Charge gap in the one–dimensional dimerized Hubbard model at quarter-filling

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Abstract

We propose a quantitative estimate of the charge gap that opens in the one-dimensional dimerized Hubbard model at quarter-filling due to dimerization, which makes the system effectively half-filled, and to repulsion, which induces umklapp scattering processes. Our estimate is expected to be valid for any value of the repulsion and of the parameter describing the dimerization. It is based on analytical results obtained in various limits (weak coupling, strong coupling, large dimerization) and on numerical results obtained by exact diagonalization of small clusters. We consider two models of dimerization: alternating hopping integrals and alternating on-site energies. The former should be appropriate for the Bechgaard salts, the latter for compounds where the stacks are made of alternating $TMTSF$ and $TMTTF$ molecules.
I. INTRODUCTION

A large number of compounds exhibit one-dimensional electronic properties that can be described by a quarter-filled Hubbard model with some kind of dimerization. For instance, the Bechgaard salts \((TMTSF)_2X\) and \((TMTTF)_2X\), where \(X\) denotes an anion like \(ClO_4^{-}\), \(PF_6^{-}\), \(Br^{-}\), etc... can be regarded concerning their electronic structure as being essentially one-dimensional systems above a crossover temperature \(T_x\) of the order of 30K\(^1\). From stoichiometry it is known that there are 3 electrons in the HOMO for each pair \((TMTSF)_2\), so that the system is 3/4-filled in terms of electrons or quarter-filled in terms of holes. In the following we will always use hole notation and consider quarter-filled systems. A reasonable description of these properties should be provided by the dimerized Hubbard model defined by the Hamiltonian

\[
H = H_0 + H_{\text{int}} ,
\]

where the kinetic part of the Hamiltonian is (see Fig. \[1\])

\[
H_0 = -t_1 \sum_{i \text{even}, \sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) - t_2 \sum_{i \text{odd}, \sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) .
\]

The operators \(c_{i,\sigma}^\dagger\) create particles in the HOMO of \(TMTSF\) or \(TMTTF\) with spin \(\sigma\). We have included two hopping integrals \(t_1\) and \(t_2\) \((t_1 > t_2)\) to describe the dimerization along the stacks\[^2\]. The dispersion of this model is given by \(\varepsilon(k) = \sqrt{t_1^2 + t_2^2 + 2t_1t_2\cos k}\) and is depicted in Fig. \[2\]. The important parameters are the dimerization gap \(\Delta_D = 2(t_1 - t_2)\) that opens at the Brillouin zone boundary and the total bandwidth \(W = 2(t_1 + t_2)\).

To the hopping part of the Hamiltonian we have to add an interaction part to describe the correlation between the electrons. For simplicity, we have chosen the form of the standard Hubbard model

\[
H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow} ,
\]

where \(U\) is the on-site Coulomb repulsion and \(n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}\).
This model should also provide a good description of salts like \((FA)_2PF_6\), where \(FA\) stands for Fluoranthenyl, which undergo a Peierls transition leading to dimerization along the stacks at a temperature of order 190K. There is another class of materials however for which a modified version of the previous model is more appropriate. These materials are related to the Bechgaard salts, but the stacks now consist of alternating \(TMTTF\) and \(TMTSF\) molecules. A minimal model in this case would be a Hubbard model with alternating atomic on–site energies, with a kinetic part of the form

\[
H_0 = -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma}^{\phantom{\dagger}} + \text{h.c.)} - \varepsilon_0 \sum_{\text{seven, }\sigma} (c_{i,\sigma}^\dagger c_{i,\sigma}^{\phantom{\dagger}} - c_{i+1,\sigma}^\dagger c_{i+1,\sigma}^{\phantom{\dagger}}),
\]  

where \(2\varepsilon_0\) is the energy splitting between the HOMO of the \(TMTSF\) and \(TMTTF\). The dispersion relation is given by \(\varepsilon(k) = \sqrt{\varepsilon_0^2 + 2t^2 + 2t^2 \cos k}\). It has the same form as in the previous case. The dimerization gap is now given by \(\Delta_D = \sqrt{\varepsilon_0^2 + 4t^2}\) and the bandwidth by \(W = 2\varepsilon_0\). However, although the dispersion relations are the same, the two models are different because the interaction part will not be the same when expressed in terms of the operators that diagonalize the kinetic part of the Hamiltonian. Let us also note that a similar model has been recently proposed by Sudbø et al. as a one dimensional analog of the copper oxide layers in the high temperature superconductors. A model where dimerization is induced via alternating on–site repulsions has also been studied.

It is clear from Fig. 2 that, due to dimerization, the system is effectively half–filled. In this case, it is known from the general theory of one–dimensional models with umklapp scattering that an on–site repulsion of arbitrary size will open a gap in the charge sector. This has been shown explicitly in the case of the Hubbard model for which exact results are available from the Bethe ansatz solution. In the general case, where no exact solution is known, a quantitative estimate of the gap is not available so far. This is unfortunate because such an estimate is necessary to interprete the activated behaviour of the resistivity observed at relatively low temperatures in several compounds, which in turn provides an estimate of the magnitude of the Coulomb repulsions. An analysis of that sort has already been performed for the Bechgaard salts of the \(TMTTF\) family on the basis of a preliminary
determination of the charge gap in the model with alternating hopping amplitudes.

In this paper, we propose a quantitative estimate of the gap in the case of the dimerized models described above that should be valid in the whole range of parameters. This estimate is based on approximations that provide analytical expressions in various limits, and on numerical calculations using Lánczos diagonalization of small clusters. As we think that the results might be useful to readers that do not want to go through the details of the calculation, we start in Sec. II with a detailed account of the results, including analytical expressions, tables and curves, that can be used independently of the rest of the paper. Then, in Sec. III we explain how and for which values of the parameters numerical estimates can be obtained on the basis of exact diagonalization of small clusters. The following sections are devoted to the approximate expressions that can be obtained analytically in various limits: Sec. IV summarizes exact results in a few trivial limits, Sec. V deals with the large dimerization case, where the dimerization gap is larger than both the repulsion and the Fermi velocity, and Secs. VI and VII with the case of weak and strong coupling, respectively. The summary can be found in Section II. Throughout the paper, subsections A will deal with the model with alternating hopping amplitudes, and subsections B with the model with alternating on–site energies.

II. SUMMARY OF RESULTS

In Fig. 3 we have illustrated the different regimes in which analytical results have been obtained as a function of the model parameters. In this section, we give a summary of these results for each model.

A. Alternating hopping amplitudes
1. **Numerical estimates:**

Using exact diagonalization of small clusters, we have obtained estimates of the charge gap for intermediate values of repulsion $U$ and for $t_2 \leq 0.5 t_1$. The limitation comes from the size of the clusters (maximum 16 sites), so that only large gaps corresponding to correlation lengths smaller than 16 sites could be extracted. The numerical results are shown in Fig. 4a. They are in good agreement with analytical approximations in different limits, as we will show in the subsequent paragraphs.

2. **Large dimerization:**

In this limit we have mapped our model onto the exactly solvable Hubbard model at half-filling and we found that the gap is given by:

$$\Delta_c = \begin{cases} 
\frac{t_2 8}{2\pi} \sqrt{\frac{U}{t_2} e^{-2\pi t_2/U} e^{-\pi t_2/4t_1}}, & \text{if } t_1 \gg t_2 \gg U; \\
\frac{U}{2} - \frac{U^2}{16t_1} - 2t_2, & \text{if } t_1 \gg U \gg t_2.
\end{cases} \quad (2.1)
$$

In Fig. 5 we have compared our estimate with numerical results (curve a) for $t_2 = 0.1$, where we can see the crossover from the exponential regime (curve d) to the linear one (curves b and c, b is without the quadratic term $U^2/16t_1$) for $U/t_1 \sim 0.5$.

3. **Weak coupling limit**

In the weak coupling limit ($U \ll t_1, t_2$), using the RG group method and results from the large dimerization limit, we found that the gap is exponentially small [see Eq. (6.24)]:

$$\Delta_c = at_1 \sqrt{\frac{U}{t_1}} \exp \left( -bt_1 \frac{U}{U} \right), \quad (2.2)$$

where the parameters $a$ and $b$ can be found in Table I for different values of $t_2/t_1$. 
In Fig. [6] we compare the numerical values of the gap for $t_2 = 0.3$ and $t_2 = 0.4$ with the weak coupling approximation Eq. (2.2). We can see that up to $U/t_1 = 4$ the weak coupling formula gives very good results.

4. Strong coupling limit

When the on-site repulsion is large enough ($U \gg t_1, t_2, 4t_1^2/t_2$), the effective Hamiltonian of our model is a $t-J$ like Hamiltonian. Applying degenerate perturbation theory, we found that the charge gap is equal to the dimerization gap with a $1/U$ correction [see Eq. (7.20)]:

$$\Delta_c = \Delta_D \left(1 - \frac{t_1}{U}\right),$$

(2.3)

where the parameters $\Delta_D/t_1$ and $c$ can be found for different values of $t_2/t_1$ in Table [IV].

5. Intermediate region

On the basis of the previous results, we can propose an estimate of the gap for any value of the parameters. This can be achieved by using Padé approximants to connect the exact results we have obtained for $U$ small and $U$ large respectively. For $t_2 \geq 0.2$, we have used the weak coupling expression up to $U_0$, where $U_0$ is not too large (actually we choose $U_0/t_1 = b$ for $t_2/t_1 \leq 0.5$ and $U_0/t_1 = 4$ for $t_2/t_1 > 0.5$) and Padé approximants of the form

$$f(U) = \frac{a_1 U + \Delta_D U^2}{b_2 + b_1 U + U^2}$$

(2.4)

for $U > U_0$. The coefficients are chosen in such a way that, for $U \rightarrow +\infty$, the Padé approximant gives the correct large $U$ behavior given by Eq. (2.3) and that, at $U = U_0$, the resulting curve and its derivative be continuous. The curves depend weakly on the value of $U_0$: Changing the value of $U_0$ by 50% affects the value of the gap by less than 10%. In Table [IV] we give the values of the coefficients and of $U_0$ for different values of $t_2/t_1$.

For $t_2 = 0.1t_1$ we have also used a Padé approximant, but now the limiting behaviors were determined by the second equation in (2.1), which is valid for the intermediate values
of $U$ for $t_2$ small, and by Eq. (2.3) in the large $U$ limit. At the crossing point of the weak-coupling expression and the Padé approximant, we have got rid of the kink (see Fig. 3) by a linear interpolation. The resulting curves for $t_2/t_1$ ranging from 0.1 to 0.9 are presented in Fig. 4.

