

# One-dimensional fermions with incommensurate hopping close to dimerization

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We study the spectrum 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 small. For free fermions, we use a continuum Dirac theory to show that there are an infinite number of bands which meet at zero energy as  $q$  approaches zero. In the limit that the ratio  $q/\delta \rightarrow 0$ , the number of states lying inside the  $q = 0$  gap is nonzero and equal to  $2\delta/\pi^2$ . Thus the limit  $q \rightarrow 0$  differs from  $q = 0$ ; this can be seen clearly in the behavior of the specific heat at low temperature. For interacting fermions or the  $XXZ$  spin-1/2 chain, we use bosonization to argue that similar results hold.

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One-dimensional lattice models with incommensurate hopping elements or on-site potentials have been studied for many years from different points of view<sup>1-3</sup>. Many unusual properties of the quantum spectra and wave functions have been discovered for various kinds of aperiodicity<sup>4</sup>. Physically, such models have applications to several problems such as incommensurate crystals<sup>5</sup> and semiconductor heterojunctions<sup>6</sup>. If the incommensuration is close to dimerization (wave number  $\pi$ ), then the models have an additional interest in the context of metal-insulator transitions or spin-Peierls compounds<sup>7,8</sup>. 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, particularly inside the gap which exists *exactly* at dimerization. The major surprise is that states appear inside the gap *as soon as* we move away from dimerization. These states carry a finite weight, and therefore contribute to quantities like the specific heat at low temperatures. The bulk of our discussion is for free fermions or the  $XY$  spin-1/2 chain for which quantitatively accurate results can be obtained by analytical methods. However, we will argue at the end that the same results should hold for interacting fermions or the  $XXZ$  spin-1/2 chain, which is the more general and interesting case.

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

$$H = -\frac{1}{2} \sum_n J_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \mu \sum_n c_n^\dagger c_n ,$$
$$J_n = 1 + \delta \cos (\pi + q)n , \tag{1}$$

where we will assume that  $\delta \ll 1$  and  $q \ll \pi$ . We set the chemical potential  $\mu = 0$  as we are interested in

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energies close to zero. If  $\delta = 0$ , the model can be easily solved; the dispersion relation is  $E(k) = -\cos k$ . In the ground state, all the states with momenta lying in the range  $[-k_F, k_F]$  are filled, where the Fermi momentum  $k_F = \pi/2$ . The Fermi velocity is equal to  $\sin k_F = 1$ .

If  $\delta \neq 0$  but  $q = 0$ , i.e., with dimerization, the model can still be solved analytically. There is an energy gap extending from  $-\delta$  to  $\delta$ . Let us now consider nonzero values of  $q$ . [Since  $\cos(\pi+q)n = \cos(qn)\cos(\pi n)$ , we see that a small value of  $q$  is equivalent to dimerization term whose amplitude  $\delta \cos(qn)$  varies slowly with  $n$ ]. 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  $2N$  if  $M + N$  is odd. The one-particle spectrum of Eq. (1) can be found by computing a  $2 \times 2$  transfer matrix  $M(q, E)$  obtained by multiplying together  $P$  matrices<sup>4</sup>,

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

If  $|\text{tr } M(q, E)| \leq 2$ , the energy  $E$  is allowed in the spectrum; otherwise that energy is not allowed. By following this method and sweeping through a large number of values of  $q$  and  $E$ , 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 sampled the energy values with a resolution of  $dE = 10^{-6}$ ). We have scaled both  $E$  and  $q$  in units of  $\delta$  because the pictures turn out to depend only on those two ratios. We immediately see that the pictures look much more complicated than the situation in which  $q$  is *exactly* equal to zero; in that case, there is precisely one gap extending from  $E/\delta = 0$  to 1. [We will consider only positive values of  $q$  and  $E$  since it can be shown that the spectrum is invariant under either  $q \rightarrow -q$  or  $E \rightarrow -E$ . Thus the energy bands shown in Figs. 1 and 2 should be understood as continuing to negative values of both  $E$  and  $q$  by reflection about those two axis].

