Mesoscopic fluctuations of the Density of States and Conductivity in the middle of the band of Disordered Lattices

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The mesoscopic fluctuations of the Density of electronic States (DoS) and of the conductivity of two- and three-dimensional lattices with randomly distributed substitutional impurities are studied. Correlations of the levels lying above (or below) the Fermi surface, in addition to the correlations of the levels lying on opposite sides of the Fermi surface, take place at half filling due to nesting. The Bragg reflections mediate to increase static fluctuations of the conductivity in the middle of the band which change the distribution function of the conductivity at half-filling.

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Recent studies of electronic level statistics in disordered systems have shown [2,11] that existence of repulsions between the levels in metallic phase results in a realization of the Wigner-Dyson statistics, [8]. Energy levels in a sufficiently doped $d > 2$ dimensional electron gas become uncorrelated in an insulator phase and the level distribution obeys to Poisson statistics, [9]. However, overlapping of one-particle states with different energies leads to level correlations which change their distribution.

Our recent studies of weak localization effects in two-dimensional (2D) square lattice and in three-dimensional (3D) cubic lattice with substitutional impurities have revealed that Bragg reflections (BR) due to commensurability of the electronic wavelength, $\lambda$, and a lattice spacing, $a$, strongly change the localization picture, [10,12]. The DoS vanishes on the Fermi surface for non-interacting electrons in a 2D lattice and it acquires a small dip on the Fermi surface of 3D simple cubic lattice with approaching half-filling, [11]. Nevertheless, electron-electron (e-e) interactions give a positive quantum correction to the DoS, [13], which compensates the Altshuler-Aronov’s negative logarithmic corrections to the DoS of 2D systems, [11]. Therefore it is interesting to clarify how static fluctuations of physical parameters of 2D disordered lattice with nested Fermi surface are changed by BR as the half-filling is approached.

In this paper we consider the effect of BR on the level statistics and on conductivity fluctuations of 2D and 3D disordered lattices with a half-filled band. A particular characteristics of level spectra is the two-level correlation function,

$$R(\epsilon, \epsilon') = \frac{1}{\rho_{od}} \langle \rho(\epsilon) \rho(\epsilon') \rangle - \langle \rho(\epsilon) \rangle \langle \rho(\epsilon') \rangle,$$  \hspace{1cm} (1)

where $\langle ... \rangle$ means averaging over impurity realizations. $\rho_{od}$ is the DoS of the $d$-dimensional ($d = 2,3$) lattice calculated in the Born approximation:

$$\rho_{od} = \frac{2}{(2\pi)^{d+1}} \ln(\epsilon F \min \{\tau_0, |t|/|t_o| \}),$$

and $\rho_{od}$ is the 'volume' and $\rho$ is the factor of spin degeneracy. For $d = 2$ tunneling integral for nearest-neighbor sites and the retarded ($RA$) and advanced ($AA$) Green’s functions, $R(\epsilon, \epsilon')$ can be expressed as,

$$R(\epsilon, \epsilon') = -\frac{8}{2\pi v^2 \rho_{od}^2} \int dr \int dr' \{\langle G_A(r, r'; \epsilon) G_A(r', r'; \epsilon') \rangle + \langle G_R(r, r; \epsilon) G_R(r', r'; \epsilon') \rangle - \langle G_R(r, r; \epsilon) G_A(r', r'; \epsilon') \rangle - \langle G_A(r, r; \epsilon) G_R(r', r'; \epsilon') \rangle \} - 4Re \langle G_R(r, r; \epsilon) \rangle | Re \langle G_A(r', r'; \epsilon') \rangle |,$$  \hspace{1cm} (2)

