Finite Temperature Spectral Function of Mott Insulators and Charge Density Wave States

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We calculate the low-temperature spectral function of one-dimensional incommensurate charge density wave states and half filled Mott insulators. At $T = 0$ there are two dispersing features associated with the spin and charge degrees of freedom, respectively. We show that already at very low temperatures (compared to the gap) one of these features gets severely damped. We comment on implications of this result for photoemission experiments.

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The determination of the finite temperature single-electron Green's function in strongly interacting one-dimensional (1D) electron systems with a spectral gap is a problem of significant interest as the spectral function $A(\omega, q)$ is expected to exhibit the celebrated property of spin-charge separation. Rather than a single coherent quasiparticle peak, one expects to see two broad features in $A(\omega, q)$, which are associated with the independent dispersion of spin and charge collective modes. This phenomenon also occurs in the case of a 1D metallic Luttinger liquid state. The great advantage of the insulating state is that due to the presence of a gap it is much more robust against the effects of 3D couplings, temperature, or impurities. Hence the chances to observe spin-charge separation by means of angle resolved photoemission spectroscopy (ARPES) are higher in Mott insulators (MI) or charge density wave (CDW) insulators than in metallic systems. Unfortunately it is much more difficult to determine dynamical correlation functions in these states. The very existence of a gap prohibits the application of methods based on conformal field theory such as the Luttinger liquid approach. A further complication is that the gap is dynamically generated, which invalidates mean-field approximations to the problem. In light of these difficulties, $1/N$ expansions have been a method of choice, where N is a large parameter introduced by enlarging the spin rotational symmetry of the Hamiltonian from SU(2) to SU(N).

In this Letter we derive asymptotically exact expressions for the spectral function and the tunneling density of states for incommensurate CDW states and half filled MI in the field theory limit. The reason to treat both cases at once is that the results for the MI can be obtained from those for the CDW state. At $T = 0$ we perform our calculations for general N, which allows us to see how the large-N result progressively loses its accuracy as N decreases and for $N = 2$ no longer reproduces even qualitative features of the solution. We demonstrate that Luttinger's theorem continues to hold despite the absence of a Fermi surface. Finally we consider the effects of temperature in the physically relevant case $N = 2$ by means of a systematic expansion in $\exp(-\Delta/T)$, where Δ is the spectral gap. There has been much previous work on determining the $T = 0$ spectral function of 1D MI and CDW states. In Ref. [1] a conjecture for $A(\omega, q)$ was put forward, which agrees with the result we obtain in the field theory limit by means of an exact, systematic method. Expressions for the spectral function have also been obtained in the limit where the single-particle gap is much larger than the bandwidth [2]. This regime is complementary to the case we address here. Finally there also have been extensive numerical studies on t-J and Hubbard models, e.g., Refs. [3,4].

Incommensurate CDW state.—As a starting point for a microscopic description of the CDW state one may choose a model of noninteracting electrons at some incommensurate band filling, coupled to 1D phonons. Examples are the Su-Schrieffer-Heeger [5] and Holstein [6] Hamiltonians. The electronic low-energy degrees of freedom have momenta close to the Fermi momenta $\pm k_F$. In the low-energy sector the electron operators can therefore be represented as

$$c_{n,\sigma} = \sqrt{a_0}[e^{ik_F x} R_\sigma(x) + e^{-ik_F x} L_\sigma(x)], \tag{1}$$

where a_0 is the lattice spacing, $x = na_0$, and R and L are slowly varying Fermi fields. In three spatial dimensions the presence of an electronic spectral gap would automatically imply the formation of an anomalous average $\langle R^\dagger_\sigma(x) L_\sigma(x)\rangle \neq 0$. In one dimension the average is not formed even at $T = 0$; instead correlation functions of the operator $R^\dagger_\sigma L_\sigma$ decay in a power-law fashion. In the limit of infinite phonon frequency ω_0 the phonons can be integrated out without inducing retardation effects in the resulting effective electron Hamiltonian [7]. The case of large but finite ω_0 can be treated similarly, as long as one is interested only in low energies $\omega \ll \omega_0$ [8]. In this regime the electronic model obtained by integrating over the phonon degrees of freedom is described by the following universal Hamiltonian:

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_s, \tag{2}$$

$$\mathcal{H}_c = \frac{v_c}{16\pi}[K_c^{-1}(\partial_x \Phi_c)^2 + K_c(\partial_x \Theta_c)^2], \tag{3}$$

$$\mathcal{H}_s = \frac{2\pi v_s}{3}[:J^a J^a: + :\bar{J}^a \bar{J}^a:] + v_s g J^a \bar{J}^a. \quad (4)$$

