Non-linear excitations in 1D correlated insulators

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Abstract

In this work we investigate charge transport in one-dimensional (1D) insulators via semi-classical and perturbative renormalization group (RG) methods. We consider the problem of electron-electron, electron-phonon and electron-two-level system interactions. We show that non-linear collective modes such as polarons and solitons are responsible for transport. We find a new excitation in the Mott insulator: the polaronic soliton. We discuss the differences between band and Mott insulators in terms of their spin spectrum and obtain the charge and spin gaps in each one of these systems. We show that electron-electron interactions provide strong renormalizations of the energy scales in the problem.
I. INTRODUCTION

It is with joy that we celebrate Michael Pollak’s birthday. One of us (A.H.C.N.) had the honor of inheriting Mike’s office after his retirement. In this office we had long and exciting conversations about many aspects of condensed matter physics and especially one of Mike’s early interests: DNA electronics. It turns out that Mike worked for a few years as an experimentalist and he was probably one of the first researchers to look into the problem of DNA stability with condensed matter experimental tools [1]. These were probably one of the first systematic studies of DNA molecules from the condensed matter point of view. In fact, Mike went ahead and also worked on some theoretical aspects of DNA [2]. Besides being a complete scientist, theorist and experimentalist, Mike’s interest in DNA was far ahead of his own time. Mike’s broad vision of science can also be seen in his beautiful and important work on the insulator-metal transition [3]. Perhaps because of his knowledge and experience, Mike was always convinced that DNA was not a simple band insulator but a more exotic Mott insulator. At this point in time it is not clear if a DNA molecule is an ordinary band insulator or the more complex Mott insulator. We believe that the evidences that DNA is an insulator are quite strong: DNA is transparent to light and transport measurements have shown a charge gap of the order of a few volts [4,5]. From the theoretical point of view the question that remains is: is DNA a band insulator or a Mott insulator? While naive electron counting and LDA calculations [6] seem to indicate that DNA is a band insulator with a very narrow bandwidth, there are some experimental indications that DNA is not an ordinary band insulator. The first comes from the fact that antiferromagnetic excitations have been observed in DNA [7] (see our discussion of magnetic fluctuations in Mott insulators below) and DNA seems to be able to conduct supercurrents when connected to superconducting electrodes via a proximity effect [8]. These effects cannot be observed in ordinary insulators where the gap to charge excitations produces a vanishing density of states at the chemical potential. So, maybe, once again Mike was right and DNA is hiding a few surprises. However, the field of DNA electronics is still in its infancy. Many more
experiments are needed in order to understand the real nature of electron propagation in DNA and the theoretical effort is intense [9–12]. It is with an eye to these possibilities that in the last few years we have been trying to understand the problem of conduction in 1D insulators, which is the main theme of this paper. We are thankful to Mike for pointing the way.

Band insulators cannot transport charge at low temperatures because of a charge gap in the excitation spectrum. When doped with acceptors and/or donors impurities, a band insulator can conduct charge as in the case of semiconductors. But the periodicity of the lattice is broken and impurity bands can only be formed at high density of dopants. There is, therefore, a competition between the disorder (which localizes the carriers), and the overlap between the impurities wave-function (which delocalizes the carriers). In band insulators electron-electron interactions are supposed to be weak and are not usually discussed. While in three dimensions this is certainly true, 1D systems are clearly strongly interacting because electrons cannot avoid each other in their motion, in other words, interactions are enhanced in 1D because of phase space constraints. In this paper we are going to discuss the case of clean insulators in one dimension that can only transport charge via non-linear excitations. By their nature these non-linear excitations only exist if the electronic system interacts with itself or with another set of degrees of freedom that can provide feedback effects and hence nonlinearity.

The classical example of a non-linear excitation in a insulator is a polaron: the dressing of a single electron in the conduction band by phonons. Because of non-linear effects the polaron problem is equivalent to the self-trapping of the electron and the creation of a bound state below the conduction band (very much like a donor state in a semiconductor). The polaron problem has a long history and it is a well-known non-linear problem [13]. Another famous problem is the propagation of solitons in polymers like polyacetylene. While polyacetylene is an insulator because of the Peierls mechanism that leads to the doubling of the unit cell, doping can produce lattice-soliton states in the middle of the gap that in principle can carry charge [14,15]. As in the case of band insulators, the Peierls mechanism does not
require any electron-electron interactions and usually the lattice distortion is assumed to be static so polaronic band effects are not usually discussed. In systems where insulating behavior is driven by electron-electron interactions, that is in the case of the so-called Mott insulators, charge-solitons are known to exist \[16,17\]. Usually charge-solitons are again only discussed in the context of a static lattice without any polaronic effects. These are collective excitations associated with the electronic charge density and, like polarons and lattice-solitons, they are energetically costly since these are topological defects of the field theory that describes them in the first place. As we will show there are many similarities between polaron and soliton conduction and in general these two types of excitations play an important role in 1D systems.

In this paper we generalize the problem of soliton formation in 1D insulators by taking into account not only the electron-electron interaction (which is unavoidable in these systems) but also the electron-phonon interaction and the interaction between electrons and two-level systems. Our interest in discussing the interaction between two-level systems and electrons arises from three main sources. The first is the electron interaction with hydrogen bonds in biological systems such as DNA \[18\], the second is the interaction between electrons and dangling bonds of atoms in 1D nano-structures \[19\], and finally two level systems appear in problems of magnetic moments in 1D metals - the so-called Kondo chain \[20\]. In all cases the electronic scattering by localized two-level systems can lead to new effects such as unitary scattering and Kondo resonance. Thus, two-level systems behave like pseudo-spins. As is expected, the level of complexity of the systems we are going to discuss is quite high but, as we are going to show, the interplay between the electrons with these degrees of freedom leads to new effects that cannot be observed in their absence. As we are going to see the energy for creation of non-linear excitations is greatly reduced by feedback effects \[21\] and this might be at the core of the problem of electron propagation in DNA molecules \[22\].

The paper is organized as follows: in Section I we describe the model; in Section II we describe the problem of a 1D non-interacting band insulator (this is a somewhat idealized
situation but will illustrate very well the main concepts in polaron physics and how they apply in one-dimension); in Section IV we discuss the problem of non-linear transport in a Mott insulator and compare with its non-interacting counterpart; in Section V we show that along the so-called Luther-Emery line, where the interacting electronic problem is exactly solvable, that the electron-phonon coupling reduces to the problem of polaron dressing of the soliton excitations (the polaronic soliton); Section VI contains our conclusions and a discussion of the interplay between electron-electron interaction and the lattice potential.

II. DESCRIPTION OF THE MODEL

Our system of interest can be broken into three different pieces: electrons, phonons and pseudo-spins (two-level systems). The electrons are described in term of creation, $\psi_\sigma^\dagger(x)$, and annihilation, $\psi_\sigma(x)$, operators at position $x$ with spin $\sigma$ ($\sigma = \uparrow, \downarrow$) and obey anti-commutation relations: $\{\psi_\sigma(x), \psi^\dagger_{\sigma'}(x')\} = \delta(x - x') \delta_{\sigma,\sigma'}$. In the absence of interactions the Hamiltonian describing the electron motion is simply:

$$H_0 = \int dx \sum_\sigma \left\{ \frac{\hbar^2}{2m} \frac{\partial \psi_\sigma^\dagger}{\partial x} \frac{\partial \psi_\sigma}{\partial x} + V(x) \psi^\dagger_\sigma(x) \psi_\sigma(x) \right\}, \quad (2.1)$$

where $m$ is the electron mass and $V(x)$ is the lattice potential. If $V(x)$ is periodic then a gap opens up in the spectrum and if the number of electrons per unit cell is 2 the problem is described as a band insulator.

