Short Range Interaction Effects on the Density of States of Disordered Two Dimensional Crystals with a half–filled band

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The Density of electronic States (DoS) of a two–dimensional square lattice with substitutional impurities is calculated in the presence of short–range electron–electron interactions. In the middle of the energy band, the Bragg reflections off the Brillouin zone boundary are shown to lead to additional quantum corrections to the DoS, the sign of which is opposite to the sign of the Altshuler–Aronov's logarithmic correction. The resulting quantum correction to the DoS at half–filling is positive, i.e. the DoS increases logarithmically as the Fermi energy is approached. However, far from the commensurate points where the Bragg reflections are suppressed, the negative logarithmic corrections to the DoS survive.

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The competition of the effects of interaction and randomness in one–dimensional ($1D$) and two–dimensional ($2D$) electronic systems is one of the most intriguing problems in low temperature physics. Impurities of arbitrary concentration in a $1D$ metal off half–filling have been shown to localise all electronic states of a non–interacting electron gas, [1]. However, the Bragg reflections appearing at half–filling delocalise the states and enhance the density of states (DoS) in the middle of the band, an effect known as 'Dyson singularity', [2,3]. A $1D$ correlated electron gas without disorder is described by the Luttinger liquid theory, [4]. In a half–filled band, charge excitations with gap (Mott insulator) may be relevant in $1D$ systems as a consequence of commensurability, [5], whereas the localization length for coherent propagation of two interacting particles in a $1D$ random electronic system has been shown [6] to be larger than the one–particle localization length, i.e., interaction leads to a significant delocalization of the pair.

The problem of the interplay of interaction and disorder in $2D$ systems is as complicated as it is in $1D$ systems. Indeed, all states of a $2D$ electron gas have been proved to be localized irrespective of how small the impurity concentration is, [7]. Weak Coulomb interactions between electrons moving diffusively in a $2D$ disordered metal away from half–filling have been shown to increase the localization effect, [8–10]. The ground state of a clean $2D$ lattice with nested Fermi surface becomes unstable with respect to formation of antiferromagnetic spin gap under an arbitrarily small Coulomb interaction [11], and developes a Mott gap at strong interactions. Our recent studies of the DoS and of conductivity of a $2D$ electron gas on a lattice with substitutional impurities [12,13] have shown that the commensurability effects at half–filling for the noninteracting case are opposite to those obtained for $1D$ systems, [14–16], so that the impurity scatterings with coherent Bragg reflections have been found to lower the electronic density of states around the Fermi level. Interaction effects in commensurate weakly disordered $2D$ electronic systems have not yet been studied properly. Notice that, the recently observed metal–insulator transition (MIT) in $2D$ electronic systems,which occurs at low temperatures ($\sim T \leq 2K$), [17,18], cannot be explained in the framework of the 'conventional' localization theory and still is one of the puzzling issues of central importance in the physics of disordered systems. Measurements of resistivity in high–mobility Si–MOSFET's show that the insulator behavior at low particle densities, $n < n_c$, crosses over to the metallic one as the particle density n reaches the critical value $n_c = 9,02 \times 10^{10} cm^{-2}$ (for $n > n_c$). The observation of the MIT in $GaAs/AlGaAs$, [19], where e-e interactions are estimated to be weak, shows that the effect of correlations, although crucial, is not the only factor leading to MIT.

In this Letter we study the effect of short–range repulsive interactions on the one–particle DoS of a 2D square lattice with substitutional impurities for half–filled energy band. We will show that a class of quantum corrections to the DoS, negative far from half–filling, changes its sign as the center of the band is approached. Such a behavior of the DoS is similar to that observed for the conductivity $\sigma(T)$ [17–19]. A recent computation of the conductivity in the half–filled Hubbard model with disorder also displays a change in the sign of $d\sigma/dT$ as the system acquires particle–hole symmetry, [20].

The Hamiltonian of interacting electrons in the random field of substitutional impurities can be written in the Bloch–state representation in the following form,

$$\hat{\mathbf{H}} = \sum_{\mathbf{p},\sigma} \epsilon(\mathbf{p}) c^{+}_{\mathbf{p},\sigma} c_{\mathbf{p},\sigma} + \\ + \sum_{\mathbf{p},\mathbf{q},\mathbf{G},\sigma} \rho_{imp}(\mathbf{q}) V_{imp}(\mathbf{q}+\mathbf{G}) c^{+}_{\mathbf{p},\sigma} c_{\mathbf{p}+\mathbf{q}+\mathbf{G},\sigma} +$$

