa a \cos(pa) + \sinh(\kappa a)) - \kappa a - \cos(pa)\sinh(\kappa a)}{(\cosh(\kappa a) - \cos(pa))^2}. \qquad (41)
\end{aligned}$$

Hence

$$M = UDU^\dagger, \qquad (42)$$

where the columns of U are $\vec{v}(p)$, and D is diagonal with entries $\lambda(p)$.

Next, we calculate $M^{-1/2} = U \frac{1}{\sqrt{D}} U^\dagger$. We assume that the exponentially decaying bound states are strongly bound, or equivalently, $\kappa a \gg 1$, then (41) implies

$$\begin{aligned}
\lambda(p) &\approx \frac{\cosh(\kappa a)\Big(\kappa a \cos(pa) + \sinh(\kappa a)\Big)}{\cosh^2(\kappa a)} \\
&\approx \frac{\kappa a \cos(pa) + \sinh(\kappa a)}{\cosh(\kappa a)} \\
&\approx \frac{\kappa a \cos(pa) + e^{\kappa a}/2}{e^{\kappa a}/2} \\
&= 1 + 2\kappa a e^{-\kappa a} \cos(pa). \qquad (43)
\end{aligned}$$

As expected, $\lambda(p)$ are precisely the eigenvalues of the matrix M when $\kappa a \gg 1$, where

$$\begin{aligned}
M_{nm} &= (1 + \kappa|n-m|a) e^{-\kappa|n-m|a} \\
&\approx \begin{cases} 1, & n = m, \\ (1+\kappa a) e^{-\kappa a}, & |n-m| = 1, \\ 0, & |n-m| > 1. \end{cases} \\
&\approx \begin{cases} 1, & n = m, \\ \kappa a e^{-\kappa a}, & |n-m| = 1, \\ 0, & |n-m| > 1. \end{cases} \qquad (44)
\end{aligned}$$

Then

$$\begin{aligned}
\frac{1}{\sqrt{\lambda(p)}} &= \frac{1}{\sqrt{1 + 2\kappa a e^{-\kappa a} \cos(pa)}} \\
&\approx 1 - \kappa a e^{-\kappa a} \cos(pa). \qquad (45)
\end{aligned}$$

Observe that (45) is (43) with the coefficient 2κ in front of the cosine term replaced by $-\kappa$. Hence,

$$(M^{-1/2})_{nm} \approx \begin{cases} 1, & n = m, \\ -\frac{1}{2}\kappa a e^{-\kappa a}, & |n-m| = 1, \\ 0, & |n-m| > 1, \end{cases} \tag{46}$$

and

$$\begin{aligned} \phi_n(r) &= \sum_m (M^{-1/2})_{nm} \psi(x - ma) \\ &= \psi(x - na) - \frac{1}{2}\kappa e^{-\kappa a}\Big[\psi\Big(x - (n-1)a\Big) + \psi\Big(x - (n+1)a\Big)\Big]. \end{aligned} \tag{47}$$

(e) We first calculate H in the $\psi(x)$ basis,

$$\begin{aligned} h_{nm} &= \int_{-\infty}^{\infty} dx\ \psi^*(x - na)(H_m + V_{m,\text{pert}})\psi(x - ma) \\ &= -\epsilon M_{nm} - \int_{-\infty}^{\infty} dx\ \psi^*(x - na)\Big(\sum_{l \neq m} V_0 \delta(x - la)\Big)\psi(x - ma) \\ &= -\epsilon M_{nm} - V_0 \sum_{l \neq m} \psi^*\Big((l-n)a\Big)\psi\Big((l-m)a\Big) \\ &= -\epsilon M_{nm} - V_0 \sum_{l \neq m} \kappa e^{-\kappa\big(|l-n|+|l-m|\big)a} \\ &= -\epsilon M_{nm} - V_0 \kappa \left(\frac{2e^{-\kappa a|m-n|}}{e^{2\kappa a} - 1} + |m-n| e^{-\kappa a|m-n|}\right) \\ &\approx -(\epsilon + \frac{2\kappa V_0}{e^{2\kappa a} - 1})\delta_{n,m} - \kappa e^{-\kappa a}\left(\epsilon a + V_0\right)\delta_{n\pm1,m} \end{aligned} \tag{48}$$

The matrix representation of H in the Fourier basis

$$|p\rangle = \sum_n e^{inap}\phi_n(x) = \sum_n U^*_{np}\phi_n(x) = \sum_n (U^\dagger)_{pn}\phi_n(x) \tag{49}$$

is given by

$$\begin{aligned} H_{\text{Fourier}} &= U^\dagger H_{\text{eff}} U \\ &= U^\dagger M^{-1/2} H M^{-1/2} U \\ &= U^\dagger U \frac{1}{\sqrt{D}} U^\dagger H U \frac{1}{\sqrt{D}} U^\dagger U \\ &= \frac{1}{\sqrt{D}} U^\dagger H U \frac{1}{\sqrt{D}}. \end{aligned} \tag{50}$$

