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Recalculation of $4k_F$ correlations in one-dimensional systems

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The $4k_F$ response function is recalculated for the one-dimensional electron system in the presence of the umklapp matrix element g_3. It is shown that the $1/\omega^{2-4\gamma_c}$ singularity is replaced by a finite value below the energy gap set by g_3.

Correlated one-dimensional systems with weak interactions have been studied intensively over the last decades, and their theory is fairly well understood by now. Particular attention was devoted to the interesting case of a half-filled electron band where in addition to the backward and forward scattering g_1 and g_2, the umklapp matrix element g_3 is also important.

As it is well known, the $2k_F$ and $4k_F$ charge-density wave, the $2k_F$ spin-density wave, the singlet and triplet superconducting response functions were calculated with and without g_3. In general, the power laws were found[1,2] and the powers in absence and presence of g_3 were related.[3,4] In the case of the $4k_F$ response function this lead to the assertion that for the half-filled band it behaves[1] as ω^{-2} at $T=0$ and ω small with respect to the umklapp gap Δ_3, whereas for larger ω the singularity is weaker or even absent. Analogous effects were predicted at $\omega=0$ in a function of the temperature.

A good physical realization of the described model was found in Bechgaard salts.[5,6] These materials are characterized by g_3 small[4,5] (originating[4,7] from anions that are arranged periodically near the chains) with respect to g_1 and g_2 and by very small interchain couplings. A crossover is therefore expected in the one-dimensional regime on the temperature and the frequency scale $\Delta_3 \sim g_3$.

The strong T^{-2} singularity of the $4k_F$ response function has not been observed however.[6] The latter is coupled to the dimerization of the lattice through the linear dependence of g_3 on dimerization.[4,7] The enhancement of the singularity below Δ_3 should therefore result in the fast increase of dimerization on lowering the temperature. Empirically, however, instead of increasing, the dimerization tends to saturate[6] below Δ_3. This means that the $4k_F$ response function saturates in this temperature and frequency range. It was asserted recently[8] (without proof) that the saturation and not the enhancement is the theoretically correct behavior of χ_4. Here we wish to prove this assertion, limiting ourselves to the physically interesting regime $|g_3| < g_2 - g_1/2$. What actually happens is that although defined as a response function χ_4 is usually calculated as a correlation function. When the long-range order becomes important (below Δ_3) these two functions differ essentially: The response function is finite as will be shown here in contrast to the correlation function which contains the long-range order singularity. As already mentioned, it is the response function that couples to the lattice.

The one-dimensional system, usually modeled[1,2] through the matrix elements for the forward (g_2,g_4) and backward (g_1) scattering, is conveniently treated in the bosonization formalism in which the charge and spin degrees of freedom separate.[9] When the electronic band is half-filled the umklapp process described by g_3 also becomes important. The bosonized form of the electron Hamiltonian in the charge channel then has a form[1,10]

$$H_c^{(b)} = \tfrac{1}{2}\int dx\{P_c(x)^2[v_F-(2g_2-g_1)/2\pi-g_4/\pi]+(\partial\phi_c/\partial x)^2[v_F+(2g_2-g_1)/2\pi-g_4/\pi]\} + \int dx[2|g_3|/(2\pi a)^2]\cos(2\sqrt{2\pi}\phi_c)\,. \tag{1}$$

Only the charge phase ϕ_c enters in the representation of the $4k_F$ operator

$$O_{4c}^{(b)} = 2(2\pi a)^{-2}\cos(2\sqrt{2\pi}\phi_c) \tag{2}$$

(the wave vector in O_4 is measured relative to $4k_F$; $a=1/\Lambda\sim k_F$ is a momentum cutoff in a theory). Therefore the calculation of the $4k_F$ response function requires only the consideration of $H_c^{(b)}$ of the Hamiltonian. It should be emphasized that in Eq. (1) we assumed that g_3 is a real positive number. For complex g_3 the operator $O_{4s}^{(b)} = [2/(2\pi a)^2]\sin(2\sqrt{2\pi}\phi_c)$ also enters into the Hamiltonian. On the other hand, the form given in Eq. (1) always may be obtained after the constant shift in the charge phase, $\phi_c \to \phi_c + \arg(g_3)/2\sqrt{2\pi}$. As a consequence, the energy of the electronic system depends only on the absolute magnitude of g_3, the well-known fact. However, if we are interested in the response of the electronic system to the lattice dimerization which couples to it through

$$g_3(u) = g_{30} + au\,, \tag{3}$$

both response functions,

$$\chi_{4c}(k,\omega)=\mathcal{F}((-i)\langle[O_{4c}(x,t),O_{4c}(0,0)]\rangle) \tag{4}$$

and

$$\chi_{4s}(k,\omega)=\mathcal{F}((-1)\langle[O_{4s}(x,t),O_{4s}(0,0)]\rangle) \tag{5}$$

