One-dimensional fermions with incommensuration close to dimerization

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Abstract. – We study a model of fermions hopping on a chain with a weak incommensuration close to dimerization; both $q$, the deviation of the wave number from $\pi$, and $\delta$, the strength of the incommensuration, are assumed to be small. For free fermions, we show that there are an infinite number of energy bands which meet at zero energy as $q$ approaches zero. The number of states lying inside the $q = 0$ gap remains nonzero as $q/\delta \to 0$. Thus the limit $q \to 0$ differs from $q = 0$, as can be seen clearly in the low-temperature specific heat. For interacting fermions or the $XXZ$ spin-$(1/2)$ chain, we use bosonization to argue that similar results hold. Finally, our results can be applied to the Azbel-Hofstadter problem of particles hopping on a two-dimensional lattice in the presence of a magnetic field.

One-dimensional lattice models with an incommensurate hopping or on-site potential have been studied extensively using a variety of methods [1]. If interactions between the particles are ignored, many unusual properties of the quantum spectra have been discovered in models with strong incommensuration, such as an infinite number of bands, and wave functions which exhibit power law scaling [2]. Physically, such models arise in several problems such as incommensurate crystals [3], semiconductor heterojunctions [4], the incommensurate phase of spin-Peierls systems such as CuGeO$_3$ [5], and the Azbel-Hofstadter problem of particles hopping on a two-dimensional lattice in the presence of a perpendicular magnetic field [6]. If the incommensuration is close to dimerization (wave number $\pi$), the models have an additional interest in the context of metal-insulator transitions near half-filling and spin-Peierls systems near zero magnetization [7,8].

In this paper, we study a model of fermions with a hopping which has a small incommensurate term close to dimerization. We will show that this has some unusual properties inside the gap which exists exactly at dimerization. Namely, states appear inside the gap as soon as we move away from dimerization. We first discuss free fermions for which accurate results can be obtained by analytical continuum methods. Our work differs from earlier ones which have concentrated on the effects of incommensuration which are either large or close to "highly" irrational numbers such as the golden ratio [1–3,6]. Further, we will use techniques from continuum field theory which have not been used much in this area. We will then argue

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that similar peculiarities occur as soon as we move away from dimerization for interacting fermions (or, equivalently, for the $XXZ$ spin-$(1/2)$ chain) which is the more general and interesting case. Our results show that an incommensuration close to dimerization constitutes an interesting kind of perturbation which dramatically alters the low-energy properties of a Luttinger liquid \[9\].

We begin with the following Hamiltonian for noninteracting and spinless fermions on a lattice:

$$H = -\frac{1}{2} \sum_n J_n \left( c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right),$$

$$J_n = 1 + \delta \cos (Qn), \quad (1)$$

where we assume that $\delta \ll 1$, and $Q = \pi + q$ with $q \ll \pi$. We are interested in energies close to zero, i.e., the half-filled case. If $\delta = 0$, the dispersion relation is $E(k) = -\cos k$. In the ground state, all states with momenta lying in the range $[-\pi/2, \pi/2]$ are filled. The Fermi velocity is equal to $\sin \pi/2 = 1$; we set the lattice spacing equal to 1.

With dimerization, i.e., $\delta \neq 0$ but $q = 0$, there is a single energy gap extending from $-\delta$ to $\delta$. We now consider nonzero values of $q$. For any rational value of $q/\pi = M/N$, where $M$ and $N$ are relatively prime integers, we have a periodic system with period $P$ equal to $N$ if $M + N$ is even and $2N$ is $M + N$ is odd. The one-particle spectrum of eq. (1) is found by computing a transfer matrix $M(q, E)$ obtained by multiplying together $P$ matrices \[2\],

$$M(q, E) = \prod_{n=1}^{P} \left( \begin{array}{cc} -2E/J_n & -J_{n-1}/J_n \\ 1 & 0 \end{array} \right). \quad (2)$$

If $|\text{tr} \, M(q, E)| \leq 2$, the energy $E$ is allowed in the spectrum; otherwise that energy is not allowed. By sweeping through a large number of values of $q$ and $E$ (with a resolution of $dE = 10^{-6}$), we obtain the picture of energy bands and gaps (shaded and unshaded regions, respectively) shown in figs. 1 and 2, taking $\delta = 0.05$. We have scaled $E$ and $q$ in units of $\delta$. 