Fig. 1 shows that as  $q/\delta$  increases, the gaps shrink rapidly. We will show that this can be understood using perturbation theory to  $n^{\text{th}}$  order, where  $n$  is an odd integer, and that the gaps shrink as  $(\delta/q)^n$ . We have therefore labeled the gaps in Fig. 1 by the integers  $n = 1, 3, 5, \dots$ . 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  $q/\delta \rightarrow 0$  as we will argue from a WKB analysis. This makes it impossible to find these portions of the bands by looking for energies satisfying  $|\text{tr } M(q, E)| \leq 2$  using any reasonable energy resolution  $dE$ . We therefore find these thin portions of the bands by looking for minima of  $\text{tr} M^2(q, E)$  as functions of  $E$ ; these minima yield single points in energy which lie within a distance of  $dE$  of the band. We are thus able to find the locations of the thin regions without having to use a resolution smaller than  $dE = 10^{-6}$ . In Fig. 2, we show these points (thin regions) which smoothly join on to the wider regions of the bands. We also show six curves which are the analytical results of a low-energy theory of the model which involves solving a  $1 + 1$ -dimensional Dirac equation in a periodic potential. We will also prove that the number of bands in the region  $0 \leq E/\delta \leq 1$  increases as  $2\delta/\pi q$  as  $q/\delta \rightarrow 0$ , while the number of states in each band is equal to  $q/\pi$  when normalized appropriately in the thermodynamic limit, i.e., the number of sites  $L \rightarrow \infty$ . This will show that the number of states lying inside the  $q = 0$  gap is finite and equal to  $2\delta/\pi^2$  in the limit  $q \rightarrow 0$ ; this implies that  $q = 0$  is a rather singular point.

To begin with, let us understand 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  $\pm(\pi + q)$ , we see that 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  $n = 1, 3, 5, \dots$ . 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 we must have  $k_{i+1} - k_i = \pm(\pi + q) \text{ mod } 2\pi$ . 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 two-fold degeneracy (at the energy  $E_1 = E_{n+1} \simeq nq/2$ ) gets broken at the  $n^{\text{th}}$  order in perturbation theory to produce a gap of the order of  $\delta^n/q^{n-1}$ . To be explicit, we find that the upper and lower edges of the two gaps labeled by  $n = 1$  and 3 in Fig. 1 are given by

$$\begin{aligned}\frac{E_{\pm}(1)}{\delta} &= \frac{q}{2\delta} \pm \frac{1}{2}, \\ \frac{E_{\pm}(3)}{\delta} &= \frac{3q}{2\delta} + \frac{3\delta}{16q} \pm \frac{\delta^2}{32q^2},\end{aligned}\tag{3}$$

and we have verified that this agrees well with the numerically obtained boundaries. We will show elsewhere that the general formula for the gap  $\Delta E(n) = E_+(n) - E_-(n)$  labeled by the odd integer  $n = 2p + 1$  is given by

$$\frac{\Delta E(n)}{\delta} = \frac{(\delta/4q)^{2p}}{(p!)^2}\tag{4}$$

to lowest order in  $\delta$ .

We can count the number of states in the band lying between gaps  $n$  and  $n+2$  as follows. For  $\delta = 0$ , let us normalize the number of states so that the total number is 1; since the momentum  $k$  goes from  $-\pi$  to  $\pi$  in that case, the density of states in momentum space is  $1/2\pi$ . If we now turn on a very small value of  $\delta$ , we find that the band lying between the gaps  $n$  and  $n+2$  is made up of linear combinations of the states lying between the two momenta intervals  $[\pi/2 + nq/2, \pi/2 + (n+2)q/2]$  and  $[-\pi/2 - nq/2, -\pi/2 - (n+2)q/2]$ . The total number of states in these two intervals is  $2(q/2\pi) = q/\pi$ . Thus each band contains  $q/\pi$  states. Now, this number cannot change if we change  $\delta$ , and we can therefore use the same number below in the opposite limit where  $q/\delta$  is small.

