Solid State Theory
Solution Sheet 7

Exercise 7.1 Bound and Antibound States in One Dimension

Expressing the real-space operators $\hat{c}_j$ through momentum-space operators $\hat{c}_k$ via

$$\hat{c}_j = \frac{1}{\sqrt{N}} \sum_k e^{ikj} \hat{c}_k \tag{1}$$

and obtain the Hamiltonian

$$\mathcal{H} = \sum_k (-2t \cos k) \hat{c}_k^\dagger \hat{c}_k + \frac{1}{N} \sum_k \sum_{k'} (-\Delta t)(e^{ik'} + e^{-ik}) \hat{c}_k^\dagger \hat{c}_{k'}. \tag{2}$$

We make the most general Ansatz for a state in momentum-space

$$|\Psi\rangle = \sum_q A_q \hat{c}_q^\dagger |0\rangle \tag{3}$$

This state should satisfy the Schrödinger equation

$$\mathcal{H}|\Psi\rangle = E|\Psi_\pm\rangle. \tag{4}$$

From this equation, we obtain

$$\sum_k (-2t \cos k) A_k \hat{c}_k^\dagger |0\rangle + \frac{1}{N} \sum_k \sum_q (-\Delta t) A_q (e^{iq} + e^{-ik}) \hat{c}_k^\dagger |0\rangle = \sum_k E A_k \hat{c}_k^\dagger |0\rangle. \tag{5}$$

In order that $|\Psi\rangle$ is an eigenstate, the condition

$$\frac{1}{N} \sum_q (-\Delta t) A_q (e^{iq} + e^{-ik}) = (E + 2t \cos k) A_k \tag{6}$$

has to be fulfilled for all k, which can be rewritten as

$$\frac{(-\Delta t)}{E + 2t \cos k} \frac{1}{N} \sum_q A_q e^{iq} + \frac{(-\Delta t) e^{-ik}}{E + 2t \cos k} \frac{1}{N} \sum_q A_q = A_k. \tag{7}$$

We once sum this equation over k and once multiply this equation by e^{ik} and obtain the set of equations

$$\frac{1}{N} \sum_k \frac{(-\Delta t)}{E + 2t \cos k} \frac{1}{N} \sum_q A_q e^{iq} + \frac{1}{N} \sum_k \frac{(-\Delta t) e^{-ik}}{E + 2t \cos k} \frac{1}{N} \sum_q A_q = \frac{1}{N} \sum_k A_k \tag{8}$$

$$\frac{1}{N} \sum_k \frac{(-\Delta t) e^{ik}}{E + 2t \cos k} \frac{1}{N} \sum_q A_q e^{iq} + \frac{1}{N} \sum_k \frac{(-\Delta t)}{E + 2t \cos k} \frac{1}{N} \sum_q A_q = \frac{1}{N} \sum_k e^{ik} A_k. \tag{9}$$

By introducing $c_0 = \sum_k A_k$ and $c_1 = \sum_k A_k e^{ik}$, we can write this set of equations as a matrix equation

$$\begin{pmatrix} 1 - \frac{1}{N} \sum_k \frac{(-\Delta t) e^{-ik}}{E + 2t \cos k} & -\frac{1}{N} \sum_k \frac{(-\Delta t)}{E + 2t \cos k} \\ -\frac{1}{N} \sum_k \frac{(-\Delta t)}{E + 2t \cos k} & 1 - \frac{1}{N} \sum_k \frac{(-\Delta t) e^{ik}}{E + 2t \cos k} \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{10}$$

As the sum runs in the range $[-\pi, \pi]$ only the even part of the integrand survives and we have a matrix equation of the form

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{11}$$

with

$$a = 1 - \frac{1}{N} \sum_k \frac{(-\Delta t) \cos k}{E + 2t \cos k}, \tag{12}$$

$$b = -\frac{1}{N} \sum_k \frac{(-\Delta t)}{E + 2t \cos k}. \tag{13}$$

In order to have a solution, the determinant of the matrix above should vanish, i.e. $a^2 - b^2 = 0$, from which follows that $a = \pm b$. We now perform the continuum limit such that

$$a = 1 - \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{(-\Delta t) \cos k}{E + 2t \cos k}, \tag{14}$$

$$b = -\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{(-\Delta t)}{E + 2t \cos k}. \tag{15}$$

and we obtain the condition

$$1 = (-\Delta t) \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\pm 1 + \cos k}{E + 2t \cos k} \tag{16}$$