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Fig. 1 – The bands as a function of the energy $E$ and the wave number $q$, both in units of $\delta$, taking $\delta = 0.05$. The numbers 1, 3 and 5 labeling the three biggest gaps are explained in the text.
and have considered only positive values of $E$ and $q$ since the spectrum is separately invariant under $E \to -E$ and $q \to -q$.

Figure 1 shows that, as $q/\delta$ increases, the gaps shrink rapidly. As indicated below, this can be understood using perturbation theory to $n$-th order, where $n$ is an odd integer. We therefore label the gaps in fig. 1 by the value of $n = 1, 3, 5, \ldots$. More interestingly, we observe that all the bands approach the origin $(q, E) = (0, 0)$. The widths of the low-lying bands vanish exponentially fast as $q/\delta \to 0$. In fig. 2, we show these thin portions of the bands which smoothly join on to the wider regions. We also show six curves which are the analytical results of a low-energy continuum Dirac theory discussed below. We will argue that, in the thermodynamic limit $L \to \infty$, the number of states per site in the region $0 \leq E/\delta \leq 1$ has the nonzero limit $2\delta/\pi^2$ as $q/\delta \to 0$. Thus the number of states lying inside the $q = 0$ gap is finite in the limit $q \to 0$, which implies that $q = 0$ is a rather singular point. (Note that we always take the limit $L \to \infty$ before letting $q \to 0$.)

Let us first examine the gaps for large values of $q/\delta$ by using perturbation theory about $\delta = 0$. If $q$ and $\delta$ are both small, the states close to zero energy are dominated by momenta near $\pm \pi/2$. Since the incommensuration has Fourier components at momenta $\pm(\pi + q)$, the gaps above zero energy result from the breaking of the energy degeneracy between the two states with momenta $k_1 = \pi/2 + nq/2$ and $k_{n+1} = -\pi/2 - nq/2$, where $n = 1, 3, 5, \ldots$. These two states are connected to each other through the $n-1$ successive intermediate states with momenta $k_2 = -\pi/2 + (n-2)q/2$, $k_3 = \pi/2 + (n-4)q/2$, $k_4 = -\pi/2 + (n-6)q/2$, ..., $k_n = \pi/2 - (n-2)q/2$. Since all the relevant matrix elements are equal to $\delta/2$, and the energy denominators are of the order of $q$ each, we see that the twofold degeneracy (at the energy $E_1 = E_{n+1} \simeq nq/2$) gets broken at the $n$-th order in perturbation theory to produce a gap of the order of $\delta^n/q^{n-1}$. We will present an explicit formula elsewhere for the width of the $n$-th gap which agrees well with the numerically obtained gaps in fig. 1 [10].

We now examine the regime where $q/\delta$ is small and $E/\delta < 1$. In the continuum limit, the Fermi field $\psi(x) = c_n$ can be written as

$$\psi(x) = \psi_R(x) \exp \left[ i \frac{\pi}{2} x \right] + \psi_L(x) \exp \left[ -i \frac{\pi}{2} x \right],$$

(3)
where \(\psi_R\) and \(\psi_L\) denote the right- and left-moving fields, respectively; these fields vary slowly on the scale of the lattice spacing, and they contain the modes near the momenta \(\pm \pi/2\) for which a linear dependence of the energy on the momenta is assumed (with the velocities \(\partial E/\partial k\) being equal to \(\pm 1\) for the right- and left-moving fields). We substitute (3) in the equations of motion following from eq. (1), and drop terms like \(\exp[\pm i\pi x]\) which vary rapidly. We find the following equations for the time-dependent (Heisenberg) fields:

\[
i (\partial/\partial t + \partial/\partial x) \psi_R - i\delta \cos(qx) \psi_L = 0,
\]

\[
i (\partial/\partial t - \partial/\partial x) \psi_L + i\delta \cos(qx) \psi_R = 0.
\]

We define \(\psi_\pm = \psi_R \pm \psi_L\); then \(\psi_+\) satisfies the time-independent equation

\[
[-\partial^2/\partial x^2 + \delta^2 \cos^2(qx) - q\delta \sin(qx)] \psi_+ = E^2 \psi_+.
\]

It is sufficient to solve this equation since \(\psi_-\) is given by \(\psi_-(x) = (i/E)[-\partial/\partial x + \delta \cos(qx)]\psi_+(x)\) if \(E \neq 0\).

