Spectral Function and Self-Energy of the One-Dimensional Hubbard Model in the $U \to \infty$ Limit

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The interpretation of the $k$ dependent spectral functions of the one-dimensional, infinite $U$ Hubbard model obtained by using the factorized wave-function of Ogata and Shiba is revisited. The well-defined feature which appears in addition to low energy features typical of Luttinger liquids, and which, close to the Fermi energy, can be interpreted as the shadow band resulting from $2k_F$ spin fluctuations, is further investigated. A calculation of the self-energy shows that, not too close to the Fermi energy, this feature corresponds to a band, i.e. to a solution of the Dyson equation $\omega - \epsilon(k) - \text{Re} \Sigma(k, \omega) = 0$.

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In the study of systems of interacting electrons, the dynamical correlation functions play a central role because they correspond to the response functions that can be measured in several experiments (infrared reflectivity, inelastic neutron scattering, nuclear magnetic resonance, etc...) The most basic of these correlation functions is the time-ordered Green’s function, which can be defined by its spectral representation according to

$$ G(k, \omega) = \int_{-\infty}^{+\infty} d\omega' \frac{A(k, \omega')}{\omega - \omega' + i\delta} + \int_{-\infty}^{\mu} d\omega' \frac{B(k, \omega')}{\omega - \omega' - i\delta} $$

(1)

The spectral functions $A(k, \omega)$ and $B(k, \omega)$ are defined by

$$ A(k, \omega) = \sum_{f, \sigma} \left| \langle f, N+1 | c_{k, \sigma}^\dagger | 0, N \rangle \right|^2 \delta(\omega - E_f^{N+1} + E_0^N) $$

$$ B(k, \omega) = \sum_{f, \sigma} \left| \langle f, N-1 | c_{k, \sigma} | 0, N \rangle \right|^2 \delta(\omega - E_f^N + E_0^{N-1}) $$

in the standard notation, and in principle they can be measured in angular-resolved inverse photoemission and photoemission experiments, respectively. The effect of electron-electron interactions on the spectral functions of the three-dimensional Coulomb gas has been investigated in much detail several years ago [1]. With respect to the simple $\delta(\omega - \varepsilon_k)$ structure of the non-interacting case, the main differences are: i) A shift of the energy of the quasi-particle band; ii) A broadening of the quasi-particle peak; iii) A renormalization of the weight of the quasi-particle peak, compensated by the appearance of an incoherent background; iv) The presence of another band - a plasmon band - due to the long-range nature of the Coulomb potential. For a short-range repulsion, such as the on-site interaction of the Hubbard model, there is no plasmon band, and the spectral function is expected to have only one well-defined feature, the quasi-particle band, on top of an incoherent background. The validity of this simple picture in lower dimensional systems is currently under intense discussion. In two dimensions (2D), there are at least two important issues: 1. the actual existence of a quasiparticle peak, and 2. the generation by antiferromagnetic short-range fluctuations close to half-filling of additional well-defined features in the spectral functions, called generically “shadow bands” [2]. The absence of exact results in 2D for correlated models makes the interpretation of the experimental results quite difficult. For high-$T_c$ cuprates, these issues are still controversial [3].

In 1D, a number of analytical approaches are available. For instance, models having both charge and spin low-lying excitations belong to the universality class of the Luttinger liquid, and bosonization gives an accurate description of their low-energy properties. The consequence for the spectral functions is that there is no quasi-particle peak but two divergences due to spin-charge separation [4]. A lot of insight has also been obtained by the Bethe ansatz solution of integrable models, the prototype being the Hubbard model defined by:

$$ \mathcal{H} = -t \sum_{i, \sigma} (c_{i, \sigma}^\dagger c_{i+1, \sigma} + h.c.) + U \sum_{i} n_{i, \uparrow} n_{i, \downarrow} $$

(2)

where $c_{i, \sigma}$ and $c_{i, \sigma}$ are electron creation and annihilation operators, and $n_{i, \sigma} = c_{i, \sigma}^\dagger c_{i, \sigma}$ is the density operator. The Bethe ansatz wave-functions are so complicated that it is not possible to use them to calculate correlation functions. However, Ogata and Shiba showed a few years ago that, in the limit $U \to +\infty$, the ground-state wave function can be written as a product of a spinless fermion wave-function $|\psi\rangle$ and a squeezed spin wave-function $|\chi\rangle$, and that this wave function allows a very precise evaluation of the momentum distribution function [3]. More recently, Penc et al. [5] used the same representation for the excited states to calculate the spectral functions $A(k, \omega)$ and $B(k, \omega)$. The results for $n = 1/4$ are shown in Fig. 1.