$$+\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{G},\sigma,\sigma'} U(\mathbf{q}+\mathbf{G}) c^{+}_{\mathbf{k},\sigma} c^{+}_{\mathbf{k}',\sigma'} c_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q}+\mathbf{G},\sigma}, \quad (1)$$

where

$$\epsilon(\mathbf{p}) = t[2-\cos(p_x a)-\cos(p_y a)], \quad (2)$$

with t and a being the tunnelling integral for nearest–neighbor sites and the lattice spacing, respectively. $V_{imp}(\mathbf{q})$ and $U(\mathbf{q})$ in Eq.(1) are the Fourier–transforms of a single impurity potential and of the short–range e-e interaction potential respectively; $\mathbf{G}$ is a reciprocal lattice-vector. $\rho_{imp}(\mathbf{q}) = L^{-2}\sum_\alpha exp(i\mathbf{q}\mathbf{R}_\alpha)$, where L is a linear dimension of the system, and $\mathbf{R}_\alpha$ is the coordinate of an impurity, randomly located on a lattice site. The impurity concentration is assumed to be small, and scatterings on the δ–correlated impurity potential can be estimated in the framework of the Born approximation, [21]. For a metallic system $p_F l \gg 1$ and crossed impurity lines of higher order in $(p_F l)^{-1}$ are ignored; p_F and l are the Fermi momentum and mean free path, respectively.

By varying the band filling, Bragg reflections of the electronic wave off the Brillouin zone boundary are intensified for commensurate values of the electron wavelength,λ, and the lattice constant,a. We will study the effects of Bragg reflections at half–filling, since they become essential as the middle of the band is approached. The Fermi surface for the energy dispersion given by Eq.(2) is flat at half–filling, and its whole section is nested, with vectors $\mathbf{Q} = \{\pm\frac{\pi}{a},\frac{\pi}{a}\}$. The perfect nesting of the Fermi surface gives rise to the following electron-hole symmetry relation for the electron dispersion with respect to $\mathbf{Q}$:

$$\epsilon(\mathbf{p}+\mathbf{Q})-\epsilon_F = -[\epsilon(\mathbf{p})-\epsilon_F], \quad (3)$$

where ϵ_F is the Fermi energy and $\epsilon_F = 2t$ for the half–filling case. Notice that introducing the next–nearest–neighbor hopping term with amplitude t' destroys the perfect nesting of the Fermi surface. However, an optimal nesting takes place with $\mathbf{Q}^* = 0.91\mathbf{Q}$ for $t'/t = 0.165$, [22].

For a small band filling and far from the rational points, the Fermi surface of the model we are studying looks like a sphere, so that the effects of periodicity can be incorporated into the electronic effective mass. This situation does not differ from that of an electron gas moving in the random field of impurities. The quantum corrections to the DoS for this model have been calculated in [8–10]. The lowest order quantum correction to the DoS resulting from the interactions in the diffusion channel can be expressed in the following form, [8,9]:

$$\delta\rho_N^{(D)}(\epsilon,T) = -\rho_o^{(2d)}\frac{[U(0,0)-2\overline{U(\mathbf{p}-\mathbf{p}',0)}]}{4\pi^2\hbar D} \times \ln\frac{1}{\tau_o max\{\epsilon,T\}}, \quad (4)$$

where D is the diffusion coefficient, $D = \frac{{v_F}^2\tau_o}{2}$, with v_F and τ_o being the Fermi velocity and the impurity relaxation time for Normal scattering, respectively, and $\rho_0^{(2d)} = \frac{2}{(\pi a)^2 t}\ln(\epsilon_F min\{\tau_o,\frac{1}{|\epsilon|}\})$. The bar over the interaction potential U denotes the average over the Fermi surface, and the additional prefactor 2 in the Hartree correction term comes from the spin degeneracy. Interactions in the Cooper channel give the following contribution to the DoS far from half–filling,

$$\delta\rho_N^{(C)}(\epsilon,T) = -\frac{1}{2\pi^2\hbar D}\ln\frac{\ln T_c\tau_o/\hbar}{\ln T_c/max\{\epsilon,T\}}, \quad (5)$$

where $T_c = \epsilon_F\exp(1/\lambda)$ and $\lambda = \rho_o^{(2d)}U$ is the dimensionless interaction constant. Notice that the dynamical screening of a short–range interaction in the diffusion channel far from half–filling does not change the bare interaction potential considerably, whereas a short range potential is strongly renormalized in the Cooper channel, [21,24] as seen performing the summation of a ladder series in the bare interaction, which replaces the logarithmic energy or temperature dependence of the quantum correction by the rather weak double logarithmic dependence given by Eq.(5).