Since eq. (5) has the form of a Schrödinger equation (with “energy” \(E^2\)) in the presence of a periodic potential, we expect bands to form. To simplify the notation, let us shift \(x\) of a periodic potential, we expect bands to form. To simplify the notation, let us shift \(x\) by \(\pi/2q\) and then scale it by a factor of \(q\) to make the period equal to \(2\pi\). We get

\[
\left[-\partial^2/\partial x^2 + \delta^2 \sin^2 x - \delta \cos x \right] \psi_+ = \frac{E^2}{q^2} \psi_+.
\]

By Floquet’s theorem, the solutions must satisfy \(\psi_+(x + 2\pi) = e^{i\theta}\psi_+(x)\), where \(\theta\) goes from 0 to \(\pm \pi\) from the bottom of a band to the top. (Note that there is an exact zero energy state with \(\psi_+(x) = \exp[\pi q \cos x]\) and \(\psi_-(x) = 0\) for which \(\theta = 0\).) If \(q/\delta\) is large, the positions of the low-lying bands (with \(E^2/q^2 \ll \delta/q\)) can be found analytically as follows. For energies much lower than the maxima of the potential, we first ignore tunneling between the different wells. Near the bottom of a single well, we have a simple harmonic potential with small anharmonic corrections. Ignoring the anharmonic terms, the energy levels are simply given by \(E_n^2 = 2nq\delta\), where \(n = 0, 1, 2, \ldots\). Including the anharmonic corrections, we get the more accurate expression

\[
E_n = \sqrt{2nq\delta} \left[ 1 - \frac{nq}{8\delta} - \frac{5n^2 + 2q^2}{128\delta^2} \right]
\]

up to second-order in perturbation theory. We now include tunneling between wells; a WKB analysis shows that each of the above energies splits into a band whose width \(\Delta E_n/\delta\) is of the order of \(\exp[-2\delta/q]\). This explains why the bands rapidly become thin and shrink to isolated points as \(q \to 0\) in fig. 2. In that figure, we have shown the six curves corresponding to \(n = 1\) to 6 in eq. (7); for \(n = 0\), we get a straight line lying at zero energy. The curves agree extremely well with the numerical data, even up to \(E_n\) of the order of \(\delta\) where the harmonic approximation breaks down and the band widths become large.

For large \(\delta/q\), we can use a semiclassical phase space argument to count how many states lie below any given energy. The “Hamiltonian” on the left-hand side of (5) has the form

\(p^2 + V(x)\),

where \(V(x) = \delta^2 \cos^2(qx) - q\delta \sin(qx)\). Hence the number of states per site up to energy \(E\) is given by

\[
\nu(E) = \frac{1}{L} \int \frac{dx dp}{2\pi} \Theta(E^2 - p^2 - V(x)),
\]

where we have divided by the number of sites \(L\), and \(\Theta(y) = 1\) and 0 if \(y\) is positive and negative, respectively. On doing the momentum integral, we get

\[
\nu(E) = \int_0^{2\pi/q} \frac{q dx}{2\pi^2} \sqrt{E^2 - V(x)} \Theta(E^2 - V(x)),
\]

and then scale it by a factor of \(q\) to make the period equal to \(2\pi\).
where \( V(x) \) has period \( 2\pi/q \). The number of states per site lying between \( E = 0 \) and \( \delta \) is therefore \( \nu(\delta) = 2\delta/\pi^2 \), which is independent of \( q \), provided that \( q/\delta \) is very small. We will show elsewhere that each band contains \( q/\pi \) states per site, and therefore the number of bands lying between \( E = 0 \) and \( \delta \) is about \( 2\delta/(\pi q) \) [10]. This diverges as \( q/\delta \to 0 \).

