Exact results for the optical absorption of strongly correlated electrons in a half-filled Peierls-distorted chain

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Abstract

In this second of three articles on the optical absorption of electrons in a half-filled Peierls-distorted chain we present exact results for strongly correlated tight-binding electrons. In the limit of a strong on-site interaction $U$ we map the Hubbard model onto the Harris-Lange model which can be solved exactly in one dimension in terms of spinless fermions for the charge excitations. The exact solution allows for an interpretation of the charge dynamics in terms of parallel Hubbard bands with a free-electron dispersion of band-width $W$, separated by the Hubbard interaction $U$. The spin degrees of freedom enter the expressions for the optical absorption only via a momentum dependent but static ground state expectation value. The remaining spin problem can be traced out exactly since the eigenstates of the Harris-Lange model are spin-degenerate. This corresponds to the Hubbard model at temperatures large compared to the spin exchange energy.

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Explicit results are given for the optical absorption in the presence of a lattice distortion $\delta$ and a nearest-neighbor interaction $V$. We find that the optical absorption for $V = 0$ is dominated by a peak at $\omega = U$ and broad but weak absorption bands for $|\omega - U| \leq W$. For an appreciable nearest-neighbor interaction, $V > W/2$, almost all spectral weight is transferred to Simpson’s exciton band which is eventually Peierls-split.

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I. INTRODUCTION

Some charge-transfer salts are understood as strongly correlated one-dimensional electron systems for half-filled bands (Mott-Hubbard insulators) (Farges 1994); (Alcácer, Brau, and Farges 1994). The extended Hubbard model for interacting electrons on a Peierls-distorted chain at half-filling is considered appropriate for these materials (Mazumdar and Dixit 1986); (Fritsch and Ducasse 1991); (Mila 1995). There are only few studies of the optical, i.e., finite frequency properties of correlated electron systems since their calculation is a formidable task (Kohn 1964); (Maldague 1977); (Lyo and Galinar 1977); (Lyo 1978); (Galinar 1979); (Campbell, Gammel, and Loh 1988); (Mahan 1990); (Shastry and Sutherland 1990); (Stafford, Millis, and Shastry 1991); (Fye, Martins, Scalapino, Wagner, and Hanke 1992); (Stafford and Millis 1993).

In this second article on the optical absorption of electrons in half-filled Peierls-distorted chains we present a detailed analysis of the optical absorption in the limit of strong correlations and for a half-filled band where the charge and spin dynamics decouple. We find that the physics of the half-filled Hubbard model at strong correlations is determined by the upper and lower Hubbard band for the charges which are parallel bands. This essential feature and its significant consequences have been missed in earlier analytical and numerical investigations. In this work we include a finite lattice dimerization and nearest-neighbor interaction between the electrons, i.e., we analyze the extended dimerized Hubbard model at strong correlations.

The paper is organized as follows. In section I we address the Hubbard model at strong coupling from which we derive the Harris-Lange model which determines the motion of the charge degrees of freedom. In the ground state there are no free charges but only singly occupied lattice sites. The exact spectrum and eigenstates of the Harris-Lange model are presented in section II for the translational invariant and the dimerized case. The results can be interpreted in terms of two parallel Hubbard bands for the charges which are eventually split into Peierls subbands. Optical absorption can now formally be treated as if we had
independent (spinless) Fermions.

Unfortunately, this simple band structure interpretation is blurred by the spin degrees of freedom which enter the expressions for the optical absorption in terms of a very complicated ground state expectation value. In section IV we treat the case of the Harris-Lange model where all spin configurations are equally possible ground states. This corresponds to the Hubbard model at temperatures large compared to the spin exchange energy. It allows the calculation of the optical absorption even in the presence of a Peierls distortion and a nearest-neighbor interaction between the charges. A summary and outlook closes our presentation. Some details of the calculations are left to the appendices.

II. STRONGLY CORRELATED MOTT-HUBBARD INSULATORS

A. Tight-binding electrons on a Peierls-distorted chain

For narrow-band materials the electron transfer is limited to nearest neighbors only. In standard notation of second quantization the Hamiltonian for electrons in the tight-binding approximation reads

\[
\hat{T}(\delta) = -t \sum_{l=1,\sigma}^{L} \left( 1 + (-1)^l \delta \right) \left( \hat{c}_{l,\sigma}^{+} \hat{c}_{l+1,\sigma} + \hat{c}_{l+1,\sigma}^{+} \hat{c}_{l,\sigma} \right)
\]

(1)

where \( \delta \) describes the effect of bond-length alternation on the electron transfer amplitudes. As usual the Hamiltonian can be diagonalized in momentum space. We apply periodic boundary conditions, and introduce the Fourier transformed electron operators as \( \hat{c}_{k,\sigma}^{+} = \sqrt{1/L} \sum_{l=1}^{L} \exp(ikla) \hat{c}_{l,\sigma}^{+} \) for the \( L \) momenta \( k = 2\pi m/(La) \), \( m = -(L/2), \ldots, (L/2) - 1 \). We may thus write

\[
\hat{T}(\delta) = \sum_{|k| \leq \pi/(2a),\sigma} \epsilon(k) \left( \hat{c}_{k,\sigma}^{+} \hat{c}_{k,\sigma} - \hat{c}_{k+\pi/a,\sigma}^{+} \hat{c}_{k+\pi/a,\sigma} \right) - i \Delta(k) \left( \hat{c}_{k+\pi/a,\sigma}^{+} \hat{c}_{k,\sigma} - \hat{c}_{k,\sigma}^{+} \hat{c}_{k+\pi/a,\sigma} \right)
\]

(2)

with the dispersion relation \( \epsilon(k) \) and hybridization function \( \Delta(k) \) defined as

\[
\epsilon(k) = -2t \cos(ka)
\]

(3a)

\[
\Delta(k) = 2t\delta \sin(ka)
\]

(3b)
The Hamiltonian can easily be diagonalized in $k$-space. The result is (Gebhard, Bott, Scheidler, Thomas, and Koch I 1996)

$$
\hat{T}(\delta) = \sum_{|k| \leq \pi/(2a),\sigma} E(k)(\hat{a}_{k,\sigma,+} \hat{a}_{k,\sigma,+} - \hat{a}_{k,\sigma,-} \hat{a}_{k,\sigma,-}) .
$$  \hfill (4)

Here, $\pm E(k)$ is the dispersion relation for the upper (+) and lower (−) Peierls band,

$$
E(k) = \sqrt{\epsilon(k)^2 + \Delta(k)^2} .
$$  \hfill (5)

The new Fermion quasi-particle operators $\hat{a}_{k,\sigma,\pm}$ for these two bands are related to the original electron operators by

$$
\hat{a}_{k,\sigma,-} = \alpha_k \hat{c}_{k,\sigma} + i \beta_k \hat{c}_{k+\pi,\sigma},
$$  \hfill (6a)

$$
\hat{a}_{k,\sigma,+} = \beta_k \hat{c}_{k,\sigma} - i \alpha_k \hat{c}_{k+\pi,\sigma},
$$  \hfill (6b)

with

$$
\alpha_k = \sqrt{\frac{1}{2} \left( 1 - \frac{\epsilon(k)}{E(k)} \right)}
$$  \hfill (7a)

$$
\beta_k = -\sqrt{\frac{1}{2} \left( 1 + \frac{\epsilon(k)}{E(k)} \right)} \text{sgn}(\Delta(k))
$$  \hfill (7b)

Details of the upper transformation and the optical absorption of this model are presented in (Gebhard et al. I 1996).

### B. Hubbard model

The only spinful interacting electron model that can be solved exactly for all values of the interaction strength is the Hubbard model in one dimension (Hubbard 1963); (Gebhard and Ruckenstein 1992); (Essler and Korepin 1994); (Gebhard, Girndt, and Ruckenstein 1994); (Bares and Gebhard 1995). For narrow-band materials the electron transfer is limited to nearest neighbors only, and the interaction is supposed to be described by the purely local (Hubbard-)interaction of strength $U$. 


\[ \hat{H}_{\text{Hubbard}} = \hat{T} + U \hat{D} \]
\[ \hat{D} = \sum_l \hat{D}_l = \sum_l \hat{n}_{l,\uparrow} \hat{n}_{l,\downarrow}, \]
where \( \hat{n}_{l,\sigma} = \hat{c}_{l,\sigma}^\dagger \hat{c}_{l,\sigma} \) is the local density of \( \sigma \)-electrons, and \( \hat{T} = \hat{T}(\delta = 0) \).

The model (8) poses a very difficult many-body problem. Its spectrum and, in particular, its elementary excitations can be obtained from the Bethe Ansatz solution (Lieb and Wu 1968); (Shastry, Jha, and Singh 1985); (Andrei 1995). Its low-energy properties including the DC-conductivity, \( \sigma_{\text{DC}} = \text{Re}\{\sigma(\omega = 0)\} \), can explicitly be obtained from the corresponding \( g \)-ology Hamiltonian (Schulz 1990); (Schulz 1991) or from conformal field theory (Frahm and Korepin 1990); (Frahm and Korepin 1991); (Kawakami and Yang 1990); (Kawakami and Yang 1991). The Hubbard model describes a (correlated) metal for all \( U > 0 \) for less than half-filling. Unfortunately, the Bethe Ansatz solution does not allow the direct calculation of transport properties at finite frequencies.

At half-filling the one-dimensional Hubbard model describes a Mott-insulator which implies that \( \sigma_{\text{DC}} = 0 \) for all \( U > 0 \). The density of states for charge excitations displays two bands, the upper and lower Hubbard band, separated by the Mott-Hubbard gap. This gap is defined as the jump in the chemical potential at half filling,

\[ \Delta_{\text{MH}} = \mu^+(N = L) - \mu^-(N = L) \]
\[ = [E(N = L + 1) - E(N = L)] - [E(N = L) - E(N = L - 1)] \quad \text{.} \]

As shown by Ovchinnicov (Ovchinnicov 1969) the Mott-Hubbard gap can be obtained from the Lieb-Wu solution (Lieb \textit{et al}. 1968) in the form

\[ \Delta_{\text{MH}} = \frac{16t}{U} \int_1^\infty \frac{dy \sqrt{y^2 - 1}}{\sinh(2\pi ty/U)} \quad \text{(9b)} \]
\[ = \begin{cases} 
(2W/\pi)\sqrt{4U/W} \exp(-\pi W/(2U)) & \text{for } U \ll W = 4t \\
U - W + \ln(2)W^2/(2U) + \mathcal{O}(W^3/U^2) & \text{for } U \gg W = 4t 
\end{cases} \quad \text{(9c)} \]

It is obvious that optical absorption is only possible if \( \omega \geq \Delta_{\text{MH}} \). It is further seen that the upper and lower Hubbard band are well separated for \( U \gg W \).
One might expect that the optical absorption for large interactions, $U \gg W$, and high temperatures, $k_B T \gg J = \mathcal{O}(W^2/U)$, shows the signature of a broad band-to-band transition for $U - W \leq \omega \leq U + W$ (units $\hbar \equiv 1$), similar to the Peierls insulator (Gebhard et al. 1996). Such considerations seemed to be supported by analytical (Lyo et al. 1977); (Lyo 1978); (Galinar 1979) and numerical calculations (Campbell, Gammel, and Loh 1989). Below we will calculate $\sigma(\omega > 0)$ in the limit $U \gg W$, and show that the linear absorption is actually dominated by a singular contribution at $\omega = U$ because the upper and lower Hubbard band are in fact parallel bands. The situation changes for $k_B T \ll J$ which we will consider in (Gebhard, Bott, Scheidler, Thomas, and Koch III 1996).

### C. Harris-Lange model

In the following we will address the limit $W/U \to 0$ where matters considerably simplify since the charge and spin degrees of freedom completely decouple (Ogata and Shiba 1990); (Parola and Sorella 1990). For example, for less than half-filling, $N \leq L$, and $U = \infty$ the eigenenergies become those of a Fermi gas of $N_h = L - N$ holes with dispersion $\epsilon(k)$, and each energy level is $2^N$-fold degenerate in the thermodynamical limit (Beni, Pincus, and Holstein 1973); (Klein 1973); (Ogata et al. 1990); (Parola et al. 1990).

To facilitate the discussion of the strong coupling limit we map the Hubbard model onto a problem for which the number of double occupancies is conserved. For a large on-site Coulomb repulsion $W/U \to 0$ it is natural to start with a spectral decomposition of operators into those which solely act in the upper or lower Hubbard band, and to perturbatively eliminate those parts in $\hat{H}_{\text{Hubbard}}$ which couple the two bands. For the Hubbard model this has first been achieved by Harris and Lange (Harris and Lange 1967); (van Dongen 1994), and the resulting effective Hamiltonian to lowest order in $W/U$ will thus be called the “Harris-Lange” model. It offers several advantages, both for analytical and numerical calculations.

To carry out the spectral decomposition we start from the case $t = 0$. The Fermi
annihilation operator can be split into a part which destroys an electron on a single occupied site and does not change the energy of the state, and another part which destroys an electron on a double occupied site and thus decreases the energy by $U$,

$$\hat{c}_{l,\sigma} = \hat{n}_{l,-\sigma} \hat{c}_{l,\sigma} + (1 - \hat{n}_{l,-\sigma}) \hat{c}_{l,\sigma}$$  \hspace{1cm} (10)

The corresponding creation operator can be treated accordingly.