For $|E| > 2t$, this integral can be calculated using the integral

$$\int_0^{\pi} \frac{dq}{2\pi} \frac{1}{x + \cos q} = \begin{cases} \frac{1}{2\sqrt{x^2-1}} & x > 1 \\ -\frac{1}{2\sqrt{x^2-1}} & x < -1 \end{cases} \tag{17}$$

and we obtain for $E > 2t$

$$1 = \frac{\Delta t}{2t}(-1 + \sqrt{\frac{E \mp 2t}{E \pm 2t}}) \tag{18}$$

which has a solution only for the lower sign and we obtain

$$E = 2t + \frac{\Delta t^2}{t + \Delta t}. \tag{19}$$

In the same way, we find for $E < -2t$ a solution

$$E = -2t - \frac{\Delta t^2}{t + \Delta t}. \tag{20}$$

Exercise 7.2 Peierls' Instability in 1D

We set the lattice constant for the whole task to $a = 1$.
For the eigenstates of our system we first only consider the electronic part of the Hamiltonian,

$$\mathcal{H}_{\text{el}} = \sum_{i,s} (c^{\dagger}_{i+1s} c_{is} + h.c.)(-t + \alpha \delta u_i). \tag{21}$$

We change to momentum space by introducing the corresponding electronic operators,

$$c_{is}^\dagger = \frac{1}{\sqrt{L}} \sum_k e^{-ikr_i} c_{ks}^\dagger. \tag{22}$$

While the first part of the sum obviously yields

$$\mathcal{H}_{\text{diag}} = \sum_{k,s} (-2t \cos k) c_{ks}^\dagger c_{ks}, \tag{23}$$

more care has to be taken for the calculation of the second term: by using

$$\delta u_i = u_0 \cos q r_i. \tag{24}$$

we find

$$\mathcal{H}_{\text{offd}} = \frac{\alpha u_0}{2} \sum_k \left[(e^{i(k+q)} + e^{-ik}) c_{ks}^\dagger c_{k+qs} + (e^{i(k)} + e^{-i(k+q)}) c_{k+qs}^\dagger . c_{ks} \right]. \tag{25}$$

a) We now want to consider the half filled case, i.e. $n = 1$. In this case, the Fermi energy is exactly $\epsilon_{\text{F}} = 0$ and we have a nesting vector $q = \pi$. This results in a periodicity of twice the lattice constant, the unit cell is doubled and thus the first Brillouin zone is folded back. We can thus write the Hamiltonian as

$$\mathcal{H} = {\sum_{k,s}}' \boldsymbol{c}_{ks}^\dagger \mathcal{H}_k \boldsymbol{c}_{ks} \tag{26}$$

where

$$\mathcal{H}_k = \begin{pmatrix} -2t \cos k & -2i\alpha u_0 \sin k \\ 2i\alpha u_0 \sin k & 2t \cos k \end{pmatrix} \tag{27}$$

and the primed sum $\sum'$ only runs over the reduced Brillouin zone, $k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$. We can now write the $\mathcal{H}_k$ in terms of Pauli spin-matrices,

$$\mathcal{H}_k = \sigma_y 2\alpha u_0 \sin k - \sigma_z 2t \cos k. \tag{28}$$

The diagonalization of this matrix thus corresponds to a rotation of the vector $(0, 2\alpha u_0 \sin k, -2t \cos k)$ around the x-axis. The angle of rotation is given by

$$\omega(k) = -\arctan(\frac{\alpha u_0}{t} \tan(k)). \tag{29}$$

We thus immediately find the eigenenergies which are just the length of the vector:

$$\xi_{k\pm} = \pm 2\sqrt{t^2 \cos^2 k + \alpha^2 u_0^2 \sin^2 k}. \tag{30}$$

With this trick, it is also straight forward to find the transformation matrix: Since a rotation in the spin space is in general given by

$$U_{\boldsymbol{\omega}} = e^{-i\boldsymbol{\sigma}\cdot\boldsymbol{\omega}} = \cos\frac{\omega}{2} - i\hat{\omega}\cdot\boldsymbol{\sigma} \sin\frac{\omega}{2} \tag{31}$$

with $\omega = |\boldsymbol{\omega}|$ and $\hat{\omega} = \boldsymbol{\omega}/\omega$, we find for our new operators

$$\begin{pmatrix} b_{ks-} \\ b_{ks+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\omega}{2} & -i\sin\frac{\omega}{2} \\ -i\sin\frac{\omega}{2} & \cos\frac{\omega}{2} \end{pmatrix} \begin{pmatrix} c_{ks} \\ c_{k+\pi s} \end{pmatrix}. \tag{32}$$

Eventually, we can now calculate the density of states using

$$k = \arccos\left(\sqrt{\frac{\xi^2 - 4t^2}{4\alpha^2 u_0^2 - 4t^2}}\right) \tag{33}$$

which follows directly from eq. (30). Thus the density of states yields

$$\rho(\xi) = 2 \cdot 2\frac{L}{2\pi}\left|\frac{\partial k}{\partial \xi}\right| = \frac{2L}{\pi}\left|\frac{\xi}{\sqrt{(\xi^2 - 4t^2)(\xi^2 - 4\alpha^2 u_0^2)}}\right| \tag{34}$$

with squareroot singularities at the band edges. The results of this part are summarized in fig. 1.