While the above description is satisfactory for a system where the electronic wave-function is extended (and therefore the system is well-described by an electron gas), in systems where the coupling with the ions is strong a tight-binding description is usually a better starting point. In fact this kind of description is the starting point for the description of the Mott insulator. The electron Hamiltonian including the electron-electron interactions can be generically written as:

$$H_e = -t_e \sum_{i,\sigma} C_{i,\sigma}^+ C_{i+1,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{i,\sigma,\sigma'} n_{i,\sigma} n_{i+1,\sigma'}, \quad (2.2)$$
where \( C_{i,\sigma} \) (\( C_{i,\sigma}^+ \)) is the annihilation (creation) electron operator at unit cell \( i \) with spin \( \sigma \) and \( n_{i,\sigma} = C_{i,\sigma}^+ C_{i,\sigma} \) is the electron number operator. \( t_e \) is the hopping energy of the electron between different sites and \( U \) and \( V \) describe the on-site and the nearest neighbor electron-electron interactions, respectively.

In the non-interacting limit the electron energy is \( E_k = -2t_e \cos(ka) \), where \( a \) is the lattice spacing. For a finite density of electrons all the states up to the Fermi energy, \( E_F \), are filled generating two Fermi points defined by \( E_{\pm k_F} = E_F \), where \( k_F = \pi n/2 \) is the Fermi momentum (\( n \) is the number of electrons per unit of length). Close to the Fermi points the spectrum is \( E_{k_F + q} - E_F = v_F q \) where \( v_F = 2t_e a \sin (k_F a) \), is the Fermi velocity. The linearization of the spectrum close to the Fermi points can also be translated into operator language. We rewrite the electron operator as the product of a rapidly varying part \( (e^{\pm ik_F x}) \) and a slowly varying part:

\[
\psi_\sigma(x) = \psi_{R,\sigma}(x)e^{ik_F x} + \psi_{L,\sigma}(x)e^{-ik_F x},
\]  

(2.3)

where \( \psi_{R,\sigma}(x) \) (\( \psi_{L,\sigma}(x) \)) creates a right (left) moving electron in the system. Because of the chiral nature of these excitations they can be described in terms of bosonic operators \( [23] \):

\[
\psi_{(R,L),\sigma}(s) = \frac{1}{\sqrt{2\pi a}} e^{\pm i\sqrt{\pi} \phi_{(R,L),\sigma}(s)}. 
\]  

(2.4)

In turn, the bosonic modes \( \phi_{(R,L),\sigma} \) can be described in terms of new fields, \( \phi_\sigma \) and \( \theta_\sigma \), as \( \phi_{(R,L),\sigma}(x) = \phi_\sigma(x) \mp \theta_\sigma(x) \). The bosonic fields can then be rewritten in terms of charge and spin bosonic modes:

\[
\Phi_{\rho,\sigma} = \frac{1}{\sqrt{2}} (\phi_\uparrow \pm \phi_\downarrow) \\
\Theta_{\rho,\sigma} = \frac{1}{\sqrt{2}} (\theta_\uparrow \pm \theta_\downarrow). 
\]  

(2.5)

The procedure of writing electron operators in terms of bosons is called bosonization. It can be shown that the charge density operator \( \rho(x) \) is related to \( \Phi_{\rho}(x) \) by

\[
\rho(x) = -\sqrt{2} \frac{\partial \Phi_{\rho}(x)}{\partial x}. 
\]  

(2.6)
The non-interacting Hamiltonian and all the scattering process in the 1D system can now be rewritten in terms of bosons. There are three main types of scattering in 1D: forward scattering (with small momentum transfer), backscattering (with $2k_F$ momentum transfer) and Umklapp scattering (with $4k_F$ momentum transfer). While the forward and backscattering do not require the lattice to participate, the Umklapp scattering requires, by momentum conservation, that $4k_F = G$ where $G = 2\pi/a$ is the reciprocal lattice vector. Because of this constraint the Umklapp scattering is only important at commensurate filling factors and is responsible for the opening of the Mott gap in the half-filled system ($n = 1/a$).

The model (2.2) can be bosonized using the fields $\Phi_\rho(x)$ and $\Phi_\sigma(x)$. The Hamiltonian of the problem breaks into two main parts, $H = H_s + H_c$, describing spin $H_s$ and charge $H_c$ [23]:

$$H_s = H_\sigma + \frac{2g_1}{(2\pi a)^2} \int dx \cos \left[ \sqrt{8} \Phi_\sigma(x) \right]$$

$$H_c = H_\rho + \frac{2g_3}{(2\pi a)^2} \int dx \cos \left[ \sqrt{8} \Phi_\rho(x) + 4k_F x \right].$$

(2.7)

In the above Hamiltonian we have

$$H_v = \frac{1}{2\pi} \int dx \left[ (u_v K_v) \pi^2 \Pi^2_v(x) + \frac{u_v}{K_v} \left( \frac{\partial \Phi_v(x)}{\partial x} \right)^2 \right], \quad v = \rho, \sigma$$

(2.8)

describing a gapless Luttinger liquid involving only the forward scattering processes. Here, $u_v$ are the velocity of the bosonic fields, $K_v$ are the Luttinger parameters, and $\Pi_v(x)$ is the momentum field operator that is canonically conjugate to $\Phi_v(x) : [\Phi_v(x), \Pi_{v'}(x')] = i\delta_{v,v'} \delta(x - x')$.

In (2.7) the coupling constants $g_1$ and $g_3$ represent the backward scattering and the Umklapp process. One can relate the parameters in the bosonized Hamiltonian with the ones in (2.2) by [24]:

$$u_\rho K_\rho = u_\sigma K_\sigma = v_F - \frac{V a}{\pi}$$

$$\frac{u_\rho}{K_\rho} = v_F + \frac{(U + 5V) a}{\pi}$$

$$\frac{u_\sigma}{K_\sigma} = v_F - \frac{(U - V) a}{\pi}$$

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This relation between the coupling constants in the bosonic theory and the interactions in the electron problem allow us to change freely from one representation to the other. Notice that the bosonization procedure is not a good starting point for the problem of the band insulator because \( n = 2/a \) and therefore \( v_F = 0 \), implying that we cannot define right and left moving particles (this is just the trivial statement that when the band is full there is no electronic motion).

Observe that the bosonic fields in (2.7) separate completely into the spin and charge parts. This is called spin-charge separation and it is a generic property of one dimensional systems. Namely, while an isolated electron carries both spin and charge, in the 1D system the electron decays into the bosonic collective modes described above that carry spin and charge separately. Since we are only considering the properties of insulators, the spin degrees of freedom decouple from the problem and are completely described by \( H_s \) in (2.7). From this result we can immediately draw some conclusions about the nature of the spin excitations in these systems.