Here Φ_c is a canonical Bose field, Θ_c is its dual field, and $J^a = L^\dagger_\sigma \tau^a_{\sigma\sigma'} L_{\sigma'}$, $\bar{J}^a = R^\dagger_\sigma \tau^a_{\sigma\sigma'} R_{\sigma'}$ are current operators satisfying the level-1 SU(2) Kac-Moody algebra. The parameters $v_{c,s}$ (charge and spin velocities), Δ (spin gap), and K_c (Luttinger liquid parameter) depend on the details of the underlying microscopic lattice model and, in particular, on ω_0. The parameter K_c controls the scaling dimensions in the charge sector.

Half filled MI.—The Hamiltonian (2)–(4) is identical to the low-energy theory for a half filled MI like the Hubbard model, provided we interchange charge and spin sectors $c \leftrightarrow s$ and then set $K_s = 1$, $k_F = \pi/2$. Below we present results for the more general CDW case with the understanding that the corresponding results for the MI are obtained by the aforementioned mapping.

Zero temperature.—The model (2)–(4) is generalized to SU(N) by replacing the currents in (4) by their SU(N) analogs. The spectrum in the charge sector is gapless $E_c(k) = v_c|k|$, whereas the spectrum in the spin sector consists of scattering states of electrically neutral, massive solitons with dispersion $E_s(k) = \sqrt{\Delta^2 + (v_s k)^2}$ and their bound states for $N > 2$; the presence of bound states does not affect the results presented here. For small $g \ll 1$ we have $\Delta = Dg^{1/N} e^{-2\pi/Ng}$, where $D \sim \omega_0$ is the ultraviolet cutoff. The electron operators can be expressed as products of (vertex) operators acting in the charge and spin sectors, respectively,

$$\langle L_\sigma(\tau, x) L^\dagger_\sigma(0)\rangle = \prod_{\alpha=c,s} \langle \mathcal{O}_\alpha(\tau, x) \mathcal{O}^\dagger_\alpha(0)\rangle. \quad (5)$$

Using the results of [9,10] we obtain the following result for the asymptotics of the single-particle Green's function at zero temperature:

$$G(\tau, x) = e^{-ik_F x} G_R(\tau, x) + e^{ik_F x} G_L(\tau, x), \quad (6)$$

$$G_L(\tau, x) \simeq \frac{Z_N \Delta}{\sqrt{\pi v_s v_c} 2\pi} \left[\frac{2v_c/\Delta}{(v_c\tau + ix)}\right]^{1/N} \left[\frac{(2v_c/\Delta)^2}{x^2 + v_c^2\tau^2}\right]^{\theta/2} \times \left(\frac{v_s\tau - ix}{v_s\tau + ix}\right)^{[(N-1)/(2N)]} K_{1-(1/N)}(\Delta r), \quad (7)$$

where $r = \sqrt{\tau^2 + x^2 v_s^{-2}}$, Z_N is a nonuniversal constant, and $\theta = (1/2N)[K_c + (1/K_c) - 2]$. We note that $G_R(\tau, x) = G_L(\tau, -x)$. Equation (7) is derived by taking into account processes with emission of an arbitrary number of charge excitations and *only one* massive spin excitation. The corrections to (7) are of order $\mathcal{O}(e^{-3\Delta r})$ for $N = 2$. However, due to the fact that matrix elements corresponding to the emission of multisoliton states are numerically small, the accuracy achieved by this approximation is very good. The smallness of matrix elements also allows us to generalize our calculations to finite T. In the case of equal velocities $v_s = v_c = v$ the retarded Green's function at $T = 0$ for right moving fermions is

$$G_R(\omega, k_F + q) = \frac{Z_N}{\pi^{1/2}} \Gamma\left(1 - \frac{\theta}{2}\right) \Gamma\left(2 - \frac{1}{N} - \frac{\theta}{2}\right) \frac{\omega + vq}{\Delta^2} \times F\left(1 - \frac{\theta}{2}, 2 - \frac{1}{N} - \frac{\theta}{2}, 2; \frac{s^2}{\Delta^2}\right), \quad (8)$$