appear, where $\mathcal{F}$ denotes Fourier transform. The components of u which couple to χ_{4c} and χ_{4s} are respectively (for g_{30} and a real) its real and imaginary part, $u=u'+iu''$. In the absence of umklapp ($g_{30}=0$) there is no difference between these two response functions. In that case the calculation of χ_4 is particularly straightforward within the bosonization approach giving the well-known power-law decay in (x,t) space[1,11] which corresponds to the Fourier transform

$$\chi_4(k=0,\omega)\sim[E_F/\max(\omega,T)]^{2(1-2\gamma_c)} \tag{6}$$

for

$$2(1-2\gamma_c)\ln[E_F/\max(\omega,T)]>1 \tag{7}$$

and with γ_c defined by

$$\gamma_c\equiv\left[\frac{1-(2g_2-g_1)/2\pi\tilde{v}}{1+(2g_2-g_1)/2\pi\tilde{v}}\right]^{1/2},\quad \tilde{v}\equiv v_F+g_4/\pi. \tag{8}$$

The same power law is found for the correlation function $\langle TO_4(x,t)O_4(0,0)\rangle$.

The introduction of g_3 causes the freezing[1-3] of charge degrees of freedom at low temperatures and the absence of the power-law decay of the correlation function in the (x,t) space. However, it can be argued immediately that the corresponding $4k_F$ response function χ_4 is finite. Regarding the au term in H_c [Eqs. (1) and (3)] as a perturbation the well-known relation (at $T=0$)

$$\chi_{4c}(\omega=0)=(\partial\langle O_{4c}\rangle/\partial a u')_{u=0}=(\partial\langle O_{4c}\rangle/\partial|g_3|)_{u=0}$$
$$=(\partial^2\delta E_{\text{g.s.}}(|g_3|)/\partial|g_3|^2)_{u=0}, \tag{9}$$

expresses χ_{4c} through $\delta E_{\text{g.s.}}(g_3)$, the change of the ground-state energy per unit length caused by g_3O_{4c}. It is reasonable to expect $\partial^2\delta E_{\text{g.s.}}(g_3)/\partial|g_3|^2$ and thus χ_4 is finite in some range of values of g_3. A similar argument applies for χ_{4s}. In the latter case the equation

$$\chi_{4s}(\omega=0)=(\partial\langle O_{4s}\rangle/\partial a u'')_{u=0}$$
$$=(1/|g_{30}|)(\partial\delta E_{\text{g.s.}}(|g_3|)/\partial|g_3|)_{u=0}, \tag{10}$$

follows immediately from the fact that $\delta E_{\text{g.s.}}$ depends only on the absolute value of g_3. Equations (9) and (10) can be further substantiated by calculating the actual functional dependence of $\delta E_{\text{g.s.}}$ on g_3. This is a question to which we now turn.

The expression for $\delta E_{\text{g.s.}}(g_3)$ may be obtained using the Bethe-Ansatz (BA) solution[12] for the massive Thirring model after the inverse bosonization transformation which maps the charge Hamiltonian H_c to the Thirring Hamiltonian H_T. The result is

$$\delta E_{\text{g.s.}}(g_3)=-\frac{C}{2\pi v}\frac{\sinh[(1-2\gamma_{\text{BA}})\ln(2v\Lambda/\Delta_3)]}{1-2\gamma_{\text{BA}}}$$
$$\times(2v\Lambda/\Delta_3)^{1-2\gamma_{\text{BA}}}\Delta_3^2 \tag{11}$$

where

$$1-2\gamma_{\text{BA}}\equiv[1+\pi/2\arctan(g/2v)]^{-1} \tag{12}$$

and where m, g, and v are parameters of the Thirring Hamiltonian in usual notation,

$$m=\Delta_3\equiv|g_3|/2\pi a,\quad g=(5\tilde{v}\pi/4)[(2g_2-g_1)/2\pi\tilde{v}-\tfrac{3}{5}],$$
$$v=(4\tilde{v}/5)\{1-\tfrac{15}{16}[(2g_2-g_1)/2\pi\tilde{v}-\tfrac{3}{5}]\}. \tag{13}$$

C is a function of g/v that goes to unity on the Luther-Emery (LE) line (where $g=0$).

Using Eq. (9) the response function is obtained showing the power-law dependence on Δ_3,

$$\chi_{4c}(\omega=0)\approx-\frac{C}{(2\pi a)^2 2\pi v}\frac{4\gamma_{\text{BA}}(4\gamma_{\text{BA}}-1)}{1-2\gamma_{\text{BA}}}$$
$$\times\left(\frac{2v\Lambda}{\Delta_3}\right)^{2(1-2\gamma_{\text{BA}})} \tag{14}$$

for

$$2(1-2\gamma_{\text{BA}})\ln(2v\Lambda/\Delta_3)\gg 1. \tag{15}$$

It should be noted that near the Luther-Emery line ($g/v\ll 1$) the exponent $2(1-2\gamma_{\text{BA}})$ has the same limiting behavior as the exponent $2(1-2\gamma_c)$ in χ_4 obtained in the high-temperature region,

$$2(1-2\gamma_c),2(1-2\gamma_{\text{BA}}),2g/\pi v$$
$$\to\tfrac{25}{8}[(2g_2-g_1)/2\pi\tilde{v}-\tfrac{3}{5}]. \tag{16}$$