The simplest way to understand the importance of these terms is to perform a perturbative renormalization group (RG) calculation by assuming that the non-linear terms in (2.7) are small compared to the Luttinger liquid terms in (2.8). We can study how these non-linear terms affect the physics of the Luttinger liquid. The RG procedure is defined by introducing a cut-off \( \Lambda \) in momentum space so that all the momenta, \( k \), are defined in \(-\Lambda < k < \Lambda\). We now trace all degrees of freedom in the region of high momenta around the cut-off, say, \( \Lambda/b < |k| < \Lambda \) (\( b > 1 \)), and rescale the frequencies and momenta so that the Luttinger liquid Hamiltonian (2.8) becomes invariant under rescaling (\( \omega \to b\omega \) and \( k \to bk \)). As we rescale the system to lower energies the coupling constants change with the scale. This change is given by the RG equations. For the backscattering problem it can be shown that [23]:

\[
\frac{\partial g_1(\ell)}{\partial \ell} = 2(1 - K_\sigma)g_1(\ell),
\] (2.10)
where \( \ell = \ln(1/\Lambda) \). Notice that for \( K_\sigma > 1 \), the backscattering term scales to zero and therefore it is irrelevant under the RG. The spin degrees of freedom are completely described by the Luttinger liquid Hamiltonian (2.8). The spin excitations are gapless and propagate with velocity \( v_\sigma \). However, when \( K_\sigma < 1 \), the backscattering term grows under the RG, implying that the non-linear terms are becoming stronger at low energies: the backscattering is relevant. The relevance of this term can be easily understood if we consider only the non-linear part of the Hamiltonian:

\[
H_I = \frac{g_1}{2(\pi a)^2} \int dx \cos(\sqrt{8}\Phi_\sigma(x)).
\]  

(2.11)

If \( g_1 \to \infty \) at long length scales we see that the coefficient of the cosine grows and becomes much bigger than the energy scale of the Luttinger liquid in (2.8). If we now ignore completely the Luttinger liquid part of the Hamiltonian (as the RG procedure tells us we should do), we see that the energy of the problem is minimized when the field \( \Phi_\sigma(x) = 0 \) for \( g_1 < 0 \) or \( \Phi_\sigma(x) = \sqrt{\pi/8} \) when \( g_1 > 0 \). Thus, in the ground state the field is uniform. Let us allow the field \( \Phi_\sigma \) to fluctuate around its minimum value. Expanding \( H_I \) up to second order in \( \Phi_\sigma \) we find

\[
H_I \approx -\frac{|g_1| L}{2(\pi a)^2} + \frac{2|g_1|}{(\pi a)^2} \int dx \Phi_\sigma^2(x),
\]

(2.12)

where \( L \) is the size of the system. The first term in (2.12) is the ground state energy of the uniform state. Adding now the Luttinger liquid part of the Hamiltonian, Eq.(2.8), we find that the action that describes the system is:

\[
S \approx -\frac{|g_1| L}{2(\pi a)^2} + \int dx \int d\tau \left[ \frac{1}{2K_\sigma v_\sigma} (\partial_\tau \Phi_\sigma(x))^2 + \frac{v_\sigma}{2K_\sigma} (\partial_\xi \Phi_\sigma)^2 + \frac{2|g_1|}{(\pi a)^2} \Phi_\sigma^2(x) \right] \\
\approx -\frac{|g_1| L}{2(\pi a)^2} + \int dq \int d\omega \frac{1}{2\pi} \left[ \frac{1}{2K_\sigma v_\sigma} \omega^2 + \frac{v_\sigma}{2K_\sigma} q^2 + \frac{2|g_1|}{(\pi a)^2} \right] |\Phi_\sigma(q, \omega)|^2,
\]

(2.13)

where we have Fourier transformed the fields in the last line. Notice that the excitation spectrum has changed from \( \omega(q) = \pm v_\sigma |q| \) to

\[
\omega(q) = \pm v_\sigma \sqrt{q^2 + m^2} \\
= \frac{2}{\pi a} \sqrt{K_\sigma |g_1| v_\sigma}.
\]

(2.14)
This result indicates that a gap of energy

\[ \Delta_S = \nu m = 2 \sqrt{\frac{K_\sigma \nu |g_1|}{\pi a}} \]  

(2.15)

opens in the spectrum at \( q = 0 \) (\( k = k_F \) in terms of the original electrons). We can define a correlation length \( \xi = 1/m = \nu / \Delta_0 \) which tells us that the correlations decay exponentially over \( \xi \) and that for distances larger than \( \xi \) no correlations are possible. Thus, the relevance of the operators under the RG implies that the low lying spin excitations of the system are gapped (in contrast to the Luttinger liquid). This is the so-called spin gap and is a sign of Cooper pairing in the system since for \( K_\sigma < 1 \) the interactions become effectively attractive.

To understand the origin of this result we notice that when two electrons form a Cooper pair in a singlet state it costs energy to break the pair and make a spin excitation.

Let us focus on the charge part of the Hamiltonian that can be written as:

\[ H_e = \frac{1}{2\pi} \int dx \left[ (u_\rho K_\rho) \pi^2 \Pi_\rho^2 + \frac{u_\rho}{K_\rho} \left( \frac{\partial \Phi_\rho}{\partial x} \right)^2 \right] + \frac{2g_3}{(2\pi \alpha)^2} \int dx \cos \left[ \sqrt{8} \Phi_\rho + 4k_Fx \right]. \] (2.16)

The problem described by (2.16) is well understood and it can be shown that when \( 4k_Fa \neq 2\pi \) the Umklapp term is irrelevant and the problem is described by a gapless Luttinger liquid. However, when the system becomes commensurate with the lattice (\( n = 1/a \)) the Umklapp term in (2.16) is important. In fact, an RG calculation gives [23]:

\[ \frac{\partial g_3(\ell)}{\partial \ell} = 2(1 - K_\rho)g_3(\ell). \] (2.17)

In complete analogy with the backscattering problem, this result shows that a gap opens in the charge spectrum (the so-called Mott gap) if \( K_\rho < 1 \). The Umklapp term is irrelevant when \( K_\rho > 1 \). Thus, a correlated insulator has two major requirements. Namely, the electron-electron interactions have to be repulsive and the charge density has to be commensurate with the lattice.

In fact the calculation of the gap in (2.15) is incorrect because we have not taken into account the fluctuations in the problem by expanding the fields close to its minimum. We can learn more about the actual value of the Mott gap by looking at the RG equation (2.17)
more closely. That RG predicted that for $K_\rho < 1$ the system scales to strong coupling and $g_3$ grows without bound. The maximum value $g_3$ can attain in our theory is the largest energy scale, that is, the electron bandwidth, $W \approx 4t_e$. Beyond this energy scale the perturbative RG calculation breakdown. In our linearized theory it is easy to see that $W \approx v_F\Lambda_0$, where $\Lambda_0 \approx 1/a$ is the bare cut-off in the theory. When $g_3(\ell)$ becomes of the order of $W$ the variable $\ell$ reaches its maximum value $\ell^* = \ln(\Lambda_0/\Lambda^*)$. Here $\Lambda^*$, which has dimensions of inverse length, becomes of the order of the inverse of correlation length, that is, $\Lambda^* \approx 1/\xi_\rho \approx \Delta/v_\rho$. However, accordingly to (2.17) we must have

$$\ell^* = \frac{1}{2(1-K_\rho)} \ln(g(\ell^*)/g_3(0))$$

$$\ln(W/\Delta) \approx \frac{1}{2(1-K_\rho)} \ln(W/|g_3|),$$

(2.18)

which can be solved for $\Delta$ as

$$\Delta_M = W \left( \frac{|g_3|}{W} \right)^{1/(1-K_\rho)}$$

(2.19)

showing that the gap is proportional to $|g_3|^{1/(2(1-K_\rho))}$ instead of $|g_3|^{1/2}$ as predicted by our naive expansion (2.13). In fact the square root behavior of the gap with the coupling constant is only obtained when $K_\rho = 0$ which is equivalent to the strong coupling regime where the interaction becomes of the order of the bandwidth of the original problem (see (2.9)). The exact value of $\Delta_M$ can be obtained by the mapping, via a Jordan-Wigner transformation, the Umklapp problem into the anisotropic Heisenberg model [25]. This model can be solved exactly by Bethe ansatz and the gap calculated without approximations [16]. It is found that the power law dependence of the Mott gap with the coupling constant in (2.19) is exact. This result shows the importance of the RG calculation. Observe that the bandwidth $W$ which appears in (2.19) is a non-universal number that cannot be obtained from the RG. By comparing (2.19) with (2.15), however, we find $W \approx 4v_F/(\pi a)$.