**B. Alternating on-site energies**

1. **Large dimerization:**

   In this limit we have mapped our model to the exactly solvable Hubbard model at half-filling and we found that the gap is given by:

   $\Delta_c = \begin{cases} \frac{8}{\pi} t \sqrt{\frac{U}{2\varepsilon_0}} \exp\left(-\frac{\pi t^2}{U \varepsilon_0}\right), & \text{if } \varepsilon_0 \gg t \gg U; \\ \frac{U - \frac{2t^2}{\varepsilon_0}}{\varepsilon_0}, & \text{if } \varepsilon_0 \gg U \gg t. \end{cases}$

   (2.5)

2. **Weak coupling limit**

   In the weak coupling limit ($U \ll \varepsilon_0, t$), on the basis of renormalization group analysis and results from the large dimerization limit, the gap is exponentially small and is given by [see also Eq. (6.38)]:

   $\Delta_c = \sqrt{\frac{U}{t}} \exp\left(-b \frac{t}{U}\right).$  

   (2.6)

   The parameters $a$ and $b$ are given in Table III for some values of $\varepsilon_0/t$.

3. **Strong coupling limit**

   When the on-site repulsion is large enough ($U \gg \varepsilon_0, t, 4t^2/\varepsilon_0$), the effective Hamiltonian of our model is again a $t-J$ like Hamiltonian and we found that the charge gap is [see also Eq. (7.36)]:

   $\Delta_c = \ldots$
\[ \Delta_c = \Delta_D \left( 1 - \frac{t}{U} \right) . \]  

(2.7)

The parameters \( \Delta_D \) and \( c \) are given in Table III for some values of \( \varepsilon_0/t \).

III. NUMERICAL SIMULATIONS

We have done intensive numerical simulations based on Lánczos diagonalization of small clusters for the model with alternating hopping integrals. Our numerical estimation for the gap was based on the usual formula

\[ \Delta_c = \lim_{N \rightarrow +\infty} \Delta_c(N) , \]

\[ \Delta_c(N) = E(N + 1; 2N) + E(N - 1; 2N) - 2E(N; 2N) , \]

(3.1)

where \( E(M; L) \) is the ground state energy for \( M \) particles on \( L \) sites. We have obtained results for systems of 4, 8, 12 and 16 sites. Periodic (resp. antiperiodic) boundary conditions have been used for \( L=8 \) and 16 (resp. \( L=4 \) and 12) to have open-shell systems. Typical results are shown on Fig. 7, where we have plotted \( \Delta_c(N) \) as a function of \( 1/N \). Good estimates can be obtained only when the exponential regime \( \Delta_c(N) \sim \exp(-cst/N) \) has been reached for \( N = 16 \). But the exponential regime is obtained when \( \nu_c/N < \Delta_c \), that is \( N > \nu_c/\Delta_c \). So we can only obtain good numerical estimates of the gap when \( \Delta_c \) is not too small, i.e. when \( U \) and \( \Delta_D \) are not too small. The gap can then be extracted by use of the Shanks transformation\(^{13}\) given by

\[ \Delta_c = \frac{\Delta(N_1)\Delta(N_3) - \Delta(N_2)^2}{\Delta(N_1) + \Delta(N_3) - 2\Delta(N_2)} . \]

(3.2)

This procedure has been shown to work very well in the case of the Haldane gap of spin-1 chains\(^{14}\). Applying it for \( (N_1, N_2, N_3) = (4, 8, 12) \) and \( (8, 12, 16) \) respectively gave similar results. The results quoted throughout this paper are those obtained for \( (8, 12, 16) \) because they are a priori better.

Another limitation comes from the size of the repulsion. When \( U \) is very large, the convergence of the Lánczos algorithm becomes very slow, and it is no longer possible to get
good values of the energy. So, in summary, good estimates have been obtained for $\Delta_D \gtrsim t_1$ and $1 \lesssim U/t_1 \lesssim 60$. This does not cover the range of parameters for actual compounds, for which one often has $\Delta_D/t_1$, or $U/t_1 \ll 1$, and analytical methods are clearly needed to complement these numerical results. In fact, the analytical methods developed in the rest of the paper provide an estimate of the gap for any value of the parameters, and the numerical simulations have been only used to check the analytical results.

IV. EXACT RESULTS

A schematic picture of the regions of interest as a function of the model parameters are given in Fig. 3 for each model. Exact, although trivial, results can be deduced on the boundaries and they are summarized in this section.

A. Alternating hopping amplitudes

(i) $t_1 = t_2$: This is a quarter–filled Hubbard model and we know from the Bethe ansatz solution that there is no gap in the spectrum.

(ii) $t_2 = 0$: The Hamiltonian describes a set of independent systems, each system consisting of two sites. At 1/4 filling there is one electron for each pair of sites in the ground state. The gap is then given by $\Delta_c = E_0(0) + E_0(2) - 2E_0(1)$, where $E_0(n)$ is the ground state energy of $n$ electron on a pair of sites. These energies are $E_0(0) = 0$, $E_0(1) = -2t_1$ and $E_0(2) = (U - \sqrt{U^2 + 16t_1^2})/2$ and the charge gap is

$$
\Delta_c = 2t_1 + \frac{U}{2} - \sqrt{\frac{U^2}{4} + 4t_1^2} = \begin{cases} 
\frac{U}{2} - \frac{U^2}{16t_1}, & \text{if } t_1 \gg U; \\
2t_1 - \frac{4t_1^2}{U}, & \text{if } t_1 \ll U.
\end{cases}
$$

(iii) $U = 0$: The band structure is given on Fig. 2. The Fermi energy is in the middle of the lower band, and $\Delta_c = 0$. 

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(iv) $U = +\infty$: The energies that enter Eq. (3.1) are the same as for free spinless fermions at half–filling, because the energy is independent of the spin when $U = +\infty$ for open boundary conditions (or for periodic one in the limit $N \to +\infty$). So, the charge gap is actually the same as for a system of spinless fermions described by the kinetic part of the Hamiltonian at half–filling, which is nothing but the dimerization gap (see Fig. 2). So $\Delta_c = \Delta_D$.

B. Alternating on–site energies

(i) $\varepsilon_0 = 0$: This is a quarter filled Hubbard model, and there is no gap.

(ii) $\varepsilon_0 = +\infty$: The odd sites are outside the Hilbert space. The ground state has one particle per even site, and the first excited state has a doubly occupied site. So clearly $\Delta_c = U$.

(iii) $U = 0$: The Fermi energy is in the middle of the band, and $\Delta_c = 0$.

(iv) $U = +\infty$: The dimerization gap $2\varepsilon_0$ and the charge gap coincides, like in the case of alternating hoppings.

(v) In the atomic limit ($t = 0$) the charge gap is given by $\Delta_c = \min(U, 2\varepsilon_0)$.

V. THE LIMIT OF LARGE DIMERIZATION

In this section, we consider the limit of large dimerization, that is the limit where the dimerization gap $\Delta_D$ is much larger than both the width of each subband and the repulsion $U$. This limit corresponds to $t_1 \gg t_2, U$ for the model with alternating hoppings and to $\varepsilon_0 \gg t, U$ for the model with alternating on–site energies. It is particularly interesting because in both cases the model can be mapped onto the half–filled Hubbard model, so that we can use the exact result provided by the Bethe Ansatz for the charge gap.
A. Alternating hopping amplitudes

To diagonalize the part of the Hamiltonian corresponding to the hopping terms \( t_1 \), we introduce bonding and antibonding operators defined by:

\[
b_{j,\sigma} = \frac{1}{\sqrt{2}} \left[c_{j,\sigma} + c_{j+1,\sigma}\right], \quad a_{j,\sigma} = \frac{1}{\sqrt{2}} \left[c_{j,\sigma} - c_{j+1,\sigma}\right],
\]

(5.1)

where \( j \) is now even. In terms of these operators, the Hamiltonian becomes

\[
H = -t_1 \sum_{\text{even},\sigma} \left( b_{j,\sigma}^\dagger b_{j,\sigma} - a_{j,\sigma}^\dagger a_{j,\sigma} \right) - \frac{t_2}{2} \sum_{\text{even},\sigma} \left( b_{j,\sigma}^\dagger b_{j+2,\sigma} + b_{j+2,\sigma}^\dagger b_{j,\sigma} + b_{j,\sigma}^\dagger a_{j+2,\sigma} + a_{j+2,\sigma}^\dagger b_{j,\sigma} - a_{j,\sigma}^\dagger a_{j+2,\sigma} - a_{j+2,\sigma}^\dagger a_{j,\sigma} \right) + \frac{U}{2} \sum_{\text{even}} \left( n_{d,j}\uparrow + n_{f,j}\downarrow \right) \left( n_{d,j}\downarrow + n_{f,j}\uparrow \right) + \left( b_{j,\uparrow}^\dagger a_{j,\uparrow} + a_{j,\uparrow}^\dagger b_{j,\uparrow} \right) \left( b_{j,\downarrow}^\dagger a_{j,\downarrow} + a_{j,\downarrow}^\dagger b_{j,\downarrow} \right).
\]

(5.2)

The bonding and the antibonding bands are separated by a large energy \( 2t_1 \). The occupation of the upper band is thus negligible and to zeroth order in \( 1/t_1 \) we get

\[
H_{\text{eff}} = -\frac{t_2}{2} \sum_{\text{even},\sigma} \left( b_{j,\sigma}^\dagger b_{j+2,\sigma} + \text{h.c.} \right) + \frac{U}{2} \sum_{\text{even}} n_{b,j}\uparrow n_{b,j}\downarrow + O(1/t_1),
\]

(5.3)

which is nothing but the regular Hubbard model with a repulsion \( \tilde{U} = U/2 \) and a hopping integral \( \tilde{t} = t_2/2 \). Here the Hamiltonian acts on a Hilbert space where the antibonding states are all empty. The value of the gap in the half–filled Hubbard model is known exactly from the Bethe Ansatz solution. For small interaction (\( \tilde{U} \ll \tilde{t} \)), it is given by \( \Delta_c = (8\tilde{t}/\pi)\sqrt{\tilde{U}/\tilde{t}}\exp(-2\pi\tilde{U}/\tilde{t}) \), which, with our notations, reads

\[
\Delta_c = \frac{t_2}{2} 8 \frac{\sqrt{U}}{\pi} e^{-2\pi t_2/U}.
\]

(5.4)

For large interaction (\( U \gg t_2 \) but still \( U \ll t_1 \)), the exact expression becomes \( \Delta_c = U/2 - 2t_2 \).

