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Weak Localization in Disordered Two-dimensional Crystals with Half-Filled Band

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Abstract

Effect of subtitutional impurities on electron localization in two dimensional (2D) lattice near the middle of the band is studied. Calculation of density of the electronic states, $\rho(\varepsilon)$, increases logaritmically in the middle of the band. This singularity in the density of states of noninteracting electron gas on lattice gives rise to anomalous dependencies of thermodynamic quantities on the temperature.

The quantum correction to the conductivity of a nonintreracting electron gas due to *Umklapp* electron–impurity scattering is calculated. This correction to the conductivity is shown to compete with that from the localization corrrection for a *Normal* scattering process. As a result the conductivity has a finite value at the middle of the band. With a small offset from the middle of the band all states again become localized.

Introduction

The great advance has been made in the theory of disordered metals after the pioneer work of Abrahams et al [1]. According to this paper all electron states in one and two dimensional (1D and 2D) disordered systems are localized irrespective of degree of randomness,and there exists no minimum metallic conductivity in three-dimensional (3D) disordered systems. As regards to 1D systems, the properties of 1D electron gas, moving in the potential of randomly distributed impurities, have been studied by means of the exact solvable diagrammatic method [2] which confirm the Mott's statement [3]that all states are localized due to repeated backscattering with localization length $\xi_{loc} \simeq l_{-}$,where l_{-} is the backscattering mean free path.

Relatively explicit calculation for a 2D disordered electronic system can be carried out in the weakly disordered limit,when the criterion of smallness of the electronic wavelength λ compared to the mean free path l is satisfied $\lambda \ll l$. Effect of randomness on the conductivity of a 2D noninteracting electron gas in the weakly disordered limit has been investigated from a first principle by Gor'kov et al. [4] Calculation of the conductivity, σ, according to the Kubo formula shows the existence of significant quantum corrections to

the Drude's expression. These corrections nontrivially depend on temperature,external fields and sample size and σ is shown to decrease with temperature or with increasing the sample size [4,5]. Another aspect in the theory of disordered metals is electron-electron interactions [6,7].The study of correlation effects in the framework of Fermi-liquid theory gives rise to finite renormalization of the thermodynamic parameters of the system. In contrast to the Fermi-liquid theory, treating electron-electron interaction in a disordered metal by means of perturbation theory [8,9] results in nontrivial corrections to the conductivity, which are similar to the localization corrections obtained for noninterecting electron gas. The existence of electron correlations in disordered systems also gives rise to singularity of the density of electronic states and termodynamics quantities near the Fermi level.

Studies of the correlation effects drastically change the classical understanding of the theory of disordered metals. Indeed, according to Matthiessen's rule, if there exist several mechanisms of collision in the system with the relaxation times τ_i, then the total relaxation time is given by $\frac{1}{\tau} = \sum \frac{1}{\tau_i}$, making the resistivities additive, i.e. there is no interference between the different relaxation mechanisms. However, the results, obtained in [8,9] show that the Matthiessen's rule is failed for a disordered correlated system at low temperatures.

Disordered metal in all above mentioned papers is modeled as a free electron gas moving in the random field of rigid impurities. However, at low concentrations of impurities the crystal usually has a periodical structure and impurity atoms in most of the case substitute the host atoms of the lattice. In this case the effects of commensurability of the electron wavelength, λ, and the lattice constant a become essential in the scattering processes. The role of the commensurability seems to be important for a half-filled band. The commensurability effect for 1D disordered crystal near the middle of the band have been studied by many authors near the middle of the band[$10-15$]. Here we shall study the effects of periodicity on the density of states and the conductivity of 2D disordered crystals.

The simplest electron spectrum for a 2D square lattice can be written in the tight-binding approximation as,

$$\varepsilon(\overrightarrow{k}) = t[2 - \cos(k_x a) - \cos(k_y a)]; k_{x,y} = \frac{2\pi}{aN_{x,y}} n_{x,y}; -\frac{N_{x,y}}{2} \leq n_{x,y} \leq \frac{N_{x,y}}{2} \qquad (1)$$

where only electron tunneling between the nearest-neighboring sites with the tunneling integral t is involved. The bandwidth is w=4t. Since we shall study the half-filled band case the Fermi energy has ε_F=2t. The Fermi surface for an infinite 2D lattice is changed with band-filling which is shown in Fig.1 (see, [16,17]). As it is shown from Fig.1, the Fermi surface corresponding to the half-filling is flatness and the relation $\varepsilon(\overrightarrow{k}) - \varepsilon_F = -t[cos(k_x a + cos(k_y a)]$ is satisfied. In this case , there exists a reciprocal lattice vector $\overrightarrow{P}_0 = (\pm\frac{\pi}{a}, \frac{\pi}{a})$ that maps an entire section of the Fermi surface onto another, i.e. the Fermi surface is perfectly "nested" for the half-filled band case. The nesting means that all electrons might excite from one side of the Fermi surface to the other with a single wave-vector $\overrightarrow{P}_0$ and very little energy required. The reciprocal lattice vector $\overrightarrow{P}_0$ connects

opposite sides of the Fermi surface, having parallel tangents of all connected points on the Fermi surface. There exists the following inversion symmetry of the electron dispersion with respect to the vector $\overrightarrow{P}_0 = (\pm\frac{\pi}{a}, \frac{\pi}{a})$ for a half-filled electronic band.

