A Pseudogap in the Single-Particle Density of States of a Tomonaga-Luttinger Liquid

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We study a single-particle density of states (DOS) in a model of Tomonaga-Luttinger liquid with small (large) values of the Luttinger parameter $K_c < 0.17, (K_c > 5.82)$, in the charge sector. We explain that such values of $K_c$ may be achieved by electron-phonon interactions without generating the spin gap. We suggest that electron-phonon interactions can be partially incorporated into the Tomonaga-Luttinger liquid scheme by introducing frequency dependent $K_c(\omega)$. We demonstrate that when the low-frequency asymptotic value $K_c(0) < 0.17$ or $K_c(0) > 5.82$, the single-particle DOS has a pseudogap behavior in frequency where $\rho(\omega)/\omega$ vanishes at small frequencies. The DOS exhibits a peak the position of which scales as $|K(0) + K^{-1}(0)|\omega_0/2$ where $\omega_0$ is the characteristic phonon frequency.

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The Tomonaga-Luttinger liquid theory predicts a power-law frequency dependence of the single-particle density of states (DOS). In an apparent contradiction with this prediction many quasi-one-dimensional materials (see, for example, \[1\]) exhibit a pseudo-gap type behavior (5). Below we calculate the DOS for a model of Tomonaga-Luttinger liquid with electron-phonon interactions.

At small frequencies this integral is dominated by the asymptotics \[4\] when $\theta < 1$. Then we have

$$G(\omega_n) \approx 2i A \int_0^{\infty} d\tau \frac{\sin(\omega_n \tau)}{\tau^{1+\theta}} \sim (\omega_n)^{\theta}$$ \[4\]

The analytic continuation is quite straightforward in this case and one gets

$$\Im G^{(R)}(\omega) = A(\omega)^{\theta} \sin[\pi(1-\theta/2)] \sin[\pi(\theta-1)/2] \Gamma(2-\theta) \theta(\theta-1).$$ \[5\]

When $\theta > 1$ the integral \[3\] converges at large Matsubara times. However, at $\theta < 2$ its second derivative with respect to $\omega_n$ is still determined by the asymptotics at large $\tau$ such that we get

$$G(\omega_n) = -i\omega_n g(0) - 2(\omega_n)^{\theta} \frac{\sin[\pi(1-\theta/2)] \Gamma(2-\theta)}{\theta(\theta-1)} ...$$ \[6\]

After the analytic continuation only the second term contributes to the imaginary part and we find that Eq. \[3\] is still valid. Thus the value $\theta = 1$ corresponding either to $K_c = 3 - 2\sqrt{2} \approx 0.17$ or $K_c = 3 + 2\sqrt{2} \approx 5.83$ marks a crossover into a pseudogap phase where $\rho(\omega)/\omega$ vanishes at $\omega \to 0$.

Small values of $K_c$ can be achieved in systems with strong retardation effects such as systems with electron-phonon interactions or Kondo lattices \[3\]. In all these systems small values of $K_c$ are achieved asymptotically at small frequencies. Therefore it is interesting to learn what is the area of validity of the universal power law behavior \[6\]. Below we calculate the DOS for a model with electron-phonon interactions.

The influence of phonons on the electron subsystem in quasi-one-dimensional metals have been studied by different authors; mostly for the case of noninteracting electron-phonon interactions (see \[1\], \[2\] and references therein). The combined effects of the Coulomb and electron-phonon interactions...
was studied in [1], [2] using the renormalization group approach. In [3] these effects have been studied in the framework of Tomonaga-Luttinger theory.

Here we briefly repeat the derivation given in [3]. The lattice effects can be included in the Hubbard Hamiltonian by making the hopping integral $t$ dependent on the intersite distance:

$$ t_{ij} \approx t + \frac{1}{2a} \kappa (u_i - u_j) \ . $$

(It has been proposed for the first time by Su, Schriefer and Heeger to describe the essential physics of conducting polymers [4]). Then the Hamiltonian takes the form:

$$ H = -t \sum_{j,\sigma} \left( c^+_j c_{j+1,\sigma} + c^+_j c_{j+1,\sigma} \right) + U \sum_j n_{j\up} n_{j\dn} - \frac{1}{2a} \kappa \sum_{j,\sigma} (u_j - u_{j+1}) \left( c^+_j c_{j+1,\sigma} + c^+_j c_{j+1,\sigma} \right) + H_{ph} \ , $$

where $u_j$ is dimensionless and $\kappa$ has dimensions of energy. The $c_{j,\sigma}$ operators are the usual creation and annihilation operators for the electrons with spin $\sigma$ in the Wannier orbitals at site $j$ and $n_{j,\sigma}$ is the number of electrons. $U$ is the repulsion of two electrons on the same site.