If we now turn on the hopping of electrons ($t \neq 0$) we may split the kinetic energy operator into

$$\hat{T} = \hat{T}_{LHB} + \hat{T}_{UHB} + \hat{T}^+ + \hat{T}^-$$  \hspace{1cm} (11a)

$$\hat{T}_{LHB} = (-t) \sum_{l,\sigma} (1 - \hat{n}_{l,-\sigma}) (\hat{c}_{l,\sigma}^+ \hat{c}_{l+1,\sigma} + \hat{c}_{l+1,\sigma}^+ \hat{c}_{l,\sigma}) (1 - \hat{n}_{l+1,-\sigma})$$  \hspace{1cm} (11b)

$$\hat{T}_{UHB} = (-t) \sum_{l,\sigma} \hat{n}_{l,-\sigma} (\hat{c}_{l,\sigma}^+ \hat{c}_{l+1,\sigma} + \hat{c}_{l+1,\sigma}^+ \hat{c}_{l,\sigma}) \hat{n}_{l+1,-\sigma}$$  \hspace{1cm} (11c)

$$\hat{T}^+ = (-t) \sum_{l,\sigma} \left[ \hat{n}_{l,-\sigma} \hat{c}_{l,\sigma}^+ \hat{c}_{l+1,\sigma} (1 - \hat{n}_{l+1,-\sigma}) + \hat{n}_{l+1,-\sigma} \hat{c}_{l+1,\sigma}^+ \hat{c}_{l,\sigma} (1 - \hat{n}_{l,-\sigma}) \right]$$  \hspace{1cm} (11d)

$$\hat{T}^- = (\hat{T}^+)^+$$  \hspace{1cm} (11e)

The operator $\hat{T}_{LHB}$ for the lower Hubbard band describes the hopping of holes while doubly occupied sites can move in the upper Hubbard band via $\hat{T}_{UHB}$. Their number is conserved by both hopping processes. These two bands will constitute the basis for our approach. The operator $\hat{T}^+$ ($\hat{T}^-$) increases (decreases) the number of double occupancies by one.

Similar to the Foldy-Wouthuysen transformation for the Dirac equation (Bjorken and Drell 1964) we apply a canonical transformation that eliminates the operators $\hat{T}^\pm$ to a given order in $t/U$,

$$\hat{c}_{l,\sigma} = e^{i\hat{S}(\bar{\psi})} \hat{c}_{l,\sigma} e^{-i\hat{S}(\psi)}$$  \hspace{1cm} (12)

with $\left(\hat{S}(\bar{\psi})\right)^+ = \hat{S}(\psi)$. As shown by Harris and Lange (Harris et al. 1967); (van Dongen 1994) the operator to lowest order in $t/U$ reads

$$\hat{S}(\bar{\psi}) = \frac{i t}{U} \left( \hat{T}^{\bar{\psi},+} - \hat{T}^{\bar{\psi},-} \right)$$  \hspace{1cm} (13)
which can easily be verified since \([-\hat{D}, \hat{T}^\pm] = \pm \hat{T}^\pm\).

The transformed Hamilton operator in the new Fermions becomes the Harris-Lange model

\[
\hat{H}^e_{\text{HL}} = \hat{T}^e_{\text{LHB}} + \hat{T}^e_{\text{UHB}} + U\hat{D}^e ,
\]

if we neglect all correction terms to order \(t/U\) and higher. The energies obtained from the Harris-Lange model thus agree with those of the Hubbard model to order \(t(t/U)^{-1}\) and \(t(t/U)^0\). For all other physical operators which do not contain a factor of \(U/t\) we may replace

\[
\hat{c}_{l,\sigma} = \bar{c}_{l,\sigma} .
\]

because the error is only of order \((t/U)\). In the following we will thus make no distinction between the operators \(\hat{c}_{l,\sigma}\) and \(\bar{c}_{l,\sigma}\) to lowest order in \(t/U\).

The Hamiltonian has the following symmetry. The particle-hole transformation

\[
T_{\text{ph}}\hat{c}_{l,\sigma}^{+}T_{\text{ph}}^{-1} = i\lambda_{\sigma}e^{i\pi l}\hat{c}_{l,-\sigma}
\]

\[
T_{\text{ph}}\hat{c}_{k,\sigma}^{+}T_{\text{ph}}^{-1} = i\lambda_{\sigma}\hat{c}_{\pi/a-k,-\sigma}
\]

with \(\lambda_\uparrow = -\lambda_\downarrow = 1\) is generated with the help of

\[
T_{\text{ph}} = e^{i\pi/2(\hat{C}^+ + \hat{C}^-)} = \prod_l \left[ 1 - \left(\hat{D}_l + \hat{H}_l\right) + i(\hat{C}^+_l + \hat{C}^-_l) \right]
\]

\[
\hat{C}^+ = (\hat{C}^-)^+ = \sum_l \hat{C}^+_l = \sum_l (-1)^l\hat{c}_{l,\uparrow}^+\hat{c}_{l,\downarrow}^+ ; \quad \hat{H}_l = (1 - \hat{n}_{l,\uparrow})(1 - \hat{n}_{l,\downarrow}) .
\]

The additional phase factors \(i\lambda_{\sigma}\) are irrelevant global phases, and can be ignored since there is always an equal number of Fermion creation and annihilation operators of each spin species. The operators for the motion of holes and double occupancies are mapped into each other,

\[
\hat{T}_{\text{UHB}} \mapsto \hat{T}_{\text{LHB}} \quad \hat{T}_{\text{LHB}} \mapsto \hat{T}_{\text{UHB}} .
\]
Furthermore, $[\hat{T}_{\text{UHB}} + \hat{T}_{\text{LHB}}, \hat{C}^\pm]_\pm = 0$. This symmetry allows for an exact solution of the model since there is essentially no difference in the motion of double occupancies in the upper Hubbard band and holes in the lower Hubbard band.

The discussion above is readily generalized to the case of dimerization in the Harris-Lange model. The model Hamiltonian reads

$$\hat{H}^\text{dim}_{\text{HL}} = \hat{T}_{\text{LHB}}(\delta) + \hat{T}_{\text{UHB}}(\delta) + U \hat{D}$$

in an obvious generalization of the kinetic operators for the upper and lower Hubbard bands.

### D. Optical absorption and optical conductivity

The dielectric function $\tilde{\varepsilon}(\omega)$ and the coefficient for the linear optical absorption $\tilde{\alpha}(\omega)$ are given by (Haug and Koch 1990)

$$\tilde{\varepsilon}(\omega) = 1 + \frac{4\pi i \sigma(\omega)}{\omega}$$

$$\tilde{\alpha}(\omega) = \frac{4\pi \text{Re}\{\sigma(\omega)\}}{n_b c}$$

where $\text{Re}\{\ldots\}$ denotes the real part and $n_b$ is the background refractive index. It is supposed to be frequency independent near a resonance. Hence, the real part of the optical conductivity directly gives the absorption spectrum of the system.

The standard result (Maldague 1977); (Mahan 1990) for the real part of the optical conductivity in terms of the current-current correlation function $\chi(\omega)$ is

$$\text{Re}\{\sigma(\omega)\} = \frac{\text{Im}\{\chi(\omega)\}}{\omega}$$

$$\chi(\omega) = \frac{\mathcal{N}_\perp}{La} \int_0^\infty dt e^{i\omega t} \langle [\hat{j}(t), \hat{j}]_\perp \rangle$$

where $\mathcal{N}_\perp$ is the number of chains per unit area perpendicular to the chain direction.

The current-current correlation function can be spectrally decomposed in terms of exact eigenstates of the system as
\[ \chi(\omega) = \frac{N_1}{L\omega} \sum_n |\langle 0|j|n \rangle|^2 \left[ \frac{1}{\omega + (E_n - E_0) + i\gamma} - \frac{1}{\omega - (E_n - E_0) + i\gamma} \right]. \tag{22} \]

Here, \(|0\rangle\) is the exact ground state (energy \(E_0\)), \(|n\rangle\) are exact excited states (energy \(E_n\)), and \(|\langle 0|j|n \rangle|^2\) are the oscillator strengths for optical transitions between them. Although \(\gamma = 0^+\) is infinitesimal we may introduce \(\gamma > 0\) as a phenomenological broadening of the resonances at \(\omega = \pm (E_n - E_0)\). The spectral decomposition of the real part of the optical conductivity reads

\[ \text{Re}\{\sigma(\omega)\} = \frac{N_1 \pi}{L\omega} \sum_n |\langle 0|j|n \rangle|^2 \left[ \delta(\omega - (E_n - E_0)) - \delta(\omega + (E_n - E_0)) \right] \tag{23} \]

which is positive for all \(\omega\).

In the following we will always plot the dimensionless reduced optical conductivity

\[ \sigma_{\text{red}}(\omega > 0) = \frac{\omega \text{Re}\{\sigma(\omega > 0)\}}{N_1 ae^2 W}. \tag{24} \]

Furthermore we replace the energy conservation \(\delta(x)\) by the smeared function

\[ \tilde{\delta}(x) = \frac{\gamma}{\pi(x^2 + \gamma^2)} \tag{25} \]

to include effects of phonons, and experimental resolution. For all figures we graphically checked that the sum rules of appendix A were fulfilled.

### E. Current operator

As derived in (Gebhard et al. I 1996) the current operator is given by

\[ \hat{j} = -e \sum_{l,\sigma} i\tau_0 \left( 1 + (-1)^l \delta \right) \left( 1 + (-1)^l \eta \right) \left( \hat{c}_{l+1,\sigma} \hat{c}_{l,\sigma} - \hat{c}_{l,\sigma} \hat{c}_{l+1,\sigma} \right) \tag{26} \]

where \(\eta = -|R_{l+1} - R_l - a|/a < 0\) is the relative change of lattice distances due to the Peierls distortion. Note that \(\delta\) and \(\eta\) always have opposite sign. The current operator can be split into two parts, \(\hat{j} = \hat{j}^\text{H}_{\text{intra}} + \hat{j}^\text{H}_{\text{inter}}\), where \(\hat{j}^\text{H}_{\text{intra}}\) moves electrons between neighboring sites without changing the number of double occupancies or holes. This (Hubbard-)intraband current does not change the number of double occupancies. Hence it can be ignored for the
optical absorption in the Harris-Lange model at half-filling. The current operator between
the two Hubbard bands $j_{\text{inter}}^H$ can be written as

$$j_{\text{inter}}^H = j_{\text{inter},+}^H + j_{\text{inter},-}^H$$  \hspace{1cm} (27a)

$$j_{\text{inter},+}^H = -i(e\alpha \sum_{l,\sigma} \left(1 + (-1)^\delta\right) \left(1 + (-1)^\eta\right) \hat{n}_{l+1,-\sigma} \hat{c}_{l+1,\sigma}^+ \hat{c}_{l,\sigma} - \hat{n}_{l,-\sigma} \hat{c}_{l,\sigma}^+ \hat{c}_{l+1,\sigma} \left(1 - \hat{n}_{l+1,-\sigma}\right) \right)$$  \hspace{1cm} (27b)

$$j_{\text{inter},-}^H = -i(e\alpha \sum_{l,\sigma} \left(1 + (-1)^\delta\right) \left(1 + (-1)^\eta\right) \left(1 - \hat{n}_{l+1,-\sigma}\right) \hat{c}_{l+1,\sigma}^+ \hat{c}_{l-\sigma} - \left(1 - \hat{n}_{l,-\sigma}\right) \hat{c}_{l,\sigma}^+ \hat{c}_{l+1,\sigma} \hat{n}_{l+1,-\sigma} \right)$$  \hspace{1cm} (27c)

where $j_{\text{inter},\pm}$ create and destroy a neighboring pair of double occupancy and hole, respectively.

Next we study the action of $j_{\text{inter},+}^H$ on a pair of neighboring spins in a state $|\Psi\rangle$ in position
space. It is a sequence of singly occupied sites ($\sigma$), holes ($\circ$), and double occupancies ($\bullet$)
from site 1 to $L$, e.g.,

$$|\Psi\rangle = |\uparrow_1, \circ_2, \circ_3, \circ_4, \downarrow_5, \ldots \downarrow_{L-3}, \bullet_{L-2}, \downarrow_{L-1}, \bullet_L\rangle.$$  \hspace{1cm} (28)

We introduce the notations

$$|\ldots, (\uparrow_l, \downarrow_{l+1} \pm \downarrow_l, \uparrow_{l+1}), \ldots\rangle = |\ldots, \uparrow_l, \downarrow_{l+1}, \ldots\rangle \pm |\ldots, \downarrow_l, \uparrow_{l+1}, \ldots\rangle$$  \hspace{1cm} (29a)

$$|S_{l,l+1} = 1, S_{l,l+1}^z = 1\rangle = |\ldots, \uparrow_l, \uparrow_{l+1}, \ldots\rangle$$ \hspace{1cm} (29b)

$$|S_{l,l+1} = 1, S_{l,l+1}^z = 0\rangle = |\ldots, (\uparrow_l, \downarrow_{l+1} + \downarrow_l, \uparrow_{l+1}), \ldots\rangle$$ \hspace{1cm} (29c)

$$|S_{l,l+1} = 1, S_{l,l+1}^z = -1\rangle = |\ldots, \downarrow_l, \downarrow_{l+1}, \ldots\rangle$$ \hspace{1cm} (29d)

$$|S_{l,l+1} = 0, S_{l,l+1}^z = 0\rangle = |\ldots, (\uparrow_l, \downarrow_{l+1} - \downarrow_l, \uparrow_{l+1}), \ldots\rangle$$ \hspace{1cm} (29e)

as the local spin triplet and spin singlet states. Furthermore,

$$|C_{l,l+1} = 1, C_{l,l+1}^z = 0\rangle = |\ldots, (\bullet_l, \circ_{l+1} - \circ_l, \bullet_{l+1}), \ldots\rangle$$ \hspace{1cm} (29f)

denotes the local charge triplet state since $\hat{C}^+|C_{l,l+1} = 1, C_{l,l+1}^z = 0\rangle \neq 0$. With these
definitions one finds
\[ \hat{j}_{\text{inter}, +}^{\text{H}} |S_{t, t+1} = 1\rangle = 0 \]  
\[ \hat{j}_{\text{inter}, +}^{\text{H}} |S_{t, t+1} = 0\rangle = -itea(1 + (-1)^{l}\delta)(1 + (-1)^{l}\eta)(-2)|C_{t, t+1} = 1, C_{t, t+1}^{z} = 0\rangle . \]  

It is thus seen that \( \hat{j}_{\text{inter}}^{\text{H}} \) preserves the spin of a neighboring pair such that \( \Delta S = \Delta S^{z} = 0 \) is the selection rule for the spin sector. The selection rule for the charge sector is found as \( \Delta C = 1, \Delta C^{z} = 0 \). Note that the current operator does \textit{not} commute with \( \hat{C}^{\pm} \) as defined in eq. (16d).