where $v$ is the 'volume' and $\sigma$ is the factor of spin degeneracy. Far from half-filling the correlators $RA$ and $AR$ in Eq.(2) give only contributions to the two-level correlation function, [13]. However, existence of the electron-hole symmetry for nested Fermi surfaces gives rise to considerable contributions of the $RR$ and $AA$ correlators to $R(\epsilon, \epsilon')$ in Eq.(2). The Fermi surface of a $d$-dimensional lattice with the energy spectrum of $\epsilon(p) = t \sum_{\alpha=1}^{d} [1 - \cos(p\alpha)]$ becomes nested at half-filling, when $\epsilon_F = dt$, which permits an electron-hole symmetry, $\epsilon(p + Q) - \epsilon_F = -\epsilon(p) - \epsilon_F$, with respect to the nesting vectors $Q = \{\pm \pi/a, \pi/a \}$ for 2D and $Q = \{\pm \pi/a, \pm \pi/a, \pi/a \}$ for 3D lattices. New singular impurity blocks take place at half-filling with particle-hole symmetry, which are referred to as the $\pi$-Diffuson ($D_\pi$) and the $\pi$-Cooperon ($C_\pi$). The $\pi$-Diffuson ($\pi$-Cooperon) has a diffusion pole at large $\infty Q$ momenta differences (total momenta) and small total energies of the electron and the hole (of two electrons), [10].

As it is known, an interference between the self-intersecting trajectories leads to the weak localization of an
electron wave function, (see, [13]). The electron passing the loop (e.g. in Fig.1a), which is formed on the trajectory due to multiple scattering on impurities with small tilted angles, in clock- and counterclockwise, reduces its transmission probability. However, for a nested Fermi surface each act of impurity scattering is accompanied by BR with large (π) scattering angle (see Fig.1b), which strongly changes the weak localization picture of free electron gas. Worthwhile to notice that the electron-hole symmetry effects in the 2D case strongly differ from that in the one-dimensional (1D) case, where BR act as a destructive factor of localization and result in big effects (like the Dyson singularity in the 1D DoS, [13]) only in the absence of forward scattering (see,e.g. [10]) reversing backward scattering to forward one.

The expression for the two particle impurity block \( C_\pi(q, \epsilon + \epsilon') \) in the particle–particle channel due to Umklapp scatterings with the particles’ energies \( \epsilon \) and \( \epsilon' \) is given as, \([10],[12]\):

\[
C_\pi(q, \epsilon + \epsilon') = \frac{1}{2\pi \rho_\text{od} \tau_o} \left\{ \theta(-\epsilon\epsilon') + \frac{\theta(\epsilon\epsilon')}{(1 - i\tau_o|\epsilon + \epsilon'| + \gamma \tau_o)^2 + \frac{2}{\beta}(ql)^2 - 1} \right\},
\]

where the phenomenological parameter \( \gamma \) is introduced to signify an inelastic processes rate. The \( \pi \)-Diffusion \( D_\pi(q, \epsilon + \epsilon') \) is also expressed by Eq.\( [3]\) with exception that \( q \) will now be the momenta difference of a particle and a hole with accuracy of the nesting vector \( Q \). Notice that the ‘normal’ Cooperon and Diffuson blocks depend on the difference of the energies \( \epsilon \) and \( \epsilon' \) instead of sum in Eq.\( [3]\).

New diagrams (see, Fig.2) appear at half-filling due to BR which give contributions to \( R(\epsilon, \epsilon') \) in addition to that coming from normal scattering in a diffusive system. The study of the diffusive regime assumes that the linear length \( L \) of the system is larger than the elastic mean free path \( l \) and smaller than the localization length, the latter of which is exponentially large. By considering the energy scales as the Thouless energy, \( E_c = \hbar D/L^2 \) with the diffusion coefficient \( D = \frac{\hbar^2}{2m} \) of \( d \) dimensional system, and the average level spacing, \( \Delta = \frac{1}{\rho_o d L^d} \), it is possible to see that \( E_c = \hbar D/L^d = \frac{\pi^2}{(\pi L_d)^d} \) is a dimensionless conductance. Since \( g > 1 \) for the metallic case, the diffusive system can be characterized by the condition \( \Delta \ll E_c \ll \hbar/\tau_o \). By summing up contributions of the diagrams in Fig.2 the correlator \( R(\epsilon, \epsilon') \) is expressed as,