Let us examine the more interesting regime where  $q/\delta$  is small and  $E/\delta < 1$ . For analyzing this, it is useful to consider the continuum limit. In this limit, the Fermi field  $\psi(x) = c_n$  can be written as

$$\psi(x) = \psi_R(x) \exp(i\frac{\pi}{2}x) + \psi_L(x) \exp(-i\frac{\pi}{2}x),\tag{5}$$

where  $\psi_R$  and  $\psi_L$  denote the right- and left-moving fields, respectively; they vary slowly on the scale of the lattice spacing (which is set equal to 1 here). We substitute (5) in Eq. (1) and drop terms like  $\exp(\pm i\pi x)$  which vary rapidly. We then find the following Dirac-like equations for the two time-dependent (Heisenberg) fields

$$\begin{aligned}i(\partial/\partial t + \partial/\partial x)\psi_R - i\delta \cos(qx)\psi_L &= 0, \\ i(\partial/\partial t - \partial/\partial x)\psi_L + i\delta \cos(qx)\psi_R &= 0.\end{aligned}\tag{6}$$

Eq. (6) can be solved by defining  $\psi_{\pm} = \psi_R \pm \psi_L$  which satisfy the second-order equations

$$\begin{aligned}[\partial^2/\partial t^2 - \partial^2/\partial x^2 + \delta^2 \cos^2(qx) - \delta q \sin(qx)]\psi_+ &= 0, \\ [\partial^2/\partial t^2 - \partial^2/\partial x^2 + \delta^2 \cos^2(qx) + \delta q \sin(qx)]\psi_- &= 0.\end{aligned}\tag{7}$$

It is sufficient to solve one of these equations, say, for  $\psi_+$ , since  $\psi_-$  is related to  $\psi_+$ . The energy spectrum can be found by solving the time-independent equation

$$[-\partial^2/\partial x^2 + \delta^2 \cos^2(qx) - \delta q \sin(qx)]\psi_+ = E^2 \psi_+.\tag{8}$$

Eq. (8) has the form of a Schrödinger equation (with “energy”  $E^2$ ) in the presence of a periodic potential. The potential is similar but not identical to Mathieu’s equation<sup>9</sup>. We therefore again 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 then get

$$[-\partial^2/\partial x^2 + \frac{\delta^2}{q^2} \sin^2 x - \frac{\delta}{q} \cos x]\psi_+ = \frac{E^2}{q^2} \psi_+.\tag{9}$$

By Floquet's theorem<sup>9</sup>, 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. We observe that there is an exact zero energy state with  $\psi_+(x) = \exp(\frac{\delta}{q} \cos x)$  and  $\psi_-(x) = 0$  for which  $\theta = 0$ . In general, the nonzero energy states can only be found numerically. But 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 can ignore tunneling between the different wells to begin with. Near the bottom of a single well, we have a simple harmonic potential with small anharmonic corrections. Ignoring the anharmonic terms, we find the energy levels to be simply given by

$$E_n^2 = 2nq\delta, \quad (10)$$

where  $n = 0, 1, 2, \dots$ . Next, we include the anharmonic corrections perturbatively. Up to second-order in perturbation theory, we get the more accurate expression

$$E_n = \sqrt{2nq\delta} \left[ 1 - \frac{nq}{8\delta} - \frac{5n^2 + 2q^2}{128} \frac{q^2}{\delta^2} \right]. \quad (11)$$

We can now include tunneling between wells; a WKB analysis shows that each of the above energies should split into a band whose width  $\Delta E_n$  is of the order of  $\delta$  times  $\exp(-2\delta/q)$ . This explains why the bands rapidly become thin and shrink to isolated points as  $q \rightarrow 0$  in Fig. 2. In that figure, we have shown the six curves corresponding to  $n = 1$  to 6 in Eq. (11); for  $n = 0$ , we simply get a straight line lying at zero energy. We see that all 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 noticeable.