where F is a hypergeometric function and $s^2 = \omega^2 - (vq)^2$. As might be expected, the gap in the spectral function is "clean," i.e., $A_R(\omega, k_F + q) = -\text{Im}G_R(\omega, k_F + q)/\pi$ vanishes for $|\omega| \le \sqrt{\Delta^2 + v^2 q^2}$. The zero temperature tunneling density of states is

$$\rho(\omega) \simeq A_N \int_0^{\text{arccosh}(\omega/\Delta)} dx \frac{\cosh(x[1 - 1/N])}{(\omega/\Delta - \cosh x)^{1-\theta-1/N}}, \quad (9)$$

where $A_N = (Z_N 2^{1+(1/N)+\theta})[\sqrt{\pi v_s v_c}\Gamma(\Theta + 1/N)]^{-1}$. We see that at $T = 0$, $\rho(\omega)$ vanishes inside the gap. The singularity just above the threshold $[0 < (\omega/\Delta) - 1 \ll 1]$ is

$$\rho(\omega) \simeq \frac{A_N B(\theta + \frac{1}{N}, \frac{1}{2})}{\sqrt{2}} (\omega/\Delta - 1)^{\theta+(1/N)-(1/2)}. \quad (10)$$

We note that for the physical case $N = 2$ the "asymptotic" result (10) is actually equal to (9). According to (10) the behavior of $\rho(\omega)$ above the gap is determined by the scaling exponent $1/2 - 1/N + \theta$. The nonuniversal part θ is small for large phonon frequencies. On the other hand, the remaining part is determined only by the Lorentz spin of the spinon creation operator and therefore is universal. Equations (9) and (10) show that a $1/N$ expansion fails completely in the physically relevant case $N = 2$, where the tunneling density of states experiences a qualitative change and becomes nonsingular at the threshold. As we have alluded to earlier, the $N \to \infty$ limit agrees with the mean-field results of Ref. [11].

Luttinger's theorem.—The Green's function (8) has branch cuts, but no poles. In particular, there are no poles at zero frequency and thus no Fermi surface. Nevertheless Luttinger's theorem as stated in Ref. [12] is fulfilled since the logarithm of the Green's function $\ln G(\omega = 0, k_F + p)$ is still singular at the noninteracting Fermi surface, because the Green's function (8) has *zeroes*. This property follows from (i) the fact that the charge sector is gapless, which implies that $\langle R_\sigma(\tau, x) L^\dagger_\sigma(0)\rangle = 0$ and (ii) Lorentz invariance of the low-energy effective theory, which implies that

$$\langle \Psi_\sigma(\tau, x) \Psi^\dagger_\sigma(0)\rangle \sim \exp(\pm i\phi)\mathcal{R}(r); \qquad \Psi = R, L. \quad (11)$$

Here r and ϕ are polar coordinates and $\mathcal{R}$ denotes the radial part of the correlation function. As we are dealing with an insulating state we have $\mathcal{R}(r) \propto \exp(-\Delta r)$ at large distances and hence $\int dr \mathcal{R}(r) r$ is finite. Thus

$$G_{R,L}(0, 0) = \int_{-\pi}^{\pi} d\phi \exp(\pm i\phi) \int dr \mathcal{R}(r) r = 0. \quad (12)$$

For a metallic state the r integral would diverge and the

Green's function would have a singularity rather than a zero.

Finite temperature.—Let us now turn to the general case $v_c \neq v_s$ and finite temperatures. We will restrict the discussion to $N = 2$. The spectral function is conveniently expressed as a convolution

$$A_R(\omega, k_F + q) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} d\omega' dq' \tilde{g}_s(\omega', q')[\tilde{g}_c(\omega - \omega', q - q') + \tilde{g}_c(-\omega - \omega', -q - q')], \quad (13)$$

where $\tilde{g}_{c,s}(\omega, q)$ are the Fourier transforms of the finite temperature correlators $\langle \mathcal{O}_{c,s}(x, t)\mathcal{O}^\dagger_{c,s}(0, 0)\rangle_T$. In the charge sector we can use the standard conformal mapping to obtain (see, e.g., [13])

$$\tilde{g}_c(\omega, q) = C(T) f\left(\frac{\omega + v_c q}{2\pi T}, \frac{1+\theta}{2}\right) f\left(\frac{\omega - v_c q}{2\pi T}, \frac{\theta}{2}\right), \qquad f(\alpha, \gamma) = \mathrm{Re}\left[(-2i)^\gamma B\left(\frac{\gamma - i\alpha}{2}, 1 - \gamma\right)\right], \quad (14)$$