A new kind of quantum corrections to the DoS takes place in the correlated disordered system due to the Bragg reflection, which enhances the number of electronic states at half–filling.

As it is well known, the quantum interference corrections to the thermodynamic and kinetic coefficients come from the singular impurity ladder series referred to as the *diffuson* and the *Cooperon* blocks, [9].The diffuson (Cooperon) block has the diffusion pole when the difference $\mathbf{q}$ of the momenta of the electron and the hole (total sum $\mathbf{k}$ of the momenta of the electrons) and their energies difference $|\omega_m|$ are small, i.e. the block acquires the pole in the diffusion regime when $ql \ll 1$ ($kl \ll 1$) and $|\omega_m|\tau_o \ll 1$.

New singular impurity blocks take place at half–filling with particle–hole symmetry, which are referred to as π–Diffuson and π–Cooperon, [12,13]. The π–Diffuson (π–Cooperon) has a diffusion pole at large $\propto \mathbf{Q}$ momenta differences (total momenta) and small total energies of the electron and the hole (of two electrons). The diagram equations for the π–Cooperon, $C_\pi(\mathbf{q},i\omega_m)$, and for the π–Diffuson, $D_\pi(\mathbf{q},i\omega_m)$, are given in Fig.1e,f. The bare Green's function G_0 is indicated in the diagrams by a straight line, and $G_0(\mathbf{p},i\epsilon_n) = \frac{1}{i\epsilon_n-(\epsilon(\mathbf{p})-\epsilon_F)+\frac{i}{2\tau_o}sign\epsilon_n}$. The Green's function of an electron with large momentum is represented by a dashed line. Notice that the dashing of the line has a physical meaning only for an impurity vertex or an interaction one when a large momentum transfer ($\propto \mathbf{Q}$ due to the Bragg reflection) is involved in the scattering process, [12,13]. Therefore, the new selection of diagrams to be included in the summation is performed according to the rule that a straight line in each impurity or interaction point joins a dashed line and vice versa. This rule is consistent with the fact that each scattering with large momentum transfer implies also coherent Bragg reflection of the scattered electron on the boundary of the Brillouin zone. It is easy to see that the momentum conservation for impurity vertices with large momentum transfer is violated, so that they correspond to Umklapp scattering. As far as scatterings on point– like impurities are considered, these vertices are also characterised by τ_o. By summing the ladder series in Fig.1f, treating the π–scattering of an electron on impurities perturbatively, the following expression for the π–Cooperon $C_\pi(\mathbf{q}, i\omega_m)$ is obtained:

$$C_\pi(\mathbf{q}, i\omega_m) = \frac{1}{2\pi\tau_o\rho_o^{2d}}\Big\{\theta(-\epsilon_n(\omega_m - \epsilon_n)) + + \frac{\theta(\epsilon_n(\omega_m - \epsilon_n))}{(1 + |\omega_m|\tau_o)^2 + (ql)^2 - 1}\Big\} \tag{6}$$

The expression for the π–Diffuson $D_\pi(\mathbf{q}, i\omega_m)$ is also given by Eq.(6) with the exception that $\mathbf{q}$ in the equation for $D_\pi(\mathbf{q}, i\omega_m)$ denotes the differences of the momenta of a particle-hole pair.