We will now prove that the number of states lying below the line  $E/\delta = 1$  is proportional to  $\delta$ . 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 Eq. (8) has the form  $p^2 + V(x)$ , where  $V(x) = \delta^2 \cos^2(qx) - \delta q \sin(qx)$ . Hence the number of states up to energy  $E$  is given by the phase space integral

$$\nu(E) = \frac{1}{L} \int \int \frac{dx dp}{2\pi} \Theta(E^2 - p^2 - V(x)), \quad (12)$$

where we have divided by the length  $L$  of the system for normalization; the  $\Theta$ -function is defined to be 1 and 0 if its argument is positive and negative, respectively. On doing the momentum integral in (12), we get

$$\nu(E) = \frac{q}{2\pi} \int_0^{2\pi/q} dx \frac{1}{\pi} \sqrt{E^2 - V(x)} \Theta(E^2 - V(x)), \quad (13)$$

where we have used the fact that  $V(x)$  has period  $2\pi/q$ . For small values of  $q/\delta$ , we then see that the number of states lying between  $E = 0$  and  $\delta$  is

$$\nu(\delta) = \frac{2\delta}{\pi^2}, \quad (14)$$

which is *independent* of  $q$ . Incidentally, this also yields the number of bands lying below  $E = \delta$ . Since each band contains  $q/\pi$  states, Eq. (14) gives the number of bands to be  $2\delta/\pi q$ . We have verified that this estimate agrees very well with our numerical results.

The difference in the spectrum for  $q = 0$  and  $q \rightarrow 0$  should show up most clearly in the specific heat at temperatures  $T \ll \delta$ . (We set the Boltzmann constant equal to 1 for convenience). For  $q = 0$ , the energy gap from  $-\delta$  to  $+\delta$  means that the specific heat vanishes exponentially at low temperature. But

for  $q \rightarrow 0$ , the semiclassical expression in (13) shows that the density of states at any energy  $E \ll \delta$  is of the order of  $\rho(E) \sim E/\delta$ . This implies that the low-temperature specific heat goes as  $T^2/\delta$  which is very different from the exponential behavior at  $q = 0$ .

Let us pause to ask: why does the model in Eq. (1) show such different behaviors in the limit  $q \rightarrow 0$  and at  $q = 0$ ? To answer this question, it is useful to generalize the form of the incommensurate hopping in (1) from  $\delta \cos(\pi + q)n$  to  $\delta \cos[(\pi + q)n + \eta]$ , where  $\eta$  is a phase lying between 0 and  $2\pi$ . If  $q/\pi$  is *irrational* (this is the generic case to consider if  $q$  is nonzero), the spectrum does not depend on  $\eta$ . [If  $q/\pi = M/N$  is rational, the spectrum does depend on  $\eta$ , but it varies less and less with  $\eta$  as  $N \rightarrow \infty$ . In our numerical computations, we introduced a random phase  $\eta$  for each value of  $q$  and found that this had no noticeable effect on the two figures]. This insensitivity to  $\eta$  can also be seen from the continuum theory in Eq. (6) where a potential of the form  $\cos(qx + \eta)$  can be transformed to  $\cos(qx)$  by shifting  $x$  appropriately. However, *exactly* at  $q = 0$ , the hopping has a term like  $\delta \cos \eta \cos(\pi n)$  and the spectrum depends significantly on  $\eta$ ; for instance, there is a gap from  $E = 0$  up to  $|\delta \cos \eta|$ , and the number of states up to an energy  $E$  is given by

$$\nu(E, \eta) = \frac{1}{\pi} \sqrt{E^2 - \delta^2 \cos^2 \eta} \quad (15)$$

for  $|\delta \cos \eta| < E \ll 1$ . We may now consider taking an *average* of this number over all possible values of  $\eta$ . Thus, the number of states up energy  $E$  is given by Eq. (15) to be

$$\nu(E) = \int_0^{2\pi} \frac{d\eta}{2\pi^2} \sqrt{E^2 - \delta^2 \cos^2 \eta} \Theta(E^2 - \delta^2 \cos^2 \eta) . \quad (16)$$