Hence,

$$\begin{aligned} H_{\text{Fourier}}(p, p') &= \sum_{n,m} \frac{1}{\sqrt{\lambda(p)}} U^\dagger_{pn} h_{nm} U_{mp'} \frac{1}{\sqrt{\lambda(p')}} \\ &= \frac{1}{\sqrt{\lambda(p)\lambda(p')}} \sum_{n,m} e^{inap - imap'} h_{nm} \\ &= \frac{1}{\sqrt{\lambda(p)\lambda(p')}} \sum_m e^{ima(p-p')}\left[-(\epsilon + \frac{2\kappa V_0}{e^{2\kappa a} - 1}) - 2\cos{(pa)}\kappa e^{-\kappa a}(\epsilon a + V_0)\right] \\ &= \frac{1}{\lambda(p)}\left[-(\epsilon + \frac{2\kappa V_0}{e^{2\kappa a} - 1}) - 2\cos{(pa)}\kappa e^{-\kappa a}(\epsilon a + V_0)\right]\delta(p - p') \end{aligned} \tag{51}$$

Therefore, H_{Fourier} is diagonal, and the Fourier basis $|p\rangle$ are the true eigenstates of H. The energies are given by

$$\begin{aligned}
E(p) &\approx \Big(1 - 2\kappa a e^{-\kappa a}\cos(pa)\Big)\left[-(\epsilon + \frac{2\kappa V_0}{e^{2\kappa a}-1}) - 2\cos(pa)\kappa e^{-\kappa a}(\epsilon a + V_0)\right] \\
&\approx -\epsilon - 4\kappa e^{-\kappa a}\epsilon a\cos(pa) - 2\cos(pa)\kappa e^{-\kappa a}V_0 \\
&\approx -\epsilon - 2\kappa e^{-\kappa a}\cos(pa)(V_0 + 2\epsilon a).
\end{aligned} \tag{52}$$

Problem 3

(a) The number of electron states is given by

$$\begin{aligned}
N_D &= \int_{-\infty}^{\infty} \rho(\epsilon)\frac{1}{e^{\beta(\epsilon-\mu)}+1}d\epsilon \\
&= N_D\frac{1}{e^{\beta(-\delta-\mu)}+1} + \rho_0\int_0^{\infty}\frac{1}{e^{\beta(\epsilon-\mu)}+1}d\epsilon \\
&= N_D\frac{1}{e^{\beta(-\delta-\mu)}+1} + \rho_0 T\ln(1+e^{\beta\mu}).
\end{aligned} \tag{53}$$

Therefore,

$$N_D(1 - \frac{1}{e^{\beta(-\delta-\mu)}+1}) = \rho_0 T\ln(1+e^{\beta\mu}), \tag{54}$$

which implies that

$$\rho_0 T\ln(1+e^{\beta\mu}) = N_D\frac{1}{e^{\beta(\delta+\mu)}+1}. \tag{55}$$

It is worth noticing that this case is slightly different from the case discussed in Aschorft and Mermin chapter 28 where we took into account the Coulombic forces for the two spins in the same state of the donor level.

(b) When $T \ll \delta$, $-\delta < \mu < 0$, so

$$N_D\frac{1}{e^{\beta(\delta+\mu)}+1} \approx N_D e^{-\beta(\delta+\mu)}, \tag{56}$$