\[
R(\epsilon, \epsilon') = \frac{(s\Delta \tau_o)^2}{\beta \pi^2} Re \left\{ \frac{\theta(-\epsilon\epsilon')}{(\epsilon - \epsilon'| + \gamma \tau_o)^2 + \frac{2}{\beta}(ql)^2 - 1} \right\} - \theta(\epsilon\epsilon') \left\{ (1 - i\tau_o|\epsilon + \epsilon'| + \gamma \tau_o)^2 + \frac{2}{\beta}(ql)^2 - 1 \right\},
\]

where \( q^2 = \sum_{\alpha=1}^{d} q^2_{\alpha} \) and \( q_\alpha = (2\pi/aN_o)n_\alpha \) with \( (-N_o/2) < n_\alpha \leq (N_o/2) \), and \( \beta \) is the Dyson index classifying the orthogonal, unitary and symplectic ensembles with \( \beta = 1, 2, \) and \( 4 \), respectively, [8]. Far from half-filling where BR are suppressed, only the first term in the bracket of Eq.\( [4]\) contributes to \( R_\pi \).

In the ergodic regime, \( |\epsilon \pm \epsilon'| \ll E_c \), only the \( q = 0 \) term needs to be retained in the summation over \( q \) in Eq.\( [4]\). So,

\[
R(\epsilon, \epsilon') = \frac{(s\Delta)^2}{\beta \pi^2} \left( \frac{\theta(-\epsilon\epsilon')}{(\epsilon - \epsilon'| + i\gamma)^2} - \frac{\theta(\epsilon\epsilon')}{4(\epsilon - \epsilon'| + i\gamma)^2} \right),
\]

which shows that two levels on the opposite sides of the Fermi surface with energy difference \( |\epsilon - \epsilon'| > \gamma \) repel each other and they attract at energy difference of \( |\epsilon - \epsilon'| < \gamma \). On the other hand, two levels with energies \( |\epsilon + \epsilon'| > \gamma \) on the same side of the Fermi surface attract each other and they repel for the energies \( |\epsilon + \epsilon'| < \gamma \). Furthermore, attraction of two levels on the Fermi surface \( (\epsilon = \epsilon' = 0) \) weakens with approaching half-filling and the correlator.
R(0, 0) reaches its 3/4 value at half-filling. Notice that far from half-filling the levels lying only on the opposite sides of the Fermi surface interact with each other. Additional interaction of the levels on the same side of the Fermi surface appears due to BR at half-filling.

The correlator of two levels centered at ε_0 and ε_o' and averaged in an energy interval of E ≤ W, where W = 2Δ is the band width, can be obtained by integrating R(ε, ε') over the energy interval E:

\[ \langle \delta \rho_{\epsilon_o}(E) \delta \rho_{\epsilon_o'}(E) \rangle = \int_{\epsilon_o - E/2}^{\epsilon_o + E/2} \int_{\epsilon_o' - E/2}^{\epsilon_o' + E/2} d\epsilon d\epsilon' R(\epsilon, \epsilon') \]

\[ = \frac{s^2}{\beta \pi^2 \rho_{od}} \text{Re} \left\{ \ln \left[ \frac{\gamma^2}{E/2 + i\gamma} \right] \right\} - \frac{1}{4} \ln \left[ \frac{\gamma^2}{E/2 + i\gamma} \right] \right\};

\|\epsilon_o|,|\epsilon_o'| \leq E/2 \}

\[ = \frac{s^2}{\beta \pi^2 \rho_{od}} \text{Re} \left[ \frac{E}{2} \right] \left\{ \frac{\gamma^2}{|\epsilon_o| + |\epsilon_o'| + i\gamma} \right\};