This agrees with (13) if we substitute  $\eta = qx$ . Thus, the limit  $q \rightarrow 0$  agrees with the point  $q = 0$  provided that we average over  $\eta$  in the latter case. However, this statement may not have any physical significance since an experimental system sitting at  $q = 0$  (the dimerized point) is more likely to choose a particular value of  $\eta$ , rather than average over many values of  $\eta$ . We will therefore choose  $\eta = 0$  henceforth.

We will 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, i.e., for Luttinger liquids. To this end, consider adding a four-fermion interaction term like  $\sum_n c_n^\dagger c_n c_{n+1}^\dagger c_{n+1}$  to the Hamiltonian (1). Equivalently, we can consider an  $XXZ$  spin-1/2 chain governed by

$$H = \frac{1}{2} \sum_n \left[ (1 + \delta \cos(\pi + q)n) (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + \Delta S_n^z S_{n+1}^z \right] . \quad (17)$$

which is related to the interacting fermion theory by a Jordan-Wigner transformation<sup>10</sup>. If the incommensurate term is absent ( $\delta = 0$ ), it is known from the exact Bethe ansatz solution and conformal field theory<sup>11</sup> that the model in (17) is gapless at zero magnetic field if  $-1 < \Delta \leq 1$ . If we now add a dimerization ( $q = 0$  and  $\delta$  is small), then the system becomes gapped and the gap scales as

$$\Delta E = \delta^{1/(2-K)} ,$$

$$\text{where } K = \frac{\pi}{2 \cos^{-1}(-\Delta)} . \quad (18)$$

[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, and a gap is not generated]. It is useful to state the result in Eq. (18) in the language of bosonization. For  $q = 0$ , the model in (17) is equivalent, at low energies, to a bosonic sine-Gordon theory described by the Lagrangian density<sup>11</sup>

$$\mathcal{L} = \frac{1}{2\pi K} \left[ (\partial\phi/\partial t)^2 - (\partial\phi/\partial x)^2 \right] - \alpha \delta^{2/(2-K)} [1 - \cos(2\phi)] , \quad (19)$$

where  $\alpha$  is a positive constant whose numerical value is not important here; the main point is to note the exponent of  $\delta$  in the coefficient of  $\cos(2\phi)$ . (There are also factors of  $\ln \delta$  due to the presence of a marginal operator in the  $XXZ$  model<sup>12</sup>, but we will ignore such terms here). Thus, the incommensurate term which is *linear* in  $\delta$  in the original theory in (17) becomes a cosine term with a different exponent for  $\delta$  in the bosonic theory. This is because a nontrivial renormalization occurs in the process of deriving the low-energy bosonic theory from the fermionic one<sup>7,13</sup>. This renormalization occurs even if the fermions are noninteracting, i.e., for the  $XY$  spin-1/2 chain with  $\Delta = 0$  in (17) and  $K = 1$ ; the reason for this is that 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 (i.e. classical) spectrum that one obtains from the sine-Gordon theory, namely, the classical soliton mass for the fermionic excitations and the quadratic fluctuations around  $\phi = 0$  spectrum for the bosonic excitations<sup>14</sup>. The noninteracting fermionic model in (1) has no such renormalizations, which is why we did not use bosonization in the earlier part of this paper.