The other important components of the problem are the phonons. These can be of two types: acoustic or optical. Since we are only interested in the low energy physics of the 1D system we consider only the acoustic modes that can be described by the Hamiltonian [26]
\[ H_{ph} = \frac{1}{2} \int dx \left[ \frac{\Pi_L^2(x)}{\rho_L} + c_s^2 \rho_L \left( \frac{\partial \phi_L(x)}{\partial x} \right)^2 \right], \quad (2.20) \]

where \( \rho_L \) is the mass density of the system, \( c_s \) is the sound velocity, and \( \Pi_L(x) \) is the phonon momentum operator that is canonically conjugated to the phonon field \( \phi_L(x) \):

\[ [\phi_L(x), \Pi_L(x')] = i\hbar \delta(x - x'). \]

The electron-phonon coupling assumed here is of the deformation potential type, which is appropriate for acoustic phonons:

\[ H_{e-p} = \gamma_p \int dx \rho(x) \frac{\partial \phi_L(x)}{\partial x} \]
\[ = \gamma_p \int dx \psi^\dagger(x) \psi(x) \frac{\partial \phi_L(x)}{\partial x} \]
\[ = \frac{\gamma_p \sqrt{2}}{\pi} \int dx \frac{\partial \phi_p(x)}{\partial x} \frac{\partial \phi_L(x)}{\partial x}. \quad (2.21) \]

Another component in our problem is the presence of pseudo-spins (or two-level systems) that couple to the electronic charge degrees of freedom but not to the spins (this is why we term them pseudo-spins). In a real system these pseudo-spins can be dangling bonds of atoms in a nano-structure or hydrogen bonds in DNA. Because of their nature the pseudospins are assumed to be non-interacting and are described by a Hamiltonian:

\[ H_t = \frac{1}{2} \int dx \left[ -\varepsilon \sigma^z(x) + t \sigma^x(x) \right], \quad (2.22) \]

where \( \sigma^z \) and \( \sigma^x \) are Pauli matrices that obey: \( [\sigma^z(x), \sigma^z(x')] = 2i\sigma^y(x)\delta(x - x') \). In (2.22) \( \varepsilon > 0 \) is the energy difference between the ground state with pseudo-spin \( \uparrow \) and the first excited state with pseudo-spin \( \downarrow \). For generality we also allow for the quantum tunneling of the pseudo-spin between the two possible configurations and \( t \) is the energy associated with this tunneling.

As mentioned previously, the coupling between the pseudo-spins and the charge degrees of freedom has essentially the same structure as the electron-phonon coupling:

\[ H_{e-t} = \frac{\gamma_t}{2} \int dx \psi^\dagger(x) \psi(x) [\sigma^z(x) - 1] \]
\[ = \frac{\gamma_t}{\sqrt{2\pi}} \int dx \frac{\partial \phi_p(x)}{\partial x} [\sigma^z(x) - 1]. \quad (2.23) \]
The rationale for this coupling is the fact that electron polarization around a pseudo-spin can lead to its local reorientation. This is the same reasoning behind the electron-phonon coupling except that in the case of the pseudo-spin the reorientation process is quantized.

In order to simplify the problem we project out the pseudo-spin variables in terms of a new field $\theta(x)$ by writing the generic form for the pseudo-spin wavefunction,

$$
\Psi(x) = \begin{pmatrix}
\cos \theta(x) \\
\sin \theta(x)
\end{pmatrix},
$$

and rewriting the Hamiltonian as:

$$
H_t \rightarrow \langle \Psi | H_t | \Psi \rangle = \frac{1}{2} \int dx [ -\varepsilon \cos 2\theta(x) + t \sin 2\theta(x) ]
$$

$$
H_{e-t} \rightarrow \langle \Psi | H_{e-t} | \Psi \rangle = -\gamma_t \int dx \psi^\dagger(x) \psi(x) \sin^2 \theta(x).
$$

Now, all the variables in the problem are given in terms of fields that are continuous and smoothly varying in space.

**III. POLARONS IN BAND INSULATORS**

In this section we review the problem of polarons in band insulators described by the Hamiltonian (2.1). The problem reduces to a valence band which is full and a conduction band that is empty. In this case, as discussed previously, the bosonization procedure is not a good starting point since the charge density is such that the Fermi velocity vanishes and therefore the linearization around the Fermi point is a bad approximation. The problem of bosonization and band insulators for weak periodic potentials is discussed in Section VI. In this section we disregard electron-electron interactions and consider the problem of a single electron (hole) at the bottom (top) of the conduction (valence) band. The Hamiltonian for the electron in the conduction band is identical to the one in (2.1) except that we can set $V = 0$ and replace the electron bare mass $m$ by its effective band mass $m_c$. The full Hamiltonian of the problem is written as $H_p = H_0 + H_{ph} + H_t + H_{e-p} + H_{e-t}$ where:
\[ H_0 = \frac{\hbar^2}{2m_c} \int dx \frac{\partial \psi^\dagger}{\partial x} \frac{\partial \psi}{\partial x} \]

\[ H_{ph} = \frac{1}{2} \int dx \left[ \frac{\Pi^2}{\rho_L} + c^2 \rho_L \left( \frac{\partial \phi_L}{\partial x} \right)^2 \right] \]

\[ H_t = \frac{1}{2} \int dx \left[ -\varepsilon \cos 2\theta(x) + t \sin 2\theta(x) \right] \]

\[ H_{e-p} = \gamma_p \int dx \psi^\dagger \frac{\partial \phi_L}{\partial x} \]

\[ H_{e-t} = -\gamma_t \int dx \psi^\dagger(x) \psi(x) \sin^2 \theta(x). \] (3.1)

The generating function of the problem can be written as:

\[ Z = \int D\psi^* D\psi D\phi_L D\theta \ e^{-\frac{i}{\hbar} \int dt \int dx \mathcal{L}[\psi^*, \psi, \phi_L, \theta]}, \] (3.2)

where \( \psi^* \) and \( \psi \) are Grassmann variables and the Lagrangian of the problem is:

\[ \mathcal{L} = i\hbar \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) - \frac{\hbar^2}{2m_c} \left( \frac{\partial \psi^*}{\partial x} \right) \left( \frac{\partial \psi}{\partial x} \right) + \frac{\rho_L}{2} \left[ \left( \frac{\partial \phi_L}{\partial t} \right)^2 - c^2 \left( \frac{\partial \phi_L}{\partial x} \right)^2 \right] + \frac{1}{2} \left[ \varepsilon \cos 2\theta - t \sin 2\theta \right] - \left[ \gamma_p \frac{\partial \phi_L}{\partial x} - \gamma_t \sin^2 \theta(x) \right] |\psi(x)|^2. \] (3.3)