\|\epsilon_o|,|\epsilon_o'| \geq E/2 \}

Far from half-filling the second contribution in the brackets of Eqs. (3) and (4) vanishes. This case corresponds to the continuum model. However, the fact that interactions of levels lying on opposite sides of the Fermi surface do give contribution to \( \langle \delta \rho_{\epsilon_o}(E) \delta \rho_{\epsilon_o'}(E) \rangle \) has not been taken into account in [2]. As it is seen from Eqs. (5) and (6) the two-level correlation function strongly depends on center of energy strip E even a correlation is considered in the same energy interval when \( \epsilon_o = \epsilon_o' \). A logarithmical energy dependence of the variance \( \langle [\delta \rho_{\epsilon_o}(E)]^2 \rangle \) takes place for a strip centered around the Fermi level:

\[ \langle [\delta \rho_{\epsilon_o=0}(E)]^2 \rangle = \frac{2s^2(1-f)}{\beta \pi^2 \rho_{od}} \ln \frac{E}{\gamma}; \quad \frac{E}{2} < \gamma < E, \]

\[ = - \frac{2s^2(1-f)}{\beta \pi^2 \rho_{od}} \ln \frac{E}{4\gamma}; \quad \gamma < E/2, \]

where f is the parameter characterizing the BR: f = 1/4 at half-filling and f = 0 far from commensurate points. According to Eq. (8) the Dyson repulsion of levels for energies E/2 < \gamma < E turns to attraction of levels for large energy distances E > 2\gamma.

For the diffusive limit, when E ≫ E_c, summing over q in Eq. (9) can be replaced by integration. As a result we get the following expressions for the DoS variance \( \langle [\delta \rho_{\epsilon_o=0}(E)]^2 \rangle \):

\[ \langle [\delta \rho_{\epsilon_o=0}(E)]^2 \rangle_{diff} = \frac{(\sqrt{2} - 1)(1-f)s^2}{6\pi^3 \beta \rho_{od}^3} \left( \frac{E}{E_c} \right)^{3/2}; \quad d = 3 \]

\[ = - \frac{(1-f)s^2}{4\pi^3 \beta \rho_{od}^2} (E \tau_0) \left( \frac{E}{E_c} \right); \quad d = 2. \]

In the d = 2 case linear contributions in E to \( \langle [\delta \rho_{\epsilon_o=0}(E)]^2 \rangle \) in Eq. (9) are completely cancelled and the fluctuations are not as strong as in 3D systems. This seems to be connected with the localized character of levels in 2D systems.

\[ \text{FIG. 3. The diagrams which contribute to the conductivity variance due to BR. The diagrams denoted by primes differ from the presented ones through the direction of the electron lines. (\epsilon), (f) are symmetric to (\epsilon_o), (f) with respect to the single impurity line; and (\tilde{g}), (\tilde{h}) are obtained from (g), (h) by interchanging the straight and dashed lines under single impurity lines. Diagrams, similar to (e)-(\tilde{h}') exist also in the Cooper channel which are produced from (d, d').} \]
\[ \langle \delta G_{\alpha \beta} \delta G_{\gamma \mu} \rangle = G_D^2 \left\{ \delta_{\alpha \gamma} \delta_{\beta \mu} + \delta_{\alpha \mu} \delta_{\beta \gamma} \right\} + G_\rho^2 \delta_{\alpha \beta} \delta_{\gamma \mu}. \] (10)

