Solid State Theory
Solution Sheet 4

FS 12
Prof. M. Sigrist

Exercise 4.1 One-dimensional model of a semiconductor

The Hamilton operator is $H_1 = H_0 + V$ where

$$H_0 = -t \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right), \tag{1}$$

$$V = v \sum_i (-1)^i \; c_i^\dagger c_i. \tag{2}$$

[a] Let us consider the case $v = 0$. We write

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikj} c_k^\dagger, \qquad c_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k, \tag{3}$$

where $k \in [-\pi, \pi)$ and $kN = 2\pi n$, $n \in \mathbb{Z}$. The above expression is plugged into Eq. (1) and we obtain

$$H_0 = -\frac{t}{N} \sum_{k,k',j} \left(e^{i[kj - k'(j+1)]} + e^{i[k(j+1) - ik'j]} \right) c_k^\dagger c_{k'} \tag{4}$$

$$= -t \sum_{k,k'} c_k^\dagger c_{k'} \left(e^{-ik'} + e^{ik} \right) \underbrace{\frac{1}{N} \sum_j e^{i(k-k')j}}_{\delta_{k,k'}} = \sum_k \underbrace{(-2t\cos k)}_{\epsilon_k} \, c_k^\dagger c_k \;, \tag{5}$$

where we have made use of the Bravais sum.[1]

Let us define the following one-particle state: $|\phi_k\rangle = c_k^\dagger |0\rangle$ where $|0\rangle$ is the vacuum. It fulfills

$$c_k^\dagger c_k |\phi_k\rangle = c_k^\dagger c_k c_k^\dagger |0\rangle = c_k^\dagger (1 - c_k^\dagger c_k)|0\rangle = c_k^\dagger |0\rangle = |\phi_k\rangle, \tag{6}$$

and consequently

$$H_0 |\phi_k\rangle = \epsilon_k |\phi_k\rangle. \tag{7}$$

Therefore, $|\phi_k\rangle$ is an eigenstate of the Hamilton operator. Similar procedure may be performed also with any-particle states $c_{k_1}^\dagger c_{k_2}^\dagger \ldots c_{k_n}^\dagger |0\rangle$.

[b] Let's consider now the case $v \neq 0$. Again, the expression (3) is plugged into V:

$$V = v \sum_{k,k'} \Big[\underbrace{\frac{1}{N} \sum_j e^{i\pi j} \, e^{i(k-k')j}}_{\delta_{k,k'+\pi}} \Big] c_k^\dagger c_{k'} \;, \tag{8}$$

where we have used identity $(-1)^j \equiv e^{i\pi j}$ (for integer j). It follows that

$$H_1 = \sum_{k \in [-\pi/2, \pi/2]}^{\prime} \left(\epsilon_k \, c_k^\dagger c_k + \epsilon_{k+\pi} \, c_{k+\pi}^\dagger c_{k+\pi} + v \, c_k^\dagger c_{k+\pi} + v \, c_{k+\pi}^\dagger c_k \right) \;. \tag{9}$$

[1] A more precise form of the Bravais sum is $\sum_j e^{i(k-k')j} = N\delta_{k,k'+G}$, where G may be arbitrary reciprocal vector (in our case $G = 2n\pi$).

From now on we will work only in the reduced Brillouin zone ($k \in [-\pi/2, \pi/2]$), for which does stand the denotation $\sum'$. Note that

$$\epsilon_{k+\pi} = -2t\cos(k+\pi) = 2t\cos k = -\epsilon_k. \tag{10}$$

Introducing

$$\bar{c}_k = \begin{pmatrix} c_k \\ c_{k+\pi} \end{pmatrix} \tag{11}$$

the Hamilton operator is written in matrix form

$$H_1 = \sum_k{}' \bar{c}_k^\dagger \hat{H}_1 \bar{c}_k, \tag{12}$$

where

$$\hat{H}_1 = \begin{pmatrix} \epsilon_k & v \\ v & -\epsilon_k \end{pmatrix}. \tag{13}$$

We define new operators a_k and b_k according to

$$\bar{c}_k = \begin{pmatrix} c_k \\ c_{k+\pi} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k & -u_k \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} = U\bar{\alpha}_k, \tag{14}$$

$$H_1 = \sum_k{}' \bar{\alpha}_k^\dagger U^\dagger \hat{H}_1 U \bar{\alpha}_k. \tag{15}$$