Although the above Lagrangian is of relative complexity we are going to study the problem in the semiclassical limit by letting \( \hbar \to 0 \). In this limit, as one can see directly from (3.2), the problem is dominated by the saddle point equations:

\[ t \cos 2\theta = -\varepsilon \sin 2\theta + \gamma_{bs} |\psi|^2 \sin 2\theta \]

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_c} \frac{\partial^2 \psi}{\partial^2 x} + \left( \gamma_p \frac{\partial \phi_L}{\partial x} - \gamma_t \sin^2 \theta \right) \psi(x) \]

\[ \rho_L \frac{\partial^2 \phi_L}{\partial t^2} = c^2 \rho_L \frac{\partial^2 \phi_L}{\partial x^2} + \gamma_p \frac{\partial |\psi|^2}{\partial x}. \] (3.4)

The first equation in (3.4) gives:

\[ \tan 2\theta(x) = \frac{t}{\gamma_t |\psi(x)|^2 - \varepsilon}, \] (3.5)

which shows that the pseudo-spins can rearrange their orientation due to the presence of the electrons. In fact if we define a position dependent pseudo-spin energy:

\[ \varepsilon(x) = \varepsilon - \gamma_t |\psi(x)|^2 \] (3.6)
we see that the electrons decrease the effective pseudo-spin energy allowing for the tunneling of the pseudo-spins. In other words, the electrons delocalize the pseudo-spins. In what follows we are going to consider two regimes. In the first regime we have \( t \gg \bar{\varepsilon}(x) \) and therefore the pseudospins delocalize, in the second regime \( t \ll \bar{\varepsilon} \) the renormalization of the pseudo-spin energy is not enough to delocalize the pseudo-spins. As we are going to see, in both limits the physics is very similar and therefore the final behavior of the polaron is essentially independent of these limits. The expression \( (3.3) \) can also be written as:

\[
\sin^2 \theta(x) = \frac{1}{2} - \frac{\bar{\varepsilon}(x)}{2\sqrt{\bar{\varepsilon}^2(x) + t^2}}.
\]

(3.7)

For \( t \gg \bar{\varepsilon} \) we have

\[
\sin^2 \theta(x) \approx \frac{1}{2t} \left( \gamma_t |\psi(x)|^2 - \varepsilon + t \right),
\]

(3.8)

while for \( t \ll \bar{\varepsilon} \) we have

\[
\sin^2 \theta(x) \approx \frac{t^2}{2\bar{\varepsilon}^3} \left( \gamma_t |\psi(x)|^2 + \frac{\varepsilon}{2} \right).
\]

(3.9)

Substituting \( (3.8) \) or \( (3.9) \) back into \( (3.4) \) we find:

\[
\begin{align*}
\frac{i\hbar}{\partial t} \frac{\partial \psi}{\partial t} & = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \gamma_p \frac{\partial \phi_L}{\partial x} \psi - \left( D_t |\psi|^2 + E_t \right) \psi \\
\rho_L \frac{\partial^2 \phi_L}{\partial t^2} &= c_s \rho_L \frac{\partial^2 \phi_L}{\partial x^2} + \gamma_p \frac{\partial |\psi|^2}{\partial x},
\end{align*}
\]

(3.10)

where the values of \( D_t \) and \( E_t \) are giving by

\[
\begin{align*}
D_t & \approx \frac{1}{2t} \gamma_t^2 \\
E_t & \approx \frac{1}{2} \left( 1 - \frac{\varepsilon}{t} \right) \gamma_t
\end{align*}
\]

(3.11)

for \( t \gg \bar{\varepsilon} \), and

\[
\begin{align*}
D_t & \approx \frac{t^2}{2\bar{\varepsilon}^3} \gamma_t^2 \\
E_t & \approx \frac{t^2}{4\bar{\varepsilon}^2} \gamma_t
\end{align*}
\]

(3.12)
for $t \ll \varepsilon$. The form of the equations in (3.10) is similar to the ones studied by Davydov [27] in the problem of propagations of solitonic waves in biological systems by taken into account electrons and phonons. This should not be surprising since they describe non-interacting electrons interacting with harmonic excitations. We should stress, however, that our equations also include the pseudo-spin variables that were not considered in ref. [27].

The solution of the problem can now be obtained by noticing that both the electron field, $\psi$, and the phonon field, $\phi_L$, have the form of a traveling wave. Using the Galilean invariance of the problem we write:

$$
\psi(x,t) = \phi_0 (x \mp vt) \exp \left[ \frac{i}{\hbar} (mvx - E_0 t) \right],
$$

$$
\phi_L(x,t) = \phi_L (x \mp vt) = \phi_L (\lambda),
$$

(3.13)

where $\lambda = x \mp vt$. Here $E_0$ is the binding energy of the electron and $v$ is the speed of the traveling wave. After this simple transformation we find:

$$
- \frac{\hbar^2}{2m_e} \frac{d^2 \phi_0}{d\lambda^2} + \gamma_p \frac{d\phi_L}{d\lambda} \phi_0 = \left[ E_0 - \frac{m_e v^2}{2} + E_t \right] \phi_0 + D_t \phi_0^3
$$

$$
\rho_L \left( v^2 - c_s^2 \right) \frac{d\phi_L}{d\lambda} = \gamma_p \phi_0^2.
$$

(3.14)

Combining both equations, we have

$$
- \frac{\hbar^2}{2m_e} \frac{d^2 \phi_0}{d\lambda^2} = \left[ E_0 - \frac{mv^2}{2} + E_t \right] \phi_0 + \left[ D_t + \frac{\gamma_p^2}{\rho_L (c_s^2 - v^2)} \right] \phi_0^3,
$$

(3.15)

which is the non-linear Schrödinger equation supporting the propagation of a soliton in the system. This soliton is nothing but a polaron formed of the polarization of the lattice and the pseudo-spins. It is simple to show that for one electron (or hole) the solution is:

$$
\phi_0(x,t) = \sqrt{g} \frac{2}{\text{sech}} \left[ g (x - vt) \right],
$$

(3.16)

where

$$
g = \frac{m_e}{\hbar^2} \left[ D_t + \frac{\gamma_p^2}{\rho_L (c_s^2 - v^2)} \right]
$$

(3.17)

and the binding energy is
\[ E_0 = \frac{mc^2}{2} - \frac{\hbar^2 g^2}{8mc} - E_t. \] (3.18)

By comparing this result with the one found in reference \[28\] where pseudo-spins are not considered, we notice the binding energy is lowered by \( E_t \). Thus, the soliton becomes more stable due to the electron coupling with two-level systems. Moreover, since the size of the polaron is of order \( \xi \approx \frac{1}{g} \) we see that the coupling to the pseudo-spins also decreases the size of the polaron by a factor of \( D_t \). The relative lattice displacement is given by (3.14)

\[ \phi_L(x, t) = -\frac{\gamma_p}{2\rho_L (c_s^2 - \nu^2)} \tanh \left[ \frac{g(x - \nu t)}{2} \right]. \] (3.19)

IV. POLARONIC SOLITON IN MOTT INSULATORS

In the previous section we studied the problem of polaron formation in a band insulator. In this section we will study the problem of non-linear excitations in a Mott insulator where the gap is generated by correlations, not by the interaction with the lattice. Since this is an interacting problem it is clearly more involved. However, because we are considering a system where the electronic density is commensurate with the lattice and the band is not full, we can use the tools of bosonization to study it. The methods will be, however, very similar to the ones used in the previous section. This will show that the polaronic soliton formation in the Mott insulator is very similar to the problem of polaron formation in a band insulator.