To compare with other limits, it is useful to go to next order in \( 1/t_1 \). Using a Schrieffer–Wolff transformation, we can determine the \( 1/t_1 \) corrections to the zeroth order effective Hamiltonian by including scattering processes to the antibonding band and we get
\[ H_{\text{eff}} = -\frac{t_2}{2} \sum_{j \text{ even}, \sigma} (b_{j,\sigma}^\dagger b_{j+2,\sigma} + \text{h.c.}) + \left(\frac{U}{2} - \frac{U^2}{16t_1}\right) \sum_{j \text{ even}} n_{b,j,\uparrow} n_{b,j,\downarrow} \]
\[ + \frac{t_2^2}{8t_1} \sum_{j \text{ even}, \sigma} \left( b_{j-2,\sigma}^\dagger b_{j+2,\sigma} + b_{j+2,\sigma}^\dagger b_{j-2,\sigma} \right) + O\left(1/t_1^2\right). \quad (5.5) \]

The on-site repulsion is reduced by a \( U^2/16t_1 \), and a second nearest neighbor hopping appears. The formula for the gap is now modified to
\[ \Delta_c = \begin{cases} \frac{t_2}{2} \frac{8}{\pi} \sqrt{\frac{U}{t_2}} e^{-2\pi t_2/U} e^{-\pi t_2/4t_1}, & \text{if } U \ll t_2; \\ \frac{U}{2} - \frac{U^2}{16t_1} - 2t_2, & \text{if } U \gg t_2. \end{cases} \quad (5.6) \]

The second formula agrees with Eq. (4.1) when \( t_2 = 0 \). The first one will be used in Section VI. We have illustrated the above estimates of the gap on Fig. 5.

**B. Alternating on-site energies**

In the limit \( \epsilon_0 \gg U, t \) the occupation of the energetically lower lying even sites is much larger than that of the odd sites. Using this, we can again find an effective Hamiltonian starting from \( t = 0 \), in which case only the even sites are occupied. Switching on the hopping, the electrons can hop to the energetically unfavorable odd sites, and from those sites they can hop further. This second order virtual process produces an effective hopping of order \( t^2/2\epsilon_0 \) between the even sites, so that the effective Hamiltonian is given by
\[ H_{\text{eff}} = -\frac{t_2^2}{2\epsilon_0} \sum_{j \text{ even}, \sigma} (c_{j,\sigma}^\dagger c_{j+2,\sigma} + \text{h.c.}) + U \sum_{j \text{ even}} n_{j,\uparrow} n_{j,\downarrow}. \quad (5.7) \]

Here the Hamiltonian acts on a Hilbert space with empty odd sites. This effective Hamiltonian describes a half–filled Hubbard model with a hopping amplitude \( \tilde{t} = t^2/2\epsilon_0 \) and repulsion \( \tilde{U} = U \), so again we can use the expression of the charge gap for the Hubbard model. In the weak coupling limit \( U \ll t^2/\epsilon_0 \), we get
\[ \Delta_c = 8 \sqrt{\frac{\epsilon_0}{2\epsilon_0}} \exp\left(\frac{-\pi t^2}{U\epsilon_0}\right). \quad (5.8) \]

In the intermediate coupling limit, where \( U \) is larger than the effective hopping, but smaller then the energy splitting of the two bands \( \epsilon_0 \), the gap is given by \( \Delta_c = U - 2t^2/\epsilon_0 \).
VI. WEAK COUPLING LIMIT

In this limit we can first diagonalize the hopping part of the Hamiltonian and treat the interaction as a perturbation. To do that, we introduce the Fourier transforms of the electron creation and annihilation operators keeping in mind that there are two sites in the unit cell:

\[
\begin{align*}
  c_{k,\sigma} & = \sqrt{\frac{2}{L}} \sum_{j \text{ even}} e^{-ikj/2} c_{j,\sigma} \\
  \tilde{c}_{k,\sigma} & = \sqrt{\frac{2}{L}} \sum_{j \text{ odd}} e^{-ik(j-1)/2} c_{j,\sigma}.
\end{align*}
\]

(6.1)

Here \( L \) is the number of sites, \( L/2 \) is the number of unit cells, and the length of the unit cell is set to 1.

A. Alternating hopping amplitudes

The Fourier transform of the kinetic part of the Hamiltonian (1.2) is

\[
H_0 = -\sum_{k,\sigma} \left[ (t_1 + t_2 e^{-ik}) c_{k,\sigma}^\dagger \tilde{c}_{k,\sigma} + (t_1 + t_2 e^{ik}) \tilde{c}_{k,\sigma}^\dagger c_{k,\sigma} \right].
\]

(6.2)

Let us introduce annihilation operators for the electrons in the lower (\( d_{k,\sigma} \)) and upper (\( f_{k,\sigma} \)) bands by

\[
\begin{align*}
  d_{k,\sigma} & = \frac{1}{\sqrt{2}} \left[ s(k) c_{k,\sigma} + s^*(k) \tilde{c}_{k,\sigma} \right], \\
  f_{k,\sigma} & = \frac{1}{\sqrt{2}} \left[ s(k) c_{k,\sigma} - s^*(k) \tilde{c}_{k,\sigma} \right],
\end{align*}
\]

(6.3)

where \( s(k) = \exp i(\alpha_k/2 + k/4) \) and \( \alpha_k \) is defined by

\[
\tan \alpha_k = \frac{t_2 - t_1}{t_2 + t_1} \tan \frac{k}{2}, \quad \left( -\frac{\pi}{2} < \alpha_k < \frac{\pi}{2} \right).
\]

(6.4)

The hopping part of the Hamiltonian is now diagonal:

\[
H_0 = -\sum_{k,\sigma} \varepsilon(k) \left( d_{k,\sigma}^\dagger d_{k,\sigma} - f_{k,\sigma}^\dagger f_{k,\sigma} \right),
\]

(6.5)
with
\[ \varepsilon(k) = \sqrt{t_1^2 + t_2^2 + 2t_1t_2 \cos k} . \] (6.6)

The Fermi velocity \( v_F \) is given by
\[ v_F = \frac{t_1t_2}{\sqrt{t_1^2 + t_2^2}} = \frac{W^2 - \Delta_D^2}{8 \sqrt{(W^2 + \Delta_D^2)/2}} , \] (6.7)
where \( \Delta_D = 2(t_1 - t_2) \) is the dimerization gap and \( W = 2(t_1 + t_2) \) is the total bandwidth (see Section 1).

The Fourier transform of the Hamiltonian (1.3) describing the interaction is
\[ H_{\text{int}} = \frac{U}{L} \sum_{k_1,k_2,k_3,k_4} \left( c_{k_1,\uparrow}^\dagger c_{k_2,\downarrow}^\dagger c_{k_3,\downarrow} c_{k_4,\uparrow}^\dagger + c_{k_1,\uparrow}^\dagger c_{k_2,\downarrow}^\dagger \tilde{c}_{k_3,\downarrow} \tilde{c}_{k_4,\uparrow}^\dagger \right) , \] (6.8)

where \( k_1 + k_2 - k_3 - k_4 = Q \) is a vector of the reciprocal lattice. Usually \( Q = 0 \), but if one of the bands is half filled, the umklapp processes with \( Q = \pm 2\pi \) become important. Using the operators defined by Eq. (6.3), the interaction can be written as
\[ H_{\text{int}} = \frac{U}{2L} \sum_{k_1,k_2,k_3,k_4} \cos \left( \frac{\alpha_{k_1} + \alpha_{k_2} - \alpha_{k_3} - \alpha_{k_4}}{2} + \frac{Q}{4} \right) d_{k_1,\uparrow}^\dagger d_{k_2,\downarrow}^\dagger d_{k_3,\downarrow} d_{k_4,\uparrow} , \] (6.9)
where we have kept only the fermions near the Fermi energy.

From the interaction part of the Hamiltonian we can identify the interactions between the electrons near the Fermi surface, the so-called \( g \)-couplings of the \( g \)-ology. Usually these couplings are spin dependent. However, in our model the interaction is isotropic, thus we do not have to worry about the spin dependence, and they read:
\[ g_1 = g_2 = g_4 = \frac{U}{2} , \]
\[ g_3 = -\sin(2\alpha_F) \frac{U}{2} = \frac{\Delta_D}{W} \frac{2}{1 + (\Delta_D/W)^2} \frac{U}{2} . \] (6.10)

The umklapp scattering amplitude \( g_3 \) vanishes linearly with \( \Delta_D \) for small \( \Delta_D/W \), in agreement with the estimates obtained using perturbational arguments to get the strength of the umklapp scattering. Clearly, the model of Eq. (6.10) is not equivalent to the half-filled Hubbard model, for which all the \( g \) couplings are equal and given by \( U \).
In perturbation theory, the logarithmic corrections to the vertex generate the differential equations of the renormalization group (RG) approach when one integrates out the degrees of freedom far from the Fermi level. There are four differential equations altogether, but near half-filling we need only the equations which describe the charge degrees of freedom and give rise to the charge gap. As we know from Larkin and Sak, to account correctly for the fluctuations which give rise to the $\sqrt{U}$ factor in Eq. (5.4), we need the RG equations up to third order in $g$. Introducing $g = 2g_2 - g_1$ and denoting by $\tilde{g}$ the renormalized couplings corresponding to momentum cutoff $\tilde{D}$, the 3rd order RG equations we need are

$$\begin{align*}
\frac{d\tilde{g}}{d \ln \tilde{D}} &= -\frac{1}{\pi v_c} \tilde{g}^2 + \frac{1}{2\pi^2 v_c^2} \tilde{g}\tilde{g}_3^2, \\
\frac{d\tilde{g}_3}{d \ln \tilde{D}} &= -\frac{1}{\pi v_c} \tilde{g}\tilde{g}_3 + \frac{1}{4\pi^2 v_c^2} \left[ \tilde{g}^2 \tilde{g}_3 + \tilde{g}_3^3 \right],
\end{align*}$$

(6.11)

where $v_c = v_F + g_4/2\pi$ is the velocity of the charge excitations. There is a scaling invariant $C = (\tilde{g}^2 - \tilde{g}_3^2)/(2\pi v_c - \tilde{g})$, and the system of equations above can be rewritten as a single differential equation:

$$\frac{d\tilde{g}}{d \ln \tilde{D}} = \pi v_c \left( \frac{\tilde{g}^2}{\pi^2 v_c^2} + \frac{C \tilde{g}}{\pi^2 v_c^2} - \frac{2C}{\pi v_c} \right) \left( 1 - \frac{\tilde{g}}{2\pi v_c} \right).$$

(6.12)

Reducing the cutoff $\tilde{D}$, we scale towards the strong coupling region, where the RG equations are no longer valid. This cross-over occurs when the cutoff $\tilde{D}$ corresponds to an energy scale that has been identified with the charge gap. So integrating the scaling equations (6.12), we get

$$\int_{\Delta_c/v_c}^{\tilde{D}_0} d \ln \tilde{D} = -\int_{\tilde{g}(\Delta_c)}^{g} \frac{d\tilde{g}}{\pi v_c} \left( \frac{\tilde{g}^2}{\pi^2 v_c^2} + \frac{C \tilde{g}}{\pi^2 v_c^2} - \frac{2C}{\pi v_c} \right)^{-1} \left( 1 - \frac{\tilde{g}}{2\pi v_c} \right)^{-1},$$

(6.13)

where $\tilde{D}_0$ is the initial cutoff with $\tilde{g}(\tilde{D}_0) = g$ and $\tilde{g}_3(\tilde{D}_0) = g_3$. Keeping only the leading and next to leading terms of $g$, and introducing the notation $\xi = g_3/g$, one gets

$$\ln \frac{\Delta_c}{v_c} - \ln \tilde{D}_0 = \frac{1}{2} \ln \frac{\xi g}{\pi v_c} - \left( \frac{\pi v_c}{g} - \frac{1}{4} \right) \frac{\text{Arth} \sqrt{1 - \xi^2}}{\sqrt{1 - \xi^2}} + 1 + \ln C_{\Delta},$$

(6.14)

where the constant $\ln C_{\Delta}$ contains the terms like $1/\tilde{g}(\Delta_c)$ which are small compared to $1/g$, as $\tilde{g}$ scales towards the strong coupling limit. As in that region the RG equations are not
any more valid, all the possible corrections are incorporated in that constant\footnote{17}. We have separated $\frac{1}{4}$ from the constant $\ln C_\Delta$ for convenience.