The difference in the spectrum for \( q = 0 \) and \( q \to 0 \) shows up most clearly in the density of states \( \rho(E) \) for \( E < \delta \) and therefore the specific heat at low temperatures \( T \). We can obtain the density of states \( \rho(E) \) from the expression in (9) by differentiating it with respect to \( E \). In the limit \( q/\delta \to 0 \), we find that \( \rho(E) \) is proportional to \( E/\delta \) for \( E \ll \delta \). This is to be contrasted with the density of states found exactly at \( q = 0 \), where \( \rho(E) \) vanishes for \( E < \delta \). Hence, for temperatures \( T \ll \delta \), the specific heat vanishes exponentially for \( q = 0 \), but goes as \( T^2/\delta \) for \( q \to 0 \).

We now argue that the difference between small \( q \) and \( q = 0 \) (in particular, the presence of states within the \( q = 0 \) gap) persists for the more interesting case of interacting fermions [9]. Consider adding a four-fermion interaction term like \( \sum_n c_n^\dagger c_n^\dagger c_{n+1} c_{n+1} \) to the Hamiltonian (1). Equivalently, we can consider an \( XXZ \) spin-(1/2) chain governed by

\[
H = \frac{1}{2} \sum_n \left[ (1 + \delta \cos(\pi + q)n)(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + D S_n^z S_{n+1}^z \right], \tag{10}
\]

which is related to the interacting fermion theory by a Jordan-Wigner transformation [11]. If \( \delta = 0 \), it is known from the exact Bethe ansatz solution and conformal field theory [9] that the model in (10) is gapless at zero magnetic field with a linear dispersion for the low-energy excitations if \( -1 < D \leq 1 \). If we now add a weak dimerization (\( q = 0 \) and \( \delta \) is small), the system becomes gapped. A renormalization group calculation [12, 13] shows that the gap scales as

\[
\Delta E \sim \delta^{1/(2-K)}, \tag{11}
\]

where

\[
K = \frac{\pi}{2\cos^{-1}(-D)},
\]

and \( 0 < \cos^{-1}(-D) \leq \pi \). (Actually, a gap opens up only if \( K \leq 2 \). If \( K > 2 \), the dimerization term is irrelevant in the sense of the renormalization group. Note that \( K = 1 \) for noninteracting fermions.) It is useful to state this result in the language of bosonization. For \( q = 0 \), the model in (10) is equivalent, after renormalization (i.e., at low energies or long distances), to a bosonic sine-Gordon theory described by the Lagrangian density [9]

\[
\mathcal{L} = \frac{1}{2\pi v K} \left[ (\partial \phi/\partial t)^2 - v^2(\partial \phi/\partial x)^2 \right] + \gamma \delta^{2/(2-K)} \cos(2\phi), \tag{12}
\]

where \( v \) is the velocity of low-energy excitations and \( \gamma \) is a constant; their numerical values are not important here. The main point to note is the exponent of \( \delta \) in the coefficient of \( \cos(2\phi) \). Thus, the dimerization term which is linear in \( \delta \) in the microscopic fermionic theory in (10) becomes a cosine term with a nontrivial and interaction-dependent exponent for \( \delta \) in the low-energy bosonic theory. This is because a renormalization occurs in the process of deriving the low-energy bosonic theory from the original fermionic one [12, 13]. This renormalization occurs even if the fermions are noninteracting and \( K = 1 \); this is because the sine-Gordon theory is always strongly interacting. These strong interactions are also responsible for the large renormalizations of the correct quantum spectrum compared to the naive classical spectrum that one obtains from the sine-Gordon theory, namely, the classical soliton mass for the fermionic excitations and the quadratic fluctuations around \( \phi = 0 \) for the bosonic excitations [14].
Let us now change $q$ slightly away from zero. Since $\cos(\pi + q)n = \cos(\pi n)\cos(qn)$ on a lattice, we have a dimerization whose coefficient $\delta \cos qn$ varies very slowly over the system. Upon doing a similar renormalization group analysis [10], we find that the low-energy Lagrangian density is given by

$$L = \frac{1}{2\pi vK} \left[ (\partial \phi/\partial t) \right.$$

$$\left. - v^2(\partial \phi/\partial x)^2 \right] + \gamma \frac{\delta^{2/(2-K)}}{\delta \cos(qx) \cos(2\phi)}, \quad (13)$$