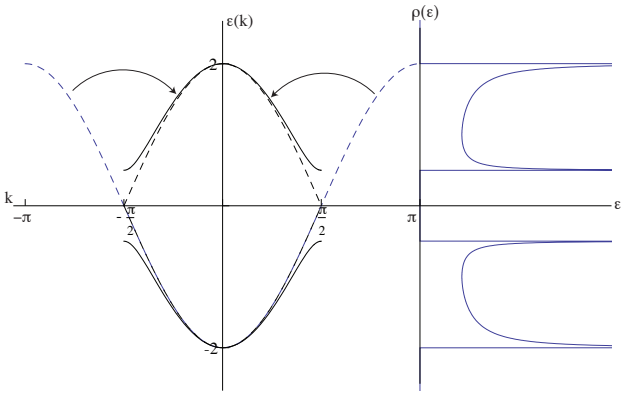

Figure 1: Combined plot of the dispersion and the density of states of the one-dimensional chain with no fixed positions for the atoms. On the left side, the arrows indicate the folding of the Brillouin zone. On the right side, one sees the square root singularities of the density of states,typical for one-dimensional systems, occurring at the band edges.

b) To calculate the total energy we first again consider the electronic part: For T=0, only the lower band is filled and thus the energy (per length) yields

$$\begin{aligned} E_{\text{el}} &= \frac{2}{L}{\sum_k}' \xi_{k-} = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} \xi_{k-} dk && (35)\\ &= -\frac{4}{\pi}\int_0^{\pi/2} \sqrt{t^2\cos^2 k + \alpha^2 u_0^2 \sin^2 k} dk && (36)\\ &= -\frac{4t}{\pi}\int_0^{\pi/2} \sqrt{1 - (1 - \frac{\alpha^2 u_0^2}{t^2})\sin^2 k} dk && (37)\\ &= -\frac{4t}{\pi} E\left(\frac{\pi}{2}, \sqrt{1 - \frac{\alpha^2 u_0^2}{t^2}}\right) && (38) \end{aligned}$$

where the first factor of two comes from the spins and in the last line we have used the elliptic function of the second kind as given on the exercise sheet.
For large λ the displacement of an atom costs a lot of energy and we only expect a

very small u_0 so that we can expand in $k' = \sqrt{1-k^2} = \alpha u_0/t$. The total energy is then

$$E_{\rm tot} \approx -\frac{4t}{\pi} - \left(\frac{2\alpha^2}{t\pi}\left(\log\frac{4t}{\alpha u_0} - \frac{1}{2}\right) - \frac{\lambda}{2}\right) u_0^2. \tag{39}$$

We see that for small enough u_0 the expression in the bracket becomes positive and the total energy is reduced with respect to the energy without any displacements.

c) We now want to calculate

(i) $\rho_i = \sum_s \langle c_{is}^\dagger c_{is}\rangle = \frac{2}{L}\sum_{k,k'} e^{-i(k-k')r_i}\langle c_{ks}^\dagger c_{k's}\rangle$

(ii) $\tilde{\rho}_i = \sum_s \langle c_{is}^\dagger c_{i+1s}\rangle = \frac{2}{L}\sum_{k,k'} e^{-i(k-k')r_i} e^{ik'}\langle c_{ks}^\dagger c_{k's}\rangle$.

where the first one is the average electron density per atom and the second one is a measure for the electron density on the bond between i and $i+1$.
Before continuing we note that the ground state of the system is given in terms of the new operators $b_{k\alpha}$ and the only expectation values not vanishing are $\langle b_{ks-}^\dagger b_{ks-}\rangle$. Since the original operators are given as

$$c_{ks} = \cos\frac{\omega(k)}{2} b_{ks-} + i\sin\frac{\omega(k)}{2} b_{ks+} \tag{40}$$

$$c_{k+\pi s} = i\sin\frac{\omega(k)}{2} b_{ks-} + \cos\frac{\omega(k)}{2} b_{ks+}, \tag{41}$$

this means that the only non vanishing matrix elements in terms of the original operators are