Finally, the current operator is invariant against translations by one unit cell and thus preserves the total momentum modulo a reciprocal lattice vector (\( Q = 2\pi/a \) for \( \delta = 0 \), \( Q = \pi/a \) for \( \delta \neq 0 \)). However, the current operator can create or destroy a charge excitation with momentum \( q \), and create or destroy a spin excitation with momentum \( -q \). Although there is charge-spin separation in the Hubbard model for strong coupling the current operator mixes both degrees of freedom. This renders the calculation of the optical absorption of the Hubbard model a very difficult problem even in the limit of strong correlations.

### III. EXACT SOLUTION OF THE HARRIS-LANGE MODEL

#### A. Translational invariant case

The Harris-Lange model can exactly be solved by an explicit construction of all eigenstates. This has recently been shown by (de Boer, Korepin, and Schadschneider 1995) and (Schadschneider 1995) for periodic, and by (Aligia and Arrachea 1994) for open boundary conditions. Since optical excitations conserve total momentum we work with periodic boundary conditions where the total momentum is a good quantum number.

The number \( N_{S} \) of sites with spin (singly occupied sites), and the number \( N_{C} = N_{d} + N_{h} \) of sites with charge (double occupancies and holes) are separately conserved in the Harris-Lange model. We have \( N_{C} + N_{S} = L \) lattice sites, \( N = N_{S} + 2N_{d} \) electrons, and choose \( L \) to be even such that our lattice is bipartite for all \( L \). In the sequence of singly occupied sites, double occupancies and holes of the state \( |\Psi\rangle \) in eq. (28) we may identify subsequences for
the spins and the charges only (independent of the position on a special site). Additionally, the indices \( l_j \) indicate the actual position of the charges \( C_j \). The positions occupied by the spins are then the ones left over by the charges:

\[
\Psi = |(l_1, l_2, \ldots, l_{N_C-1}, l_{N_C}); (C_1, C_2, \ldots C_{N_C-1}, C_{N_C}); (S_1, S_2, \ldots S_{N_S-1}, S_{N_S})\rangle
\]

where in our example

\[
(S_1, S_2, \ldots S_{N_S-1}, S_{N_S}) = (\uparrow, \downarrow, \uparrow, \downarrow)
\]

is the subsequence for the spins and

\[
(C_1, C_2, C_3, \ldots C_{N_C-1}, C_{N_C}) = (\bullet, \circ, \circ, \ldots \bullet, \bullet)
\]

for the charges. The sequence for the positions occupied by charges is

\[
(l_1, l_2, l_3, \ldots l_{N_C} - 1, l_{N_C}) = (2, 3, 4, \ldots L - 2, L)
\]

Since there is nearest-neighbor hopping only both the spin and charge subsequences are separately conserved up to cyclic permutations due to the periodic boundary conditions.

To include the boundary effect we follow (de Boer et al. 1995) and (Schadschneider 1995) and introduce the properly symmetrized spin and charge sequences. To this end we define the operator for a cyclic permutation of the spin sequence,

\[
\hat{T}_S(S_1, S_2, \ldots S_{N_S}) = (S_{N_S}, S_1, \ldots S_{N_S-1})
\]

and, equivalently, \( \hat{T}_C \) for the charge sequence. Let \( K_S \) and \( K_C \) be the smallest positive integers such that \( (\hat{T}_S)^{K_S} \) and \( (\hat{T}_C)^{K_C} \) act as identity operators on a given spin and charge sequence, respectively. Then we define the \( K_S K_C \) states

\[
\sqrt{K_S K_C}|(l_1, \ldots l_{N_C}); (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle =
\]

\[
e\sum_{l=0}^{K_S-1} \sum_{l=0}^{K_C-1} e^{i\alpha(l k_S + l k_C)} \hat{T}_S^{l} \hat{T}_C^{l} |(l_1, \ldots l_{N_C}); (C_1, \ldots C_{N_C}); (S_1, \ldots S_{N_S})\rangle
\]
with the momentum shifts \( k_S = \frac{2\pi m_S}{(K_S a)} \), \( m_S = 0, 1, \ldots (K_S - 1) \), \( k_C = \frac{2\pi m_C}{(K_C a)} \), \( m_C = 0, 1, \ldots (K_C - 1) \). An extra phase factor \((-1)^l\) for each double occupancy at site \( l \) has been included here through the operator \( \exp(\sum_i i\pi l \hat{D}_l) \). This allows to make direct contact to the model considered by (de Boer et al. 1995); (Schadschneider 1995), and (Aligia et al. 1994). There the hopping amplitudes for lower and upper Hubbard band have opposite signs.

We transform the states of eq. (33) into momentum space with respect to the charge coordinates. The exact eigenstates can now be classified according to their spin and charge sequence, their momentum shifts \( k_C, k_S \), and \( N_C \) momenta from the set of \( k_j = \frac{2\pi m_j}{(La)}, m_j = -(L/2), \ldots (L/2) - 1 \). The normalized eigenstates read

\[
L^{N_C/2} |k_1, \ldots k_{N_C}; (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle = \sum_{l_1<\ldots<l_{N_C}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} \exp \left( i\alpha \sum_{j=1}^{N_C} l_{\mathcal{P}(j)} (k_j + \Phi_{CS}) \right) |(l_1, \ldots l_{N_C}); (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle
\]

where the permutations \( \mathcal{P} \) generate a simple Slater determinant for the momenta and the positions of the \( N_C \) charges, and \( \Phi_{CS} = (k_C - k_S)/L \) is an additional momentum shift which vanishes in the thermodynamical limit.

It is straightforward (de Boer et al. 1995); (Schadschneider 1995) but lengthy to explicitly show that the states in eq. (34) have energy and momentum

\[
E = \sum_{j=1}^{N_C} \epsilon(k_j + \Phi_{CS}) + UN_d \quad (35a)
\]

\[
P = k_S + (\pi/a)(N_d - 1) + \sum_{j=1}^{N_C} (k_j + \Phi_{CS}) + (N \mod 2)\pi/a \quad \mod 2\pi/a \quad (35b)
\]

with \( \epsilon(k) \) given by equation (3a). The essential arguments are repeated in the appendices A2 and A3.

The above set of eigenstates is complete. After summing over the subspaces with different \( K_S, K_C \) the number of states which become degenerate in energy in the thermodynamical limit is given by \( 2^{N_S} N_C!/(N_d! N_h!) \). The number of possible choices for the momenta
is \(L/(N_C!(L - N_C)!)\) since the momenta are those of a gas of spinless Fermions. Altogether one finds for an even number of electrons \(N\)

\[
\sum_{N_d=0}^{N/2} \binom{N_C}{N_d} 2^{N-2N_d} \left( \frac{L}{L - N + 2N_d} \right) = \binom{2L}{N}
\]

(36)

where eq. (10.33.5) of (Hansen 1975) and eq. (22.2.3) of (Abramowitz and Stegun 1970) have been used. This exhausts the Hilbert space for fixed number of electrons \(N\).

**B. Dimerized Harris-Lange model**

The Harris-Lange model can also be solved in the presence of a finite lattice distortion as long as there is hopping between nearest neighbors only. For the \(U = \infty\) Hubbard model at less than half filling this has already been realized some time ago (Bernasconi, Rice, Schneider, and Strässler 1975). The exact eigenenergies are those of spinless Fermions on a dimerized chain.

For the Harris-Lange model with \(N_C\) charge excitations we choose momenta \(|k_j| \leq \pi/(2a)\) of the reduced Brillouin zone, and one of the \(2^{N_C}\) sequences \((\tau_1, \ldots \tau_{N_C})\) with \(\tau_j = \pm 1\). Let us introduce the operator \(\hat{\Pi}_r\) by

\[
\hat{\Pi}_r|k_1, \ldots k_r, \ldots k_{N_C}; (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle = |k_1, \ldots k_r + \pi/a, \ldots k_{N_C}; (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle
\]

(37)

and the four functions \(\xi_1^r(1) = \beta_{k_r}, \xi_2^r(1) = i\alpha_{k_r}, \xi_1^r(-1) = \alpha_{k_r}, \text{ and } \xi_2^r(-1) = -i\beta_{k_r}\), compare eq. (37). The eigenstates for fixed number of charge excitations \(N_C\) can then be written as

\[
|k_1, \tau_1; \ldots k_{N_C}, \tau_{N_C}; (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle = \left[ \prod_{r=1}^{N_C} (\xi_1^r(\tau_r) + \xi_2^r(\tau_r)\hat{\Pi}_r) \right] |k_1, \ldots k_{N_C}; (C_1, \ldots C_{N_C})_{k_C}; (S_1, \ldots S_{N_S})_{k_S}\rangle.
\]

(38)

This state corresponds to \((N_C + \sum_r \tau_r) ((N_C - \sum_r \tau_r)/2)\) spinless Fermions in the upper (lower) Peierls subband.
The corresponding energies and momenta of these states are obviously given by

\[ E = \sum_{j=1}^{N_C} E(k_j + \Phi_{CS})\tau_j + U_Nd \]  
\[ P = k_S + \sum_{j=1}^{N_C} (k_j + \Phi_{CS}) \mod \pi/a \]  

(39a) \hspace{1cm} (39b)

where \( E(k) \) has been given in eq. (3).

C. Band picture interpretation of the spectrum

1. Translational invariant case

The exact solution for the Harris-Lange model can be interpreted in terms of upper and lower Hubbard bands. To simplify the discussion we will ignore the momentum shift \( \Phi_{CS} \) in this subsection. For \( U > W \) the ground state of the half-filled band \( N = L \) has energy zero and is \( 2^L \)-fold degenerate, and we may choose the fully polarized ferromagnetic state as our reference state, \( |\text{FM}\rangle = |\uparrow, \ldots \uparrow\rangle \). Note that this state has momentum \( \pi/a \) on a chain with an even number of sites \( L \), see eq. (35b).

We may now add an electron. We obtain all exact eigenstates for \( N = L + 1 \) electrons, \( N_d = 1 \), and all spins up as

\[ |k; (\bullet)_{k_C=0}, (\uparrow, \ldots \uparrow)_{k_S=0}\rangle = \hat{c}^\dagger_{k,\downarrow} |\text{FM}\rangle \]  

(40a)

with momentum \( P = k + \pi/a \) and energy \( E = \epsilon(k) + U \). The state in eq. (40a) is interpreted as a particle at momentum \( k \) in the upper Hubbard band which has the dispersion relation \( \epsilon(k) + U \). The momentum \( \pi/a \) is attributed to the ferromagnetic reference state.

We may equally well take out an electron from the fully polarized state. We obtain all exact eigenstates for \( N = L - 1 \) electrons, \( N_h = 1 \), and all spins up as

\[ |k; (\circ)_{k_C=0}, (\uparrow, \ldots \uparrow)_{k_S=0}\rangle = -\hat{c}_{\pi/a-k,\uparrow} |\text{FM}\rangle \]  

(40b)

with momentum \( P = -(\pi/a - k) + \pi/a \) and energy \( E = \epsilon(k) \). Note that the states of eq. (40a) and those of eq. (40b) can be generated from each other by the particle-hole
transformation of eq. (16). Their momenta differ by $\pi/a$ since their respective numbers of double occupancies differ by one.

Since the ground state corresponds to a completely filled lower Hubbard band we interpret the state in eq. (40b) as a hole in the lower Hubbard band at $k_h = \pi/a - k$, and the momentum $\pi/a$ is again attributed to the ferromagnetic reference state. The lower Hubbard band must have the dispersion relation $\epsilon(k)$ for particles because a hole at $k_h = \pi/a - k$ has momentum $P = -(\pi/a - k)$ and energy $E = -\epsilon(k_h) = -\epsilon(-k + \pi/a) = \epsilon(k)$.

The band structure for the Harris-Lange model is depicted in figure 1. It displays the parallel upper and lower Hubbard bands with band width $W$ separated by a distance $U$. It is amusing that the celebrated Hubbard-I approximation (Hubbard 1963); (Mazumdar and Soos 1981) also gives parallel bands. Those bands, however, carry a spin index while charge-spin separation is most essential in one dimension. Furthermore, the width of those bands is only half of the exact band width $W$.