The basic Hamiltonian of the problem is given by: \( H_m = H_{ee} + H_{ph} + H_t + H_{e-p} + H_{e-t} \)

where:

\[ H_{ee} = \frac{1}{2\pi} \int dx \left[ (u_{\rho}K_{\rho}) \pi^2 \Pi_{\rho}^2 + \frac{u_{\rho}}{K_{\rho}} \left( \frac{\partial \Phi_{\rho}}{\partial x} \right)^2 \right] + \frac{2g_3}{(2\pi\alpha)^2} \int dx \cos \left[ \sqrt{8} \Phi_{\rho} \right] \]

\[ H_{ph} = \frac{1}{2} \int dx \left[ \frac{\Pi_L^2}{\rho_L} + c_s^2 \rho_L \left( \frac{\partial \phi_L}{\partial x} \right)^2 \right] \]

\[ H_t = \frac{1}{2} \int dx \left[ -\varepsilon \cos 2\theta(x) + t \sin 2\theta(x) \right] \]

\[ H_{e-p} = \gamma_p \int dx \frac{\partial \Phi_{\rho}(x)}{\partial x} \frac{\partial \phi_L(x)}{\partial x} \]
\[ H_{e-t} = -\gamma t \int dx \frac{\partial \Phi_p(x)}{\partial x} \sin^2 \theta(x). \] (4.1)

Once again the problem can be discussed in terms of the generating functional for the fields:

\[ Z = \int D\Phi_p D\phi_L D\theta e^{i \frac{\chi}{\hbar} \int dt \int dx L[\Phi_p, \phi_L, \theta]}, \] (4.2)

where the Lagrangean of the system can then be written as

\[
\mathcal{L} = \frac{1}{2\pi} \left[ \frac{u_p}{u_p K_p} \left( \frac{\partial \Phi_p}{\partial t} \right)^2 - \frac{u_p}{K_p} \left( \frac{\partial \Phi_p}{\partial x} \right)^2 \right] - \frac{2g_3}{(2\pi\alpha)^2} \cos \left[ \sqrt{8} \Phi_p \right] + \frac{\rho_L}{2} \left[ \left( \frac{\partial \phi_L}{\partial t} \right)^2 - c_s^2 \left( \frac{\partial \phi_L}{\partial x} \right)^2 \right] + \frac{1}{2} \left[ \varepsilon \cos 2\theta - t \sin 2\theta \right] - \gamma_p \frac{\partial \Phi_p}{\partial x} \frac{\partial \phi_L}{\partial x} + \gamma_t \frac{\partial \Phi_p}{\partial x} \sin^2 \theta. \] (4.3)

The equations of motion are:

\[
t \cos 2\theta = -\varepsilon \sin 2\theta + \gamma_t \frac{\partial \Phi_p}{\partial x} \sin 2\theta
\]
\[
\frac{1}{u_p \pi K_p} \frac{\partial^2 \Phi_p}{\partial t^2} = \frac{u_p}{\pi K_p} \frac{\partial^2 \Phi_p}{\partial x^2} + \frac{\sqrt{2} g_3}{(\pi\alpha)^2} \sin \left( \sqrt{8} \Phi_p \right) + \gamma_p \frac{\partial^2 \phi_L}{\partial x^2} - \gamma_t \frac{\partial \sin^2 \theta}{\partial x}
\]
\[
\rho_L \frac{\partial^2 \phi_L}{\partial t^2} = c_s^2 \rho_L \frac{\partial^2 \phi_L}{\partial x^2} + \gamma_t \frac{\partial^2 \Phi_p}{\partial x^2}. \] (4.4)

The first equation in (4.4) can be solved exactly as in (3.3) and the effective local pseudo-spin energy is replaced by

\[ \varepsilon(x) = \varepsilon - \gamma_t \frac{\partial \Phi_p}{\partial x}. \] (4.5)

We consider the same limits as before, namely \( t \gg \varepsilon \) and \( t \ll \varepsilon \). The equations of motion for the fields are:

\[
\frac{1}{u_p \pi K_p} \frac{\partial^2 \Phi_p}{\partial t^2} = \frac{u_p}{\pi K_p} \frac{\partial^2 \Phi_p}{\partial x^2} + \frac{\sqrt{2} g_3}{(\pi\alpha)^2} \sin \left( \sqrt{8} \Phi_p \right) + \gamma_p \frac{\partial^2 \phi_L}{\partial x^2} - D_t \frac{\partial^2 \Phi_p}{\partial x^2}
\]
\[
\rho_L \frac{\partial^2 \phi_L}{\partial t^2} = c_s^2 \rho_L \frac{\partial^2 \phi_L}{\partial x^2} + \gamma_p \frac{\partial^2 \Phi_p}{\partial x^2}. \] (4.6)

This set of equations is very different from the ones obtained in the case of the band insulator that is described by the Davykov’s equations (3.10). In fact these equations contain non-perturbative effects that cannot be described by the the non-interacting electron picture.
Using once again the Galilean invariance of the solutions we can write \( \Phi_\rho(x,t) = \Phi_\rho(x \mp vt) = \Phi_\rho(\lambda) \) and \( \phi_L(x,t) = \phi_L(x \mp vt) = \phi_L(\lambda) \), where \( \lambda = x \mp vt \). The equations of motion reduce to:

\[
\left( \frac{v^2}{u_\rho \pi K_\rho} - \frac{u_\rho}{\pi K_\rho} + D_t \right) \frac{d^2 \Phi_\rho}{d\lambda^2} = \frac{\sqrt{2} g_3}{(\pi \alpha)^2} \sin \left( \sqrt{8} \Phi_\rho \right) + \gamma_p \frac{d^2 \phi_L}{d\lambda^2} \\
\rho_L \left( v^2 - c_s^2 \right) \frac{d^2 \phi_L}{d\lambda^2} = \gamma_p \frac{d^2 \Phi_\rho}{d\lambda^2}.
\]

(4.7)

Combining both equations and replacing \( \Phi_\rho \) with \( \Phi = \sqrt{8} \Phi_\rho \), the equation of motion for the charge field becomes:

\[
\frac{d^2 \Phi}{d\lambda^2} = \text{sign}(\mu) \sin(\Phi(\bar{\lambda}))
\]

(4.8)

where \( \text{sign}(x) = +1 \ (-1) \) if \( x > 0 \ (x < 0) \) is a sign function,

\[
\bar{\lambda} = \pm \frac{1}{\sqrt{|\mu|}} \lambda
\]

(4.9)

with

\[
\mu = \frac{(\pi \alpha)^2}{4 g_3} \left[ \frac{\gamma^2_p}{\rho_L (c_s^2 - v^2)} - \frac{u_\rho^2 - u^2}{u_\rho \pi K_\rho} + D_t \right].
\]

(4.10)

Notice that (4.8) is a sine-Gordon equation that has soliton solutions [21]:

\[
\Phi_\rho(x,t) = \pm \sqrt{2} \tan^{-1} \left( e^{\pm \sqrt{|\mu|}(x-\nu t)} \right), \quad \text{for} \ \mu > 0
\]

\[
= \pm \sqrt{2} \tan^{-1} \left( e^{\pm \sqrt{|\mu|}(x-\nu t)} \right) + \frac{\pi}{2\sqrt{2}}, \quad \text{for} \ \mu < 0.
\]

(4.11)

The electronic density that is related to \( \Phi_\rho \) by equation (2.6) and is localized in space as in the polaron case (3.16) with a width of order \( \xi \approx 1/\sqrt{\mu} \). In the present case, however, the soliton properties are heavily dressed by the lattice and pseudo-spin. Therefore we will term this excitation a polaronic soliton.