where $C(T) = (v_c/2\pi^3)^{1/2}(2\pi/\Delta)^\theta T^{\theta - 3/2}$ and $B(x, y)$ is the Euler beta function. The correlation function in the spin sector can be determined by using exact results for the SU(2) Thirring model. We invoke a spectral representation in terms of scattering states of solitons and antisolitons, constructed by means of the Zamolodchikov-Faddeev algebra (see, e.g., Ref. [14]). We introduce an index $\epsilon = \pm$ for solitons and antisolitons, respectively, and parametrize energy and momentum by a rapidity variable θ in the usual way as $E(\theta) = \Delta \cosh\theta$, $P(\theta) = (\Delta/v_s)\sinh\theta$. In a basis of scattering states $|\theta_n \cdots \theta_1\rangle_{\epsilon_n \cdots \epsilon_1}$ of solitons and antisolitons with rapidities θ_j the following spectral representation for thermal two-point functions holds

$$\langle \mathcal{O}^\dagger(\omega, q)\mathcal{O}(-\omega, -q)\rangle_T = \sum_{n,\{\epsilon_j\}} \frac{1}{n!}\int \prod_{j=1}^n \frac{d\theta_j}{2\pi} \sum_{m,\{\epsilon'_k\}} \frac{1}{m!}\int \prod_{k=1}^m \frac{d\theta_k}{2\pi} |^{\epsilon_1 \cdots \epsilon_n}\langle \theta_1 \cdots \theta_n|\mathcal{O}(0, 0)|\theta'_m \cdots \theta'_1\rangle_{\epsilon'_m \cdots \epsilon'_1}|^2$$
$$\times\ e^{-\sum_{j=1}^n E(\theta_j)/T}(2\pi)^2 \delta\left(\omega - \sum_{j=1}^n E(\theta_j) + \sum_{k=1}^m E(\theta'_k)\right)\delta\left(q - \sum_{j=1}^n P(\theta_j) + \sum_{k=1}^m P(\theta'_k)\right). \quad (15)$$

As was shown recently, the representation (15) is suitable for carrying out a low-temperature expansion ($T \lesssim \Delta$) of correlation functions [15,16]. Taking into account the two leading terms $n = 0$, $m = 1$ and $n = 1$, $m = 0$ in (15) and combining this result with (13) and (14) we obtain

$$A_R(\omega, k_F + q) \approx \mathcal{A}\int_{-\infty}^{\infty} dz e^{z/2}\left[\tilde{g}_c(\omega - c(z), q - s(z)) + e^{-c(z)/T}\tilde{g}_c(\omega + c(z), q + s(z)) + \left\{\begin{matrix}\omega \to -\omega \\ q \to -q\end{matrix}\right\}\right], \quad (16)$$

where $\mathcal{A} = \sqrt{(\pi\Delta/v_s)}[Z_2/(2\pi)^3]$, $c(z) = \Delta\cosh z$, and $s(z) = (\Delta/v_s)\sinh z$. Let us now see how changing θ and T affects $A_R(\omega, q)$. We constrain our discussion to the cases of zero temperature and varying θ and of finite T and fixed θ. As a function of θ, $A_R(\omega, k_F + q)$ displays a strongly varying behavior. For small θ, corresponding to a high phonon frequency, the spectral function is very similar to the one of the half filled MI (see the dotted curves in Fig. 2): there are two sharp, dispersing features associated with the spin and charge degrees of freedom, respectively. For smaller phonon frequencies and concomitantly larger θ these features become less prominent until they eventually disappear altogether. We plot $A_R(\omega, k_F + q)$ at $T = 0$ for the intermediate value $\theta = 0.8$, $v_c = 0.4 v_s$ and several values of q in Fig. 1. We see that the peak associated with v_s is already quite weak. The effects of a small, finite temperature $T = 0.05\Delta$ are shown in Fig. 2 for a half filled MI (we now switch spin and charge sectors as discussed above and set $\theta = 0$, $k_F = \pi/2$). Compared to the $T = 0$ result we find that the holon peak is significantly damped although T is still quite small compared to the low-energy scale Δ. The physical reason for this is very simple: in the MI only the charge sector is protected by the gap, whereas the gapless spin sector is significantly affected by T. This leads to a damping of the peak associated with the charge degrees of freedom, whereas the spinon peak stays rather sharp.