We can choose U such that $U^\dagger \hat{H}_1 U$ is diagonal. The energies are obtained from the secular equation

$$\det \begin{pmatrix} \epsilon_k - \lambda & v \\ v & -\epsilon_k - \lambda \end{pmatrix} = \lambda^2 - \epsilon_k^2 - v^2 = 0 \tag{16}$$

which has the solutions

$$\lambda = \pm\sqrt{\epsilon_k^2 + v^2} = \pm E_k. \tag{17}$$

Furthermore, one finds

$$u_k = \frac{v}{\sqrt{2E_k(E_k+\epsilon_k)}}, \qquad v_k = -\sqrt{\frac{E_k+\epsilon_k}{2E_k}}. \tag{18}$$

Finally, the Hamilton operator is written in the eigenbasis

$$H_1 = \sum_k{}' \left(-E_k\, a_k^\dagger a_k + E_k\, b_k^\dagger b_k\right). \tag{19}$$

[c] The band structure of the alternating chain is shown in Fig. 1. The gap between valence and conduction band is $\Delta = 2E_{\pm\pi/2} = 2v$. The ground state for $N/2$ electrons on the chain is given by

$$|\Omega\rangle = \prod_{k=-\pi/2}^{\pi/2} a_k^\dagger |0\rangle. \tag{20}$$

Compared to a) we now have one fully filled band with a finite gap for all kinds of excitations.

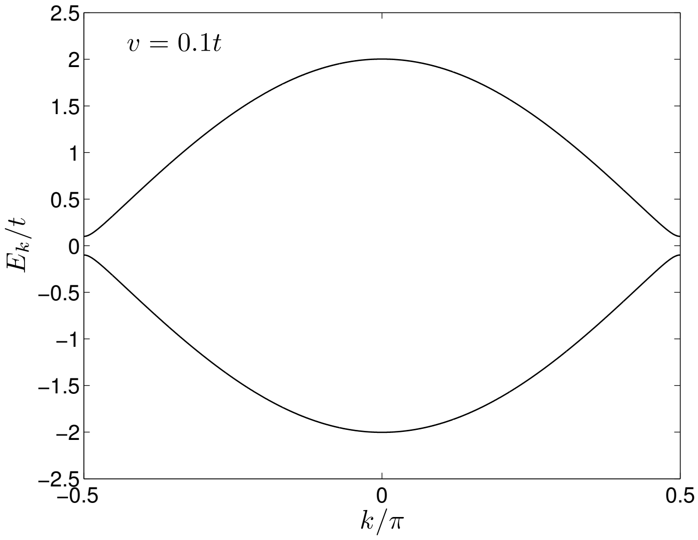

Figure 1: The two bands of the alternating chain.

Exercise 4.2 Coulomb interaction - excitons

We want to study the influence of the electron-electron interaction on the excitation spectrum of the half-filled chain.

[a] In the following we show that the repulsive interaction between the electrons leads to an attractive interaction between the electrons in the conduction band and the holes in the valence band.

We consider the following repulsive interaction:

$$U = u\sum_{i=1}^{N} n_i n_{i+1} = u\sum_{i=1}^{N/2} n_{2i}(n_{2i-1} + n_{2i+1}). \tag{21}$$

We want to find a simple expression in terms of the operators a_k and b_k. We start with the density operator $n_j = c_j^\dagger c_j$.

$$\begin{aligned}
n_{2j} &= \frac{1}{N}\sum_k\sum_{k'} e^{i(k-k')2j}\, c_k^\dagger c_{k'} \\
&= \frac{1}{N}{\sum_k}'{\sum_{k'}}' e^{i(k-k')2j}(c_k^\dagger c_{k'} + c_k^\dagger c_{k'+\pi} + c_{k+\pi}^\dagger c_{k'} + c_{k+\pi}^\dagger c_{k'+\pi}) \\
&= \frac{1}{N}{\sum_k}'{\sum_{k'}}' e^{i(k-k')2j}\, \underbrace{(c_k^\dagger + c_{k+\pi}^\dagger)}_{\approx -\sqrt{2}b_k^\dagger}\underbrace{(c_{k'} + c_{k'+\pi})}_{\approx -\sqrt{2}b_{k'}} \\
&\approx \frac{2}{N}{\sum_k}'{\sum_{k'}}' e^{i(k-k')2j}\, b_k^\dagger b_{k'}.
\end{aligned} \tag{22}$$