On the LE line the power law gives place to the logarithmic expression for χ_4 [inequality in Eq. (15) does not hold there but we always assume that $\ln(2v\Lambda/\Delta_3)\gg 1$],

$$\chi_{4c}(k=0,\omega)\approx-1/(2\pi a)^2(1/\pi v)\ln(2v\Lambda/\Delta_3) \tag{17}$$

in complete analogy with the $2k_F$ correlation function for the Peierls system of spinless fermions which is also described by the Thirring Hamiltonian for $g=0$. Moreover, the direct calculation of the commutator in Eq. (4) is easy to perform on the LE line. For finite T and ω the results familiar from the Peierls theory follow

$$\chi_{4c}(k=0,\omega)\approx-1/(2\pi a)^2(1/\pi v)$$
$$\times\ln[v\Lambda/\max(\omega,T,\Delta_3)]. \tag{18}$$

From Eqs. (18) and (14) we may finally conclude that in the system with umklapp electron-electron scattering the $4k_F$ response function $\chi_{4c}(\omega)$ at low temperature has the same form as in the high-temperature (or high-frequency) region but with the umklapp gap Δ_3 coming instead of T or ω.

The other response function of interest, χ_{4s}, is obtained, using Eq. (10), as a first derivative of $\delta E_{\text{g.s.}}$ with respect to $|g_3|$. The result may be expressed in terms of χ_{4c} as

$$\chi_{4s}(0)\approx c_1\chi_{4c}(0), \tag{19}$$

where the factor $c_1=1/(4\gamma_{\text{BA}}-1)$ goes to 1 on the LE line. It is interesting to note that the change of the ground-state energy due to umklapp may be expressed

through χ_4. Indeed, the result has the form

$$\delta E_{\text{g.s.}} \sim \tfrac{1}{2} |g_3|^2 \chi_4(\Delta_3) . \quad (20)$$

(Omitting factors like c_1, which are close to 1 near LE line.) Equation (20) is similar[8] to the umklapp contribution to the free energy for $T \gg \Delta_3$. The difference is again only in the substitution of Δ_3 for T in χ_4.

Having found the susceptibility we also may be interested in calculating the optimal value of the dimerization u. It is obtained on minimizing the sum of the electronic ground-state energy (or free energy at $T > 0$) and the lattice elastic energy $|u|^2\omega_0^2$ with respect to $u = u' + iu''$. The minimization may be done numerically for any choice of parameters. A qualitative plot of the dependence of u on g_{30} for $1 - \gamma_{BA} > 0$ is given in Fig. 1, together with the corresponding temperature dependence. The calculation is particularly simple when $|au| \ll g_{30}$. The change of the electronic ground-state energy may then be approximated by the term linear in u,

$$\delta E_{\text{g.s.}} = c_1 g_3 \chi_{4c}(\Delta_{30}) a u' , \quad (21)$$

with the result

$$u = c_1 a g_3 |\chi_{4c}(\Delta_{30})| / 2\omega_0^2 . \quad (22)$$

Let us finally mention that, although the exact solution of the massive Thirring model is an important ingredient of our result for $\chi_4(0)$ below the LE line, it is possible to calculate the same quantity using the self-consistent harmonic approximation,[13]

$$\cos(2\sqrt{2\pi}\phi_c) \approx \langle \cos(2\sqrt{2\pi}\phi_c) \rangle (1 - 4\pi\phi_c^2 + 4\pi\langle\phi_c^2\rangle) . \quad (23)$$

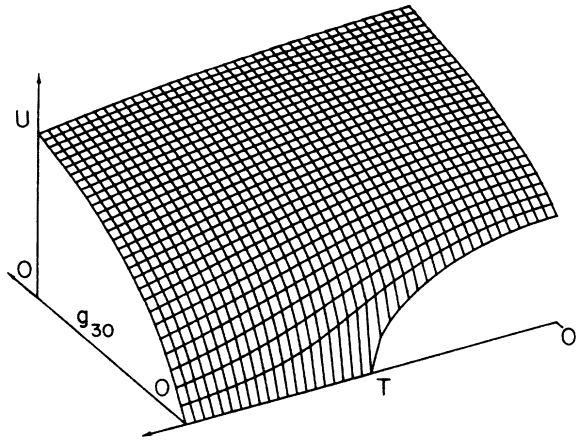

FIG. 1. The dependence of the optimal dimerization on umklapp and temperature.

It may be verified by direct calculation of the commutator in Eq. (4) that this approximation, known to give the correct low-energy spectrum of the sine-Gordon Hamiltonian in the region of intermediate[13-15] couplings [$1 > g > 1/\ln(v\Lambda/\Delta_3)$ in our notation], gives essentially the same result for $\chi_4(0)$ as obtained in Eq. (14).

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