We note that ARPES measurements on 1D cuprate Mott insulators [4] are taken at room temperature in order to avoid charging of the sample. The temperature used in Fig. 2 is chosen to reflect the ratio T/Δ in the experiments

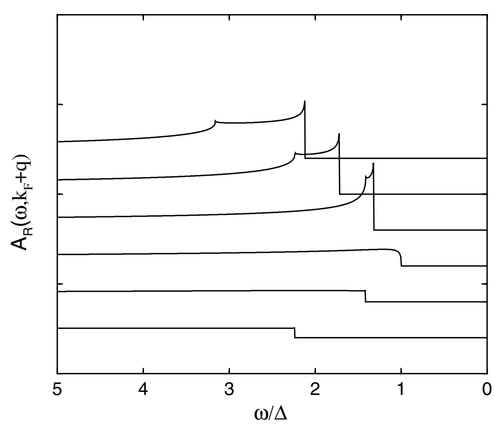

FIG. 1. Spectral function $A_R(\omega, k_F + q)$ at $T = 0$, $\theta = 0.8$, $v_c = 0.4 v_s$ for $v_s q/\Delta = -2, -1, 0, 1, 2$ (from bottom to top). The curves for different values of q have been offset.

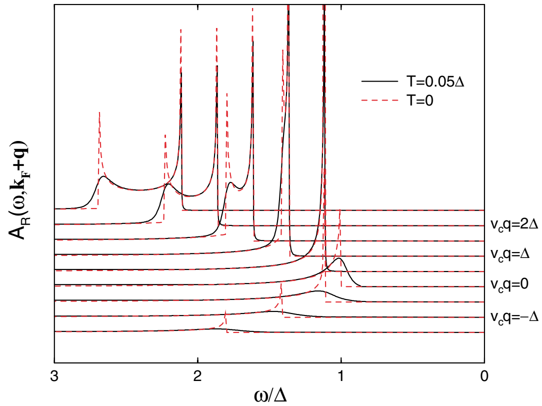

FIG. 2 (color online). Spectral function for a half filled MI ($\theta = 0$, $v_s = 0.5v_c$), $T = 0$ (dotted lines) and $T = 0.05\Delta$ (solid lines) $v_cq/\Delta = -1.5, -1, \ldots, 2.5$ (from bottom to top). The curves for different values of q have been offset.

on Sr_2CuO_3. Although the theory presented here does not describe the 1D cuprate MI quantitatively (U/t is too large in these compounds), we believe that our result gives a strong indication that temperature effects are important and at least partially account for the fact that the holon feature is barely visible in the data. The low-T behavior of the tunneling density of states can be analyzed analogously. We find

$$\rho(\omega) = \int_{-\infty}^{\infty} \frac{dx}{(2\pi)^3} \rho_s(x)\rho_c(\omega - x) + \omega \to -\omega, \quad (17)$$

where

$$\rho_c(x) = D\mathrm{Re}\Big[(-2i)^{\theta+(1/2)} B\Big(\frac{1+2\theta}{4} - i\frac{\omega}{2\pi T}, \frac{1}{2} - \theta\Big)\Big],$$

$$\rho_s(x) \simeq Z_2\sqrt{\frac{\pi}{v_s}}[\theta_H(\omega - \Delta) + e^{-|\omega|/T}\theta_H(-\omega - \Delta)] \times \Bigg[\frac{\sqrt{|\omega| - \sqrt{\omega^2 - \Delta^2}}}{\sqrt{\omega^2 - \Delta^2}} + \frac{\sqrt{|\omega| + \sqrt{\omega^2 - \Delta^2}}}{\sqrt{\omega^2 - \Delta^2}}\Bigg], \quad (18)$$

where $D = (2\pi/\Delta)^\theta (8\pi/v_c)^{1/2} T^{\theta - 1/2}$. In the regime $T \ll \omega \ll \Delta$ we may use contour techniques to extract the leading contribution to (17)

$$\rho(\omega) \approx \frac{Z_2 2^\theta}{\Gamma(\frac{1}{2} + \theta)\sqrt{v_c v_s}} \sqrt{\frac{T}{\Delta - \omega}} e^{-(\Delta - \omega)/T}. \quad (19)$$

This shows that at low temperatures only an exponentially small fraction of spectral weight gets transferred into the gap. In summary, we have calculated the low-temperature spectral function for incommensurate CDW states and half filled Mott insulators in the field theory limit. Luttinger's theorem is shown to hold despite the absence of a Fermi surface. We have studied the effects of temperature on the two dispersing features associated with spin and charge degrees of freedom. We demonstrated that already a small temperature essentially wipes out the holon peak in the half filled Mott insulator.

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