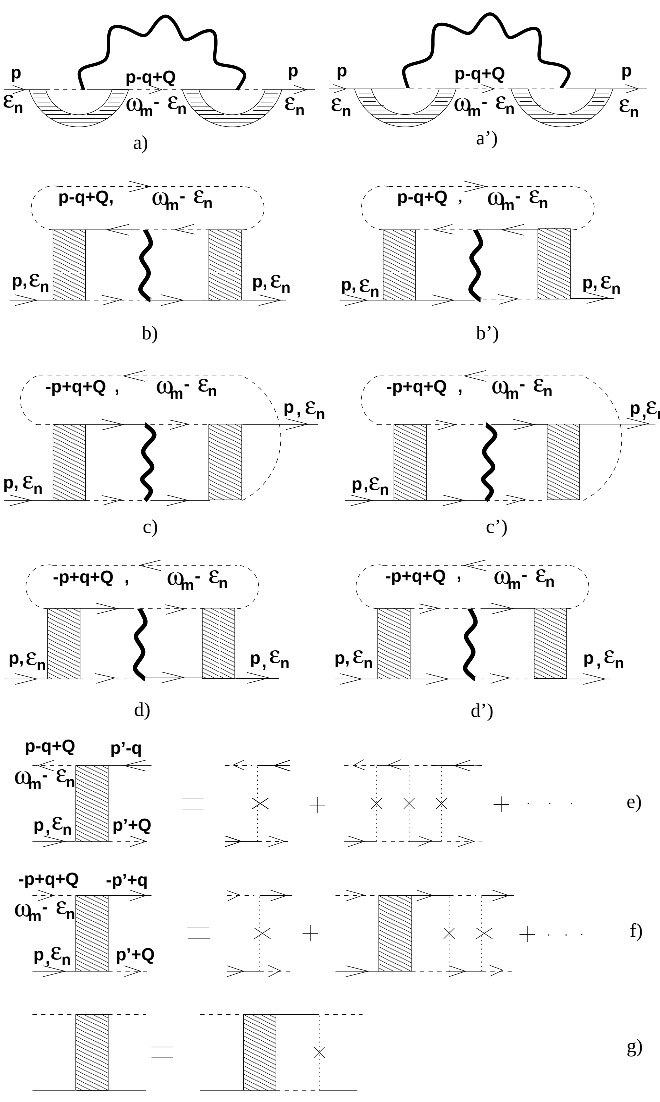

FIG. 1. Bragg reflection induced contributions to the DoS at half–filling from $(a),(a');(c),(c')$ exchange and $(b),(b');(d),(d')$ direct interactions. The diagrams obtained from the exchange ones by interchanging the straight and dashed lines joined in one interaction vertex with appropriate screening of the Coulomb interaction in particle - hole channel also give a contribution to the DOS. (e) and (f) are the impurity ladder series for the π-Diffuson,$D_\pi(\mathbf{q}, i\omega_m)$, and π- Cooperon, $C_\pi(\mathbf{q}, i\omega_m)$, respectively. (g) Diagram equation for the block $\widetilde{D}_\pi$ (or $\widetilde{C}_\pi$), obtained by adding one impurity line to the π-Diffuson (or π- Cooperon). Heavy wave line and dotted line with cross denote Coulomb potential and impurity scattering, respectively.

The additional contributions to the DoS in the middle of the band come from the diagrams shown in Fig.1a-d'. The correction to the DoS, $\delta\rho(\epsilon, T)$, due to the e-e interactions is given by the following expression,

$$\delta\rho(\epsilon, T) = -\frac{2}{\pi}\{Im\int\frac{d^2p}{(2\pi)^2}G_o^2(\mathbf{p}, i\epsilon_n)\Sigma_{ee}(\mathbf{p}, i\epsilon_n)\}_{i\epsilon_n\to\epsilon} \tag{7}$$

where Σ_{ee} is the self–energy for first order quantum corrections to the DoS given by Figs.1(a)-(d'). The expression corresponding to the diagram Fig.1a can be reduced to the following form after simple calculations,

$$\delta\rho_a(\epsilon, T) = 2\tau_o^2\rho_o^{2d}Im\int\frac{d^2q}{(2\pi)^2}\int_0^\infty\frac{d\omega}{2\pi}U(\mathbf{q} - 2\mathbf{Q}, 2\epsilon - \omega) \times\frac{\tanh\frac{\omega+\epsilon}{2T} + \tanh\frac{\omega-\epsilon}{2T}}{\left[(1 - i\omega\tau_o)^2 + (ql)^2 - 1\right]^2}. \tag{8}$$

The bare DoS $\rho_o^{(2d)}$ which is involved in the new correction (8) at half–filling is again given by $\rho_o^{(2d)} = \frac{2}{(\pi a)^2 t}\ln(\epsilon_F min\{\tau_o, 1/|\epsilon|\})$, where the van Hove singularity is cut–off due to the $i/2\tau_o$ term in the bare Green's function, [23]. Calculations of other diagrams in Fig.1 are similar to the calculation of $\delta\rho_a(\epsilon, T)$. Also, the contributions from the diagrams a'), b'), c') and d') in Fig.1 are equal to those coming from a), b), c) and d), respectively. Screening of the potential U in the diffusion and cooperon channels is realized according to the diagrammatic equations given in Fig.2.

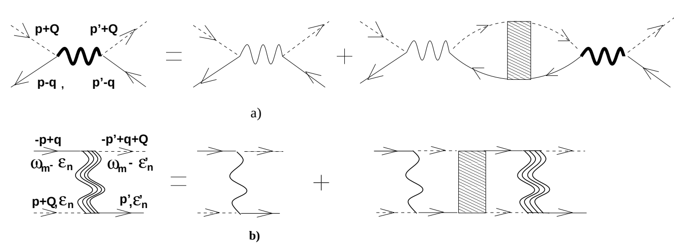

FIG. 2. Screening of the Coulomb interactions for electrons on a 2D half–filled square lattice in (a) particle–hole and (b)particle–particle channels, respectively.