In the case of an incommensurate band filling ($4k_F \neq 2\pi/a$) in the continuous approximation the electron-phonon part of this Hamiltonian generates a coupling between the lattice deformations and the $2k_F$ and $4k_F$ components of the charge density. The electron-phonon interaction contributes to an effectively retarded interaction between the electronic densities:

$$ S_{\text{int}} = -\int d\tau d\tau' dx \sum_{i=1,2} \rho(2ik_F, x) D_i(\tau - \tau') \rho(2ik_F, x) \ , $$

where $D_i(\tau)$ is the phonons Green’s function at $q = 2ik_F$ [2]. Thus the main contribution to the interaction comes from phonons with large frequency. This interaction effects both the spin and the charge sector. The phonons give a positive contribution to the current-current coupling constant in the spin sector (i.e. $g_s^{(0)} \rightarrow g_s$). In this sector the electron-phonon interaction competes with repulsive forces responsible for $g_0$. We assume that the renormalized coupling constant is still repulsive such that there is no spin gap.

In the charge sector the phonons influence the dynamics as well as the scaling dimensions, renormalizing the charge velocity $v_c$ and $K_c$. In the limit of small frequencies $|\omega| \ll \omega_1$ their renormalized values are:

$$ K_c = \left( \frac{m^*}{m} \right)^{1/2} K_c^0 \ , \quad \tilde{v}_c = \left( \frac{m^*}{m} \right)^{1/2} v_c^0 \ . $$

where $m^*$ is interpreted as renormalized electrons mass with $m$ being the bare mass.

Since we are interested not only in the long time asymptotics of the Green’s function, but in its intermediate time behavior, we shall model these behavior adopting the modified Gaussian model with the time-dependent Luttinger parameter:

$$ S = \frac{1}{2} \sum_{\omega, q} \Phi_c(-\omega, -q) \left[ \frac{1}{\nu_c} \omega^2 f(i\omega) + v_c q^2 \right] \Phi_c(\omega, q) \ , $$

where the function $f(\omega)$ takes values between $f(0) = m^*/m = K^{-2}$ and $f(\infty) = 1$. In this brief report we suggest a semi-phenomenological form for the function $f(\omega)$:

$$ f(\omega) = 1 + \frac{\omega^2}{\omega^2 + \omega_0^2} (K^{-2} - 1) \ , $$

The above model yields the following Matsubara time single-electron Green’s function

$$ G(\tau) = \frac{1}{\tau} \exp \left\{ - \int_0^{\epsilon_F/\omega_0} dx x \left[ \left( \frac{x^2 + 1}{x^2 + K^{-2}} \right)^{1/4} - \left( \frac{x^2 + K^{-2}}{x^2 + 1} \right)^{1/4} \right]^2 \sin^2(\omega_0 \tau x/2) \right\} \ . $$

where $\epsilon_F$ is the ultraviolet cut-off (recall that we consider the Green’s function at coinciding spatial points). Pictures of the single particle density of states are represented on Figure 1. They are obtained by analytic continuation of $G(\omega_{\text{in}})$ from the imaginary axis to just above the real axis.

The figures clearly show the crossover from the Luttinger-liquid type behavior with singular $d\rho/d\omega$ at $K > 0.17$ to the pseudogap behavior at $K < 0.17$. Another remarkable feature of these DOS is the peak at $\omega \approx K^{-1} \omega_0/2$ (see Fig. 2). Since the DOS is invariant under $K \rightarrow K^{-1}$ this empirical formula can be generalized as

$$ \omega_{\text{peak}} = \frac{1}{2} (K^{-1} + K) \omega_0 \ . $$

It is interesting that the peak always occurs at frequencies larger than the characteristic phonon frequency $\omega_0$. At small (large) values of $K$ this discrepancy can be quite substantial. For example, a peak in DOS has been observed in $K_{0.3}\text{MoO}_3$ at $\omega \approx 300$ meV. The behavior of DOS at smaller frequencies is almost linear in $\omega$ which suggests $K \approx 0.15$. Then Eq. (13) gives a reasonable estimate for the phonon frequency: $\omega_0 \approx 90$ meV.

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FIG. 1. Plots of the dependence of the density of states on frequency for different values of the parameters $K$ and $\omega_0$.

FIG. 2. Plots of the dependence of the density of states on frequency for different values of $\omega_0$ and fixed values of $K$. Here one can observe the placing of the peak of $\rho(\omega)$ as function of $\omega_0$. 
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