Here, we used that $u_{\pm\pi/2} = -v_{\pm\pi/2} = 1/\sqrt{2}$. Note that the above approximation is only valid in the vicinity of $k = \pm\pi/2$. However, for $u \ll v, t$ this is the region which is most affected by the interaction and the approximation is justified in this limit. In a similar way one shows

$$n_{2j\pm1} \approx \frac{2}{N}{\sum_k}'{\sum_{k'}}' e^{i(k-k')(2j\pm1)}\, a_k^\dagger a_{k'}. \tag{23}$$

In the vicinity of the band gap, namely for $k \approx \pm\pi/2$, the 'a-particles' live solely on the odd lattice sites whereas the 'b-particles' are exclusively on the even lattice sites. In other words, the electrons near the Fermi surface (for $v = 0$) have optimally arranged themselves to gain as much energy as possible from the potential V. This means that if an electron-hole pair is created we find hat the electron will mainly be on the even sites while the hole will be on the odd sites. This is in fact the reason why we need a *non-local* interaction between the electrons (as modeled by U) in order to have an attractive interaction between holes and electrons. A local interaction (which anyway is not possible for spinless fermions) would not be able to do this job.

Using Eqs. (22), (23) and (21) we obtain

$$
\begin{aligned}
U &\approx \frac{4u}{N^2} \sum_{k_1,\ldots,k_4}{}' \sum_{j=0}^{N/2} e^{i(k_1-k_2+k_3-k_4)2j} \left(e^{i(k_3-k_4)} + e^{-i(k_3-k_4)}\right) b^\dagger_{k_1} b_{k_2} a^\dagger_{k_3} a_{k_4} \qquad (24)\\
&\approx \frac{4u}{N} \sum_{k_1,\ldots,k_4}{}' \delta_{k_1+k_3,k_2+k_4} \cos(k_3-k_4) b^\dagger_{k_1} b_{k_2} a^\dagger_{k_3} a_{k_4} \ . \qquad (25)
\end{aligned}
$$

With the substitution

$$
k_1 \to k' + q \qquad k_2 \to k + q \qquad k_3 \to k \qquad k_4 \to k' \tag{26}
$$

the constraint $k_1 + k_3 = k_2 + k_4$ is automatically fulfilled and we obtain

$$
U \approx -\frac{4u}{N} \sum_{k,k',q}{}' \cos(k-k') a_{k+q} b^\dagger_k b_{k'} a^\dagger_{k'+q} \qquad \cancel{+ 4u \sum_k b^\dagger_k b_k} \tag{27}
$$

as on the exercise sheet. The minus sign in the above equation stems from the exchange of the fermionic operator $a^\dagger_{k'+q}$ with three fermionic operators. This minus sign is very important since it yields an attraction between electrons and holes. In addition, in Eq. (27) we dropped a term proportional to the total number of electrons in the conduction band which is irrelevant for the following discussion.

[b] In the following all summations run over the reduced Brillouin zone. The Hamilton operator $H = H_1 + U$ with the approximation (27) for U separately preserves the number of electrons and holes and therefore we can use the following ansatz for the wave function of the exciton:

$$
|\psi_q\rangle = \sum_k{}' A^q_k a_{k+q} b^\dagger_k |\Omega\rangle. \tag{28}
$$

Note that this ansatz yields exact eigenstates of H only in the case when U is approximated according to Eq. (27). The exact U does not preserve the number of electrons and holes separately and leads to a complicated many-body problem.

The coefficients A^q_k and the excitation energy ω_q of the exciton have to be determined such that

$$
(\tilde{H}_1 + U)|\psi_q\rangle = \omega_q |\psi_q\rangle \tag{29}
$$

where $\tilde{H}_1 = H_1 - E_0$, meaning that energies are measured with respect to the ground state energy E_0. For this we need the action of U on an exciton state,

$$
U|\psi_q\rangle = -\frac{4u}{N} \sum_{k'}{}' \sum_{k''}{}' A^q_{k'} \cos(k'-k'') a_{k''+q} b^\dagger_{k''} |\Omega\rangle, \tag{30}
$$

and the action of $\tilde{H}_1$,

$$\tilde{H}_1|\psi_q\rangle = {\sum_k}' A_k^q (E_k + E_{k+q}) a_{k+q} b_k^\dagger |\Omega\rangle. \tag{31}$$

