Friedel oscillations of density of states in a one-dimensional Mott insulator and incommensurate charge-density wave or superconductor

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Oscillations of local density of states generated by a single scalar impurity potential are calculated for one-dimensional systems with dynamically generated charge or spin gap. At zero temperature, the oscillations develop at finite wave vector (π for the Mott insulator and $2k_F$ for incommensurate charge-density wave or superconductor) and at frequencies larger than the soliton spectral gap m. Their amplitude has a broad maximum at $\omega \approx 3m$, where m is the gap magnitude.

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Modern single electron tunneling microscopy (STM) techniques provide a plephora of data by measuring minute details of coordinate dependence of the differential conductance $\sigma(\mathbf{x})=dI/dV$. An especially rich picture emerges in the presence of impurities which create Friedel oscillations in $\sigma(\mathbf{x})$. An ultimate goal for a theory is to decipher the interference pattern of these oscillations and extract from it information about the spectrum and interactions in the underlying system. Since the conductance is directly related to the single electron density of states (DOS), theory should aim at calculation of this quantity,

$$\sigma(V,\mathbf{x}) = C(\mathbf{x})\rho(\omega = eV,\mathbf{x}),$$

$$\rho(\omega,\mathbf{x}) = \frac{1}{\pi}\,\mathrm{Im}\, G^{(R)}(\omega;\mathbf{x},\mathbf{x}), \tag{1}$$

where $C(\mathbf{x})$ is an *a priori* unknown matrix element.

In majority of systems studied by now by STM, the disorder is sufficiently weak for momentum to remain a good quantum number. For instance, observing sharp peaks in the Fourier images of the STM measurements in high-T_c superconductors, like in Ref. 1, one may only conclude that the impurities are sufficiently far apart so that the Friedel oscillations from different impurities have room to develop without quenching each other. Therefore, a reasonable starting point for the theory would be to study the Friedel oscillations of DOS from a single impurity. For a d-wave superconductor, this was done in Ref. 2 using BCS theory combined with a T-matrix approximation. The results are now widely used for the analysis of STM experiments on high-T_c superconductors giving very reasonable answers for the quasiparticle spectrum not far from the nodal points. Needless to say that since the calculation is based on a picture of well-defined weakly interacting quasiparticles, it cannot hold close to the antinodal point where the STM measurements also yield very rich structure[3] which requires a careful analysis.

In general, Friedel oscillations of DOS are not very simple phenomenon and allow a straightforward interpretation only when there are well-defined quasiparticles in the system. In the first order of perturbation theory in the impurity potential V, one has

$$\delta\rho(\omega;\mathbf{r}-\mathbf{r}_0) = \sum_n \frac{e^{-\beta E_n} + e^{-\beta E_m}}{Z}\,\delta(\omega + E_n - E_m)(A_{nm} + B_{nm}), \tag{2}$$

$$A_{nm} = \sum_{m\neq k}\left\{\frac{\exp[i\mathbf{P}_{mk}(\mathbf{r}-\mathbf{r}_0)]}{E_m - E_k}\langle k|V(0)|m\rangle\langle m|\hat{\psi}^+(0)|n\rangle \times\langle n|\hat{\psi}(0)|k\rangle + \text{c.c.}\right\},$$

$$B_{nm} = \sum_{k\neq n}\left\{\frac{\exp[i\mathbf{P}_{nk}(\mathbf{r}-\mathbf{r}_0)]}{E_n - E_k}\langle n|V(0)|k\rangle\langle k|\hat{\psi}(0)|m\rangle \times\langle m|\hat{\psi}^+(0)|n\rangle + \text{c.c.}\right\}, \tag{3}$$