Our band structure picture has to be used carefully if there are more than one double occupancy or hole. Figure 1 suggests that there are $L$ states available both in the upper and in the lower Hubbard band, altogether $2L$ independent states. However, this cannot be the case because for $N_d = N_h = L/2$ we would have $L \choose L/2L \choose L/2$ states in the band picture while the Hilbert space actually has only the dimension $L \choose L/2$. The exact solution shows how an appropriate exclusion principle between particles in the upper Hubbard band and holes in the lower Hubbard band can be formulated.

For fixed spin background and fixed $k_1$, $k_2$ there are four exact eigenstates with two charges at $k_1 \neq k_2$. They all have the kinetic energy $T = \epsilon(k_1) + \epsilon(k_2)$. They correspond to four different charge excitations in the band picture: (i) two particles at momenta $k_1$, $k_2$ in the upper Hubbard band, (ii) two holes at momenta $\pi/a - k_1$, $\pi/a - k_2$ in the lower Hubbard band, (iii) a particle at momentum $k_1$ in the upper Hubbard band and a hole at momentum $\pi/a - k_2$ in the lower Hubbard band, (iv) a particle at momentum $k_2$ in the upper Hubbard band and a hole at momentum $\pi/a - k_1$ in the lower Hubbard band. The condition $k_1 \neq k_2$ is naturally fulfilled in cases (i) and (ii), if we assign a fermionic character
to our particles in the upper and holes in the lower Hubbard band, respectively. In case (iii), however, we have to explicitly demand that the momentum at which we create the hole, \( k_h = \pi/a - k_2 \), fulfills \( k_1 \neq k_2 \), i.e., \( k_h \neq \pi/a - k_1 \). This is the same condition which results from case (iv).

We thus see that a particle in the upper Hubbard band at momentum \( k \) actually blocks the creation of a hole in the lower Hubbard band at momentum \( \pi/a - k \) (this is probably the simplest example of a “statistical interaction”, see (Haldane 1991)). With this additional rule the counting of states in the band picture is correct, and the band picture interpretation gives indeed the exact results for the Harris-Lange model. The effective Hamiltonian for fermionic particles in the upper (\( \hat{u}_k \)) and lower (\( \hat{l}_k \)) Hubbard band thus reads

\[
\hat{H}_{\text{band}}^{\text{HL}} = \hat{P}_{ul} \sum_{|k| \leq \pi/a} \left[ (U + \epsilon(k))\hat{n}^u_k + \epsilon(k)\hat{n}^l_k \right] \hat{P}_{ul} \tag{41a}
\]

\[
\hat{P}_{ul} = \prod_{|k| \leq \pi/a} \left[ 1 - \left( 1 - \hat{n}^l_{\pi/a-k} \right) \hat{n}^u_k \right] \tag{41b}
\]

with \( \hat{n}^u_k = \hat{u}_k^+ \hat{u}_k \), \( \hat{n}^l_k = \hat{l}_k^+ \hat{l}_k \). The projection operators guarantee that there is no hole in the lower Hubbard band at momentum \( \pi/a - k \), if there is already a particle at momentum \( k \) in the upper Hubbard band. For half-filling at zero temperature the lower Hubbard band is completely filled.

2. Dimerized Harris-Lange model

The case of the dimerized Hubbard model can be treated accordingly. The upper and lower Hubbard band now split into two Peierls subbands with dispersion relations \( \pm E(k) \). Formally the band structure Hamiltonian for the lower band becomes (compare eq. (2))

\[
\hat{T}_{\text{LHB}}^{\text{band}}(\delta) = \sum_{|k| \leq \pi/(2a)} \epsilon(k) \left( \hat{l}_k^+ \hat{l}_k - \hat{l}_{k+\pi/a}^+ \hat{l}_{k+\pi/a} \right) - i\Delta(k) \left( \hat{l}_{k+\pi/a}^+ \hat{l}_k - \hat{l}_k^+ \hat{l}_{k+\pi/a} \right), \tag{42}
\]

and a similar expression holds for the upper Hubbard band.

The band picture Hamiltonian can easily be brought into diagonal form as in the Peierls case. The quasi-particles in the four subbands are finally described by
\[ \hat{H}^{\text{dim, band}}_{\text{HL}} = \hat{P}_{u^+l^+} + \hat{P}_{u^-l^-} \sum_{|k| \leq \pi/(2a)} \left[ (U + E(k))\hat{n}^u_{k,+} + (U - E(k))\hat{n}^u_{k,-} + E(k)\hat{n}^l_{k,+} - E(k)\hat{n}^l_{k,-} \right] \hat{P}_{u^+l^+} + \hat{P}_{u^-l^-} \]

with \( \hat{n}^u_{k,\pm} = \hat{u}^+_k \pm \hat{u}^-_{k,\pm} \), \( \hat{n}^l_{k,\pm} = \hat{l}^+_{k,\pm} \hat{l}^-_{k,\pm} \) as the number operators for the quasi-particles for the upper (\( \tau = + \)) and lower (\( \tau = - \)) Peierls subband in the upper (\( u \)) and lower (\( l \)) Hubbard band. The quasi-particles in each subband obey a fermionic exclusion principle in the same Hubbard band. In addition, a particle at momentum \( k \) in the upper Hubbard band in the upper (lower) Peierls subband blocks the creation of a hole at momentum \(-k\) in the lower Hubbard band in the upper (lower) Peierls subband. There is no hole in the lower Hubbard band at momentum \(-k\) in the upper or lower Peierls subband, if there is already a particle at momentum \( k \) in the upper Hubbard band in the corresponding Peierls subband. Note that the reciprocal lattice vector is now given by \( \pi/a \). Thereby the projection operators guarantee the proper counting of states.

The resulting band structure is shown in figure 2. The upper and lower Hubbard band are both Peierls split and display the Peierls gap \( W\delta \) at the zone boundaries \( \pm\pi/(2a) \). Note that the upper (lower) Peierls subbands are still parallel.

**D. Band picture interpretation of the current operator**

1. **Translational invariant case**

According to the spectral decomposition of the current-current correlation function, eq. (42), we need to determine the excitation energy \( E_n - E_0 \) of an exact eigenstate \( |n\rangle \) and its oscillator strength \( |\langle 0|j|n\rangle|^2 \). The respective total momenta of these states are \( P_0 \) and \( P_n \).

We are interested in optical excitations from a state with singly occupied sites only. The excited states which can be reached from this state have one pair of hole and double
occupancy, i.e.,
\[
|0\rangle = |(S_1, \ldots S_L)_{k_S}\rangle \tag{44a}
\]
\[
|n\rangle = |k_1, k_2; (\bullet\circ)_{k_C = 0}; (S_1, \ldots S_{L-2})_{k'_S}\rangle \tag{44b}
\]
where we used the fact that \( j \) creates a charge triplet with \( k_C = 0 \). Note that \( (k_1, k_2) \) is the same state as \( (k_2, k_1) \). We denote \( k_1 = k + q/2, k_2 = \pi/a - k + q/2 \) since we will finally represent the state \( |n\rangle \) by a particle in the upper Hubbard band at momentum \( k + q/2 \) and a hole in the lower Hubbard band at momentum \( k - q/2 \).

Since \( j \) conserves the total momentum we already know that \( P_0 = P_n \) which implies \( k_S = q + k'_{S(L-2)}/L \), see eq. (35). Hence, \( k'_{S} = L(k_S - q)/(L - 2) \) has to hold. Recall that \( k'_{S} \) is quantized in units of \( 2\pi/((L-2)a) \). These considerations imply that the charge sector in \( |n\rangle \) carries momentum \( q (-q) \) relative to \( |0\rangle \). In the thermodynamical limit the excitation energy is given by
\[
E(k, q) = U + \epsilon(k + q/2) - \epsilon(k - q/2) = U + 4t \sin(ka) \sin(qa/2) . \tag{45}
\]
Note that the excitation energy does not depend on the spin configuration. For this reason it is possible to find a formally equivalent band picture for the charge sector alone that gives the same optical absorption as the original model. Since \( j \) itself carries all the information on the conservation laws (momentum, charge, and spin quantum numbers) we may equally well work with the (normalized) states
\[
|k + \frac{q}{2}; \frac{\pi}{a} - k + \frac{q}{2}\rangle = \frac{1}{L} \sum_{l_1 < l_2} \left( e^{i(k+q/2)l_1 a} e^{i(\pi/a-k+q/2)l_2 a} - e^{i(k+q/2)l_2 a} e^{i(\pi/a-k+q/2)l_1 a} \right) \\
\quad \quad (-1)^{l_1} |S'_{1}, \ldots S'_{l_1-1}, \circ_{l_1}, S'_{l_1}, \ldots S'_{l_2-2}, \circ_{l_2}, S'_{l_2-1}, \ldots S'_{L-2}\rangle \tag{46}
\]
rather than the exact eigenstates of eq. (34). This will simplify the notation since we do not have to take any summation restrictions into account.

For fixed \( (k, q) \) and fixed spin configuration \( (S'_1, \ldots S'_{L-2}) \) we calculate
\[
\langle 0| j^H_{\text{inter}, -} |k + \frac{q}{2}; \frac{\pi}{a} - k + \frac{q}{2}\rangle = -ie\epsilon(k)e^{iqa/2} \\
\frac{1}{L} \sum_{l} e^{iqa} \langle 0| S'_1, \ldots S'_{L-1}, (\uparrow_{l+1} \downarrow_{l+1} - \downarrow_{l} \uparrow_{l+1}), S'_1, \ldots S'_{L-2}\rangle . \tag{47}
\]
We define the operators $\hat{x}_q^+$ and $\hat{x}_q$ via their product

$$\hat{x}_q^+ \hat{x}_q = \sum_{S_1', \ldots, S_{L-2}'} \frac{1}{L^2} \sum_{l,r} e^{iq(l-r)a} \langle 0 | S_1', \ldots, S_{L-1}', (\uparrow_{l-1} \downarrow_{l+1} - \downarrow_{l-1} \uparrow_{l+1}) , S_l' , \ldots, S_{L-2}' \rangle \langle S_{L-2}', \ldots, S_r', (\downarrow_{r+1} \uparrow_{r-1} - \uparrow_{r+1} \downarrow_{r-1}) , S_{r-1}' , \ldots, S_1' | 0 \rangle.$$  \hspace{1cm} (48)

Summed over all intermediate spin configurations the oscillator strength for fixed $(k, q)$ now becomes

$$\left| \langle 0 | \hat{J}^H_{\text{inter}} | k + \frac{q}{2}, \pi a - k + \frac{q}{2} \rangle \right|^2 = |-ie\alpha(k)\hat{x}_q^+ \hat{x}_q|^2.$$  \hspace{1cm} (49)

It is clear that we have hidden a very difficult many-body problem in the operators $\hat{x}_q$.

Nevertheless we are now in the position to identify the interband current operator in the band picture. It is given by

$$\hat{j}^{\text{band}}_{\text{inter}} = \sum_{|k|, |q| \leq \pi/a} ie\alpha(k) \left( \hat{u}_{k+q/2}^+ \hat{l}_{k-q/2} - \hat{l}_{k-q/2}^+ \hat{u}_{k+q/2} \right).$$  \hspace{1cm} (50)

This operator acts in the same space as the band Hamiltonian of section III C. It is seen that the condition $k + q/2 \neq \pi/a - (k - q/2)$ is automatically fulfilled since $\epsilon(\pi/(2a)) = 0$. Consequently, the projection operators in eq. (41) can again be ignored for the case of linear optical absorption.

2. Dimerized Harris-Lange model

For a distorted lattice the current operator can also modify the momentum of the state by $\pi/a$. Thus we address four possible states for fixed $(k, q)$ from the reduced Brillouin zone, $|k + q/2; \pi/a - k + q/2\rangle$, $|k + q/2; -k + q/2\rangle$, $|\pi/a + k + q/2; \pi/a - k + q/2\rangle$, and $|\pi/a + k + q/2; -k + q/2\rangle$. The same analysis as in the previous subsection leads us to the definition of the operators $\hat{x}_q^+ (\delta, \eta)$, $\hat{x}_q (\delta, \eta)$ with the property

22
\[ \hat{x}_q^+(\delta, \eta)\hat{x}_q^-(\delta, \eta) = \sum_{S_1' \ldots S_{L-2}'} \frac{1}{L^2} \sum_{l,r} e^{i(q_l-q_r)a} (1 + \eta \delta + (-1)^l(\delta + \eta))(1 + \eta \delta + (-1)^r(\delta + \eta)) \]

\[ \langle 0|S_1', \ldots S_{L-1}', (\uparrow_{l+1} \downarrow_{l+1} - \downarrow_{l+1} \uparrow_{l+1}), S_1', \ldots S_{L-2}' \rangle \quad (51) \]

\[ \langle S_{L-2}', \ldots S_r', (\downarrow_{r+1} \uparrow_{r+1} - \uparrow_{r+1} \downarrow_{r+1}), S_{r-1}', \ldots S_1'|0 \rangle. \]

In practice, \( q' = q \) or \( q' = q + \pi/a \).

The interband current operator becomes

\[ j^\text{band}_{\text{inter}} = j^\text{band}_{\text{inter},+} + j^\text{band}_{\text{inter},-} \]

\[ j^\text{band}_{\text{inter},+} = \left(j^\text{band}_{\text{inter},-}\right)^+ \]

\[ j^\text{band}_{\text{inter},-} = \sum_{|q|,|k| \leq \pi/(2a)} \left\{ -iea\epsilon(k) \left[ \hat{l}^+_{k-q/2} \hat{u}_{k+q/2} - \hat{l}^+_{k-q/2+\pi/a} \hat{u}_{k+q/2+\pi/a} \right] \hat{x}_q^+ \right\} \quad (52) \]

\[ + ea \frac{\Delta(k)}{\delta} \left[ \hat{l}^+_{k-q/2} \hat{u}_{k+q/2+\pi/a} - \hat{l}^+_{k-q/2+\pi/a} \hat{u}_{k+q/2} \right] \hat{x}_{q+\pi/a}. \]

Again the conditions \( k+q/2 \neq \pi/a - (k-q/2) \) and \( k+q/2 \neq -(k-q/2) \) will not be violated since \( \epsilon(\pi/(2a)) = 0 \) and \( \Delta(0) = 0 \), respectively. Consequently, the projection operators in eq. (43) can be ignored for the case of linear optical absorption.