Replacing $v_c$ by $v_F + g/2\pi$ ( $g_4 = g$ in the leading order in $U$), and exponentiating, we get

$$\Delta_c = C_\Delta \tilde{D}_0 v_F \sqrt{\frac{\xi g}{\pi v_F}} \exp \left( -\frac{\pi v_F}{g} \frac{\mathrm{Arth} \sqrt{1-\xi^2}}{\sqrt{1-\xi^2}} \right) \exp \left( -\frac{1}{4} \frac{\mathrm{Arth} \sqrt{1-\xi^2}}{\sqrt{1-\xi^2}} + \frac{1}{4} \right). \quad (6.15)$$

Its behavior in the case of small dimerization is given by

$$\Delta_c = C_\Delta \tilde{D}_0 v_F \sqrt{\frac{2g}{\pi v_F}} e^{1/4} \left( \frac{\xi}{2} \right)^{\left(\frac{\pi v_F}{g} + 3/4\right)}, \quad (6.16)$$

where we have used the fact that $\mathrm{Arth} \sqrt{1-\xi^2} \approx \ln(2/\xi)$ if $\xi \to 0$. This is the same form as found by Luther\cite{19} for the charge gap if the umklapp scattering is small compared to the $2g_2 - g_1$, which in our notation means $\xi \ll 1$ (see also Ref. \cite{10}).

Using the $g$-couplings of Eq. (6.10) in Eq. (6.15) provides us with the functional dependence of the gap on the repulsion $U$. This expression also includes a dependence on $t_2/t_1$. It does not give the full dependence on $t_2/t_1$ however. The reason is the following: Our estimate of the charge gap accounts neither for the curvature of the band (as the RG equations are based on a model with linear dispersion relation) nor for the possible processes involving the empty band. This virtual processes will contribute as higher order corrections in $U$ to the effective interactions near the Fermi surface. Since in the formula for the charge gap these effective couplings appear essentially as $\exp(-\pi v_F/g)$, the $U^2$ correction to the effective coupling will give an $O(1)$ correction, i.e. if we assume for a moment that $g = U - \gamma U^2 + O(U^3)$, then $1/g = 1/U + \gamma + O(U)$ and $\exp(-\pi v_F/g) = \exp(-\pi v_F\gamma) \exp(-\pi v_F/U)$. So the correction appears as a multiplying factor that depends on $t_2/t_1$ in the equation for the gap. Clearly, to get a quantitative estimate of the gap one has to include these contributions.

To be fully consistent with our determination of the $U$ dependence, which relies on RG equations up to third order in $g$ (see Eq. (6.11)), one should in principle calculate the vertex corrections to the coupling constants to third order in $U$. The problem with that program is that the calculation of the third order is hopelessly cumbersome. We think however that
a calculation of the vertex correction to second order in $U$ is sufficient. The procedure we have used is the following: First, we calculate the second order corrections to the effective interactions near the Fermi surface by integrating out all the electron states except those which are closer to the Fermi surface than some small cutoff $\tilde{D}_0$ in the lower band. Then, if the cut-off $\tilde{D}_0$ is small enough, the dispersion relation of the electrons within this cut-off around the Fermi surface is essentially linear and we can safely use the RG equations of Eq. (6.11) to decrease the cutoff further down to $\Delta_c/v_c$. Now, the cut-off $\tilde{D}_0$ can be taken very small: It just has to be larger than $\Delta_c/v_c$, and we already know that this quantity is exponentially small in the weak coupling limit. So this procedure should be valid. Finally, we will see that for small $\tilde{D}_0$ ($W/v_c \gg \tilde{D}_0 \gg \Delta_c/v_c$) the result for the gap is independent of the cutoff $\tilde{D}_0$.

To calculate the higher corrections in $U$, we must take into account the virtual processes that involve states in the upper band and consider the full interaction Hamiltonian instead of Eq. (6.9):

$$H_{\text{int}} = \frac{U}{2L} \sum_{k_1,k_2,k_3,k_4} \cos \left( \frac{\alpha_{k_1} + \alpha_{k_2} - \alpha_{k_3} - \alpha_{k_4}}{2} + \frac{Q}{4} \right) \times \left( d_{k_1,\uparrow}^\dagger d_{k_2,\downarrow}^\dagger d_{k_3,\downarrow} d_{k_4,\uparrow} + f_{k_1,\uparrow}^\dagger f_{k_2,\downarrow}^\dagger d_{k_3,\downarrow} d_{k_4,\uparrow} + d_{k_1,\uparrow}^\dagger d_{k_2,\downarrow}^\dagger f_{k_3,\downarrow} f_{k_4,\uparrow} + \ldots \right), \quad (6.17)$$

where we have written only the terms which are responsible for the second order corrections in $U$. To that order, the effective interactions are given by

$$g_1(\tilde{D}_0) = \frac{U}{2} - \frac{U^2}{4} (D_1 + D_3),$$

$$g_2(\tilde{D}_0) = \frac{U}{2} - \frac{U^2}{4} (D_1 + D_2 + D_3),$$

$$g_3(\tilde{D}_0) = -\sin(2\alpha_F) \frac{U}{2} - \frac{U^2}{4} (D_4 + D_5), \quad (6.18)$$

where we have denoted by $D_1, \ldots, D_5$ the diagrams contributing to the effective interaction (see Fig. 8). They are given by

$$D_1 = 2 \int_{\pi/2+\tilde{D}_0}^{\pi} \frac{dq}{2\pi} \frac{1}{2\varepsilon_F - 2\varepsilon(q)} + 2 \int_{\pi/2-\tilde{D}_0}^{\pi/2} \frac{dq}{2\pi} \frac{1}{2\varepsilon(q) - 2\varepsilon_F},$$
\[ D_2 = -2 \int_0^{\pi/2} \frac{dq}{2\pi} \cos^2(\alpha_F - (\alpha_q + \alpha_{q-q})/2) + \sin^2(\alpha_F + (\alpha_q + \alpha_{q-q})/2) \frac{\varepsilon(q) - \varepsilon(\pi - q)}{\varepsilon(q) - \varepsilon(\pi - q)}, \]
\[ D_3 = 2 \int_0^\pi \frac{dq}{2\pi 2\varepsilon_F + 2\varepsilon(q)}, \]
\[ D_4 = 4 \int_0^{\pi/2} \frac{dq}{2\pi} \cos(\alpha_F - (\alpha_q + \alpha_{q-q})/2) \sin(\alpha_F + (\alpha_q + \alpha_{q-q})/2) \frac{2\varepsilon_F + \varepsilon(q) + \varepsilon(\pi - q)}{\varepsilon(q) - \varepsilon(\pi - q)}, \]
\[ D_5 = -4 \int_0^{\pi/2} \frac{dq}{2\pi} \cos(\alpha_F - (\alpha_q + \alpha_{q-q})/2) \sin(\alpha_F + (\alpha_q + \alpha_{q-q})/2) \frac{2\varepsilon_F + \varepsilon(q) + \varepsilon(\pi - q)}{\varepsilon(q) - \varepsilon(\pi - q)}. \] (6.19)

Here \( \alpha_F \) and \( \varepsilon_F \) stands for \( \alpha(k_F) \) and \( \varepsilon(k_F) \).

The integrals \( D_1, D_2 \) and \( D_5 \) contains a logarithmic singularity \( \ln(2/\tilde{D}_0) \), and, after some algebra, one can separate these contributions, so that the effective interactions can be written as

\[ g_1(\tilde{D}_0) = \frac{U}{2} - \frac{U^2}{4} \frac{1}{\pi v_F} \left[ \ln \frac{2}{\tilde{D}_0} + \frac{A}{2} I_0^+(A) + O(\tilde{D}_0) \right], \]
\[ g_2(\tilde{D}_0) = \frac{U}{2} - \frac{U^2}{4} \frac{1}{\pi v_F} \left\{ \frac{1 - \sin^2(2\alpha_F)}{2} \ln \frac{2}{\tilde{D}_0} + \frac{A}{4} \left[ I_0^+(A) + I_0^-(A) \right] - \sin^2(2\alpha_F) \frac{A}{4} \left[ I_0^+(A) - I_0^-(A) \right] - \frac{A}{4} \sin^2(2\alpha_F) I_1(A) + O(\tilde{D}_0) \right\}, \]
\[ g_3(\tilde{D}_0) = -\sin(2\alpha_F) \left( \frac{U}{2} - \frac{U^2}{4} \frac{1}{\pi v_F} \left\{ -\ln \frac{2}{\tilde{D}_0} - \frac{A}{2} \left[ I_0^+(A) - I_0^-(A) \right] - \frac{A}{4} I_1(A) + \frac{A}{2} I_2(A) + O(\tilde{D}_0) \right\} \right), \] (6.20)

where \( A = 2t_1 t_2/(t_1^2 + t_2^2) \) and \( I_0^\pm, I_1 \) and \( I_2 \) are non–singular integrals given by:

\[ I_0^+(A) = \int_0^{\pi/2} d\varphi \frac{1}{1 + \sqrt{1 \pm A \cos(\varphi)}}, \]
\[ I_1(A) = \int_0^{\pi/2} d\varphi \left( \frac{1}{\sqrt{1 - A \cos(\varphi)}} - \frac{1}{\sqrt{1 + A \cos(\varphi)}} \right), \]
\[ I_2(A) = \int_0^{\pi/2} d\varphi \left( 1 + \frac{1}{\sqrt{1 - A^2 \cos^2(\varphi)}} \right) \frac{1}{2 + \sqrt{1 + A \cos(\varphi)} + \sqrt{1 - A \cos(\varphi)}}. \] (6.21)

For \( A \ll 1 \), they read:

\[ I_0^+(A) = \frac{\pi}{4} + \frac{A}{8} + O(A^2), \]
\[ I_1(A) = A + O(A^3) , \]
\[ I_2(A) = \pi/4 + O(A^2) . \]  

(6.22)

If it were only for a single band with linear dispersion relation these integrals near the \( \ln(2/\tilde{D}_0) \) would not appear.