and

$$\rho_0 T\ln(1+e^{\beta\mu}) \approx \rho_0 T e^{\beta\mu}. \tag{57}$$

(55) Therefore reduces to

$$\rho_0 T e^{2\beta\mu} \approx N_D e^{-\beta\delta}, \tag{58}$$

and

$$\mu \approx -\frac{\delta}{2} + \frac{T}{2}\ln\frac{N_D}{\rho_0 T}. \tag{59}$$

(c) When $T \gg \delta$,

$$N_D\frac{1}{e^{\beta(\delta+\mu)}+1} \approx \frac{1}{2}N_D, \tag{60}$$

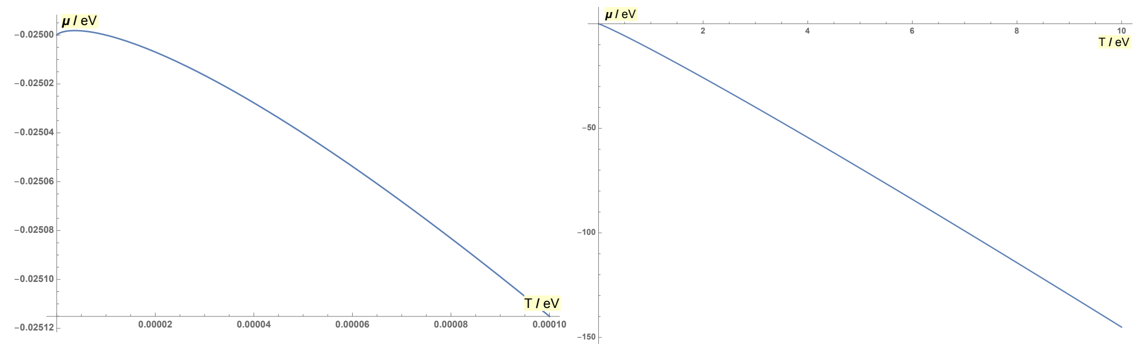
and so

$$\rho_0 T\ln(1+e^{\beta\mu}) \approx \frac{1}{2}N_D, \tag{61}$$

and

$$
\begin{aligned}
\mu &\approx T \ln(e^{N_D/(2\rho_0 T)} - 1) \\
&\approx T \ln(\frac{N_D}{2\rho_0 T}).
\end{aligned} \tag{62}
$$

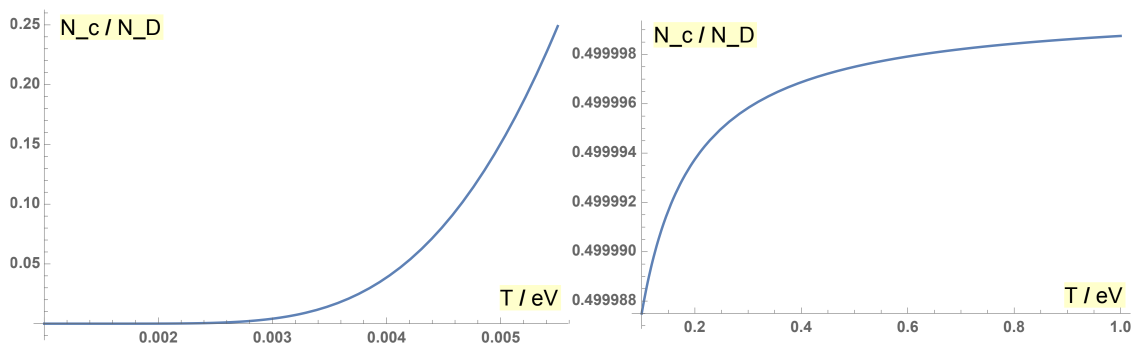
(d) See Fig. 2 and Fig. 3.



(a) $T \ll \delta$

(b) $T \gg \delta$

Figure 2: Plot of the chemical potential as a function of T in the regime $T \ll \delta$ (left), and $T \gg \delta$ (right).



(a) $T \ll \delta$

(b) $T \gg \delta$

Figure 3: Plot of the number of carriers as a function of T in the regime $T \ll \delta$ (left), and $T \gg \delta$ (right).

(e) When $T \ll \delta$,

$$
\begin{aligned}
e^{\beta\mu} &\approx \exp\Big[-\frac{\beta\delta}{2} + \frac{1}{2}\ln\frac{N_D}{\rho_0 T}\Big] \\
&= \sqrt{\frac{N_D}{\rho_0 T}} e^{-\beta\delta/2}.
\end{aligned} \tag{63}
$$

Therefore,

$$
\begin{aligned}
N_{\text{carriers}} &= \rho_0 T \ln(1 + e^{\beta\mu}) \\
&\approx \rho_0 T e^{\beta\mu} \\
&\approx \sqrt{N_D \rho_0 T} e^{-\delta/(2T)}.
\end{aligned} \tag{64}
$$

When $T \gg \delta$,

$$\begin{aligned} e^{\beta\mu} &\approx e^{\beta T \ln(\frac{N_D}{2\rho_0 T})} \\ &= \frac{N_D}{2\rho_0 T}. \end{aligned} \tag{65}$$

Therefore,

$$\begin{aligned} N_{\text{carriers}} &= \rho_0 T \ln(1 + e^{\beta\mu}) \\ &\approx \rho_0 T \ln(1 + \frac{N_D}{2\rho_0 T}) \\ &\approx \rho_0 T \left[\frac{N_D}{2\rho_0 T} - \frac{1}{2} \left(\frac{N_D}{2\rho_0 T} \right)^2 \right] \\ &\approx \frac{N_D}{2} - \frac{1}{8} \frac{N_D^2}{\rho_0 T}. \end{aligned} \tag{66}$$