In semiconductor physics one prefers to work with the dipole operator rather than the current operator to set up the perturbation theory in the electrical field (Haug et al. 1990). The corresponding expressions for the dipole operator for Hubbard interband transitions are derived in appendix A4.

**IV. OPTICAL ABSORPTION IN THE HARRIS-LANGE MODEL**

**A. Spin average**

All states with no double occupancy are possible ground states in the Harris-Lange model at half-filling. Instead of looking at the optical absorption for a specific state \(|0\rangle\) it is more reasonable to calculate the average absorption, i. e.,
\[
\text{Im}\{\chi(\omega)\} = \frac{1}{2L} \sum_{|0\rangle} \text{Im}\{\chi_{|0\rangle}(\omega)\}.
\]  

(53)

For the Hubbard model this corresponds to temperatures \(k_B T \gg J = \mathcal{O}(W^2/U)\) (“hot-spin case”). The calculation is performed in appendix [A5]. We find the result

\[
\langle \hat{x}_q^+ \hat{x}_{q'} \rangle = \frac{1}{2L} \left\{ \delta_{q,q'} \left[ (1 + \delta\eta)^2 g(q) - (\delta + \eta)^2 g(q + \frac{\pi}{a}) \right] 
+ \delta_{q,q'+\frac{\pi}{a}} (1 + \delta\eta)(\delta + \eta) \left[ g(q) + g(q + \frac{\pi}{a}) \right] \right\}.
\]

(54a)

\[g(q) = \frac{3}{5 + 4 \cos(qa)}.\]  

(54b)

The spin problem could thus be traced out completely. It is seen that \(\hat{x}_q\) keeps its operator character until we have expressed the current operator in terms of the Fermion operators for the four Peierls subbands.

**B. Optical absorption**

1. Translational invariant case

The real part of the average optical conductivity becomes

\[
\text{Re}\{\sigma(\omega > 0)\} = \frac{\pi N_\perp}{2L^2 a\omega} \sum_{|q|,|k| \leq \pi/a} (ea\epsilon(k))^2 g(q) \delta(\omega - E(k,q))
\]

(55)

with \(E(k,q)\) from equation (45). The above expression can be written as

\[
\text{\sigma}_{\text{red}}(\omega > 0) = \frac{1}{4\pi} \int_{|u|}^1 dx \frac{x^2}{\sqrt{x^2 - u^2}} \frac{3}{9 - 8x^2}
\]

(56)

for the reduced optical conductivity with \(|\omega - U|/W \leq 1\). This integral can be expressed as a sum over elliptic integrals but we rather prefer to discuss some special cases.

The optical absorption is restricted to \(|\omega - U| \leq W\). Near the band edges the absorption increases linearly which can be seen from equation (56) by a transformation \(x \rightarrow 1 - y/|u|\). The more interesting case is \(\omega = U\). Now the integrand displays a \(1/x\) singularity for \(|u| \rightarrow 0\). The parallel Hubbard bands give rise to a logarithmic divergence, \(\sigma(\omega \rightarrow U) \sim |\ln(\omega - U)|\),
since their large joint density of states for $\omega = U$ survives even in the presence of a spinon bath that provides any momentum to the charge sector.

The overall behavior of the optical absorption is shown in figure 3. The same absorption curve has been obtained earlier in (Lyo et al. 1977) for their “random” spin background. The result for their “ferromagnetic” spin background follows when we put $g(q) \equiv 1$, as expected. We will comment on their Néel state results in (Gebhard et al. III 1996).

2. Dimerized Harris-Lange model

We have to diagonalize the interband current operator of eq. (52) in terms of the Peierls operators for the lower Hubbard band

$$\hat{l}_k = \alpha_k \hat{l}_{k,-} + \beta_k \hat{l}_{k,+}$$  \hspace{1cm} (57a)

$$\hat{l}_{k+\pi/a} = -i\beta_k \hat{l}_{k,-} + i\alpha_k \hat{l}_{k,+}$$  \hspace{1cm} (57b)

for $|k| \leq \pi/(2a)$. The transformation for the upper Hubbard band is analogous. With this definition the Hamiltonian in the band picture interpretation became diagonal, see eq. (43).

The interband current operator becomes

$$\hat{j}_{\text{band inter}} = \sum_{\tau,\tau'=\pm 1} \sum_{|q|,|k|\leq \pi/(2a)} \lambda_{\tau,\tau'}(k,q) \hat{j}_{k-q/2,\tau}^+ \hat{u}_{k+q/2,\tau'}$$  \hspace{1cm} (58)

with

$$\lambda_{+,+}(k,q) = i e a \left[ \epsilon(k)(\alpha_+\alpha_-^* - \beta_+\beta_-^*)\hat{x}_q^+ + \frac{\Delta(k)}{\delta}(\alpha_+\beta_-^* + \beta_+\alpha_-^*)\hat{x}_{q+\pi/a} \right]$$  \hspace{1cm} (59a)

$$\lambda_{+,-}(k,q) = i e a \left[ -\epsilon(k)(\alpha_+\beta_-^* + \beta_+\alpha_-^*)\hat{x}_q^+ + \frac{\Delta(k)}{\delta}(\alpha_+\alpha_-^* - \beta_+\beta_-^*)\hat{x}_{q+\pi/a} \right]$$  \hspace{1cm} (59b)

and $\lambda_{-,+}(k,q) = -\lambda_{+,-}(k,q)$, $\lambda_{-,-}(k,q) = \lambda_{+,+}(k,q)$. Here we used the short-hand notation $\alpha_\pm = \alpha_{k\pm q/2}$ etc. Note that these quantities can be complex for $q \neq 0$.

The average optical conductivity becomes

$$\text{Re}\{\sigma(\omega > 0, \delta, \eta)\} = \frac{\pi N_+}{L a \omega} \sum_{\tau,\tau'=\pm 1} \sum_{|q|,|k|\leq \pi/(2a)} |\lambda_{\tau,\tau'}(k,q)|^2 \delta(\omega - E_{\tau,\tau'}(k,q))$$  \hspace{1cm} (60a)
with the absorption energies between the respective Peierls subbands

\[ E_{\tau,\tau'}(k, q) = U + \tau' E(k + q/2) - \tau E(k - q/2) , \]  

(60b)

see eq. (43) and figure 2. The transition matrix elements are given by

\[ |\lambda_{\tau,\tau'}(k, q)|^2 = \left( \frac{ea}{2L} \right)^2 \left\{ g(q) \left| (1 + \delta \eta) \epsilon(k) f_{\tau,\tau'} + \tau \tau' (\delta + \eta) \frac{\Delta(k)}{\delta} f_{\tau,-\tau'} \right|^2 + g(q + \frac{\pi}{a}) \left| (\delta + \eta) \epsilon(k) f_{\tau,\tau'} + \tau \tau' (1 + \delta \eta) \frac{\Delta(k)}{\delta} f_{\tau,-\tau'} \right|^2 \right\} \]  

(60c)

with the help functions

\[ f_{+,+}(k, q) = f_{-,-}(k, q) = \alpha_{k+q/2} \alpha_{k-q/2}^* - \beta_{k+q/2} \beta_{k-q/2}^* \]  

(61a)

\[ f_{+,-}(k, q) = f_{-,+}(k, q) = \alpha_{k+q/2} \beta_{k-q/2} + \beta_{k+q/2} \alpha_{k-q/2} \]  

(61b)

where \( \alpha_k, \beta_k \) are given in eq. (7). It can easily be checked that the case \( \delta = \eta = 0 \) is reproduced. For \( \delta = 1, \eta = 0 \) one recovers the result for the average optical conductivity of \( L/2 \) independent two-site systems since \( E(k) = 2t, \lambda_{+,+}(k, q) = 0, \) and \( |\lambda_{+,+}(k, q)|^2 = (2tea)^2 (g(q) + g(q + \pi/a))/(2L): \)

\[ \text{Re}\{\sigma(\omega > 0, \delta = 1, \eta = 0)\} = \frac{L N_{\perp}}{2 La} \pi \delta(\omega - U) \frac{(Wea)^2}{4} \]  

(62)

where we used \( \int_{-\pi}^{\pi} dq/(2\pi) g(qa) = 1. \) For the direct calculation we have to recall that only the singlet of the four spin states contributes, and the hopping between the two sites is \( 2t. \)

For general \( \delta, \eta \) it is necessary to evaluate the optical conductivity in eq. (60) numerically. An example is shown in figure 4. It is seen that now there are two side-peaks in the optical absorption spectrum. The new peaks due to the Peierls distortion are weaker than the one at \( \omega = U \) and vanish for \( \delta \to 1. \) For large lattice distortions the dominant contribution to the side peaks comes from the small-\( q \) transitions between different Peierls subbands. Their oscillator strength is maximum for \( \omega = U \pm W \sqrt{\delta} \) which determines the position of the peaks for large \( \delta. \) The Peierls gap between the bands shows up in the optical spectrum. For small lattice distortions all \( (k, q) \) contribute. The signature of the Peierls gap is smeared out and the position of the side peaks cannot be expressed in terms of a simple function of \( \delta. \)
V. OPTICAL ABSORPTION IN THE EXTENDED HARRIS-LANGE MODEL

A. Extended dimerized Harris-Lange model

Strongly isotropic, almost ideal one-dimensional systems like polymers or charge-transfer salts are not properly described by the Hubbard model of eq. (8) for two reasons: (i) the Peierls distortion is not taken into account, and (ii) the residual Coulomb interaction between charges beyond the Hubbard on-site interaction is neglected. The exponential decay of the Wannier wave functions naturally allows to limit the interactions to on-site and nearest-neighbor Hubbard terms. In the “Zero Differential Overlap Approximation” it is further assumed that only the direct Coulomb term has to be taken into account for the nearest-neighbor Coulomb interaction (Kivelson, Su, Schrieffer, and Heeger 1987); (Wu, Sun, and Nasu 1987); (Baeriswyl, Horsch, and Maki 1988); (Gammel and Campbell 1988); (Kivelson, Su, Schrieffer, and Heeger 1988); (Campbell et al. 1988); (Painelli and Girlando 1988); (Painelli and Girlando 1989); (Campbell, Gammel, and Loh 1990).

Optical absorption spectra for the extended dimerized Hubbard model could only be calculated numerically for small system sizes. Within such an approach the Hamiltonian is explicitly diagonalized (Soos and Ramesesha 1984); (Tavan and Schulten 1986); (Guo, Mazumdar, Dixit, Kajzar, Jarka, Kawabe, and Peyghambarian 1993); (Guo, Guo, and Mazumdar 1994). Since the dimension of the Hilbert space increases exponentially (dim$\hat{\mathcal{H}} = 4^L$) the numerical analysis is restricted to short chains ($L \leq 12$) due to the limited computer power.

Therefore, it is natural to analytically investigate the (dimerized) Harris-Lange model with an additional nearest-neighbor interaction. We will show below that the optical spectrum can still be calculated for this model which is equivalent to the extended dimerized Hubbard model to order $t(t/U)^{-1}$, $t(t/U)^0$, and $t(V/U)^0$. The dimerized extended Harris-Lange model reads

$$\hat{\mathcal{H}}_{\text{HL}}^{\text{dim,ext}} = \hat{T}_{\text{LHB}}(\delta) + \hat{T}_{\text{UHB}}(\delta) + U\hat{D} + V\hat{V}$$  \hfill (63a)
\[ \hat{V} = \sum_l (\hat{n}_l - 1)(\hat{n}_{l+1} - 1). \]  

(63b)

For half-filling the ground state of the extended dimerized Harris-Lange model is still \(2^L\)-fold spin degenerate because every site is singly occupied for \(|V| < U/2\). The energy of these states is zero, \(E_0 = 0\), irrespective of the dimerization value \(\delta\).

The double occupancy and the hole in the excited states now experience a nearest-neighbor attraction while the spin sector remains unchanged. Thus we may immediately translate \(\hat{V}\) into our band picture as

\[ \hat{V}^{\text{band}} = -\frac{2}{L} \sum_{|q| \leq \pi/a} \cos(qa) \sum_{|k|,|p| \leq \pi/a} \hat{u}_{k+q}^+ \hat{u}_k \hat{l}_p \hat{l}_{p-q} \]  

(64)

which describes the scattering of a hole in the lower Hubbard band with a particle in the upper Hubbard band. Again, the projection operators can be disregarded for the optical absorption.

B. Equation of motion technique

In the presence of the nearest-neighbor interaction it becomes increasingly tedious to separately calculate the exact eigenenergies and oscillator strengths. We rather prefer to directly calculate the optical conductivity from an equation of motion approach.