Consequently, the Eq.(29) written component by component has to hold

$$(E_k + E_{k+q} - \omega_q) A_k^q = \frac{4u}{N} {\sum_{k'}}' A_{k'}^q \cos(k' - k) \tag{32}$$

We assume that $u \ll v, t$. In this case the bound state will be strongly extended in real space, meaning that A_k^q is localized in k-space. Therefore, in Eq. (32) we can put the cos-factor out of the sum and approximate it by 1.[2] Then, dividing both sides by $(E_k + E_{k+q} - \omega_q)$ and summing over k yields

$$\frac{1}{4u} = \frac{1}{N} {\sum_k}' \frac{1}{E_k + E_{k+q} - \omega_q}. \tag{36}$$

The solutions of this equation for $q = 0$ for a small chain ($N = 8$) are shown in Fig. 2. For each $0 < u < \infty$ there is an exciton excitation with energy smaller then the gap Δ. Now we have revealed a bound state called exciton.

[c] In the following we want to calculate the energy dispersion ω_q of the excitons for small q. For this we write the sum as an integral

$$\frac{1}{4u} = I := \frac{1}{2} \frac{1}{N/2} {\sum_k}' \frac{1}{E_k + E_{k+q} - \omega_q} = \frac{1}{2} \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \frac{dk}{E_k + E_{k+q} - \omega_q}. \tag{37}$$

For small u the integral has to become large. Since the exciton energy lies within the gap the main contributions to the integral are from the vicinity of $k = \pm\pi/2$. We therefore expand the denominator around $k = \pm\pi/2$ and for small q's:

$$E_k + E_{k+q} \approx 2v + \frac{2t^2}{v} \underbrace{\left((k \mp \frac{\pi}{2})^2 + (k + q \mp \frac{\pi}{2})^2 \right)}_{2(k \mp \frac{\pi}{2} + \frac{q}{2})^2 + \frac{q^2}{2}} \tag{38}$$

[2] Note that setting the cos-factor to 1 does mean on-site Coulomb interaction instead of nearest-neighbor interaction. The proper way how to solve the Eq. (32) is to use

$$\cos(k - k') = \cos k \cos k' - \sin k \sin k' \ , \tag{33}$$

and write down two self-consistent equations for $F_1^q \equiv \sum_{k'}' A_{k'}^q \cos k'$ and $F_2^q \equiv \sum_{k'}' A_{k'}^q \sin k'$ by dividing Eq. (32) by $(E_k + E_{k+q} - \omega_q)$, multiplying by $\cos k$ (or $\sin k$) and subsequent summation over k:

$$F_1^q = \frac{4u}{N} {\sum_k}' \frac{F_1^q \cos^2 k + F_2^q \cos k \sin k}{E_k + E_{k+q} - \omega_q} \ , \tag{34}$$

$$F_2^q = \frac{4u}{N} {\sum_k}' \frac{F_1^q \cos k \sin k + F_2^q \sin^2 k}{E_k + E_{k+q} - \omega_q} \ , \tag{35}$$

and the non-trivial solution of this homogeneous set of equations exist only if the determinant does vanish... As you see the approximation does greatly simplify the further analysis.

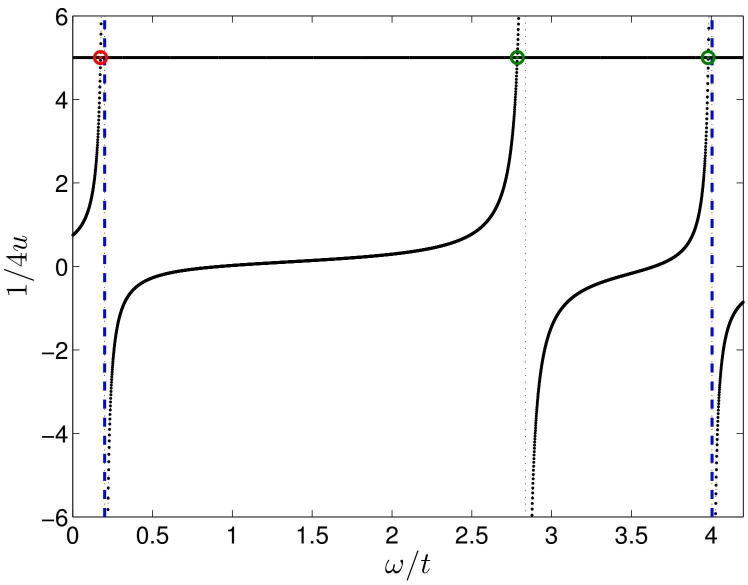

Figure 2: Graphical solution of Eq. (36), for $q = 0$, $v = 0.1$ and $N = 8$. The circles mark the solutions for $1/4u = 5$ and the dashed lines denote the band edges. Note that there is exactly one solution (red circle; corresponding to the exciton excitation) below the particle-hole continuum (which is in this plot discrete due to finiteness of N).