Here we followed the notations in [3], where the contributions from the diffusion coefficient and the DoS fluctuations to the conductance variance \( \langle \delta G_{\alpha \beta} \delta G_{\gamma \mu} \rangle \) were denoted by the temperature dependent coefficients \( G_D^2 \) and \( G_\rho^2 \), respectively. The expressions for \( G_D^2 \) and \( G_\rho^2 \) can be presented as:

\[ G_D^2 = \frac{s^2}{2} \left( \frac{e^2}{h} \right)^2 \int \frac{d\epsilon}{2T} f(\epsilon) \frac{1}{\left| Dq^2 - i\epsilon \right|^2} + \frac{\tau_0}{(1 - i\epsilon\tau_0)^2 + \frac{2}{d}(q\ell)^2 - 1} \] (11)

and

\[ G_\rho^2 = \frac{s^2}{2} \left( \frac{e^2}{h} \right)^2 \int \frac{d\epsilon}{2T} f(\epsilon) \frac{1}{\left| Dq^2 - i\epsilon \right|^2} \] (12)

where \( f(x) = \frac{\cosh x - 1}{\sinh x} \). The second term in the brackets in Eq. (11) comes from the diagrams given in Fig. 2 due to \( \pi \)-scatterings. However BR give no contribution to \( G_\rho^2 \). According to Thouless picture [10], only \( \pi \)-states lying in an interval of \( E_c \) centered on the Fermi level give contributions to the conductivity. Contributions to \( G_D^2 \) from the levels correlated on the same side of the Fermi level seem to cancel each other.

At small temperatures \( T \ll E_c \) the coefficients \( G_D^2 \) and \( G_\rho^2 \) do not depend on temperature:

\[ G_D^2 = (s^2/\beta)(e^2/\pi^3 h^2)b_d \quad \text{and} \quad G_\rho^2 = (1 + f)G_\rho^2 \] (13)

where \( b_d \) is a constant, which depends on the system dimension. In the case when \( T \gg E_c \) the values of \( G_D^2 \) and \( G_\rho^2 \) strongly differ from each other and depend on temperature:

\[ G_D^2 = (s^2/\beta)(e^2/2\pi h)^2 a_d (E_c/T)^{(4 - d)/2}, \] (14)

and,

\[ G_\rho^2 = \frac{1}{2}(1 + f)G_\rho; \quad d = 3 \]
\[ = (1 + f)(s^2/\beta)(e^2/2\pi h)^2 E_c T \ln \frac{T}{\max\{E_c, \bar{\gamma} \}}; \quad d = 2, \] (15)

where \( a_d \) is some coefficient, \( \bar{\gamma} \). As can be seen from Eqs. (14) and (15) the main contribution to the conductance variance comes from the fluctuations of the diffusion coefficient, which are intensified at half-filling.

Multiplication of the variance by the additional prefactor \( (1 + f) \) means that Umklapp scatterings of electron on impurities change the distribution function of \( G \). In the language of the random matrix theory, an insulating phase of a disordered system can be prescribed by an ensemble of \( N \times N \) diagonal matrices with random elements. Existence of off-diagonal terms in \( N \times N \) matrices due to overlapping states of different energy in diffusive systems transform the distribution function from Poisson function to Wigner-Dyson one. Umklapp scatterings on impurities give additional contributions to the off-diagonal matrix elements. Therefore, the change in the distribution function due to Umklapp scattering is reasonable. Two-level correlations are sensitive to whether the levels attract or repel each other and to the relative position of these levels, either on the same side or on the opposite sides of the Fermi surface. However, the conductance fluctuations seem not to be sensitive to the character of level interactions and the level positions; both attraction and repulsion give similar contributions to \( \langle \delta G_{\alpha \beta} \delta G_{\gamma \mu} \rangle \). This fact seems to be the reason why Eqs. (8)–(9) for \( \langle \delta \rho_{\text{loc}}(E) \rangle^2 \) and Eqs. (13), (14), (15) contain the factor \( f \) coming from BR in different way.

Recently fabricated \( C_{60} \)-based novel field-effect devices allow one to control the band filling by changing the gate potential. Half-filling is reached for 3 electrons doping per \( C_{60} \) molecule [10]. The possibility of doping the fullerites by substitutional impurities, while preserving the periodicity of the Bravais lattice, will allow the observation of the commensurability effects on the mesoscopic fluctuations at half-filling in these devices.

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