Let us now change  $q$  slightly away from 0. Then bosonization again yields a theory of the sine-Gordon type, except that the coefficient of the  $\cos(2\phi)$  term in Eq. (19) gets modified to produce

$$\mathcal{L} = \frac{1}{2\pi K} \left[ (\partial\phi/\partial t)^2 - (\partial\phi/\partial x)^2 \right] - \alpha |\delta \sin(qx)|^{2/(2-K)} [1 - \cos(2\phi)] , \quad (20)$$

where we have again shifted  $x$  to convert  $\cos(qx)$  to  $\sin(qx)$ . Unlike (19), the theory in Eq. (20) cannot be solved analytically, either in classical or in quantum mechanics. However we can make some qualitative statements about the low-energy spectrum if  $q/\delta \ll 1$ . When calculating the spectrum of small oscillations about a classical ground state  $\phi = 0$ , we find it convenient to scale  $x$  by a factor of

$$a = (q\delta)^{1/(3-K)} . \quad (21)$$

This gives the eigenvalue equation

$$-\frac{\partial^2 \phi}{\partial x^2} + 4\pi K \alpha |x|^{2/(2-K)} \phi = \left(\frac{E}{a}\right)^2 \phi \quad (22)$$

for eigenstates lying close to the origin  $x = 0$ ; we have approximated  $\sin(qx)$  by  $qx$  and  $\sin(2\phi)$  by  $2\phi$ . Since (22) is the Schrödinger equation with a confining potential, we see that the energy can take several discrete values which are given by numerical factors multiplying  $a$ . [Note that our earlier results for noninteracting fermions agree with this scaling argument if we set  $K = 1$ ]. These discrete values will then spread out into bands once we include tunneling between the different wells centered at the points  $x = n\pi$ . Similarly, we can find the energy of a classical soliton which goes from  $\phi = 0$  at  $x \rightarrow -\infty$  to  $\phi = \pi$  at  $x \rightarrow \infty$ ; once again we can show by scaling that this will be given by  $a$  times some numerical factor. [Of course, all the numerical factors will get renormalized due to quantum corrections, but the power-law dependence on  $q\delta$  is not expected to change]. We therefore see that all the low-lying excitations have energies of the order of  $(q\delta)^{1/(3-K)}$ ; this is much smaller than the gap which exists exactly at  $q = 0$  given by  $\Delta E$  in Eq. (18), since we are assuming that  $q/\delta$  is small. We thus see that in the limit  $q \rightarrow 0$ , there are many states which lie within the gap  $\Delta E$ .

We can use semiclassical arguments as in Eq. (13) to estimate the density of states  $\rho(E)$  at energies much smaller than the  $q = 0$  gap. If  $E \ll \delta^{1/(2-K)}$ , the wave function for that state lies in a region where we can approximate  $\sin(qx)$  by  $qx$ . Ignoring various numerical factors, we then get

$$\rho(E) = \frac{d}{dE} \int_0^{2\pi/q} \frac{qdx}{\pi} \sqrt{E^2 - (\delta qx)^{2/(2-K)}} \Theta(E^2 - (\delta qx)^{2/(2-K)}) \sim \frac{E^{2-K}}{\delta} . \quad (23)$$

The specific heat at temperatures much lower than the  $q = 0$  gap therefore scales as  $T^{3-K}/\delta$ , which is again much larger than the exponential dependence which occurs at  $q = 0$ .

Before ending this paper, we should remark that the peculiar difference between the limit  $q \rightarrow 0$  and  $q = 0$  only occurs near dimerization, i.e., near wave number  $\pi$ . If we take the incommensurate term in Eq. (1) to be of the form  $\delta \cos(Q + q)n$ , where  $Q/\pi$  is equal to some simple rational number *different* from 1, then there is no such singularity at  $q = 0$ . Let us see this for the case of noninteracting fermions. Imagine filling up the Fermi sea up to a Fermi energy  $E_F = -\cos k_F$  where  $k_F = Q/2$ ; the Fermi velocity is then  $v_F = \sin k_F$ . We define the continuum Dirac field as