So the denominator has minima $2v + t^2q^2/v$ at $k = \pm\pi/2 - q/2$. For small u, ω_q is only little less then the minimum and almost all the contributions come from the vicinity of the minimum. Therefore, we introduce a cutoff Λ and write the integral symmetrically around 0,

$$I \approx \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda}\frac{dk}{2v + \frac{t^2q^2}{v} - \omega_q + \frac{4t^2k^2}{v}} = \frac{1}{2\pi}\sqrt{\frac{v}{4t^2}}\int_{-\tilde{\Lambda}}^{\tilde{\Lambda}}\frac{dx}{a^2+x^2}, \tag{39}$$

where we have defined $a^2 = 2v - \omega_q + t^2q^2/v$. Finally, we obtain

$$I \approx \frac{1}{2\pi}\sqrt{\frac{v}{4t^2}}\frac{1}{a}\arctan\left(\frac{x}{a}\right)\Big|_{-\tilde{\Lambda}}^{\tilde{\Lambda}} \approx \sqrt{\frac{v}{4t^2}}\frac{1}{2a}\ . \tag{40}$$

Here we let the cutoff to infinity. Solution ω_q of Eq. (37) yields the dispersion

$$\omega_q = 2v - \frac{u^2v}{t^2} + \frac{t^2}{v^2}q^2 = 2v - \frac{u^2v}{t^2} + \frac{q^2}{2(2m^*)} \tag{41}$$

where $m^* = v/(4t^2)$ is the effective mass near the energy gap. Thus, the electron-hole pair has twice the mass of a single electron or hole.

[d] To show how $f(r - r')$ is related to A_k^0, we insert the Fourier expansion of

$$a_k = \frac{1}{2L}\int_{-L}^{L} dr e^{ikr}\ a\ (r)\ , \qquad b_k^\dagger = \frac{1}{2L}\int_{-L}^{L} dr'\ e^{-ikr'}\ b^\dagger(r')\ , \tag{42}$$

into the continuous form of the exciton state (for now considering finite volume, thus $k = n\pi/L$),

$$|\psi_{q=0}\rangle = \sum_k A_k^0 a_k b_k^\dagger|\Omega\rangle = \frac{1}{2L}\int_{-L}^{L} dx\, dx'\ \underbrace{\frac{1}{2L}\sum_k A_k^0 e^{ik(r-r')}}_{f(r-r')}\ a\ (r) b^\dagger(r')\ . \tag{43}$$

Now we do a limit $L \to \infty$ to conclude that

$$f(\rho) = \frac{1}{2\pi} \int_{\mathbb{R}} dk A_k^0 e^{ik\rho} \ . \tag{44}$$

In order to evaluate $f(\rho)$, we use eq. (32) (note that the right-hand-side is a constant), so that $A_k^0 \propto (2E_k - \omega_0)^{-1}$; plugging into Eq. (44) yields to

$$f(\rho) \propto m^* \int_{-\infty}^{\infty} dk \frac{e^{ik\rho}}{k^2 + m^* \left(2v - \omega_0\right)} \ ; \qquad 2v - \omega_0 > 0 \ ; \tag{45}$$

which can be evaluated using the method of residues. Note that $f(\rho)$ is real due to antisymmetry of the imaginary part of the integral. Moreover, $f(\rho)$ is symmetric, as $f(-\rho) = f(\rho)^* = f(\rho)$. For $\rho > 0$, the contour may be closed in the upper half of the complex plane where there is a single simple pole located at $\tilde{k} = i\sqrt{m^* \left(2v - \omega_0\right)}$,

$$f(\rho) \propto m^*(2\pi i) \frac{e^{i\tilde{k}|\rho|}}{2\tilde{k}} \propto e^{-|\rho|\sqrt{m^*(2v-\omega_0)}} \ , \tag{46}$$

so that $\lambda = \left[m^* \left(2v - \omega_0\right)\right]^{-1/2}$.