where Z is the partition function, $|n\rangle$, $|m\rangle$, $|k\rangle$, $E_{n,m,k}$, and $\mathbf{P}_{n,m,k}$ are eigenfunctions and energy and momentum eigenvalues of the many-body Hamiltonian governing the system. $\hat{\psi}^+$, $\hat{\psi}$ are electron creation and annihilation operators. All operators are taken at the same spatial point 0. As follows from these expressions, the relation between the Friedel oscillations and the excitation spectrum is not that straightforward. The situation is simplified only at small temperatures and when the many-body states in question can be approximated as quasiparticle ones. To see that, let us consider $\omega > 0$. At $\beta^{-1} \equiv T = 0$, $|n\rangle = |0\rangle$ is the ground state and $E_m = \omega$. Taking the Fourier transform of Eq. (2) in real space, one fixes $\mathbf{P}_{km}$ to be the external wave vector. Fixing $\mathbf{P}_{km}$ may fix E_k and lead to singularity in the Friedel oscillation amplitude but only in one dimension and only if the eigenenergies in question belong to quasiparticles. In $D>1$, equation $E_m = \omega$ determines a surface in momentum space and the singularity is smeared by integration along this surface. In the same way, the singularities are weakened when the eigenenergies $E_{n,k}$ belong to the continuum of states which cannot be parametrized by a single momentum. Therefore, one is driven to the conclusion that in order to decipher the interference pattern, concrete and model dependent expressions for DOS are necessary.

In this Brief Report, I describe Friedel oscillations of local DOS for two strongly correlated systems—one-dimensional

Mott insulator and one-dimensional incommensurate charge-density wave (ICDW) or superconductor. The motivation behind the calculations is twofold. First, these are strongly correlated systems which require nonperturbative approach. Nonperturbative results in this area predominantly concern Tomonaga-Luttinger liquids (see Ref. 4). In the systems of choice where spectral gaps are generated dynamically and the long lange order is destroyed by gapless fluctuations, the only available result is Ref. 5. Second, in my previous publication with Tsvelik and Chubukov,[6] we suggested that the dynamics of the antinodal regions in high-T_c superconductors is essentially one dimensional. Therefore, these calculations may be even relevant to the high-T_c problem after all.

I will study the case when the spectral gap (be it the charge gap in the Mott insulator or the spin gap in ICDW or superconductor) is small compared to the bandwidth. The chemical potential is in the middle of the gap. The relative smallness of the gap enables me to employ field theory methods and bosonization. These methods together with the background information on the models in question are described in many review articles and books, in particular, in Ref. 7. In the continuum limit, both the Mott insulator and ICDW or superconductor (SC) are described by a universal Hamiltonian. The corresponding Hamiltonian density is a sum of two commuting parts governing dynamics of the charge and the spin collective modes. For the Mott insulator, we have

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_s, \tag{4}$$

$$\mathcal{H}_c = \frac{v_c}{2}[K_c(\partial_x\theta_c)^2 + K_c^{-1}(\partial_x\phi_c)^2] - \mu\cos(\sqrt{8\pi}\phi_c), \tag{5}$$

$$\mathcal{H}_s = \frac{v_s}{2}[K_s(\partial_x\theta_s)^2 + K_s^{-1}(\partial_x\phi_s)^2], \tag{6}$$

where $K_c<1$, K_s and v_c, v_s are the Luttinger parameters and the velocities in the charge and spin sector, respectively, and $\mu>0$ is the coupling constant. Fields ϕ_a, θ_a obey the standard commutation relations

$$[\theta_a(x), \phi_b(y)] = -i\delta_{ab}\Theta_H(x-y), \tag{7}$$

where $\Theta_H(x)$ is the Heaviside function. For ICDW/SC, one has to interchange charge and spin indices. Then, K_s becomes the Luttinger parameter in the charge channel. For $1/2<K_s<2$, both $2k_F$ charge susceptibility and pairing susceptibility are singular at zero frequency and temperature, diverging as

$$\chi(2k_F, \omega=0) \sim T^{-2+K_s}, \quad \chi_{pair}(\omega=0) \sim T^{-2+1/K_s}. \tag{8}$$

What order will eventually emerge when such one-dimensional systems are coupled together depends on whether K_s is greater or smaller than 1 and to some extent on the strength of the interchain interactions. Since both CDW and SC channels are singular, I do not distinguish between the two and label the model ICDW/SC. However, to avoid confusion from now on, I will discuss only the Mott insulator reserving the ICDW/SC system for the final discussion.