Using the couplings of Eq. (6.20) in Eq. (6.15), we get

\[
\Delta_c = 2C_\Delta v_F \sqrt{\frac{2U}{\pi v_F}} (1 - A^2)^{1/4} \exp \left( -\frac{2\pi v_F \text{Arth}A}{U} \right) \times \exp \left( -\frac{1}{4} \frac{\text{Arth}A}{A} + \frac{1}{4} \right) e^{\tilde{C}(A)} [1 + O(\tilde{D}_0)] ,
\]

(6.23)

where, to first order, \( \tilde{D}_0 \) disappeared from the expression of the gap. This expression now describes the full functional dependence of \( \Delta_c \) on \( U/t_1 \) and \( t_2/t_1 \). The only thing that remains is to determine the prefactor \( C_\Delta \). This can be done as follows: From the Bethe ansatz solution of the Hubbard model, we know the value of the gap exactly in the limit of large dimerization [see Eq. (5.4)]. It is easily checked that in the limit \( t_2 \to 0 \) the functional dependence of Eq. (6.23) is the same as in Eq. (5.4). So we can use the result of Eq. (5.4) to determine the prefactor, and this gives

\[ C_\Delta = 2\sqrt{2/\pi} . \]

Our final expression for the gap in the weak coupling limit is thus

\[
\Delta_c = \frac{4v_F}{\pi} \sqrt{\frac{U}{v_F}} (1 - A^2)^{1/4} \exp \left( -\frac{2\pi v_F \text{Arth}A}{U} \right) \times \exp \left( -\frac{1}{4} \frac{\text{Arth}A}{A} + \frac{1}{4} \right) e^{\tilde{C}(A)} ,
\]

(6.24)

where \( A = 2t_1t_2/(t_1^2 + t_2^2) \) and \( \tilde{C}(A) \) is given by

\[
\tilde{C}(A) = \frac{1}{4A} \left[ 2(1 - A^2) I_0^- (A) + 2A^2 I_0^+ (A) - (1 - 2A^2) I_1 (A) - 2I_2 (A) \right] \\
+ \frac{\text{Arth}A}{4A^2} \left[ -2I_0^- (A) + (1 - A^2) I_1 (A) + 2(1 - A^2) I_2 (A) \right] .
\]

(6.25)

It is interesting to compare this approach with that of Larkin and Sak\textsuperscript{17}, who used slightly different arguments when they calculated the gap in the negative \( U \) Hubbard model in the small \( U \) limit. It can be shown very easily that our method is equivalent to theirs and gives the same result for the attractive Hubbard model.
B. Alternating on–site energies

The Fourier transform of the kinetic Hamiltonian (1.4) using the Fourier transforms of the operators defined in Eq. (6.1) is

\[ H_0 = -\varepsilon_0 \sum_{k,\sigma} \left( c_{k,\sigma}^\dagger c_{k,\sigma} - \tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma} \right) - 2t \cos(k/2) \sum_{k,\sigma} \left( e^{-ik/2} \tilde{c}_{k,\sigma}^\dagger \tilde{c}_{k,\sigma} + e^{ik/2} c_{k,\sigma}^\dagger c_{k,\sigma} \right) . \]  

(6.26)

It can be diagonalized in terms of new creation and annihilation operators defined by

\[ d_{k,\sigma} = c_{k,\sigma} \cos \beta_k + e^{-ik/2} \tilde{c}_{k,\sigma} \sin \beta_k , \]
\[ f_{k,\sigma} = c_{k,\sigma} \sin \beta_k - e^{-ik/2} \tilde{c}_{k,\sigma} \cos \beta_k , \]  

(6.27)

where \( \beta_k \) is given by

\[ \tan 2\beta_k = \frac{2t}{\varepsilon_0} \cos \frac{k}{2} , \quad \left( \frac{-\pi}{4} < \beta_k < \frac{\pi}{4} \right) . \]  

(6.28)

The kinetic part of the Hamiltonian reads

\[ H_0 = -\sum_{k,\sigma} \varepsilon(k) \left( d_{k,\sigma}^\dagger d_{k,\sigma} - f_{k,\sigma}^\dagger f_{k,\sigma} \right) , \]  

(6.29)

with

\[ \varepsilon(k) = \sqrt{\varepsilon_0^2 + 2t^2 + 2t^2 \cos k} . \]  

(6.30)

The dimerization gap opening at the Brillouin zone boundary is \( \Delta_D = 2\varepsilon_0 \), the 'total' bandwidth is \( W = 2\sqrt{\varepsilon_0^2 + 4t^2} \) and the Fermi velocity is

\[ v_F = \frac{t^2}{\sqrt{\varepsilon_0^2 + 2t^2}} . \]  

(6.31)

Replacing the new operators defined in Eq. (6.27) for the lower and upper band into the interaction Hamiltonian (6.8) we get:

\[ H_{\text{int}} = \frac{1}{L} \sum_{k_1,k_2,k_3,k_4} \left[ (\cos \beta_{k_1} \cos \beta_{k_2} \cos \beta_{k_3} \cos \beta_{k_4} \pm \sin \beta_{k_1} \sin \beta_{k_2} \sin \beta_{k_3} \sin \beta_{k_4}) \left( d_{k_1,\uparrow}^\dagger d_{k_2,\downarrow}^\dagger d_{k_3,\downarrow}^\dagger d_{k_4,\uparrow} \right) \\
+ (\sin \beta_{k_1} \cos \beta_{k_2} \cos \beta_{k_3} \cos \beta_{k_4} \mp \cos \beta_{k_1} \sin \beta_{k_2} \sin \beta_{k_3} \sin \beta_{k_4}) \right] \]  

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\begin{align}
\times & \left( f_{k_{1},\uparrow}^\dagger d_{k_{2},\downarrow} d_{k_{3},\downarrow} d_{k_{4},\uparrow} + f_{k_{1},\downarrow}^\dagger d_{k_{2},\uparrow} d_{k_{3},\uparrow} d_{k_{4},\downarrow} + d_{k_{1},\uparrow}^\dagger d_{k_{2},\uparrow} d_{k_{3},\downarrow} f_{k_{1},\uparrow} + d_{k_{1},\downarrow}^\dagger d_{k_{2},\downarrow} d_{k_{3},\uparrow} f_{k_{1},\downarrow} \right) \\
+ & \left( \cos \beta_{k_{1}} \cos \beta_{k_{2}} \sin \beta_{k_{3}} \sin \beta_{k_{4}} \pm \cos \beta_{k_{1}} \cos \beta_{k_{2}} \sin \beta_{k_{3}} \sin \beta_{k_{4}} \right) \\
\times & \left( f_{k_{1},\uparrow}^\dagger f_{k_{2},\downarrow}^\dagger d_{k_{3},\downarrow} d_{k_{4},\uparrow} + d_{k_{1},\uparrow}^\dagger d_{k_{2},\downarrow} d_{k_{3},\uparrow} f_{k_{1},\uparrow} \right) \\
+ & \ldots \right] , \tag{6.32}
\end{align}

with the constraint $k_{1} + k_{2} - k_{3} - k_{4} = Q$ and the upper (lower) signs stand for the normal $Q = 0$ (umklapp, $Q = \pm 2\pi$) scattering, respectively. There are altogether 16 terms, but we have kept only the terms which we need to calculate the $g$'s near the Fermi surface up to second order in $U$.

Like in the case of alternating hopping amplitudes, to determine the effective couplings $g$, we first integrate out the high energy processes up to some cutoff $\bar{D}_{0}$:

\begin{align}
g_{1}(\bar{D}_{0}) & = U(\cos^{4} \beta_{F} + \sin^{4} \beta_{F}) - U^{2} \left( D_{1} + 2D_{2} + D_{3} + 2D_{4} \right) , \\
g_{2}(\bar{D}_{0}) & = U(\cos^{4} \beta_{F} + \sin^{4} \beta_{F}) - U^{2} \left( D_{1} + 2D_{2} + D_{3} + D_{5} + 2D_{6} \right) , \\
g_{3}(\bar{D}_{0}) & = U(\cos^{4} \beta_{F} - \sin^{4} \beta_{F}) - U^{2} \left( 2D_{7} + D_{8} + D_{9} + 2D_{10} \right) , \tag{6.33}
\end{align}

where we have denoted by $D_{1}, \ldots, D_{10}$ the diagrams contributing to the effective interactions (see Fig. 3) which are given by

\begin{align}
D_{1} & = 2 \int_{\pi/2+\bar{D}_{0}}^{\pi} \frac{dq}{2\pi} \frac{\left( \cos^{2} \beta_{F} \cos^{2} \beta_{q} + \sin^{2} \beta_{F} \sin^{2} \beta_{q} \right)^{2}}{2\varepsilon_{F} - 2\varepsilon(q)} , \\
D_{2} & = 2 \int_{\pi/2}^{\pi} \frac{dq}{2\pi} \frac{\left( \cos^{2} \beta_{F} \cos \beta_{q} \sin \beta_{q} - \sin^{2} \beta_{F} \sin \beta_{q} \cos \beta_{q} \right)^{2}}{2\varepsilon_{F}} , \\
D_{3} & = 2 \int_{0}^{\pi/2} \frac{dq}{2\pi} \frac{\left( \cos^{2} \beta_{F} \sin^{2} \beta_{q} + \sin^{2} \beta_{F} \cos^{2} \beta_{q} \right)^{2}}{2\varepsilon_{F} + 2\varepsilon(q)} , \\
D_{4} & = -2 \int_{0}^{\pi/2} \frac{dq}{2\pi} \frac{\left( \cos^{2} \beta_{F} \sin \beta_{q} \cos \beta_{q} - \sin^{2} \beta_{F} \sin \beta_{q} \cos \beta_{q} \right)^{2}}{2\varepsilon(q)} , \\
D_{5} & = -2 \int_{0}^{\pi/2-\bar{D}_{0}} \frac{dq}{2\pi} \frac{2 \cos^{4} \beta_{F} \cos^{2} \beta_{q} \cos^{2} \beta_{F_{\pi-q}} + 2 \sin^{4} \beta_{F} \sin^{2} \beta_{q} \sin^{2} \beta_{F_{\pi-q}}}{\varepsilon(q) - \varepsilon(\pi - q)} , \\
D_{6} & = -2 \int_{0}^{\pi/2} \frac{dq}{2\pi} \frac{2 \cos^{4} \beta_{F} \cos^{2} \beta_{q} \sin^{2} \beta_{F_{\pi-q}} + 2 \sin^{4} \beta_{F} \sin^{2} \beta_{q} \cos^{2} \beta_{F_{\pi-q}}}{\varepsilon(q) + \varepsilon(\pi - q)} ,
\end{align}
\[ D_7 = 2 \int_{\pi/2}^{\pi} \frac{dq}{2\pi} \cos^4 \beta_F \cos^2 \beta_q \sin^2 \beta_{\pi-q} - \sin^4 \beta_F \sin^2 \beta_q \cos^2 \beta_{\pi-q}, \]
\[ D_8 = 2 \int_0^\pi \frac{dq}{2\pi} \cos^4 \beta_F \sin^2 \beta_q \sin^2 \beta_{\pi-q} - \sin^4 \beta_F \sin^2 \beta_q \sin^2 \beta_{\pi-q}, \]
\[ D_9 = -4 \int_{\pi/2-\tilde{\theta}_0}^{\pi/2} \frac{dq}{2\pi} \cos^4 \beta_F \cos^2 \beta_q \cos^2 \beta_{\pi-q} - \sin^4 \beta_F \sin^2 \beta_q \sin^2 \beta_{\pi-q}, \]
\[ D_{10} = -2 \int_{\pi/2}^{\pi} \frac{dq}{2\pi} \cos^4 \beta_F \cos^2 \beta_q \sin^2 \beta_{\pi-q} - \sin^4 \beta_F \sin^2 \beta_q \cos^2 \beta_{\pi-q}. \]  