1. Translational invariant case

Since we are interested in the real part of the optical conductivity we can concentrate on the particle current density,

\[ \langle \hat{j}_t \rangle = \frac{\mathcal{N}_L}{La} (\langle 0(t)|\hat{j}\Psi(t) \rangle + \text{h.c.}) \]  

(65)

where \(|0(t)\rangle\) and \(|\Psi(t)\rangle\) are the time evolution of the ground state with and without the external perturbation and thus obey the corresponding Schrödinger equations. We have already used the fact that we want to calculate the linear absorption.
We write
\[ \langle 0(t)|j|\Psi(t)\rangle = \sum_{k,q} -ie\epsilon(k)\hat{x}_q^+ \langle 0(t)|\hat{J}_{k-q/2}^+ \hat{u}_{k+q/2}|\Psi(t)\rangle \]
\[ \equiv \sum_{k,q} \lambda(k, q) j_{k,q}(t) . \]  
(66)

Upon Fourier transformation we obtain
\[ \langle \hat{\chi}_\omega \rangle = N_\perp \Lambda \left( \sum_{k,q} \lambda(k, q) j_{k,q}(\omega) + \lambda^+(k, q) j_{k,q}^*(-\omega) \right) . \]  
(67)

Since we are interested in the optical conductivity for positive frequencies (optical absorption) we may disregard the second term which contributes to \( \omega < 0 \).

The equation of motion for \( j_{k,q}(t) \) becomes
\[ \frac{i}{\hbar} \frac{\partial j_{k,q}(t)}{\partial t} = \langle 0(t) | [\hat{J}_{k-q/2}^+ \hat{u}_{k+q/2}, \hat{H}_{\text{band}}]_\text{−} |\Psi(t)\rangle - \frac{A(t)}{c} \langle 0(t) | \hat{J}_{k-q/2}^+ \hat{u}_{k+q/2} | 0(t) \rangle - \lambda^+(k, q) \frac{A(\omega)}{c} \]  
(68a)
\[ \omega j_{k,q}(\omega) = E(k, q) j_{k,q}(\omega) - 2V \left( \cos(ka) j_q^+(\omega) + \sin(ka) j_q^*(\omega) \right) - \lambda^+(k, q) \frac{A(\omega)}{c} \]  
(68b)

where we kept the expansion linear in the external perturbation, and performed the Fourier transformation. Furthermore, we introduced the abbreviations
\[ j_q^{c,s}(\omega) = \frac{1}{L} \sum_k \begin{pmatrix} \cos(ka) \\ \sin(ka) \end{pmatrix} j_{k,q}(\omega) . \]  
(69)

For our calculations we only need \( j_q^c(\omega) \) since our current operator preserves parity. The particle current density for positive frequencies becomes
\[ \langle \hat{j}_{\omega > 0} \rangle = \frac{N_\perp}{a} (2tiea) \sum_q \hat{x}_q^+ j_q^c(\omega) \]  
(70)

which is proportional to the external field.

We introduce the function
\[ F(q) = \frac{2}{L} \sum_{|k| \leq \pi/a} \frac{(\cos ka)^2}{\omega - E(k, q)} \]  
(71)

which allows us to finally express the optical conductivity as
\[ \text{Re}\{\sigma(\omega > 0, V)\} = -\frac{(Wea)^2 N_\perp}{16a\omega} \frac{1}{L} \sum_{|q| \leq \pi/a} g(q) \text{Im}\left\{ \frac{F(q)}{1 + VF(q)} \right\} . \]  
(72)

The result will be discussed in the next subsection.
2. Extended dimerized Harris-Lange model

The same procedure can be applied to the dimerized case where it is best to start from the diagonalized Hamiltonian in the form of eq. (41), and the current operator in the form of eq. (58). The calculations are outlined in appendix B.

We introduce the three functions $F_{1,2,3}$ as

$$F_1(q) = \frac{2}{L} \sum_{|k| \leq \pi/(2a)} \cos^2(ka) \left[ |f_{+,\tau}|^2 \left( \frac{1}{\omega - E_{\tau,-}} + \frac{1}{\omega - E_{\tau,+}} \right) + |f_{+,\tau'}|^2 \left( \frac{1}{\omega - E_{\tau',-}} + \frac{1}{\omega - E_{\tau',+}} \right) \right]$$  \hspace{1cm} (73a)

$$F_2(q) = \frac{2}{L} \sum_{|k| \leq \pi/(2a)} \sin^2(ka) \left[ |f_{\tau,-}|^2 \left( \frac{1}{\omega - E_{\tau,-}} + \frac{1}{\omega - E_{\tau,+}} \right) + |f_{\tau,\tau'}|^2 \left( \frac{1}{\omega - E_{\tau',-}} + \frac{1}{\omega - E_{\tau',+}} \right) \right]$$  \hspace{1cm} (73b)

$$F_3(q) = \frac{2}{L} \sum_{|k| \leq \pi/(2a)} \cos(ka) \sin(ka) \left\{ f_{\tau,-} f_{\tau,-}^* \left[ \frac{1}{\omega - E_{\tau,+}} + \frac{1}{\omega - E_{\tau,-}} \right] - f_{\tau,+} f_{\tau,+}^* \left[ \frac{1}{\omega - E_{\tau,-}} + \frac{1}{\omega - E_{\tau,+}} \right] \right\}$$  \hspace{1cm} (73c)

where $f_{\tau,\tau'} = f_{\tau,\tau'}(k,q)$ and $E_{\tau,\tau'} = E_{\tau,\tau'}(k,q)$ were introduced in eq. (41) and eq. (58). Furthermore, we abbreviate $A_j = (1 + \delta \eta)F_j - (\eta + \delta)F_3$, $B_j = (\delta + \eta)F_j - (1 + \delta \eta)F_3$ ($j = 1, 2$), $C_1 = (1 + \delta \eta)^2F_1 + (\delta + \eta)^2F_2 - 2(1 + \delta \eta)(\delta + \eta)F_3$, and $C_2 = (1 + \delta \eta)^2F_2 + (\delta + \eta)^2F_1 - 2(1 + \delta \eta)(\delta + \eta)F_3$. The real part of the average optical conductivity can then be expressed as

$$\text{Re}\{\sigma(\omega > 0, V, \delta, \eta)\} = \text{Re}\{\sigma(\omega > 0, \delta, \eta)\}$$

$$+ \frac{VN_a(W ea)^2}{16a^2 \omega L} \text{Im}\left\{ \sum_{|q| \leq \pi/(2a)} \frac{1}{(1 + VF_1)(1 + VF_2) - (VF_3)^2} \left\{ g(q) \left[ A_1^2 + B_2^2 + V(F_1 F_2 - F_3^2)C_1 \right] + g(q + \pi/a) \left[ A_2^2 + B_1^2 + V(F_1 F_2 - F_3^2)C_2 \right] \right\} \right\} .$$
The result for $V = 0$ is given in eq. (60). In the following we will discuss the results for the average optical absorption in the presence of a nearest-neighbor interaction.

C. Optical absorption

1. Translational invariant case

The help function $F(q)$ can be calculated analytically with the help of eqs. (2.267,1), (2.266), and (2.261) of (Gradshteyhn and Ryzhik 1980). The result is

$$F(q) = \frac{2}{[4t \sin(qa/2)]^2} \begin{cases} 
\omega - U - \sqrt{(\omega - U)^2 - (4t \sin(qa/2))^2} & \text{for } |\omega - U| \geq |4t \sin(qa/2)| \\
-i \sqrt{(4t \sin(qa/2))^2 - (\omega - U)^2} & \text{for } |\omega - U| < |4t \sin(qa/2)|
\end{cases} .$$

(75)

The result for $V = 0$, eq. (56), follows after the substitution of $x = \sin(qa/2)$ into equation (72).

The total optical absorption is shown in figure 5. For arbitrarily small $V > 0$ there is a bound exciton which is the standard situation for one-dimensional short-range attractive potentials between a positive (hole) and negative charge (double occupancy). This is evident from the form of $F(q)$ which allows for excitons with momenta $q$ if $|\omega - U| \geq |4t \sin(qa/2)|$ which is fulfilled for $q = 0$ for all $V > 0$.

When the attraction between the two opposite charges is strong, the full exciton band with width $W_{\text{exc}} = 4t^2/V$ is formed. This can be seen from the zeros of the denominator in eq. (72) in the region $|\omega - (U - V - W_{\text{exc}}/2)| \leq W_{\text{exc}}/2$. One finds from $1 + VF(q) = 0$ that

$$\omega = U - V - \frac{W_{\text{exc}}}{2} + \frac{W_{\text{exc}}}{2} \cos qa .$$

(76)

This is precisely the dispersion relation for bound pairs in one dimension with nearest-neighbor hopping of strength $t_{\text{exc}} = t(t/V)$: at large $V$ the excitons are essentially nearest-neighbor pairs of opposite charges which coherently move with the hopping amplitude $t_{\text{exc}}$. Note that this motion requires an intermediate (“virtual”) configuration where the two
charges are not nearest neighbors. Consequently, the hopping integral of the individual constituents, $t$, is reduced by the factor $t/V$ for the motion of the pair. The full band becomes apparent when $W_{\text{exc}} + V > W$ or $V > W/2$, see figure 5. Recall that the spin sector provides any momentum to the charge sector. The momentum transfer, however, is modulated by the function $g(q)$ which is maximum at $q = \pi/a$ and reflects the fact that states with antiferromagnetic spin correlations are best suited for optical absorptions since they contain many neighboring singlet pairs. Hence, the $q = \pi/a$-exciton dominates over the $q = 0$-exciton for $V > W/2$.

It is amusing to see that the optical absorption of a Peierls insulator and a Mott-insulator (extended Harris-Lange model: $U \gg W$, $V > W/2$, $J = 0$) can look very similar, compare figure 2 of I and figure 5. This has already been noted long time ago by Simpson (Simpson 1951); (Simpson 1955); (Salem 1966); (Fave 1992) who explained the optical absorption spectra of short polyenes in the above exciton model. It is seen that Simpson’s model is naturally included in our strong-correlation approach. For real polymers, however, Simpson’s original approach is not satisfactory. A fully developed exciton band only exists in the presence of an incoherent spin background. Now that even the spin-Peierls effect is excluded one can by no means explain the Peierls distortion of the lattice as an electronic effect. This does not exclude other, e.g., extrinsic, explanations for a lattice distortion.

2. Extended dimerized Harris-Lange model

The full spectrum has to be determined numerically. An example for various values of $V/t$ is shown in figure 5. For large $V/t$ we have a fully developed exciton band which is itself Peierls-split into two branches. Thus one obtains four van-Hove singularities in the optical absorption spectrum. The Peierls gap is given by $\Delta_{\text{exc}}^P = \delta W_{\text{exc}} = 4t^2\delta/V$. Even for $V = W$ it is smeared out since $V/t$ is not too large yet and the phenomenological damping $\gamma$ is already of the order of the gap.

For small $V/t$ we obtain the signature of the $q = 0$ exciton for $\delta = 0$, $V > 0$. For
intermediate $V$ this peak develops into a van-Hove singularity of the upper exciton subband. The signatures of the second van-Hove singularity of the upper band are clearly visible for $V = W/2$. The peaks of the Peierls subbands for $V = 0, \delta \neq 0$ are both red-shifted. The peak at lower energy increases in intensity and finally forms the lower exciton subband while the peak at higher energy quickly loses its oscillator strength.

VI. SUMMARY AND OUTLOOK

In this paper we addressed the optical absorption of the half-filled Harris-Lange model which is equivalent to the Hubbard model at strong correlations and temperatures large compared to the spin energy scale. It is extremely difficult to analytically calculate optical properties of interacting electrons in one dimension. For strong coupling when the Hubbard interaction is large compared to the band-width matters considerably simplified since the energy scales for the charge and spin excitations are well separated. We were able to derive an exactly equivalent band structure picture for the charge degrees of freedom and found that the upper and lower Hubbard band are actually parallel bands with the band structure of free Fermions. We have taken special care of the spin background which can act as a momentum reservoir for the charge system. Since we can exactly integrate out the spin degrees of freedom for the Harris-Lange model we were able to solve the problem even in the presence of a lattice dimerization and a nearest-neighbor interaction between the electrons.

For a vanishing nearest-neighbor interaction we found a prominent absorption peak at $\omega = U$ and additional side peaks in the absorption bands $|\omega - U| \leq W$ in the presence of a lattice distortion $\delta$. When a further nearest-neighbor interaction between the charges was included, we found the formation of Simpson’s exciton band of band-width $W_{\text{exc}} = 4t^2/V$ for $V > W/2$ which is eventually Peierls-split. As usual the excitons draw almost all oscillator strength from the band.

It should be clear that the Harris-Lange model with its highly degenerate ground state is not a suitable model for the study of real materials. The results presented here are relevant
to systems for which the temperature is much larger than the spin exchange energy. Real experiments are not carried out in this “hot-spin” regime but at much lower temperatures for which the system is in an unique ground state with antiferromagnetic correlations. Unfortunately, this problem cannot be solved analytically. In the third and last paper of this series (Gebhard et al. III 1996) we will employ the analogy to an ordinary semiconductor (electrons and holes in a phonon bath) to design a “no-recoil” approximation for the chargeons in a spinon bath. It will allows us to determine the coherent absorption features of the Hubbard model at large $U/t$.