$$\psi(x) = \psi_R(x) \exp(ik_F x) + \psi_L(x) \exp(-ik_F x), \quad (24)$$

After dropping terms like  $\exp(\pm ik_F x)$  which vary rapidly, the Dirac equations take the form

$$\begin{aligned} i(\partial/\partial t + v_F \partial/\partial x) \psi_R + \frac{\delta}{2} \exp(iqx - ik_F x) \psi_L &= 0, \\ i(\partial/\partial t - v_F \partial/\partial x) \psi_L + \frac{\delta}{2} \exp(-iqx + ik_F x) \psi_R &= 0. \end{aligned} \quad (25)$$

The solutions of this equation have the plane wave form

$$\begin{pmatrix} \psi_R(x, t) \\ \psi_L(x, t) \end{pmatrix} = \exp(-iEt) \begin{pmatrix} a_R \exp(ikx + iqx/2 - ik_F/2) \\ a_L \exp(ikx - iqx/2 + ik_F/2) \end{pmatrix}. \quad (26)$$

From this, we find that there is a single energy gap extending from  $E = (v_F q - \delta)/2$  to  $E = (v_F q + \delta)/2$ ; the size of the gap is independent of  $q$ , assuming that  $q$  and  $\delta$  are both small. If  $\delta$  is held fixed and  $q$  is increased from zero, a state first appears at zero energy when  $q$  reaches the value  $\delta/v_F$ . It is instructive to express all this in the language of bosonization. Since  $K = 1$ , the sine-Gordon Lagrangian takes the form

$$\mathcal{L} = \frac{1}{2\pi v_F} (\partial\phi/\partial t)^2 - \frac{v_F}{2\pi} (\partial\phi/\partial x)^2 - \frac{\pi\delta^2}{16v_F} [1 - \cos(2\phi + qx)], \quad (27)$$

where we have fixed the coefficient of  $\cos(2\phi)$  in such a way that, for  $q = 0$ , the soliton mass, including the quantum corrections<sup>14</sup>, is exactly equal to the gap from zero energy, i.e.,  $\delta/2$ . It is convenient to scale  $x$  in the action ( $S = \int dt dx \mathcal{L}$ ) by a factor of  $v_F$ , and then shift  $\phi$  by  $qv_F x/2$ . This gives

$$\mathcal{L} = \frac{1}{2\pi} \left[ (\partial\phi/\partial t)^2 - (\partial\phi/\partial x - qv_F/2)^2 \right] - \frac{\pi\delta^2}{16} [1 - \cos(2\phi)]. \quad (28)$$

The Hamiltonian therefore contains a boundary term  $-(qv_F/2\pi)[\phi(\infty) - \phi(-\infty)]$ ; this is equal to  $-qv_F/2$  in a one-soliton state. We thus see that if  $q$  is increased from zero, the energy of the one-soliton state becomes equal to that of the ground state (whose soliton number is zero) when  $q$  reaches the value  $\delta/v_F$ . [We note that similar results appear in the context of incommensurate crystals<sup>5,7,8</sup>].

Thus, if  $Q \neq \pi$ , there is a critical and nonzero value of  $q$  at which the gap closes at zero energy. This is very different from the earlier case with  $Q = \pi$ , where there is always a band of energies lying around zero energy, so that there is no gap at zero energy for any  $q \neq 0$ . (Our results disagree with Ref. 7 which argues that there is a nonzero critical value of  $q$  for  $Q = \pi$ ).

An interesting problem for future study may be to examine what happens if the incommensuration is strong, i.e., if  $\delta$  is comparable to or larger than 1. [Both the perturbative and the continuum Dirac theory (or bosonization) approaches would then fail]. It is possible that the pattern of bands and gaps would become much more complicated in that case, perhaps with a Devil's staircase or a point spectrum structure<sup>1,2,4,5</sup>. The nature of the wave functions, namely, whether they remain extended or become localized, would also be of interest.