Again, like for the case of alternating hoppings, we separate the logarithmic divergencies from integrals \( D_1, D_5 \) and \( D_9 \), and we write the effective couplings as

\[ g_1(\tilde{D}_0) = \frac{\varepsilon_0^2 + t^2}{\varepsilon_0^2 + 2t^2} U - \frac{U^2}{\pi v_F} \left[ \frac{\varepsilon_0^2 + t^2}{\varepsilon_0^2 + 2t^2} \right]^2 \ln \frac{2}{D_0 + I_1}, \]
\[ g_2(\tilde{D}_0) = \frac{\varepsilon_0^2 + t^2}{\varepsilon_0^2 + 2t^2} U - \frac{U^2}{\pi v_F} \left( \frac{t^4}{2(\varepsilon_0^2 + 2t^2)} \right) \ln \frac{2}{D_0 + I_2}, \]
\[ g_3(\tilde{D}_0) = \frac{\varepsilon_0}{\sqrt{\varepsilon_0^2 + 2t^2}} U - \frac{U^2}{\pi v_F} \left[ \frac{-\varepsilon_0(\varepsilon_0^2 + t^2)}{(\varepsilon_0^2 + 2t^2)^{3/2}} \right] \ln \frac{2}{D_0 + I_3}. \]

The expressions for the \( \tilde{I} \)'s are rather complicated and, for brevity, we will give here only their value in the limit of large dimerization (the compounds which can be described by this model presumably have parameters which lie in this limit):

\[ I_1 = \frac{32 + 13\pi t^6}{32 \varepsilon_0^6} + O(t^8/\varepsilon_0^8), \]
\[ I_2 = \frac{t^4}{4 \varepsilon_0^6} - \frac{48 + 3\pi t^6}{32 \varepsilon_0^6} + O(t^8/\varepsilon_0^8), \]
\[ I_3 = \frac{t^2}{4 \varepsilon_0^6} - \frac{48 + 5\pi t^6}{32 \varepsilon_0^6} + O(t^8/\varepsilon_0^8). \]

We have calculated numerically the \( \tilde{I} \)-s for a few values of \( \varepsilon_0/t \) and they are presented in Table IV.

For \( g_4 \), it is sufficient to take the value without the \( U^2 \) corrections:

\[ g_4 = U \frac{\varepsilon_0^2 + t^2}{\varepsilon_0^2 + 2t^2}. \]

Replacing the effective interactions into Eq. (6.15), we get

\[ \Delta_c = \frac{8}{\pi} \sqrt{\frac{U \varepsilon_0}{2(\varepsilon_0^2 + 2t^2)}} \exp \left( -\frac{\pi}{U} \sqrt{\varepsilon_0^2 + 2t^2} \text{Arth} \frac{t^2}{\varepsilon_0^2 + t^2} \right) \exp \left[ \frac{1}{4} - \frac{t^2 + \varepsilon_0^2}{4t^2} \frac{U}{\varepsilon_0^2 + t^2} \text{Arth} \frac{t^2}{\varepsilon_0^2 + t^2} \right] e^{\tilde{C}}, \]

(6.38)
where the constant has been fixed so that for large dimerization \((\varepsilon_0 \gg t)\) we get Eq. (5.8).

Here \(\tilde{C}\) is given by

\[
\tilde{C} = (2\tilde{I}_2 - \tilde{I}_1) \left( \frac{(2t^2 + \varepsilon_0^2)^2}{t^4} \left[ 1 - \frac{t^2 + \varepsilon_0^2}{t^2} \arctanh \frac{t^2}{\varepsilon_0^2 + t^2} \right] \right) - \tilde{I}_3 \left( \frac{(2t^2 + \varepsilon_0^2)^{3/2}}{t^2 \varepsilon_0} \left[ \frac{\varepsilon_0^2 + t^2}{t^2} - \frac{\varepsilon_0^2 (2t^2 + \varepsilon_0^2)}{t^4} \arctanh \frac{t^2}{\varepsilon_0^2 + t^2} \right] \right) .
\] 

\((6.39)\)

**VII. LARGE U LIMIT**

In the large \(U\) limit a canonical transformation can be applied to obtain an effective Hamiltonian analog to the \(t - J\) Hamiltonian of the non dimerized Hubbard model. We know already that if there are two alternating hoppings, a dimerization gap \(\Delta_D\) opens at the Brillouin zone boundary, and, in the limit \(U \to +\infty\), this gap becomes the charge gap. This will be modified by the spin interaction, which will give corrections of order \(1/U\).

**A. Alternating hoppings**

If \(U \gg t_1, t_2\), and since we have two different hopping amplitudes, the effective model will be a \(t - J\) model with alternating \(t_1\) and \(t_2\) hoppings and alternating \(J_1\) and \(J_2\) exchange interactions:

\[
H_{tJ} = -t_1 \sum_{i\text{ even}, \sigma} \hat{P} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) \hat{P} - t_2 \sum_{i\text{ odd}, \sigma} \hat{P} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) \hat{P} + J_1 \sum_{i \text{ even}} (S_i S_{i+1} - \frac{1}{4} n_i n_{i+1}) + J_2 \sum_{i \text{ odd}} (S_i S_{i+1} - \frac{1}{4} n_i n_{i+1}) + \frac{J}{4} \sum_{i, \sigma} \hat{P} (c_{i,\sigma}^\dagger c_{i,\sigma}^\dagger c_{i+1,\sigma} c_{i+1,\sigma} + \text{h.c.}) \hat{P} + \mathcal{O}(t^3/U^2) .
\] 

\((7.1)\)

Here the projector \(\hat{P} = \prod_i [1 - n_{i,\uparrow} n_{i,\downarrow}]\) ensures that there are no doubly occupied sites, \(n_i = n_{i,\uparrow} + n_{i,\downarrow}\), and the generated exchange couplings are \(J_1 = 4t_1^2/U\), \(J_2 = 4t_2^2/U\) and \(J = 4t_1 t_2/U\).

To go further, let us follow the scheme developed by Shiba and Ogata in their study of the correlation functions for the large \(U\) Hubbard model. The basic idea is to treat the
exchange part as a perturbation. This is possible if the exchange integrals are smaller than
the hopping integrals, which reduces to the condition $J_1 \ll t_2$ (remember that $t_2 < t_1$, and
thus that $J, J_2 < J_1$), or, in terms of the original parameters, $U \gg 4t_1^2/t_2$. In this limit,
the part describing essentially hopping of spinless fermions can be solved exactly and the
exchange part is then treated as a perturbation. This can be achieved by assuming that
the wave function is the product of a charge and a spin wave function, where the spin wave
function is defined in a Hilbert space of dimension $2^N$, i.e every charge has the additional
freedom of having its spin up or down:

$$|\Psi\rangle = |sf\rangle \otimes |\Phi\rangle .$$  \hspace{1cm} (7.2)

Here $|\Phi\rangle$ is the spin part of the wave function, while $|sf\rangle$, the wave function of the N spinless
fermions, is the ground state of the kinetic Hamiltonian. Following standard perturbation
technique for the case of a degenerate ground state, we will have to diagonalize the following
$2^N \times 2^N$ Hamiltonian to lift the degeneracy of $|\Phi\rangle$ and get the $1/U$ energy corrections:

$$\langle H_{tJ} \rangle' / L = -t_1 \langle c_0^\dagger c_1 \rangle' - t_2 \langle c_1^\dagger c_2 \rangle'$$
$$+ \left( \frac{J_1}{2} \langle n_0 n_1 \rangle' + \frac{J_2}{2} \langle n_1 n_2 \rangle' - J \langle c_0^\dagger c_1^\dagger c_1 c_2 \rangle' \right) \frac{1}{N} \sum_{j=1}^{N} (S_j S_{j+1} - \frac{1}{4}),$$  \hspace{1cm} (7.3)

where the $\langle \hat{A} \rangle'$ denotes the expectation value of the operator $\hat{A}$ in the Fermi sea of spinless
fermions, i.e. $\langle \hat{A} \rangle' = \langle sf | \hat{A} | sf \rangle$.

Before we continue with the calculation of the gap, we need to know the expectation
values of electron operators in the Fermi see of spinless fermions, where $k_{F,sf} = 2k_F$. Using
the translational symmetry of the system, it is enough to calculate the following basic
expectation values

$$\langle c_0^\dagger c_j \rangle' = \frac{2}{L} \sum_k e^{ikj/2} \langle c_k^\dagger c_k \rangle',$$
$$\langle c_1^\dagger c_{j+1} \rangle' = \frac{2}{L} \sum_k e^{ikj/2} \langle c_k^\dagger c_k \rangle',$$
$$\langle c_1^\dagger c_j \rangle' = \frac{2}{L} \sum_k e^{ikj/2} \langle c_k^\dagger c_k \rangle',$$  \hspace{1cm} (7.4)
where \( j \) is even everywhere. More complicated expressions can be calculated by using Wick’s theorem, i.e. by constructing all possible pairings. For example:

\[
\langle n_1n_j \rangle' = \langle c_1^\dagger c_1 \rangle' \langle c_j^\dagger c_j \rangle' - \langle c_1^\dagger c_j \rangle' \langle c_j^\dagger c_1 \rangle' = n^2 - \langle c_1^\dagger c_j \rangle'^2,
\]

\[
\langle c_0^\dagger c_1^\dagger c_1 c_2 \rangle' = n \langle c_0^\dagger c_2 \rangle' - \langle c_0^\dagger c_1 \rangle' \langle c_1^\dagger c_2 \rangle'.
\]

(7.5)

In the following, the sums above will be replaced by integrals,

\[
\frac{2}{L} \sum_k \rightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} dk.
\]

(7.6)