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APPENDIX A: THE HARRIS-LANGE MODEL

1. Sum rules

We briefly account for the sum rules. We have

\[ \int_0^{\infty} \, d\omega \, \text{Im}\{\chi(\omega)\} = \pi \frac{N_1}{L a} \sum_n |\langle 0 | j^2 | n \rangle|^2 = \pi \frac{N_1}{L a} \langle 0 | j^2 | 0 \rangle . \quad (A1) \]

It is a standard exercise to show that

\[ \langle 0 | j^2 | 0 \rangle = (2 \text{tea})^2 \sum_l \left( 1 + (-1)^l \delta \right)^2 \left( 1 + (-1)^l \eta \right)^2 \langle 0 | \left( \frac{1}{4} - \hat{S}_l \hat{S}_{l+1} + 1 \right) | 0 \rangle . \quad (A2) \]

We define the positive quantities

\[ C_\text{even,odd}_S = \frac{1}{L} \sum_l \frac{1 \pm (-1)^l}{2} \langle 0 | \left( \frac{1}{4} - \hat{S}_l \hat{S}_{l+1} + 1 \right) | 0 \rangle \quad (A3) \]

and may then write

\[ \int_0^{\infty} \, d\omega \, \text{Im}\{\chi(\omega)\} = \pi N_1 a (2 \text{tea})^2 \left[ (1 + \delta)^2 (1 + \eta)^2 C_\text{even}_S + (1 - \delta)^2 (1 - \eta)^2 C_\text{odd}_S \right] . \quad (A4) \]

If we average over all possible states \( |0\rangle \) we obtain \( C_\text{even,odd}_S = 1/8 \) since only the singlet configuration contributes. Hence,

\[ \int_0^{\infty} \, d\omega \, \text{Im}\{\chi(\omega)\} = \pi N_1 a (\text{tea})^2 \left[ (1 + \delta \eta)^2 + (\delta + \eta)^2 \right] . \quad (A5) \]

The area under the curves for \( \sigma_{\text{red}}(\omega) \), eq. (24), are thus given by

\[ \int_0^{\infty} \frac{d\omega}{W} \sigma_{\text{red}}(\omega) = \pi \frac{1}{4} \left[ (1 + \delta)^2 (1 + \eta)^2 C_\text{even}_S + (1 - \delta)^2 (1 - \eta)^2 C_\text{odd}_S \right] \quad (A6a) \]

\[ \int_0^{\infty} \frac{d\omega}{W} \sigma_{\text{red}}(\omega) = \pi \frac{1}{16} \left[ (1 + \delta \eta)^2 + (\delta + \eta)^2 \right] . \quad (A6b) \]

2. Momentum of eigenstates

First we will assume that the number of sites and the number of particles is even. \( N_C \) and \( N_S \) will thus also be even. Let \( \hat{T} \) be the translation operator by one site, i. e., \( \hat{T} \hat{c}_{l,\sigma} \hat{T}^{-1} = \hat{c}_{l+1,\sigma} \). We have to show that
\[
\hat{T} |\Psi\rangle = e^{-iPa} |\Psi\rangle \tag{A7}
\]

holds. We have to distinguish two cases: (i) a spin is at site \(L\) in \(|\Psi\rangle\) or (ii) a charge is at site \(L\) in \(|\Psi\rangle\).

\textit{a. case (i):} the operator \(\hat{T}\) shifts the spin from site \(L\) to the first site. This results in a phase factor \((-1)\) since one has to commute the Fermion operator \((N - 1)\)-times to obtain the proper order in \(|\Psi\rangle\). Furthermore, the states in \(|\Psi\rangle\) have, relative to those in \(\hat{T} |\Psi\rangle\),

1. shifted the spin sequence by one unit. This results in a phase factor \(\exp(ik_{Sa})\);
2. an additional factor \((-1)\) for each doubly occupied site. This gives a phase factor \(\exp(i\pi N_d)\);
3. a Slater determinant in which each site index is shifted by one. This results in a phase factor \(\exp(i \sum_{j=1}^{NC} (k_j + \Phi_{CS})a)\).

In sum we obtain

\[
(-1) = e^{-iPa} e^{ik_{Sa}} e^{i\pi N_d} e^{i \sum_{j=1}^{NC} (k_j + \Phi_{CS})a} = e^{iPa} e^{i\pi N_d} e^{i \sum_{j=1}^{NC} (k_j + \Phi_{CS})a}.
\tag{A8}
\]

\[
P = k_S + (\pi/a)(N_d - 1) + \sum_{j=1}^{NC} (k_j + \Phi_{CS}) \mod 2\pi/a.
\]

\textit{b. case (ii):} the operator \(\hat{T}\) shifts the charge from site \(L\) to the first site. The states in \(|\Psi\rangle\) have, relative to those in \(\hat{T} |\Psi\rangle\),

1. shifted the charge sequence by one unit. This results in a phase factor \(\exp(ik_{Ca})\);
2. an additional factor \((-1)\) for each doubly occupied site. This gives a phase factor \(\exp(i\pi N_d)\);
3. a Slater determinant in which

(a) each site index is shifted by one. This results in a phase factor \(\exp(i \sum_{j=1}^{NC} (k_j + \Phi_{CS})a)\);
(b) the last row and the first row are interchanged. This gives an additional factor 
\((-1)^{N_C - 1} = -1;\)

(c) the first row is \((1, \ldots, 1)\) instead of \((\exp(i(k_1 + \Phi_{CS})La), \ldots, \exp(i(k_{N_C} + \Phi_{CS})La))\)
\[= (1, \ldots, 1) \exp(i(k_C - k_S)a).\] This gives an additional phase factor \(\exp(-i(k_C - k_S)a).\)

In sum we obtain
\[
1 = e^{-iP a} e^{ik_C a} e^{i\pi N_d} e^{i\sum_{j=1}^{N_C} (k_j + \Phi_{CS}) a} (-1) e^{-i(k_C - k_S)a}
\]
\[P = k_S + (\pi/a)(N_d - 1) + \sum_{j=1}^{N_C} (k_j + \Phi_{CS}) \mod 2\pi/a \tag{A9}\]
as before. If the number of particles \(N\) is odd, the momentum is shifted by another factor of \(\pi/a\), if one repeats the above arguments. This proves that the total momentum of the state \(|\Psi\rangle\) is indeed given by eq. (35b).

3. Energy of eigenstates

We want to prove that
\[
\hat{H}_{HL}|\Psi\rangle = E|\Psi\rangle \quad ; \quad E = \sum_{j=1}^{N_C} \epsilon(k_j + \Phi_{CS}) + UN_d. \tag{A10}\]

Again we restrict ourselves to even \(N\). The bulk terms are simple since there is no hopping across the boundary. A hopping process of a double occupancy and a hole are equivalent:

\[
(-1)^l |\ldots \sigma_l \sigma_{l+1} \ldots \rangle \mapsto -(1)^l |\ldots \sigma_l \sigma_{l+1} \ldots \rangle = (-1)^{l+1} |\ldots \sigma_l \sigma_{l+1} \ldots \rangle \tag{A11a}
\]
\[
|\ldots \sigma_l \sigma_{l+1} \ldots \rangle \mapsto |\ldots \sigma_l \sigma_{l+1} \ldots \rangle. \tag{A11b}
\]

The extra minus sign which appears when a double occupancy moves has been taken care of in the wave function by the phase factor \((-1)^l\) for a double occupancy at site \(l\). Now that there is no difference in the motion of double occupied sites and holes they dynamically behave as spinless Fermions. Since the Slater determinant is the proper phase factor for
non-interacting Fermions eq. (A10) holds for the bulk terms. This also shows that only the Harris-Lange model with hopping amplitudes $|t_{LHB}| = |t_{UHB}|$ can be solved. Another integrable but trivial case is $t_{LHB} = 0$, $t_{UHB} \neq 0$ and vice versa.

We now address the boundary terms. A typical configuration for which transport across the boundary is possible is $|S_1, \ldots C_L\rangle$. The phase of the configuration is given by a Slater determinant in which the last row has the entry $(\exp(i(k_1 + \Phi_{CS})La), \ldots \exp(i(k_{N_C} + \Phi_{CS})La)) = (1, \ldots 1) \exp(i(k_C - k_S)La)$. The action of $\hat{H}_{HL}$ moves the charge from site $L$ to the first position by which an extra minus sign occurs since the electron operator for the spin had to be commuted with $(N - 1)$ other electron operators. These phase factors have to be compared to the corresponding configuration in $E|\Psi\rangle$. Relative to the configuration in $\hat{H}_{HL}|\Psi\rangle$ it has

1. shifted the spin sequence by minus one unit. This results in a phase factor $\exp(-ik_{Sa})$;
2. shifted the charge sequence by one unit. This results in a phase factor $\exp(ik_{Ca})$;
3. a Slater determinant which has $(\exp(i(k_1 + \Phi_{CS})a), \ldots \exp(i(k_{N_C} + \Phi_{CS})a))$ in the first row.

The boundary terms should give the same result as the bulk terms. This leads to the condition

$$- e^{i(k_C - k_S)La} = e^{-ik_{Sa}}e^{ik_{Ca}}(-1)^{N_C-1}$$

(A12)

which is obviously fulfilled. The proof for odd $N$ is analogous, and eq. (A10) holds for all $N$.

4. Electrical dipole operator for the Harris-Lange model

We can derive the electrical dipole operator for the Harris-Lange model from its definition in equation (A.22) of I. We use the Hamilton operator in the band picture interpretation, eq. (A11), and the corresponding current operator, eq. (50). Since $\hat{x}_q$ can be replaced by its average value $\sqrt{g(q)/(2L)}$ one easily sees that the dipole operator becomes
\[ \hat{\mathcal{P}}_{\text{inter}}^{\text{HL}} = \sum_{|k|,|q|\leq \pi/a} \mu_{\text{inter}}^{\text{HL}}(k, q) \left( \hat{u}_{k+q/2}^+ \hat{l}_{k-q/2} + \hat{l}_{k-q/2}^+ \hat{u}_{k+q/2} \right) \]  
(A13a)
\[ \mu_{\text{inter}}^{\text{HL}}(k, q) = i \frac{\lambda(k, q)}{E(k, q)} = ea \sqrt{\frac{g(q)}{2L}} \frac{\epsilon(k)}{E(k, q)} \]  
(A13b)

with \( E(k, q) = U + \epsilon(k + q/2) - \epsilon(k - q/2) \). One sees that the dipole matrix element is of the order \( t/U \) as it should be for interband transitions. Furthermore, for small momentum transfer we obtain
\[ \mu_{\text{inter}}^{\text{HL}}(k; q \rightarrow 0) \sim \epsilon(k). \]  
(A14)

This is the correct form since we create a neighboring hole and double occupancy which corresponds to an electric dipole between nearest neighbors.

The procedure is readily generalized to the dimerized Harris-Lange model. The interband current operator in terms of the Fermion operators for the four Peierls subbands is given in eq. (58), and the diagonalized Hamiltonian can be found in eq. (43). One readily finds
\[ \hat{\mathcal{P}}_{\text{inter}}^{\text{dim. HL}} = \sum_{\tau,\tau'=\pm 1} \sum_{|k|,|q|\leq \pi/(2a)} \mu_{\text{inter;}\tau,\tau'}^{\text{dim. HL}}(k, q) \left( \hat{u}_{k+q/2,\tau}^+ \hat{l}_{k-q/2,\tau'} + \hat{l}_{k-q/2,\tau'}^+ \hat{u}_{k+q/2,\tau} \right) \]  
(A15a)
\[ \mu_{\text{inter;}\tau,\tau'}^{\text{dim. HL}}(k, q) = i \frac{\lambda_{\tau,\tau'}(k, q)}{E_{\tau,\tau'}(k, q)} \]  
(A15b)

with \( \lambda_{\tau,\tau'}(k, q) \) as the root of eq. (60c), and \( E_{\tau,\tau'}(k, q) = U + \tau' E(k + q/2) - \tau E(k - q/2) \), see eq. (59).

The dipole matrix elements again simplify for small \( q \). Note that one obtains both contributions from \( q \rightarrow 0 \) and \( q \rightarrow \pi/a \). After some calculations one obtains
\[ |\lambda_{+,+}(k; q = 0)|^2 = \frac{1}{2L} \left[ \frac{1}{3} \left( ea \left( E(k) + \delta \eta \frac{(2t)^2}{E(k)} \right) \right)^2 + 3 \left( ea \left( \eta E(k) - \delta \frac{(2t)^2}{E(k)} \right) \right)^2 \right] \]  
(A16a)
\[ |\lambda_{+,+}(k; q = 0)|^2 = \frac{1}{2L} \left( ea \frac{\epsilon(k) \Delta(k)(1 - \delta^2)}{\delta E(k)} \right)^2 \left( \frac{\eta^2}{3} + 3 \right). \]  
(A16b)

Note that the dipole matrix elements \( |\lambda_{+,+}(k; q = 0)|^2 \) contain the contributions from \( q = \pi/a \) for \( \delta = \eta = 0 \). Eqs. (A16) have to be compared to the corresponding expressions for the
Peierls chain. It is seen that the expressions display some similarities but they show subtle differences. Even for $q = 0$ the expressions (A16) could not have been guessed.

The corresponding dipole matrix elements become

$$|\mu_{+,+}(k; q \rightarrow 0)|^2 = \frac{1}{U^2} |\lambda_{+,+}(k; q \rightarrow 0)|^2$$  \hspace{1cm} (A17a)

$$|\mu_{+,-}(k; q \rightarrow 0)|^2 = \frac{1}{(U - 2E(k))^2} |\lambda_{+,-}(k; q \rightarrow 0)|^2$$  \hspace{1cm} (A17b)

$$|\mu_{-,+}(k; q \rightarrow 0)|^2 = \frac{1}{(U + 2E(k))^2} |\lambda_{-,+}(k; q \rightarrow 0)|^2 .$$  \hspace{1cm} (A17c)

The dipole matrix elements between the same Peierls subbands are always strong, irrespective of $k$ or $\delta$. However, the dipole matrix elements for transitions between different subbands are small for strong dimerization. Furthermore, they are small in the vicinity of the center and the edge of the reduced Brillouin zone.