V. THE POLARONIC SOLITON AT THE LUTHER-EMERY LINE

In the previous section we described the physics of the polaronic soliton formation in terms of the bosonized theory. Since the connection between the electrons and boson fields
is not linear, it is not straightforward to interpret the formation of solitons in the bosonic language as formation of solitons in the fermionic language. Moreover, it is not clear what is the dressing process that changes an electronic soliton into a polaronic soliton. To make the connection more explicit we are going to study the problem of electron-phonon coupling along the so-called Luther-Emery line. Along this line the bosonic degrees of freedom can be re-fermionized. To do so we re-introduce the backscattering terms into the Hamiltonian and the parameters in the Hamiltonian are chosen so that \[24,29,30\]:

\[
\frac{g_1 - 2g_2}{\pi v_F + g_4} = \frac{6}{5},
\]

where

\[
\frac{g_2}{a} = \frac{g_4}{a} = U + 2V.
\]

This is equivalent to choosing \( K_\rho = 1/2 \). The charge part of the problem can be exactly diagonalized via an unitary transformation and the final Hamiltonian reads \[24\]:

\[
\tilde{H}_{LE} = \sum_k E_k \left( \tilde{C}_{1pk}^\dagger \tilde{C}_{1pk} - \tilde{C}_{2pk}^\dagger \tilde{C}_{2pk} \right),
\]

where \( \tilde{C}_{1pk}^\dagger \) \( \tilde{C}_{2pk}^\dagger \) is the transformed annihilation (creation) operator for momentum \( k \) for left (right) moving electrons. The energy spectrum is given by

\[
E_q = \pm \frac{4}{5\pi} \left[ (\pi v_F + g_4)^2 q^2 + \left( \frac{g_3}{2a} \right)^2 \right]^{1/2}.
\]

(5.1)

Obviously the spectrum has a gap of magnitude \( \Delta_M = \frac{4g_3}{5\pi a} \). This is the Mott gap. Notice that because \( K_\rho = 1/2 \) this value of the gap is in agreement with the RG result in (2.19).

We now add electron-phonon interaction (2.21) into the Hamiltonian as

\[
H_{LE-ph} = \sum_k E_k \left( \tilde{C}_{1pk}^\dagger \tilde{C}_{1pk} - \tilde{C}_{2pk}^\dagger \tilde{C}_{2pk} \right) - \frac{\pi \gamma_p}{2} \sum_p \sqrt{\frac{\hbar}{2M \omega(p)}} p \rho(p) \left( a_p + a_{-p}^\dagger \right),
\]

(5.2)

where \( a_p^\dagger \) (or \( a_p \)) is the phonon creation (or annihilation) operator, \( M \) is the mass of a unit cell, and

\[
\rho(p) = \sum_k \left( \tilde{C}_{1pk+p}^\dagger \tilde{C}_{1pk} + \tilde{C}_{2pk+p}^\dagger \tilde{C}_{2pk} \right)
\]

(5.3)
is the transformed fermionic density. Notice that the unitary transformation that diagonalizes the problem does not modify the form of the density operator. What this result shows is that at the Luther-Emery problem becomes identical to the polaron problem discussed in Section II. Since the operators $\bar{C}$ produce the solitonic excitations in the electronic system it becomes clear that the polaronic soliton is formed in two steps: (1) the electron-electron interaction generates collective non-linear modes; (2) these non-linear modes are dressed by the lattice fluctuations.

Let us make this description more concrete and assume that a soliton is created in the upper band of the Mott insulator. We can expand (5.1) for small $q$ as:

$$E_0^q \approx \frac{\Delta M^2}{2} + \frac{q^2}{2m^*},$$  \hspace{1cm} (5.4)

where

$$m^* = \left(\frac{5\pi}{4}\right)^2 \frac{\Delta M}{2(\pi v_F + g_4)^2}$$  \hspace{1cm} (5.5)

is the effective mass of the carrier. Let us assume that the electron-phonon coupling is weak and compute the change in energy of the ground state due to this coupling. It is a trivial exercise in second order perturbation theory to show that for a state with momentum $q$ the energy changes by:

$$\delta E_q = -\frac{\pi m^* \gamma_p^2}{2} \sum_p \frac{\hbar p^2}{2ML \omega (p)} \ln \left\{ \frac{\hbar}{2\alpha (m^* c_s + \hbar q)} + 1 \right\} \ln \left\{ \frac{\hbar}{2\alpha (m^* c_s - \hbar q)} + 1 \right\},$$  \hspace{1cm} (5.6)

where the integral was cut-off at $\Lambda \approx 1/\alpha$. For $\hbar q \ll m^* c_s$, this simplifies to

$$\delta E_q = -\frac{\pi m^* \gamma_p^2}{2\hbar c_s} \ln \left( \frac{\hbar}{2\alpha m^* c_s} + 1 \right) - \frac{\pi \gamma_p^2 (\hbar + 4\alpha m^* c_s)}{4\alpha M m^* c_s^2 (\hbar + 2\alpha m^* c_s)^2} \hbar q^2.$$  \hspace{1cm} (5.7)

By comparing (5.7) with (5.4) we conclude that the energy of the carriers can be written as:

$$E_q = \frac{\Delta R}{2} + \frac{\hbar^2 q^2}{2m_R}.$$  \hspace{1cm} (5.8)

The Mott gap, $\Delta_R$, and the effective mass of the carriers, $m_R$, have been renormalized by the polaronic effect and are given by:
\[ \Delta_R = \Delta_M - \frac{\pi m^* \gamma_p^2}{2M\hbar c_s} \ln \left( \frac{\hbar}{2\alpha m^* c_s} + 1 \right) \]

\[ m_R = m^* \left[ 1 + \frac{\pi \hbar \gamma_p^2 g_3^2}{8 m^* M c_s^2 a^2 (\pi v_F + g_4)^2 (\hbar + 4\alpha m^* c_s)^2} \frac{\hbar}{\hbar + 4\alpha m^* c_s} \right]. \tag{5.9} \]

and we conclude that the Mott gap is substantially reduced and the mass of the carriers increased because of the polaronic effect.

VI. CONCLUSIONS

In this paper we have studied the problem of charge transport via non-linear excitation in a band and Mott insulators. The insulating behavior in band insulator is due to the periodicity of the lattice and the electron-ion interaction opens a gap in the charge spectrum. Mott insulators, on the other hand, are dominated by electron-electron interactions and the gap is produced by correlation effects when the electronic density is commensurate with the lattice. We argue that in band insulators the main propagating excitation is a polaron that is described by an electron dressed by the polarization cloud. In the Mott insulator, because of the strong electron-electron interactions, the main non-linear excitation is the polaronic soliton, a non-linear excitation of the Luttinger liquid that is dressed by a polarization cloud.