In the middle of the band, it can be shown that the screening of a short–range interaction arises in the diffusion channel, instead of the screening of the potential in the Cooper channel which takes place in the electron gas model, [21,24]. It follows that a dynamical screening of the interaction in the diagrams $(c) - (d')$ of Fig.1 does not essentially change the value of the bare potential, and the contribution to the DoS from these diagrams is calculated according to Eq.(8),

$$\delta\rho_{\pi}^{(C)}(\epsilon, T) = \rho_o^{(2d)} \frac{[U(2\mathbf{Q}, 0) + 2\overline{U(\mathbf{p} - \mathbf{p}' + 2\mathbf{Q}, 0)}]}{4\pi^2\hbar D} \times \ln\Big(\frac{1}{\tau_o max\{\epsilon, T\}}\Big) \quad (9)$$

The screening of the interaction in the diffusion channel is realized according to the diagrammatic equation in Fig.2,

$$U(\mathbf{q} - \mathbf{2Q}, \omega_m) = \frac{2}{\rho_o^{(2d)}\big[\ln\frac{T_c}{T} - \psi(\frac{|\omega_m| + Dq^2}{4\pi T} + \frac{1}{2}) + \psi(\frac{1}{2})\big]} \quad (10)$$

The correction to the DoS from the diagrams in Fig.1(a, a') is calculated by putting Eq.(10) into Eq.(8). The contribution from these diagrams is given by the corresponding expression for $\delta\rho_N^{(C)}(\epsilon, T)$, expressed by Eq.(5). The potential of the other diagrams in the diffusion channel, given by Fig.1(b, b'), carries zero energy and large momentum $\sim \mathbf{p}' - \mathbf{p}'' + \mathbf{2Q}$. Therefore screening is not effective and these diagrams give logarithmic contribution to the DoS. Therefore, the total quantum correction to the DoS in the diffusion channel can be presented as:

$$\delta\rho_{\pi}^{(D)}(\epsilon, T) = -\frac{1}{2\pi^2\hbar D}\ln\frac{\ln T_c\tau_o/\hbar}{\ln T_c/max\{\epsilon, T\}} + \rho_o^{(2d)}\frac{\overline{U(\mathbf{p} - \mathbf{p}' + 2\mathbf{Q}, 0)}}{2\pi^2\hbar D}\ln\Big(\frac{1}{\tau_o max\{\epsilon, T\}}\Big) \quad (11)$$

It is seen from Eqs.(9) and (11) that the Bragg reflection contribution to the DoS $\delta\rho_{\pi} = \delta\rho_{\pi}^{(C)} + \delta\rho_{\pi}^{(D)}$ increases as ϵ approaches the Fermi level.

The total quantum correction to the DoS $\delta\rho(\epsilon, T)$ in the middle of the band can be expressed as $\delta\rho(\epsilon, T) = \delta\rho_N(\epsilon, T) + \delta\rho_{\pi}(\epsilon, T)$. Both contributions to the DoS have the same energy or temperature dependences. However, they differ in sign and by the values of the interaction potentials $U(0, 0)$ and $U(2\mathbf{Q}, 0)$. Since the short–range interaction is a screened Coulomb interaction, the potentials $U(0, 0)$ and $U(2\mathbf{Q}, 0)$ being included in Eq.(4) and Eq.(9) respectively cannot differ strongly from each other if the Thomas–Fermi screening number is of the order of the reciprocal lattice vector $2\mathbf{Q}$. As a result, the total quantum corrections to the DoS become positive at half–filling. Far from half–filling the Bragg reflections are destroyed and the dominant contribution to the DoS is the logarithmically decreasing Altshuler–Aronov contribution [8,9] given by Eq.(4). Notice that an anomaly in the one–particle DoS is experimentally observable by measuring the tunneling conductivity in a contact as a function of the bias voltage. This dependence completely reflects an energy dependence of the DoS.

In conclusion, we showed that the DoS of a $2D$ disordered lattice with flat Fermi surface is enhanced close to half–filling due to quantum corrections mediated by Bragg reflections. Since similar quantum corrections exist for all commensurate points, the DoS seems to show oscillating behavior with maximum amplitude at half–filling. It is appropriate to emphasize that, although the Bragg reflection results in the decreasing the DoS of a non–interacting system, [12,13], it gives rise to an increase of the DoS in the presence of $e - e$ correlations.

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