$4k_F$ CORRELATIONS IN 1D SYSTEMS, REVISITED

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Abstract

The $4k_F$ response function χ_4 is calculated for the 1d electron system in the presence the Umklapp electron-electron scattering. It is shown that the power law behaviour of χ_4 on high temperatures and frequencies gives place to the saturation below the Umklapp gap Δ_3.

The 1d system with weak electron-electron coupling has been extensively studied in last decades both theoretically and experimentally (in the framework of quasi one dimensional materials). Various instabilities were found in these systems depending on the strength of various electron-electron scattering processes, usually described trough corresponding matrix elements g_1, g_2, g_3, g_4 [1]. A particular situation occurs when the electronic band is half filled and the Fermi wave length $\lambda_F=2\pi/k_F$ is four times the lattice constant. This leads to the Umklapp electron-electron scattering described by g_3. Physical realisations of such system may be found in Bechgaard salts where the Umklapp originates from the potential produced by anions which are periodically arranged along the chains [2].

The effect of the Umklapp is to introduce a gap Δ_3 into the excitation spectrum for the charge degrees of freedom. As a consequence various (CDW, SDW, singlet and triplet superconductivity) response functions of the system change their behaviour for $\omega,T<\Delta_3$. Generally, these response functions are described by power laws and a thumb rule was established [1],[3] relating the exponents in absence and presence of g_3. In particular, for the $4k_F$ response function

$$\chi_4(k,\omega)= \text{F.T. of } (-i)\langle[O_4(x,t),O_4(0,0)]\rangle ,$$
$$O_4(x) \equiv \psi_{1\downarrow}^{+}(x)\psi_{1\uparrow}^{+}(x)\psi_{2\uparrow}(x)\psi_{2\downarrow}(x) + \text{h.c.}$$

it says that the $\omega^{4\delta_c-2}$ behaviour[1],[3] (at T=0) should be replaced [3] by ω^{-2} divergence in the presence of g_3. Similar behaviour is predicted as a function of temperature for ω=0. Experimentally the behaviour of $\chi_4(T)$ should be seen through the temperature dependence of the lattice dimerization since the dimerization field u couples to the electronic $4k_F$ operator O_4 as [3]

$$H_{dim} = \alpha\int dx\, u\, O_4(x) + \text{H.C.}$$

leading to the effective Umklapp $g_3=g_{30}+\alpha u$. However, the T^{-2} divergence was not observed experimentally [4]. Here we reexamine the effect of the Umklapp on χ_4 and show that, actually, the gap Δ_3 removes the divergence in χ_4 instead of strengthening it. To illustrate the main point we consider here only χ_4 at ω=0 and T=0 (Exact frequency and temperature dependences may be obtained for the special values of the electron-electron coupling constants (Luther-Emery line) [5]). The change of the ground state energy δE_{GS} of the system due to the Umklapp may be in fact found exactly for g_3 small with respect to g_1 and g_2

(received December 31, 1989)

and for $g_2-g_1/2$ positive which corresponds presumably to the situation in organic conductors [2]. Two steps are involved in the calculation. First is the bosonisation of the electronic Hamiltonian which leads to the separation of spin and charge degrees of freedom [6]. Umklapp enters in the charge part only. Second step is the mapping of the charge part of the Hamiltonian on the massive Thirring model for which the ground state was found using the Bethe Ansatz [7]. More detailed calculation will be published elsewhere [5]. Here we give only the final result for χ_4 which is obtained as a second derivative of the ground state energy with respect to g_3,

$$\chi_4(\omega=0) = \partial\langle O_4\rangle/\partial g_3 = \partial^2\delta E_{GS}(g_3)/\partial g_3^2$$

$$\approx -\frac{C}{(2\pi a)^2\, 2\pi v}\,\frac{2\gamma_{BA}(4\gamma_{BA}-1)}{1-2\gamma_{BA}}\left(\frac{2v\Lambda}{\Delta_3}\right)^{2(1-2\gamma_{BA})}$$

for

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

Here $\Delta_3=g_3/8\pi\lambda_F$ and γ_{BA} and C are known functions of g_1, g_2, g_4 and v_F. In the vicinity of the LE line γ_{BA} coincides with γ_σ that enters in the high temperature (frequency) exponents [1],[3] and C is close to 1. It should be noted that the obtained response function χ_4 is of the same form as in the system without the Umklapp but with Δ_3 substituted for T or ω. For $1-2\gamma_{BA}=0$ (LE line) the problem is analogous [6] to the Peierls problem for spinless fermions and δE_{GS} and χ_4 may be found without resorting to the Bethe Ansatz solution. The same substitution works in that case.

Using the result for χ_4 the change of the ground state energy due to Umklapp may be expressed as $\delta E_{GS}\sim(1/2)\cdot g_3^2\cdot\chi_4(\Delta_3)$. This resembles to the expression for the contribution of the Umklapp to the free energy at $T\gg\Delta_3$, the difference is again just in the substitution[8] of Δ_3 for T in χ_4. Noting that δE_{GS} is linear in u for $\omega u\ll g_{3o}$ it is realized that finite χ_4 in the system with Umklapp implies finite optimal dimerization. The optimal value for u is obtained on minimizing the sum of the δE_{GS} and the lattice elastic energy $m\omega_o^2u^2$. The result may be expressed in terms of χ_4 as

$$u = \alpha g_3 |\chi_4(\Delta_{30})| /2m\omega_o^2(4\gamma_{BA} - 1)$$

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