5. Spin average in the Harris-Lange model

We need to calculate

$$\langle \hat{x}^+_q \hat{x}_{q'} \rangle = \frac{1}{2L} \sum_{|0\rangle} \hat{x}^+_q \hat{x}_{q'}$$  \hspace{1cm} (A18)

where

$$\hat{x}^+_q(\delta, \eta)\hat{x}_{q'}(\delta, \eta) = \sum_{S_1', \ldots, S_{L-2}'} \frac{1}{L^2} \sum_{l,r} e^{i(ql-q'r)a}(1 + \eta \delta + (-1)^l(\delta + \eta))(1 + \eta \delta + (-1)^r(\delta + \eta))$$

$$\langle 0|S_1', \ldots, S_{L-2}', (\uparrow_{l-1} \downarrow_{l+1} - \downarrow_{l-1} \uparrow_{l+1}), S_{L-2}', \ldots S_1'|0 \rangle$$

$$\langle S_{L-2}', \ldots S_r', (\downarrow_{r+1} \uparrow_{r+1} - \uparrow_{r+1} \downarrow_{r+1}), S_{r-1}', \ldots S_1'|0 \rangle .$$  \hspace{1cm} (A19)

Since the set of spin states $|0\rangle$ is complete we may exactly trace it out and are left with the calculation of the spin matrix elements.
$$M(l, r) = \frac{1}{2L} \sum_{S'_1, \ldots, S'_{L-2}} \langle S'_{L-2}, \ldots, S'_r, (\downarrow r+1 \uparrow r - \uparrow r+1 \downarrow r), S'_{r-1}, \ldots, S'_{L-1}, (\uparrow l+1 \downarrow l - \downarrow l+1 \uparrow l), S'_l, \ldots, S'_{L-2} \rangle. \quad (A20)$$

The value of all spins between the sites $l$ and $r$ is fixed by the singlet operators at $(l, l+1)$ and $(r, r+1)$. We find

$$M(l, r) = 2(-1)^{r-l}2^{-|r-l|-2} \quad (A21)$$

which shows that the correlation function for finding two singlet pairs at distance $n = |r-l|$ exponentially decays with correlation length $\xi_S = 1/\ln(2)$.

Since $M(l, r)$ only depends on the distance between the two sites we may carry out one of the lattice sums in equation (A19). This gives

$$\langle \hat{x}^+_q \hat{x}_{q'} \rangle = \frac{1}{2L} \left\{ \delta_{q,q'} \sum_{n=-L/2}^{L/2-1} e^{i nqa} 2^{-|n|}(-1)^n \left[ (1 + \delta \eta)^2 + (-1)^n (\delta + \eta)^2 \right] \right. \quad (A22)$$

$$+ \left. \delta_{q,q'+\pi} \sum_{n=-L/2}^{L/2-1} e^{i nqa} 2^{-|n|} (1 + \delta \eta)(\delta + \eta)(1 + (-1)^n) \right\}.$$  

The sum over $n$ is readily taken and gives the final result

$$\langle \hat{x}^+_q \hat{x}_{q'} \rangle = \frac{1}{2L} \left\{ \delta_{q,q'} \left[ (1 + \eta \delta)^2 g(q) + (\delta + \eta)^2 g(q + \frac{\pi}{a}) \right] \right. \quad (A23a)$$

$$+ \left. \delta_{q,q'+\pi} (1 + \eta \delta)(\delta + \eta) \left[ g(q) + g(q + \frac{\pi}{a}) \right] \right\}$$

with the help function

$$g(q) = \frac{3}{5 + 4 \cos(qa)}. \quad (A23b)$$

In particular, for the translational invariant case we find

$$\langle \hat{x}^+_q \hat{x}_{q'} \rangle = \delta_{q,q'} \frac{g(q)}{2L}. \quad (A24)$$

This shows that $\hat{x}_q$ can be replaced by $\sqrt{g(q)/(2L)}$ in the translational invariant case.
Here we briefly outline the calculations for the most general case \( V \neq 0, \delta \neq 0 \). We use the diagonalized band picture Hamiltonian in the form of eq. (41), and the band picture current operator in the form of eq. (58). This has the advantage that the equation of motion can directly be inverted and the contribution for \( V = 0 \) can immediately be separated.

The equations of motions give for the four currents

\[
j_{\tau,\tau'}(k, q; \omega) = -\frac{(A(\omega)/c)\lambda^+_{\tau,\tau'} + 2V(\cos(ka)X^c_{\tau,\tau'} + \sin(ka)X^s_{\tau,\tau'})}{\omega - E_{\tau,\tau'}} \quad (B1)
\]

where \( E_{\tau,\tau'} \equiv E_{\tau,\tau'}(k, q) = U + \tau' E(k + q/2) - \tau E(k - q/2) \), \( \lambda_{\tau,\tau'} \equiv \lambda_{\tau,\tau'}(k, q) \), and \( X^c_{\tau,\tau'}, X^s_{\tau,\tau'} \) come from the nearest-neighbor interaction which mixes excited pairs in the different Peierls subbands.

With the help of eq. (B1), \( \lambda_{+,+} = -\lambda_{-,-} \), and \( \lambda_{+,+} = \lambda_{-,-} \) we can immediately write

\[
\langle \hat{j}_{\omega>0}(V) \rangle = \langle \hat{j}_{\omega>0}(V = 0) \rangle - \frac{2VN_1}{La} \sum_{|q| \leq \pi/(2a), |k| \leq \pi/(2a)} \left( \frac{\cos(ka)}{\sin(ka)} \right) \left\{ \lambda_{+,+}X^{c,s}_{+,+} \left( \frac{1}{\omega - E_{+,+}} + \frac{1}{\omega - E_{-,+}} \right) 
+ \lambda_{+,+}Y^{c,s}_{+,+} \left( \frac{1}{\omega - E_{+,+}} + \frac{1}{\omega - E_{-,+}} \right) \right\}. \quad (B2)
\]

To determine \( X^{c,s} \) and \( Y^{c,s} \) we have to evaluate \( \hat{V}\hat{u}^+_{k+q/2,\tau'}\hat{l}_{k-q/2,\tau} |0\rangle \). Since \( \hat{V} \) is simple in terms of the original operators \( \hat{u}_k, \hat{l}_k \) we first have to apply the inverse transformation of eq. (B7). As next step we let \( \hat{V} \) act and then re-transform into the operators for the Peierls subbands in the last step.

The calculation shows that only four combinations of currents occur in \( X^{c,s} \) and \( Y^{c,s} \), namely,

\[
X^{c,s}(k, q) = -f^*_{+,+}(k, q)J^{c,s}_1(q) + f^*_+(-k, q)J^{s,s}_2(q) \quad (B3a)
\]
\[
Y^{c,s}(k, q) = f^*_+(k, q)J^{c,s}_1(q) + f^*_+(k, q)J^{s,s}_2(q) \quad (B3b)
\]
with
\[
J_{1}^{c,s}(q) = \frac{1}{L} \sum_{|p| \leq \pi/(2a)} \left( \frac{\cos(pa)}{\sin(pa)} \right) \left[ f_{+,+}(j_{-,+} - j_{+,+}) + f_{+,-}(j_{+,+} + j_{-,+}) \right] \tag{B4a}
\]
\[
J_{2}^{c,s}(q) = \frac{1}{L} \sum_{|p| \leq \pi/(2a)} \left( \frac{\cos(pa)}{\sin(pa)} \right) \left[ f_{+,+}(j_{+,+} + j_{-,+}) - f_{+,-}(j_{-,+} - j_{+,+}) \right]. \tag{B4b}
\]
Since the interaction is restricted to nearest-neighbors the global, i.e., only \( q \)-dependent currents \( J_{1,2}^{c,s}(q) \) appear in the problem.

Equation (B3) becomes
\[
\langle j_{\omega>0}(V) - \langle j_{\omega>0}(V = 0) = -\frac{2VN_{s}}{a} \sum_{|q| \leq \pi/(2a)} [J_{1}^{c,s}(q)G_{1}^{c,s}(q) + J_{2}^{c,s}(q)G_{2}^{c,s}(q)] \tag{B5}
\]
with \( G_{1,2}^{c,s}(q) \) given by
\[
G_{1,2}^{c,s}(q) = \frac{1}{L} \sum_{|k| \leq \pi/(2a)} \left( \frac{\cos(ka)}{\sin(ka)} \right) \left[ \left( -\frac{f^{*}_{+,+}}{f^{*}_{+,-}} \right) \lambda_{+,+} \left( \frac{1}{\omega - E_{-,+}} + \frac{1}{\omega - E_{+,+}} \right) + \left( \frac{f^{*}_{+,-}}{f^{*}_{+,+}} \right) \lambda_{+,-} \left( \frac{1}{\omega - E_{-,+}} + \frac{1}{\omega - E_{+,+}} \right) \right]. \tag{B6}
\]
The quantities \( G_{1,2}^{c,s}(q) \) are still operator valued objects since they contain \( \lambda_{r,r'}. \) Nevertheless these quantities are known. We insert eq. (B3) and use the fact that \( |f_{+,+}(k,q)|^2 = |f_{+,+}(-k,q)|^2, |f_{+,-}(k,q)|^2 = |f_{+,-}(-k,q)|^2, \) and \( f^{*}_{+,+}(-k,q) f_{+,-}(k,q) = f^{*}_{+,-}(k,q) f_{+,+}(k,q) \) to show that \( G_{1}^{c}(q) = G_{2}^{c}(q) = 0. \) We set \( G_{1}^{c}(q) \equiv G_{1}(q), G_{2}^{c}(q) \equiv G_{2}(q), J_{1}^{c}(q) \equiv J_{1}(q), J_{2}^{c}(q) \equiv J_{2}(q). \) They can be expressed in terms of the functions \( F_{1,2,3}(q) \) of eq. (73) as
\[
G_{1}(q) = \text{itea} \left[ \hat{x}_{q}^{+} F_{1}(q) - \hat{x}^{+}_{q+\pi/a} F_{3}(q) \right] \tag{B7a}
\]
\[
G_{2}(q) = \text{itea} \left[ \hat{x}_{q}^{+} F_{3}(q) + \hat{x}^{+}_{q+\pi/a} F_{2}(q) \right]. \tag{B7b}
\]
It remains to determine \( J_{1,2}(q). \) They can be obtained from their definitions in eq. (B4) and the result from the equations of motion, eq. (B3),
\[
J_{1}(q) + \frac{A(\omega)}{c} G_{1}^{+}(q) = V (-J_{1}(q)F_{1}(q) + J_{2}(q)F_{3}(q)) \tag{B8a}
\]
\[
J_{2}(q) + \frac{A(\omega)}{c} G_{2}^{+}(q) = V (-J_{2}(q)F_{2}(q) + J_{1}(q)F_{3}(q)). \tag{B8b}
\]
It is not difficult to invert these equations to obtain the currents explicitly. The result for the real part of the optical conductivity becomes

\[
\text{Re}\{\sigma(\omega > 0, V, \delta, \eta)\} = \text{Re}\{\sigma(\omega > 0, \delta, \eta)\} + \frac{2V\mathcal{N}_1}{a\omega}
\]

\[
\text{Im}\left\{ \sum_{|q| \leq \pi/(2a)} \frac{1}{(1 + VF_1)(1 + VF_2) - (VF_3)^2} \left[ G_1 G_1^+ + G_2 G_2^+ + V \left( G_1 G_1^+ F_2 + G_2 G_2^+ F_1 + (G_1 G_2^+ + G_2 G_1^+) F_3 \right) \right] \right\}.
\]

As a last step we have to factorize the products over the functions $G_{1,2}(q)$. For the Harris-Lange model we use eq. (54a). With the help of eq. (B7) it is not difficult to derive the final result for the average optical conductivity in the Harris-Lange model, eq. (74).
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FIGURES

FIG. 1. Band structure interpretation of the exact eigenenergies of the Harris-Lange model for $U=2W$.

FIG. 2. Band structure interpretation of the exact eigenenergies of the dimerized Harris-Lange model for $U=2W$, $\delta = 0.2$.

FIG. 3. Reduced average optical conductivity, $\sigma_{\text{red}}(\omega > 0)$, in the Harris-Lange model for $U = 2W$. A broadening of $\gamma = 0.01W$ has been included.

FIG. 4. Reduced average optical conductivity, $\sigma_{\text{red}}(\omega > 0, \delta, \eta)$, in the dimerized Harris-Lange model for $U = 2W$, $\delta = 0.2$ ($\delta = 0.6$), and $\eta = -0.06$. A broadening of $\gamma = 0.01W$ has been included.

FIG. 5. Reduced average optical conductivity, $\sigma_{\text{red}}(\omega > 0, V)$, in the extended Harris-Lange model for $U = 2W$ and $V = 0, W/2, W$. A broadening of $\gamma = 0.01W$ has been included.

FIG. 6. Reduced average optical conductivity, $\sigma_{\text{red}}(\omega > 0, V, \delta, \eta)$, in the extended dimerized Harris-Lange model for $U = 2W$, $\delta = 0.2$, $\eta = -0.06$, $V = 0, W/2, W$. A broadening of $\gamma = 0.01W$ has been included.
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Fig. 5: F. Gebhard et al.,

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Fig. 6: F. Gebhard et al.,

Exact results for the optical absorption of 

\[ \delta = 0.2 \]
\[ \eta = -0.06 \]
\[ \gamma = 0.01W \]