Unlike (12), the sine-Gordon theory with the space-dependent coefficient of the $\cos(2\phi)$ term in eq. (13) cannot be solved analytically. However, if $q/\delta \ll 1$, we can make some qualitative statements about the low-energy spectrum of the interacting theory by comparison with the noninteracting theory. For the noninteracting theory, bosonization followed by a renormalization group analysis yields a Lagrangian density of the same form as in (13) but with $K = 1$. In that case, we know from the earlier single-particle analysis that in the limit $q \to 0$, the low-energy density of states is proportional to $E/\delta$, while the low-temperature specific heat goes as $T^2/\delta$. Since the only effect of interactions is to alter the exponent of $\delta$ from 1 to $1/(2-K)$, we expect that the the low-energy density of states will go as $E/\delta^{1/(2-K)}$ and the low-temperature specific heat will go as $T^2/\delta^{1/(2-K)}$. Thus the power law exponent of temperature in the specific heat should be independent of the interaction strength. The power law form is again much larger than the exponential dependence found at low temperature for $q = 0$.

To conclude, we have shown that a small incommensuration very close to dimerization produces a novel gapless phase. This phase differs from a Luttinger liquid in two ways. The density of states vanishes linearly at low energies instead of approaching a constant as in a Luttinger liquid; hence the specific heat varies quadratically instead of linearly with temperature. Secondly, our model is not translationally invariant and the low-energy states are localized in those regions of space where the effective dimerization $\delta \cos(qx)$ is small.

Before ending, it may be useful to discuss whether our model can be applied to the incommensurate (I) phase of a spin-Peierls system such as CuGeO$_3$ [5]. There are several reasons why the unusual behavior which occurs in the limit $q \to 0$ may not be experimentally observable in such a system. Firstly, in a spin-Peierls system, the value of $q$ is closely tied to the magnetic field (or the chemical potential in the fermionic language). In fact, it turns out that the Fermi energy is not zero if $q \neq 0$; rather, it lies in the gap labeled as 1 in fig. 1. Secondly, the transition from the dimerized phase ($q = 0$) to the I phase ($q \neq 0$) is first-order, and $q/\delta$ jumps directly from 0 to a value of order 1. Thus, very small values of $q/\delta$ do not seem to occur in the I phase of CuGeO$_3$. This, together with the fact that the Fermi energy lies in the gap, means that the spin excitations actually have a gap of order $\delta$, and therefore their contribution to the low-temperature specific heat is exponentially small in the I phase. On the other hand, a spin-Peierls system has dynamical phonons coupled to the spins; we have ignored such phonons here by assuming that the incommensuration is static. It is known that in the I phase, the phonon modes (called phasons) contribute a $T^3$-term to the specific heat. Finally, we should note that the sinusoidal form of incommensuration which we have assumed in our work has been observed to be quite accurate in the I phase where $q/\delta$ is of the order of 1.

For small values of $\delta$, we will show elsewhere that the energy spectrum is the same whether the incommensurate term is in the hopping or in the on-site potential [10]. Hence our results for noninteracting fermions are directly applicable to Harper’s equation

$$-\frac{1}{2} [\psi_{n+1} + \psi_{n-1}] - \delta \cos(Qn)\psi_n = E\psi_n, \quad (14)$$
which appears in the Azbel-Hofstadter problem on a highly anisotropic square lattice; here, \( \delta \) is the ratio of the hoppings in the two directions, and \( Q/(2\pi) \) is the ratio of the magnetic flux quantum penetrating each square to the elementary flux quantum \( \Phi_0 \). Thus we can analytically understand why low-energy states appear when the magnetic flux per square is close to \( \Phi_0/2 \) [6].

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