The free fermion Hamiltonian (6.2) has been solved in Sec. VI. Using the diagonal electron operators \( d \) and \( f \) defined in Eq. (6.3), we get

\[
\langle c_k^\dagger c_k \rangle' = \langle \tilde{c}_k^\dagger \tilde{c}_k \rangle' = \frac{1}{2}(n_{d,k} + n_{f,k})
\]

\[
\langle \tilde{c}_k^\dagger c_k \rangle' = \frac{s^2(k)}{2}(n_{d,k} - n_{f,k}),
\]

(7.7)

where \( n_{d,k} = d_k^\dagger d_k \), similarly for \( n_{f,k} \), and the spin index of the fermion operators has been dropped. For \( j \) even, this gives

\[
\langle c_0^\dagger c_j \rangle' = \langle c_1^\dagger c_{j+1} \rangle' = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk e^{ikj/2} \frac{1}{2}(n_{b,k} + n_{f,k})
\]

\[
= \frac{\sin \pi j n}{\pi j}.
\]

(7.8)

This is the same expression as for a non–dimerized model. For \( \langle c_1^\dagger c_j \rangle' \), we get:

\[
\langle c_1^\dagger c_j \rangle' = \frac{1}{2\pi} \int_{0}^{2\pi} dk \cos(k(j - 1)/2 - \alpha_k),
\]

(7.9)

where \( \alpha_k \) is defined in Eq. (6.4) and

\[
\varphi_0 = \begin{cases} 
\pi n, & \text{if } n < 1/2; \\
\pi(1 - n), & \text{if } n > 1/2.
\end{cases}
\]

(7.10)

After some algebra, we get

\[
\langle c_1^\dagger c_j \rangle' = \frac{1}{\pi} \int_{0}^{\varphi_0} d\varphi \frac{t_1 \cos \varphi j + t_2 \cos \varphi(j - 2)}{\sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos 2\varphi}}.
\]

(7.11)
For \( j = 0 \) and \( j = 2 \), this can be written

\[
\langle c_1^\dagger c_0 \rangle' = \frac{1}{2\pi t_1} [(t_1 - t_2) F(\varphi_0, q) + (t_1 + t_2) E(\varphi_0, q)] ,
\]

\[
\langle c_1^\dagger c_2 \rangle' = \frac{1}{2\pi t_2} [(t_2 - t_1) F(\varphi_0, q) + (t_1 + t_2) E(\varphi_0, q)] ,
\]

(7.12)

where we have introduced the notation

\[
q = \frac{2\sqrt{t_1 t_2}}{t_1 + t_2} ,
\]

(7.13)

and where the elliptic integrals \( E(\varphi_0, q) \) and \( F(\varphi_0, q) \) are defined by

\[
F(\varphi_0, q) = \int_0^{\varphi_0} \frac{d\varphi}{\sqrt{1 - q^2 \sin^2 \varphi}} ,
\]

\[
E(\varphi_0, q) = \int_0^{\varphi_0} d\varphi \sqrt{1 - q^2 \sin^2 \varphi} .
\]

(7.14)

Now, let us turn back to the effective Hamiltonian (7.3). For the spin degrees of freedom, we are left with an \( N \)-site Heisenberg Hamiltonian with an effective exchange interaction \( J_{\text{eff}} \) which we can read from Eq. (7.3):

\[
J_{\text{eff}} = \frac{J_1}{2} \langle n_0 n_1 \rangle' + \frac{J_2}{2} \langle n_1 n_2 \rangle' - J \langle c_0^\dagger c_1^\dagger c_1 c_2 \rangle'
\]

\[
= \frac{2}{U} \left[ n^2(t_1^2 + t_2^2) - nt_1 t_2 \frac{2\pi n}{\pi} - \frac{(t_1 - t_2)^2}{\pi^2} E^2(\varphi_0, q) \right] ,
\]

(7.15)

where we have used Eqs. (7.4) and (7.12).

In the ground state of the AF Heisenberg model the expectation value \( \langle \Phi |(S_0 S_1 - \frac{1}{4})|\Phi \rangle \) is \(- \ln 2\) in zero magnetic field, as shown by Griffiths.\(^{21}\) The energy per site \( \langle \Psi |H_{tJ}|\Psi \rangle/L \) is then

\[
\varepsilon_{tJ} = \varepsilon_{sf} - J_{\text{eff}} \ln 2 ,
\]

(7.16)

where \( \varepsilon_{sf} = -t_1 \langle c_1^\dagger c_0 \rangle' - t_2 \langle c_1^\dagger c_2 \rangle' \) is the kinetic energy of the spinless fermions per site. From Eq. (7.12), we get

\[
\varepsilon_{sf}(n) = -\frac{t_1 + t_2}{\pi} E(\varphi_0, q) ,
\]

(7.17)

which in the non–dimerized case (\( q = 1 \)) gives the correct energy \((2t/\pi) \sin \pi n\).
For \( n = 1/2 \), we get

\[
J_{\text{eff}} = \frac{2}{U} \left[ \frac{t_1^2 + t_2^2}{4} - \frac{(t_1 - t_2)^2}{\pi^2} K^2(q) \right],
\]

(7.18)

where \( K(q) = F(\pi/2, q) \) is the complete elliptic integral defined in Eq. (7.14).

The energy \( E_{tJ}/L \) has a cusp as a function of filling at \( n = 1/2 \), and this nonanalyticity comes from the \( \varphi_0 \) [see Eq. (7.10)]. Therefore the first derivative of \( E_{tJ}/L \) has a jump at quarter filling, which is nothing but the charge gap:

\[
\Delta_c = \frac{\partial \varepsilon_{tJ}}{\partial n} \bigg|_{n=1/2^+} - \frac{\partial \varepsilon_{tJ}}{\partial n} \bigg|_{n=1/2^-}.
\]

(7.19)

In our case this gives

\[
\Delta_c = 2(t_1 - t_2) \left[ 1 - \frac{4\ln 2}{\pi} \frac{t_1 + t_2}{U} K\left( \frac{2\sqrt{t_1 t_2}}{t_1 + t_2} \right) \right],
\]

(7.20)

where we have used the following identities:

\[
\frac{\partial F(\varphi_0, q)}{\partial n} \bigg|_{n=1/2^+} - \frac{\partial F(\varphi_0, q)}{\partial n} \bigg|_{n=1/2^-} = -\frac{2\pi}{\sqrt{1 - q^2}},
\]

\[
\frac{\partial E(\varphi_0, q)}{\partial n} \bigg|_{n=1/2^+} - \frac{\partial E(\varphi_0, q)}{\partial n} \bigg|_{n=1/2^-} = -2\pi \sqrt{1 - q^2}.
\]

(7.21)

Using the limiting behavior of the elliptic function \( K(q) = \ln(4/\sqrt{1 - q^2}) \), the gap in the small dimerization limit is

\[
\Delta_c = 2(t_1 - t_2) \left[ 1 - \frac{4\ln 2}{\pi} \frac{t_1 + t_2}{U} \ln \frac{4(t_1 + t_2)}{t_1 - t_2} \right],
\]

(7.22)

or

\[
\Delta_c = \Delta_D \left[ 1 - \frac{2\ln 2}{\pi} \frac{W}{U} \ln \frac{4W}{\Delta_D} \right].
\]

(7.23)

In Fig. 10 we have compared the analytical results presented above with the numerical data. The agreement is already very good at \( U/t_1 = 10 \) for \( t_2/t_1 \) between 0.3 and 0.5. To get such a good agreement for \( t_2/t_1 = 0.1 \), one has to go to larger values of \( U \), so that the condition \( U \gg 4t_1^2/t_2 \approx 40 \) is satisfied. For large values of \( t_2 \), the gap is small and the numerical estimate is not accurate.
As \( t_2 \to 0 \), Eq. (7.20) gives \( \Delta_c = 2t_1 - (4 \ln 2)t_2^2/U \), in apparent contradiction with the second of equations (4.1), which gives \( \Delta_c = 2t_1 - 4t_2^2/U \) for \( t_2 = 0 \). The origin of the discrepancy is that Eq. (7.20) holds if \( U \gg t_2^2/t_1 \), while the second of equations (4.1) requires that \( t_2 \ll t_1/U \). These conditions are clearly incompatible. Actually the cross-over between these two regimes can be observed on Fig. 10, where the points below the solid line \( (t_1^2/U \approx 0.1) \) gives \( \Delta_c \sim 2t_1 - 4t_2^2/U \), while for larger values of \( U \) we get the correct \( 4 \ln 2 \) slope.

B. Alternating on-site energies

Like in the previous case, a canonical transformation can be applied in the limit \( U \gg t, \epsilon_0 \) to obtain a \( t - J \) like effective Hamiltonian

\[
H_{tJ} = -t \sum_{i,\sigma} \tilde{P}(c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.})\tilde{P} - \epsilon_0 \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i,\sigma} - c_{i+1,\sigma}^\dagger c_{i+1,\sigma}) \\
+ J \sum_i (S_i S_{i+1} - \frac{1}{4} n_i n_{i+1}) \\
+ \frac{J}{4} \sum_{i,\sigma} \tilde{P}(c_{i,\sigma}^\dagger c_{i+1,-\sigma} c_{i+2,\sigma} - c_{i,\sigma}^\dagger c_{i+1,-\sigma} c_{i+2,\sigma} + \text{h.c.})\tilde{P} + \mathcal{O}(t^3/U^2), (7.24)
\]

where the projector \( \tilde{P} = \prod_i [1 - n_i, n_{i+1}] \) ensures that there are no doubly occupied sites and the generated exchange coupling is \( J = 4t_2^2/U \). If the additional condition \( J \ll \epsilon_0 \) is satisfied (that is, if \( U \gg 4t_2^2/\epsilon_0 \)), we can again follow Ogata and Shiba.