Model (5) is the sine-Gordon model; it is well studied and plenty of exact results are available, including results for its correlation functions. At $K_c<1$, the spectrum has gap(s). The excitations always include solitons and antisolitons carrying electric charge $\pm e$ (for ICDW, it would be spin 1/2) and for $K_c<1/2$ also their neutral bound states (excitons). The asymptotics of the single electron Green's function is dominated by single soliton emission processes.[9]

All spectral gaps are of the same order. The Mott gap is

$$m \sim \Lambda(\mu/\Lambda)^{1/2(1-K_c)}, \tag{9}$$

where Λ is the ultraviolet cutoff and is probably of order of the bandwidth.

For a clean Mott insulator, DOS is featureless (apart from the spectral gap) and is given by [see Eqs. (9) and (10) for $N=2$ in Ref. 10]

$$\rho(\omega) \sim (|\omega|-m)^{2\gamma}, \quad \gamma = \frac{1}{4}(\sqrt{K_s} - 1/\sqrt{K_s})^2. \tag{10}$$

This is in contrast with the band insulator; for Mott insulator with spin 1/2 electrons, quantum fluctuations wipe out the singularity at the gap. We will see that impurities change this, strongly enhancing the amplitude of Friedel oscillations at frequencies of order of m.

Let us consider a single nonmagnetic impurity coupled to the total density operator and placed at point x_0. The most relevant contribution to the Hamiltonian density comes from the backward scattering and is described by the operator

$$V = U(2k_F)\cos[\sqrt{2\pi}\phi_c(x_0)]\cos[\sqrt{2\pi}\phi_s(x_0)], \tag{11}$$

where $U(2k_F)$ is proportional to the matrix element of the impurity potential. In what follows, I will replace $\cos(\sqrt{2\pi}\phi_c)$ by its vacuum expectation value. By doing so, I neglect scattering of the massive solitons on fluctuations of the potential. It is justified that when the bare scattering potential is weak, $U(2k_F) \ll \Lambda$. The alternative approach taken in Ref. 5 was to replace the entire potential [Eq. (11)] by a solid wall which is fine if the bare impurity scattering is close to the unitary limit and, in my opinion, substantially overestimates the contribution from such scattering when the potential is weak. After the above replacement, the impurity scattering acts only in the spin sector where we have the boundary sine-Gordon problem,

$$\mathcal{H}_s = \frac{v_s}{2}[K_s(\partial_x\theta_s)^2 + K_s^{-1}(\partial_x\phi_s)^2] - \lambda\delta(x-x_0)\cos[\sqrt{2\pi}\phi_s(x_0)], \tag{12}$$

where $\lambda = U(2k_F)\langle\cos[\sqrt{2\pi}\phi_c]\rangle \sim U(2k_F)(m/\Lambda)^{K_c/2}$. This model is exactly solvable[11] and at the particular value of the coupling, $K_s=1$ can be even reduced to the model of free fermions.[12] Another free fermion point (a trivial one) is $K_s=2$. However, calculation of correlation functions of bosonic exponents is not an easy problem and in its entirety has not yet been solved, even at $K_s=1$. Some help comes from the fact that at $K_s<2$, the impurity scattering potential scales to strong coupling and below the energy scale,

$$E^* \sim \Lambda(\lambda/\Lambda)^{2/(2-K_s)} \tag{13}$$

can be replaced by the Dirichlet condition

$$\phi_s(x_0) = 0. \tag{14}$$

This gives an easy way to calculate asymptotics of the correlation functions of the bosonic exponents using the method of images. In order to get a feeling for the magnitude of errors originating from deviations from the asymptotic regime, we will consider Friedel oscillations of the particle density

$$\langle \rho(x) - \rho_0 \rangle = \langle \cos(2k_F x + \sqrt{2\pi}\phi_c)\cos(\sqrt{2\pi}\phi_s)\rangle \approx \cos(2k_F x) m^{K_c/2} \langle \cos[\sqrt{2\pi}\phi_s(x)]\rangle, \tag{15}$$

where the charge cosine was replaced by its vacuum expectation value. At $K_s=1$, the average in the right hand side of Eq. (15) was calculated in Ref. 13 [see Eq. (3.12)]. Taking the Fourier transform of this formula, we obtain

$$\langle \rho(2k_F + q)\rangle \sim \frac{(1+\sqrt{1+(E^*/q)^2})^{1/2}}{\sqrt{q^2+E^{*2}}}. \tag{16}$$

One can check that a relative deviation of this function from its low-q asymptotic value $|q|^{-1/2}$ exceeds 20% only at $(q/E^*) > 2.5$.