There are several interesting features to notice. In the low energy region near $k_F$ we can identify three structures. For $k < k_F$ there are maxima at $\omega = u_c(k - k_F)$
and \( \omega \simeq 0 \) and a lot of spectral weight between them. There is also a small weight appearing on the other side of the Fermi energy for \( \omega > -u_s(k - k_F) \). If we remember that the spin velocity \( u_s \) vanishes for the infinite U Hubbard model, all these features are qualitatively consistent with the Luttinger liquid calculations \[6]. The dispersion of the charge part is exactly given by \( E(k) = -2t \cos(|k| + k_F) \).

While there is little doubt that this physical picture is essentially correct, the interpretation should be made more precise in two respects. First of all, the concept of a shadow band is no longer well defined below the energy where the charge part of the main band crosses \( k = 0 \). In fact, if we think in terms of the whole Brillouin zone \((-\pi < k < \pi)\), what we call a shadow-band for \( k > 0 \) is continuously connected to the main band for \( k < 0 \). So what we have called a shadow band is probably better thought of as a band per se which, close to the Fermi level, can be interpreted as a shadow band.

Second, the term band has a precise meaning in the context of perturbation theory. A feature of the spectral function is called a shadow-band if it corresponds to a solution of the Dyson equation \( \omega - \epsilon(k) - \text{Re}\Sigma(k, \omega) = 0 \), where \( \epsilon(k) = -2t \cos k \) is the non-interacting dispersion while the self-energy \( \Sigma(k, \omega) \) is implicitly defined by \( G(k, \omega) = 1/(\omega - \epsilon(k) - \Sigma(k, \omega)) \) and can be obtained from \( G(k, \omega) \) as \( \Sigma(k, \omega) = \omega - \epsilon(k) - G^{-1}(k, \omega) \). For 1D systems, the perturbation expansion diverges notoriously, and, even for small \( U/t \), \( \Sigma(k, \omega) \) cannot be calculated perturbatively. However, having obtained \( A(k, \omega) \) and \( B(k, \omega) \) in an essentially exact way, we can use Eq. (1) to calculate the time ordered Green’s function, and from it the self-energy. The results for the real part and the imaginary part of the self-energy for \( k = \pi/3 \) and \( k = 2\pi/3 \) are shown in Fig. 2.

To discuss the relationship between the spectral functions and the self-energy, it is useful to write \( A(k, \omega) \) and \( B(k, \omega) \) in terms of \( \Sigma(k, \omega) \) as

\[
A(k, \omega) = \pi^{-1} \frac{-\text{Im}\Sigma(k, \omega)}{\omega - \epsilon(k) - \text{Re}\Sigma(k, \omega)^2 + (\text{Im}\Sigma(k, \omega))^2}
\]

\[
B(k, \omega) = \pi^{-1} \frac{\text{Im}\Sigma(k, \omega)}{\omega - \epsilon(k) - \text{Re}\Sigma(k, \omega)^2 + (\text{Im}\Sigma(k, \omega))^2}
\]

Let us start with \( k = 2\pi/3 \). As for a non-interacting system, the Dyson equation has only one solution corresponding to the intersection of the straight line with the real part of \( \Sigma(k, \omega) \). This corresponds to the charge part of the main excitation band. The spin part, which is pinned at the Fermi energy in the present case, corresponds to a vertical slope at \( \omega = 0^+ \) in the imaginary part of the self-energy, as well as in the spectral function \( A(k, \omega) \). The “shadow” band, which appears at negative energies for that wave-vector, does not correspond to a solution of the Dyson equation, but to a maximum of the imaginary part that occurs in a region where \( \omega - \epsilon(k) - \text{Re}\Sigma(k, \omega) \) is large, so that the denominator of \( A(k, \omega) \) is dominated by \( (\omega - \epsilon(k) - \text{Re}\Sigma(k, \omega))^2 \).