Let us now calculate the expectation values for this model. The free fermion model is given by Eq. (6.26) and it has been solved using transformations Eq. (6.27). So, for the expectation values we get

\[
\langle c_k^\dagger c_k \rangle' = \frac{n_{d,k} + n_{f,k}}{2} + \frac{n_{d,k} - n_{f,k}}{2} \cos 2\beta_k, \\
\langle \tilde{c}_k^\dagger \tilde{c}_k \rangle' = \frac{n_{d,k} + n_{f,k}}{2} - \frac{n_{d,k} - n_{f,k}}{2} \cos 2\beta_k, \\
\langle \tilde{c}_k^\dagger c_k \rangle' = e^{-ik/2} \frac{n_{d,k} - n_{f,k}}{2} \sin 2\beta_k, \\
\langle c_k^\dagger \tilde{c}_k \rangle' = e^{ik/2} \frac{n_{d,k} - n_{f,k}}{2} \sin 2\beta_k. (7.25)
\]
Using the results we obtained in Eq. (7.8), for $j$ even we get

$$\langle c_0^\dagger c_j \rangle' = \sin \frac{\pi j n}{\pi j} + I_j$$

and after some algebra

$$\langle c_1^\dagger c_{j-1} \rangle' = \langle c_1^\dagger c_j \rangle' = \frac{t}{\varepsilon_0} (I_j + I_{j-2}),$$

(7.27)

where the $I_j$ denote the following integral:

$$I_j = \frac{1}{2} \int_{2\varphi_0}^{2\varphi_0} dk e^{ikj/2} \cos 2\beta_k$$

$$= \frac{1}{2\pi} \int_{2\varphi_0}^{2\varphi_0} dk \frac{\cos(kj/2)}{\sqrt{1 + (2t/\varepsilon_0)^2 \cos^2(k/2)}},$$

(7.28)

and $\varphi_0$ is defined by Eq. (7.10). These are elliptic integrals and e.g. $I_0$ and $I_2$ are given by

$$I_0 = \frac{1}{\pi} \sqrt{\varepsilon_0^2 + 4t^2} F(\varphi_0, q),$$

$$I_0 - I_2 = \frac{2}{\pi} \varepsilon_0 \frac{\sqrt{\varepsilon_0^2 + 4t^2}}{4t^2} [F(\varphi_0, q) - E(\varphi_0, q)],$$

(7.29)

where

$$q = \frac{2t}{\sqrt{\varepsilon_0^2 + 4t^2}}.$$

(7.30)

The energy of the system is $E_{tJ} = \langle \Psi | H_{tJ} | \Psi \rangle$ and the energy per site $\varepsilon_{tJ} = E_{tJ}/L$ is still given by Eq. (7.16), but now the kinetic energy of the spinless fermions per site is

$$\varepsilon_{sf}(n) = 2t \langle c_0^\dagger c_0 \rangle' - \frac{1}{2} \left( \langle c_0^\dagger c_0 \rangle' - \langle c_1^\dagger c_1 \rangle' \right)$$

$$= -\frac{2}{\pi} \varepsilon_0 \frac{\sqrt{\varepsilon_0^2 + 4t^2}}{4t^2} E(\varphi_0, q),$$

(7.31)

where we have used Eqs. (7.27) and (7.29). For the effective exchange coupling we get

$$J_{\text{eff}} = J \left[ \langle n_0 n_1 \rangle' - \frac{1}{2} \left( \langle c_0^\dagger c_1^\dagger c_2 \rangle' + \langle c_1^\dagger c_2^\dagger c_3 \rangle' \right) \right]$$

$$= \frac{4t^2}{U} \left\{ n^2 - n \frac{\sin 2n}{2\pi} - \frac{\varepsilon_0^2}{2\pi^2 t^2} F(\varphi_0, q) [F(\varphi_0, q) - E(\varphi_0, q)] \right\},$$

(7.32)
where we have used Wick’s theorem, namely:

\[
\langle n_0 n_1 \rangle' = n_0 n_1 - \langle c_0^\dag c_1 \rangle'^2,
\]
\[
\langle c_0^\dag c_1^\dag c_1 c_2 \rangle' = n_1 \langle c_0^\dag c_2 \rangle' - \langle c_0^\dag c_1 \rangle'^2,
\]
\[
\langle c_1^\dag c_2^\dag c_2 c_3 \rangle' = n_0 \langle c_1^\dag c_3 \rangle' - \langle c_0^\dag c_1 \rangle'^2,
\]
\[
\text{(7.33)}
\]

and

\[
\langle n_0 n_1 \rangle' - \frac{1}{2} (\langle c_0^\dag c_1^\dag c_2 \rangle' + \langle c_1^\dag c_2^\dag c_2 c_3 \rangle') = n_0 n_1 - \frac{1}{2} (n_1 \langle c_0^\dag c_2 \rangle' + n_0 \langle c_1^\dag c_3 \rangle')
\]
\[
= n^2 - n \frac{\sin 2\pi n}{2\pi} - I_0 (I_0 - I_2) .
\]
\[
\text{(7.34)}
\]

For \( n = 1/2 \), we get

\[
J_{\text{eff}} = \frac{1}{U} \left\{ t^2 - \frac{2\varepsilon_0^2}{\pi^2} K(q) \left[ K(q) - E(\pi/2, q) \right] \right\} .
\]
\[
\text{(7.35)}
\]

The gap, using Eq. (7.19), is

\[
\Delta_c = 2\varepsilon_0 \left\{ 1 - \frac{2 \ln 2 \sqrt{\varepsilon_0^2 + 4t^2}}{U} \left[ (1 + q^2) K(q) - E(\pi/2, q) \right] \right\},
\]
\[
\text{(7.36)}
\]

and in the small dimerization limit it is given by

\[
\Delta_c = 2\varepsilon_0 \left[ 1 - \frac{4 \ln 2 \sqrt{\varepsilon_0^2 + 4t^2}}{U} \ln \left( \frac{4\sqrt{\varepsilon_0^2 + 4t^2}}{\varepsilon_0} \right) \right].
\]
\[
\text{(7.37)}
\]

If we parametrize the gap in this limit with \( \Delta_D \) and \( W \), we can see that it is identical with Eq. (7.23).

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FIGURES

FIG. 1. Schematic representation of the model with: a) alternating hopping amplitudes $t_1$ and $t_2$; b) alternating on-site energies with energy splitting $2\varepsilon_0$.

FIG. 2. Band structure of the model with $U = 0$.

FIG. 3. Schematic picture of the different regions as a function of model parameters for the model with: a) alternating hopping amplitudes; b) alternating on-site energies.

FIG. 4. a) Approximation for the charge gap for $t_2/t_1 = 0.1$ to 0.9 in increments of 0.1 from the top to the bottom. The diamonds are the numerical data for $t_2/t_1 = 0.1$ to 0.5; b) Approximation for the gap, but now only from $t_2/t_1 = 0.6$ to 0.9 in increments of 0.1 from the top to the bottom.

FIG. 5. Numerical estimates of the gap (diamonds) for $t_2 = 0.1$ compared with the analytical results.

FIG. 6. Weak coupling expression compared to numerical estimates for $t_2 = 0.3$ (upper curve) and $t_2 = 0.4$ (lower curve).

FIG. 7. Numerical values of the gap $\Delta_c(L)$ for $L=4,8,12$ and 16 as a function of $1/L$ for $U/t_1 = 5$. Note that $\Delta_c(L)$ converges very well for small values of $t_2/t_1$.

FIG. 8. Perturbational corrections to the effective backward scattering $g_1$, forward scattering $g_2$ and umklapp scattering $g_3$ for the model with alternating hoppings shown up to the second order. The solid (dashed) line represents the fermions in the lower $d$ (upper $f$) band.

FIG. 9. Perturbational corrections to the effective backward scattering $g_1$, forward scattering $g_2$ and umklapp scattering $g_3$ for the model with alternating hoppings shown up to the second order. The solid (dashed) line represents the fermions in the lower $d$ (upper $f$) band.
FIG. 10. Numerical estimates of the gap in the large $U$ limit (diamonds) together with the analytical approximation. The results presented are for $t_2 = 0.1, 0.2, 0.3, 0.4, 0.5$ and $0.7$ from the top to bottom.
TABLES

TABLE I. The parameters of the gap equations for the weak coupling and strong coupling limit for the model with alternating hoppings.

| $t_2/t_1$ | $a$   | $b$   | $\Delta_D/t_1$ | $c$   |
|----------|-------|-------|----------------|-------|
| 0.1      | 0.36887 | 0.6336 | 1.8            | 1.6816 |
| 0.2      | 0.46782 | 1.2990 | 1.6            | 2.0167 |
| 0.3      | 0.49990 | 2.0304 | 1.4            | 2.3984 |
| 0.4      | 0.48604 | 2.8669 | 1.2            | 2.8368 |
| 0.5      | 0.43672 | 3.8588 | 1.0            | 3.3474 |
| 0.6      | 0.36100 | 5.0790 | 0.8            | 3.9555 |
| 0.7      | 0.26867 | 6.6518 | 0.6            | 4.7075 |
| 0.8      | 0.17046 | 8.8399 | 0.4            | 5.7054 |
| 0.9      | 0.07709 | 12.4449| 0.2            | 7.2658 |

TABLE II. The parameters $U_0$, $a_1$, $b_1$ and $b_2$.

| $t_2/t_1$ | $U_0/t_1$ | $a_1$   | $b_1$   | $b_2$   |
|----------|-----------|---------|---------|---------|
| 0.2      | 1.30      | 0.45312 | 1.5438  | 13.0786 |
| 0.3      | 2.03      | -0.13375| 1.6173  | 13.5738 |
| 0.4      | 2.87      | -0.97220| 1.5540  | 10.7001 |
| 0.5      | 3.86      | -1.91825| 1.4287  | 3.3094  |
| 0.6      | 4         | -1.84743| 2.6357  | 0.0736  |
| 0.7      | 4         | -1.50580| 5.3353  | -2.2707 |
| 0.8      | 4         | -1.09045| 11.5364 | -7.4996 |
| 0.9      | 4         | -0.60222| 33.3189 | -34.0969|

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TABLE III. The parameters of the gap equations for the weak coupling and strong coupling limit for the model with alternating on-site energies.

| $\varepsilon_0/t$ | \(a\) | \(b\) | $\Delta_D/t$ | \(c\) |
|------------------|-------|-------|-------------|-------|
| 0.2              | 0.60292 | 8.82123 | 0.4         | 5.63087 |
| 0.4              | 0.78553 | 6.00854 | 0.8         | 4.41422 |
| 0.6              | 0.90155 | 4.53739 | 1.2         | 3.71014 |
| 0.8              | 0.97686 | 3.61670 | 1.6         | 3.21882 |
| 1                | 1.02292 | 2.98899 | 2           | 2.84615 |
| 2                | 1.03186 | 1.56009 | 4           | 1.78537 |
| 3                | 0.93780 | 1.04544 | 6           | 1.28117 |
| 4                | 0.84788 | 0.78494 | 8           | 0.99167 |
| 5                | 0.77446 | 0.62816 | 10          | 0.80616 |

TABLE IV. The $\tilde{I}$-s for some values of $\varepsilon_0/t$.

| $\varepsilon_0/t$ | $\tilde{I}_1$ | $\tilde{I}_2$ | $\tilde{I}_3$ |
|------------------|-------|-------|-------|
| 0                | (1/8) ln 2 | 0     | 0     |
| 0.2              | 0.0832216 | 0.0007691 | 0.0020951 |
| 0.4              | 0.0739705 | 0.0026394 | 0.0039468 |
| 0.6              | 0.0613605 | 0.0046787 | 0.0053306 |
| 0.8              | 0.0480877 | 0.0061374 | 0.0061143 |
| 1                | 0.0360938 | 0.0067624 | 0.0063123 |
| 2                | 0.0066400 | 0.0038914 | 0.0035338 |
| 3                | 0.0013135 | 0.0015298 | 0.0014380 |
| 4                | 0.0003309 | 0.0006442 | 0.0006189 |
| 5                | 0.0001034 | 0.0003044 | 0.0002961 |