We have shown that in a band insulator the doped electron (or hole) is strongly dressed by the internal degrees of freedom in the system that we described in terms of phonons and pseudo-spins. We show that the polaron can propagate freely: the lattice and the two-level systems follow its motion in the system. Moreover, we have shown that the pseudo-spins lead to an extra stabilization, relative to the phonon problem, by reducing its energy and size.

In the case of the Mott insulator we have shown via a bosonization calculation that the non-linear excitations can be thought of as a soliton comprising an electron dressed by the phonons and pseudospins. We term this new excitation the polaronic soliton. Many properties of these excitation are similar to the polaron problem. Namely, the polaronic solitons are very stable and their energy is reduced relative to the problem without phonons.
and pseudo-spins.

The great qualitative difference between a Mott insulator and a band insulator is in the spin spectrum. Spin excitations in a Mott insulator are decoupled from the charge excitations (spin-charge separation) and remain gapless even when the Mott gap opens. Thus Mott insulators have strong antiferromagnetic correlations. This should be contrasted with the case of a band insulator that has both a charge and a spin gap: in order to excite an electron from the valence band to the conduction band we have to pay an energy cost to unpair two electrons with opposite spins in the valence band. In order to illustrate this point let us consider a 1D system that is at half-filling with a weak periodic potential, $U(x)$, added such that this potential doubles the unit cell. Because the system is half-filled, a potential that doubles the unit cell has to open a gap at the Fermi energy. (This mechanism is equivalent to the Peierls mechanism due to lattice distortions \cite{14,15}). Let us consider this process of opening a gap using the bosonization technique. We consider the problem before the gap opens. We can bosonize the system as explained in Section I. The coupling between the weak periodic potential and the electrons can be written as:

$$H_U = \int dx \sum_\sigma U(x) \psi_\sigma^\dagger(x) \psi_\sigma(x), \quad (6.1)$$

where, because of the periodicity,

$$U(x) = U_0 \cos(\pi x/a). \quad (6.2)$$

We now expand the electron operators as in \cite{23} in terms of right and left moving electrons and find that in $H_U$ there are terms that oscillate with $\cos(\pi x/a)$ and $\cos(\pi x/a \pm 2k_F x)$. Since $k_F = \pi/(2a)$ the terms with wave-vector $\pi/a \pm 2k_F$ do not oscillate. All the other terms vary very rapidly in space and can be disregarded. In summary, we can rewrite $H_U$ as

$$H_V = U_0 \int dx \sum_\sigma \psi_\sigma^\dagger(x) \psi_{L,\sigma}(x) + h.c.$$

$$= U_0 \int dx \sum_\sigma \cos(2\sqrt{\pi} \phi_\sigma(x))$$

$$= \frac{2U_0}{\pi a} \int dx \cos(\sqrt{2\pi} \Phi_\rho(x)) \cos(\sqrt{2\pi} \Phi_\sigma(x)), \quad (6.3)$$

[23]
where we have used the bosonization rules (2.4) and (2.5). Notice that (6.3) describes the backscattering of the electrons by the periodic potential of the lattice. In fact the condition that $\pi/a = 2k_F$ is nothing but the Bragg condition for this particular problem. We have thus learned in the bosonized language a very simple fact about electron scattering in periodic potentials. Note, however, that in the bosonic language the extra periodic potential is a highly non-linear operator in terms of the bosons. In practice, this term is not easy to treat exactly. Let us consider, however, a perturbative RG calculation like the one explained in Section I. It is easy to show that:

$$\frac{\partial U_0}{\partial \ell} = \left(2 - \frac{K_\rho}{2} - \frac{K_\sigma}{2}\right) U_0,$$

which demonstrates that the periodic potential is a relevant perturbation of the Luttinger liquid when $K_\rho + K_\sigma < 4$. Notice that when this happens (as we explained in Section I) $H_U$ becomes relevant and the fields $\Phi_\rho$ and $\Phi_\sigma$ are pinned at the minimum of the potential energy. In this case, both a charge gap and a spin gap open in the spectrum! The size of such gaps, as in (2.19), can be obtained from the RG (6.4) and read:

$$\Delta_U = W \left(\frac{U_0}{W}\right)^{\frac{1}{2}} \frac{1}{K_\rho} \frac{1}{K_\sigma}.$$  

This result shows that a gap in a correlated band insulator depends on the strength of the electron-electron interactions. In particular, in the non-interacting limit when $K_\rho = K_\sigma = 1$ we see that $\Delta^0_U = U_0$, as expected from elementary solid state physics. It is clear that in the case of a band insulator the spin gap has nothing to do with superconducting fluctuations but rather with the fact that the band is full and therefore that the electronic shells are closed.

The RG flow for the periodic potential (6.4) should be contrasted with the RG flow for the Umklapp term, Eq. (2.17), which opens the Mott gap, and is relevant for $K_\rho < 1$. Notice that there is a competition between the Umklapp term and the periodic potential: for $0 < K_\rho < K_\sigma/3$ the Umklapp term diverges faster than the periodic potential while for $K_\sigma/3 < K_\rho < 4 - K_\sigma$ the electron-ion interaction has a stronger divergence. (For
\( K_\rho > 4 - K_\sigma \) both operators are irrelevant). Since \( K_\rho \) decreases with the strength of the electron-electron interaction it becomes obvious that for strong electron-electron interaction the Umklapp term is more important than the periodic potential and a Mott gap opens in the system. The spin spectrum is gapless while the charge spectrum has a gap. On the other hand, if the electron-electron interactions are weaker, the periodic potential dominates and a band gap opens in both the spin and the charge spectrum. It is clear that we can differentiate the band gap and the Mott gap by examining the spin spectrum. The critical value of interactions, \( U_c \) and \( V_c \) in (2.2), above which a Mott gap appears in a band insulator occurs when \( K_\rho = K_\sigma / 3 \). Using (2.9) we find

\[
U_c - \frac{2}{5} V_c = \frac{4\pi v_F}{5a},
\]

which gives the critical line in the \( U \times V \) plane above which one finds a Mott insulator and below which we have a band insulator.

The applications of the formalism developed here to systems like DNA depends very much on the actual values of \( U \) and \( V \). If DNA is better described by a band insulator then the formalism developed in section \[ \text{III} \] is more appropriate and the Davydov’s equations (3.10) should apply. In this case the elementary excitations should be polarons. However, if the electron-electron interactions are strong, as we conjecture, then the polaronic soliton of the Mott insulator, as described in section \[ \text{IV} \], is the best description. While numerical simulations can provide useful information on order of magnitude of the electronic parameters, only well-controlled experiments in periodic DNA sequences can actually give the final word on the insulating nature of DNA. As we discussed previously, we believe that the correct way to find out about the insulating nature of DNA is by the study of the spin excitation spectrum and not by conductivity measurements that are insensitive to the spin degrees of freedom. While there are indications of antiferromagnetic fluctuations in DNA that would be consistent with the Mott insulator picture \[ \text{[7]} \] the experimental picture is far from complete and many more experiments are needed.

In summary, we have shown that non-linear excitations in band and Mott insulators are
very similar and have solitonic character. We show that the band gap is strongly renormalized by electron-electron interactions in 1D and that a 1D system can be driven from a band insulator type behavior to a Mott insulator behavior as a function of interactions. The correct way to distinguish between these two types of insulator it is not by studying the charge degrees of freedom, that propagate in the form of non-linear waves, but to the spin degrees of freedom that remain gapless in the Mott case and are gapped in a band insulator. We believe that the physics described here can be applied to strongly correlated systems like DNA.

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