Ph135 - Problem Set 5

November 23, 2018

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

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

(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

$$|p\rangle = \frac{1}{\sqrt{L_1 L_2}} e^{i(p_1 x + p_2 y)}, \tag{6}$$

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

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

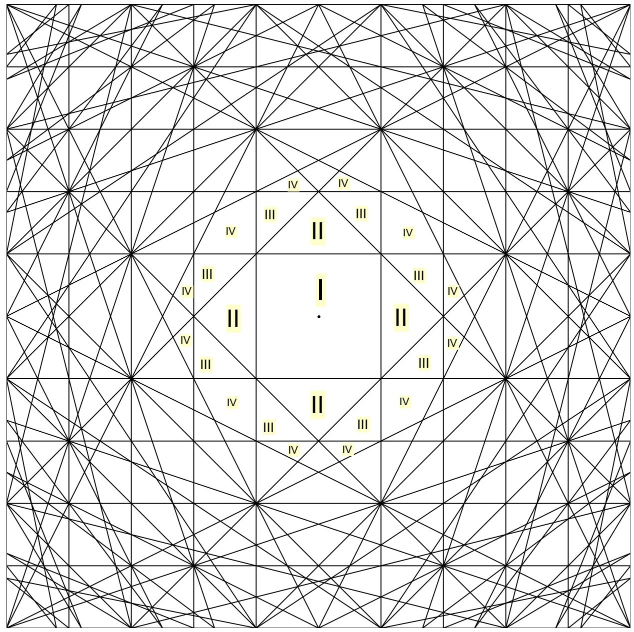

Figure 1: Illustration of the Brillouin zones.

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

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

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

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

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

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

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

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

Therefore,

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

Hence

$$
M = UDU^\dagger, \tag{42}
$$

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

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

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

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

Then

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

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,

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

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

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