For \( k = 2\pi/3 \), there are three solutions to the Dyson equation. As in the previous case, the solution for positive \( \omega \) corresponds to the charge part of the main band, and the spin part also gives rise to a singularity at \( \omega = 0^+ \). For negative frequencies, the situation is very similar to that of the plasmon band of the 3D Coulomb gas \[5\]. Decreasing \( \omega \) starting from the Fermi energy, the first solution of the Dyson equation coincides with

![Graph](image-url)
a maximum of $\text{Im} \Sigma(k, \omega)$ and does not give rise to any feature in the spectral function. On the contrary, the other solution occurs in a region where $\text{Im} \Sigma(k, \omega)$ is not particularly big. This solution gives rise to a feature in the spectral function that corresponds to what we have called the “shadow” band.

Coming back to the second point raised above, we see that the feature that crosses the Fermi energy at $3k_F$ corresponds to a band, i.e. to a solution of the Dyson equation, only far enough from the Fermi level. In that case however it can’t really be interpreted as a “shadow” band because it cannot be connected to the main band by a vector $2k_F$. Close enough to the Fermi energy, this feature can really be thought of as a shadow of the main band because it really follows the charge part of the main band at a distance $2k_F$ apart. However, this feature does not correspond any more to a solution of the Dyson equation, and strictly speaking, it should not be called a band.

To summarize, this work is the first attempt at using the self-energy to interpret the spectral functions of the Hubbard model that have been obtained in an essentially exact way in the $U \to +\infty$ limit. Extracting the self-energy from the spectral functions numerically has already allowed us to draw an interesting conclusion concerning the origin of the feature that was previously interpreted as a shadow band, namely that this feature only corresponds to a solution of the Dyson equation far enough from the Fermi level. The next step, a detailed analysis of the behaviour of the self-energy close to $(\omega = 0, k = k_F, 3k_F)$, is in progress. It might help clarify the still controversial problem of the spectral function in 2D in the presence of almost perfect nesting.

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[1] L. Hedin and S. Lundqvist, Solid State Physics 23, 1 (Academic, New York, 1969).
[2] A. P. Kampf and J. R. Schrieffer, Phys. Rev. B 42, 7967 (1990).
[3] For recent developments in 2D, see S. Haas, A. Moreo and E. Dagotto, Phys. Rev. Lett. 74, 310 (1995); R. Preuss, W. Hanke, W. von der Linden, Phys. Rev. Lett. 75, 1344 (1995); A. Chubukov, Phys. Rev. B 52, R3840 (1995); M. Langer, J. Schmalian, S. Grabowski, K. H. Bennemann, Phys. Rev. Lett. 75, 4508 (1995); J. Schmalian, M. Langer, S. Grabowski, K. H. Bennemann, Phys. Rev. B 54, 4336 (1996); D. Duffy and A. Moreo, Phys. Rev. B 52, 15607 (1995).
[4] V. Meden and K. Schönhammer, Phys. Rev. B 46, 15753 (1992); K. Schönhammer and V. Meden, ibid. 47, 16205 (1993); J. Voit, ibid. 47, 6740 (1993).
[5] M. Ogata and H. Shiba, Phys. Rev. B 41, 2326 (1990); M. Ogata, T. Sugiyama and H. Shiba, ibid. 43, 8401 (1991).
[6] K. Penc, F. Mila, H. Shiba, Phys. Rev. Lett. 75, 894 (1995).
[7] K. Penc, K. Hallberg, F. Mila, H. Shiba, Phys. Rev. Lett. 77, 1390 (1996).
[8] S. Haas and E. Dagotto, Phys. Rev. B 52, R14396 (1995).
[9] J. Favand, S. Haas, K. Penc, F. Mila and E. Dagotto, Phys. Rev. B, Rapid Comm., in press.

FIG. 2. Frequency dependence of the spectral functions and of the real and imaginary parts of the self-energy of the quarter-filled, $U \to +\infty$ Hubbard model for selected values of the momentum. The straight line corresponds to $\omega - \epsilon(k)$. a) $k = \pi/3$; b) $k = 2\pi/3$. 

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