$$\langle c_{ks}^\dagger c_{k's}\rangle = \cos^2\frac{\omega(k)}{2}\delta_{k,k'} \tag{42}$$

$$\langle c_{ks}^\dagger c_{k'+\pi s}\rangle = i\sin\frac{\omega(k)}{2}\cos\frac{\omega(k)}{2}\delta_{k,k'} \tag{43}$$

$$\langle c_{k+\pi s}^\dagger c_{k'+\pi s}\rangle = \sin^2\frac{\omega(k)}{2}\delta_{k,k'} \tag{44}$$

$$\langle c_{k+\pi s}^\dagger c_{k's}\rangle = -i\sin\frac{\omega(k)}{2}\cos\frac{\omega(k)}{2}\delta_{k,k'} \tag{45}$$

$$\tag{46}$$

We can thus write the density per site as

$$\rho_i = \frac{2}{L}\sum_{k,k'} e^{-i(k-k')r_i}\langle c_{ks}^\dagger c_{k's}\rangle \tag{47}$$

$$= \frac{2}{L}{\sum_k}'\left(\cos^2\frac{\omega(k)}{2} + \sin^2\frac{\omega(k)}{2}\right) + i\sin\frac{\omega(k)}{2}\cos\frac{\omega(k)}{2}(1-1) \tag{48}$$

$$= \frac{2}{L}{\sum_k}' = 1 \tag{49}$$

For the 'density per bond' we can again split the sum into parts with equal momentum and parts with momentum differing by π. For the first ones we find

$$\tilde{\rho}_i^{\rm const} = \frac{2}{L}{\sum_k}'\Big(e^{ik}\langle c_{ks}^\dagger c_{ks}\rangle + e^{i(k+\pi)}\langle c_{k+\pi s}^\dagger c_{k+\pi s}\rangle\Big) \tag{50}$$

$$= \frac{2}{L}{\sum_k}' e^{ik}\Big(\cos^2\frac{\omega(k)}{2} - \sin^2\frac{\omega(k)}{2}\Big) \tag{51}$$

$$= \frac{2}{L}{\sum_k}'\Big(\cos k\cos\omega(k) + i\sin k\cos\omega(k)\Big) = \frac{2}{L}{\sum_k}'\cos k\cos\omega(k) \tag{52}$$

In the last step we have used that $\cos\omega(k)$ is an even function in k (cf. eq. (29) and thus $\sin k \cos\omega(k)$ is an odd function,thus vanishing when summed over.
For the latter part we find

$$\begin{aligned}
\tilde{\rho}_i^{\text{osc}} &= \frac{2}{L}{\sum_k}' \Big(e^{i\pi r_i} e^{ik} \langle c^\dagger_{k+\pi s} c_{ks} \rangle + e^{-i\pi r_i} e^{i(k+\pi)} \langle c^\dagger_{ks} c_{k+\pi s} \rangle \Big) && (53)\\
&= \frac{2}{L}{\sum_k}' e^{ik} \cos\frac{\omega(k)}{2} \sin\frac{\omega(k)}{2} \Big(e^{-i\pi r_i} - e^{i\pi r_i} \Big) && (54)\\
&= -\frac{2\sin(\pi r_i)}{L}{\sum_k}' \Big(i\cos k \sin\omega(k) - \sin k \sin\omega(k) \Big) && (55)\\
&= \frac{2\sin(\pi r_i)}{L}{\sum_k}' \sin k \sin\omega(k) && (56)
\end{aligned}$$

Here, we used the fact that $\omega(k)$ is odd and hence is $\sin\omega(k)$.
We indeed see that the bond density is composed of a constant term and an oscillating term. We can now analyze this density in the two limits:

- $\lambda \to \infty$: In that case, the displacement of the atoms will go to zero, $u_0 \to 0$ and thus $\omega \to 0$, too. Consequenty, the oscillating term vanishes while the constant term becomes,
$$\tilde{\rho}_i = \frac{1}{\pi}. \tag{57}$$
- $\lambda \to 0$: In this case, displacement of an atom does not cost any energy and the total displacement of two atoms becomes $u_0 = \min\{\frac{t}{\alpha}, 1\}$. For the case where $\alpha \geq t$, this corresponds to a gap of $4t$ and the dispersion is completely flat, the electrons are localized. In that case $\omega = k$ and the bond density is given as
$$\tilde{\rho}_i = \tilde{\rho}_i^{\text{const}} + \tilde{\rho}_i^{\text{osc}} = \frac{1}{2}(1 + \sin\pi r_i) \tag{58}$$
which means that the bond charge is alternatively 0 or 1.