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## Figure Captions

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.
2. A finer view of the bands as a function of  $E/\delta$  and  $q/\delta$ , for  $\delta = 0.05$ . A comparison with the second-order perturbation results is indicated by the six solid lines.

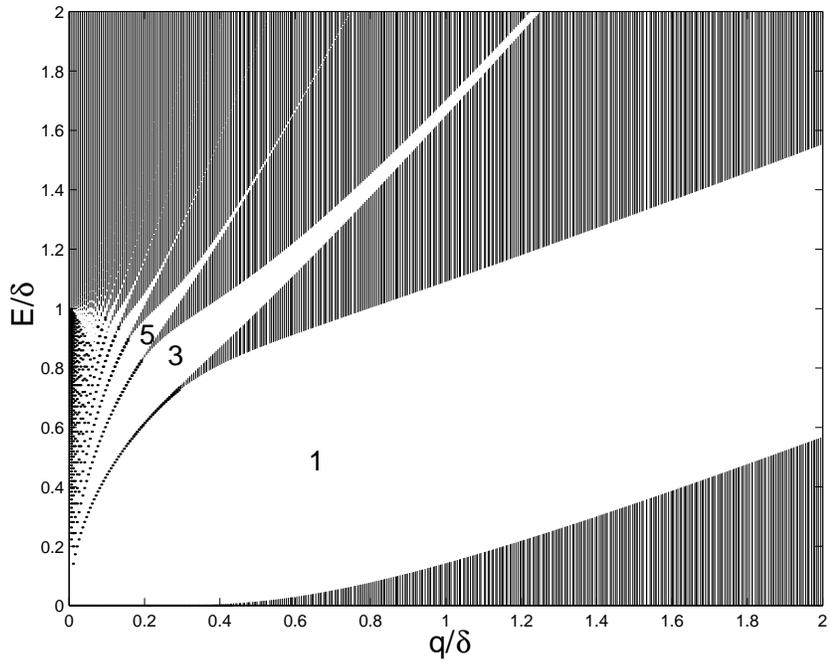


FIG. 1.

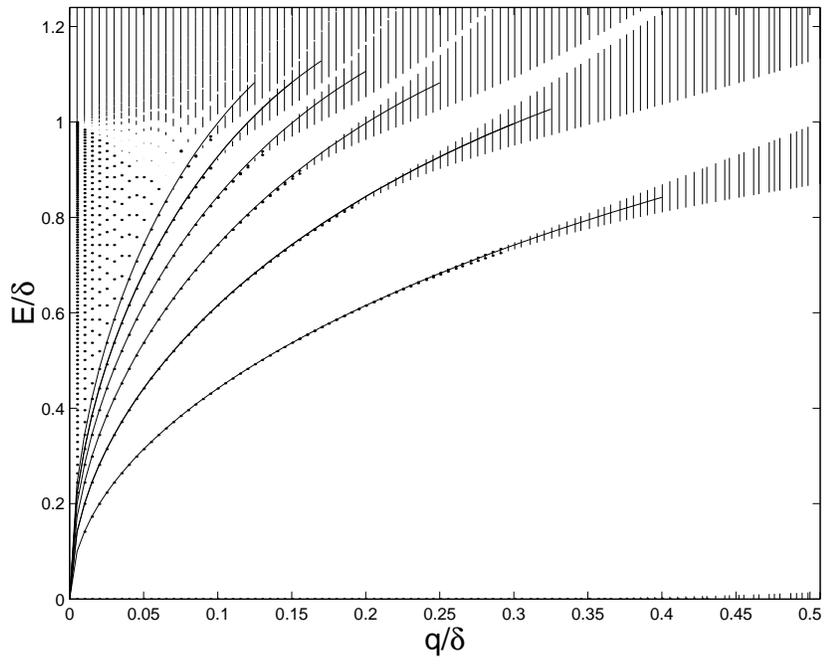


FIG. 2.