Now, let us come back to our original task: calculation of oscillations of DOS. The bosonized expression for the fermionic operator is

$$\psi_\sigma(x) = e^{-ik_F x} R_\sigma(x) + e^{ik_F x} L_\sigma(x), \tag{17}$$

$$R_\sigma = \frac{\eta_\sigma}{\pi a_0} e^{i\sqrt{\pi/2}(\phi_c+\theta_c)} e^{\sigma i\sqrt{\pi/2}(\phi_s+\theta_s)},$$

$$L_\sigma = \frac{\eta_\sigma}{\pi a_0} e^{i\sqrt{\pi/2}(-\phi_c+\theta_c)} e^{\sigma i\sqrt{\pi/2}(-\phi_s+\theta_s)}, \tag{18}$$

where η_σ are the Majorana zero modes (Klein factors), a_0 is the lattice constant, and $\sigma = \pm 1$.

The single-particle density of states is related to the single-particle Green's function at coinciding spatial points,

$$G(\tau;x,x) = G_{smooth} + G_{oscil}, \tag{19}$$

$$G_{smooth} = \langle\langle R(\tau,x)R^+(0,x)\rangle\rangle + \langle\langle L(\tau,x)L^+(0,x)\rangle\rangle, \tag{20}$$

$$G_{oscil} = [e^{2ik_F x}\langle\langle L^+(\tau,x)R(0,x)\rangle\rangle + \text{H.c.}], \tag{21}$$

where τ is Matsubara time. Let the reader note that $G_{oscil} = 0$ in a clean sample.

The operators R, L and their Hermitian conjugate factorize into charge and spin parts [Eq. (18)] governed by different Hamiltonians [Eqs. (5) and (12)], respectively. Since the impurity contributes mostly to the spin Hamiltonian, for the charge sector, one can use the results obtained in Ref. 8. Then, for the oscillatory oscillatory part [Eq. (21)] of the Green's function, we obtain

$$G_{oscil} = \alpha m^{1/2} K_0(m\tau) S(\tau, x - x_0), \tag{22}$$

$$S(\tau, x - x_0) = [e^{2ik_F x}\langle\langle e^{i\sqrt{\pi/2}(\phi_s+\theta_s)(\tau,x)} e^{i\sqrt{\pi/2}(\phi_s-\theta_s)(0,x)}\rangle\rangle + \text{c.c.}], \tag{23}$$

where α is a numerical coefficient. The K_0 function in Eq. (22) comes from the charge sector (the corresponding correlator was calculated in Ref. 8). Therefore, the fact that in the clean system object (21) vanishes altogether is due to the spin sector remaining critical. The latter means that its right and left sectors do not couple to each other and $S=0$. The scattering from the impurity connects the right and left sectors and $S(\tau,x)$ [Eq. (23)] is no longer zero. Thus, impurities reveal the parity violation which exists in the Mott insulator already in the clean case but is not directly observable for a lack of a suitable local operator.

Function (23) can be represented as

$$S(\tau,x) = \frac{1}{|x|^{2d}} \mathcal{F}\left(\frac{v_s\tau}{x}, xE^*/v_s\right), \tag{24}$$

where $d=(K+1/K)/8$ and $\mathcal{F}(y,z)$ is a scaling function. In the strong coupling limit (that is, at the distances or times much larger than $1/[E^*]$), the impurity is substituted by condition (14). This condition is equivalent to the conditions

$$\phi_s(x - x_0) = -\phi_s(x_0 - x), \quad \theta_s(x - x_0) = \theta(x_0 - x). \tag{25}$$

Then, correlation functions of bosonic exponents are calculated by the method of images, like in electrostatics. As a result in the strong coupling limit, we obtain universal (that is, independent of the bare impurity potential) asymptotics

$$G_{smooth} = \frac{Ze^{-m|\tau|}}{2\pi\tau}|\tau|^{-\gamma}\left[1 + \frac{(\tau v_s)^2}{4(x-x_0)^2}\right]^{K_s/16}, \tag{26}$$

$$G_{oscil} = \alpha\cos[2k_F(x-x_0)] \times \frac{m^{1/2}K_0(m\tau)|\tau|^{(K_s-1/K_s)/4}}{|(x-x_0)/v_s|^{K_s/4}[\tau^2 + 4(x-x_0)^2/v_s^2]^{K_s/8}}, \tag{27}$$

where factor Z was calculated in Ref. 9 and $\alpha \sim 1$. We perform a double Fourier transformation of Eq. (27), both in space and Matsubara time, and then perform the necessary analytic continuation $i\omega \to \omega + i0$. The answer can be written as

$$\delta\rho(\omega > 0; 2k_F + q) \sim |q|^{-1+K_s/2} \times \int_0^{2(\omega-m)/v_s|q|} dy A(\omega - y|q|v_s/2) f(y), \tag{28}$$

$$f(y) = \int_{-y}^{y} dz (y^2 - z^2)^{-1+K_s/8} |1+z|^{-1+K_s/4}. \tag{29}$$

Here,

$$A(\omega) = [(\omega/m)^2 - 1]^{-1/2-a}(\omega/m)^{a/2} F[-a/2, 1/2 - a/2; 1/2 - a; 1 - (m/\omega)^2], \tag{30}$$

where $a=(K_s - 1/K_s)/4$ and $F(a,b;c;x)$ is the hypergeometric function. Numerical evaluation of these integrals shows that that at $1/2 < K_s < 2$, the Friedel oscillations do not disperse and can be approximated by

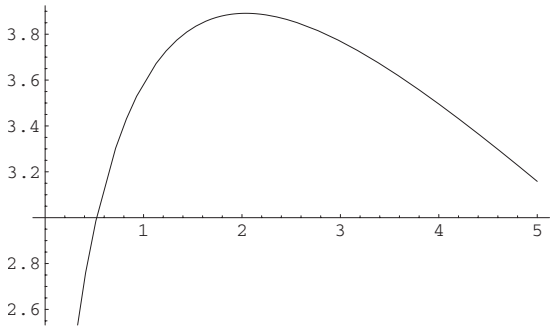

FIG. 1. Function $\mathcal{G}(x;1)$.

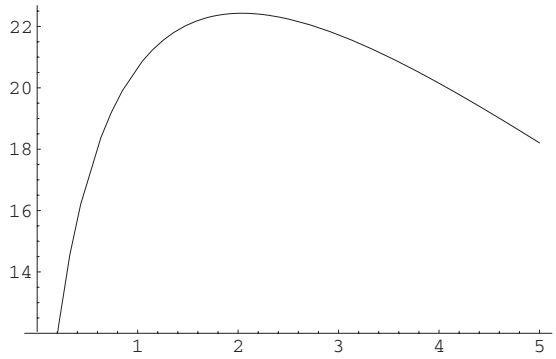

FIG. 2. Function $\mathcal{G}(x;2)$.

$$\delta\rho(\omega, q + 2k_F) \sim |q|^{-2+K_s/2}\mathcal{G}(\omega/m - 1; K_s), \qquad (31)$$

where function $\mathcal{G}(x;K_s)$ is depicted on Figs. 1 and 2 for $K_s = 1, 2$.

Thus, we have found that impurities in 1D Mott insulator (or ICDW or SC) produce $2k_F$ Friedel oscillations of DOS. These oscillations occur at frequencies larger than the Mott gap (the soliton gap) and at $T=0$ their amplitude has a maximum at $\omega \approx 3m$ and a strong singularity at $2k_F$. Near the singularity, the Fourier transform of the DOS is essentially dispersionless. In our calculations, DOS (including the Friedel oscillations) is even in frequency. This is due to the fact that the electron spectrum is linearized and the chemical potential is exactly in the middle of the gap. The latter feature can be trivially corrected by a chemical potential shift.

For Mott insulator with SU(2) symmetry in the spin sector, $K_s=1$ and $a=0$. For ICDW or SC, spin and charge sectors s and c are interchanged; then, K_s corresponds to the Luttinger parameter in the charge sector and its value is not fixed by any symmetry. The phenomenology developed for the cuprates in Ref. 6 suggests that $K_s \approx 2$. Note that at $K_s = 2$, operator (11) becomes marginal and E^* increases exponentially when the value of K_s approaches 2 from below.

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