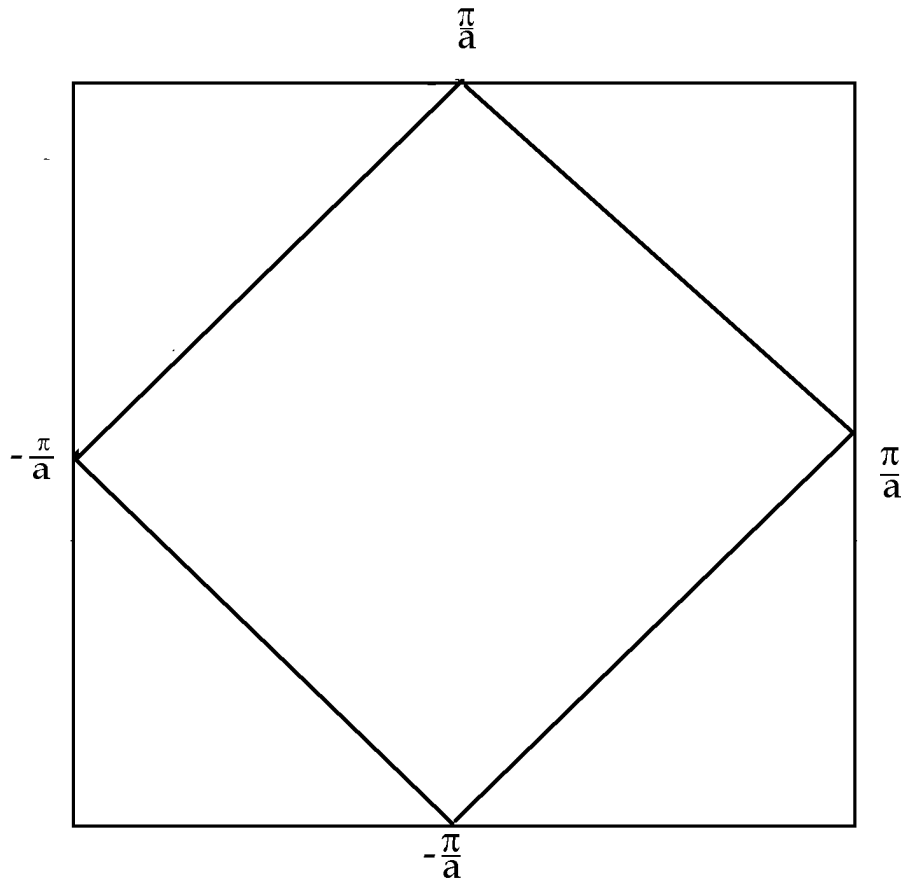

Figure 1.

$$\varepsilon(\overrightarrow{p} + \overrightarrow{p}_0) - \varepsilon_F = -[\varepsilon(\overrightarrow{p}) - \varepsilon_F] \tag{2}$$

Writing Eq (2) as $\varepsilon(\overrightarrow{p} + \frac{1}{2}\overrightarrow{P}_0) - \varepsilon_F = -[\varepsilon(\overrightarrow{p} - \frac{1}{2}\overrightarrow{P}_0) - \varepsilon_F]$ it can be seen that the inversion symmetry (2) is essentially a particle-hole symmetry through the point $\frac{\overrightarrow{P}_0}{2} = (\pm\frac{\pi}{2a}, \frac{\pi}{2a})$.

2. Density of electronic states

The one-particle density of states (DOS) of the regular lattice has been studied from the topological point of view[16] . Expressing the DOS of the regular lattice as $\rho_\circ = \frac{2}{(2\pi\hbar)^d}\int \frac{dS}{|\nabla\varepsilon(\overrightarrow{k})|_k}$ where dS is the element of isoenergetical surface in D dimensional space,it can be shown that $\rho_\circ(\varepsilon)$ should have a singularity at that points where the group velocity of the electron wave packet $V_{\overrightarrow{k}}$ vanishes. Such singularities are known as van-Hove singularity[16] . For a 3D lattice $\rho(\varepsilon)$ has integrable singularities, and for a 2D square lattice with the nearest-neighbor hopping[16, 17],

$$\rho(\varepsilon) \sim \ln(\frac{|\varepsilon - 2t|}{2t}) \tag{3}$$

The important role of the commensurability in 1Ddisordered systems for a half-filled band was first pointed out by Dyson[10]. He has shown that the density of the phonon states of a1D disordered chain has a singularity as $\rho(\varepsilon) \sim |\varepsilon|^{-1}\ln^{-3}|\varepsilon|$ near the middle of the band. Later an analogous singularity has been found in the electronic density of states of many 1D models[$10-15$] . The one electron density of states can be calculated according to the following expression:

$$\rho(\varepsilon) = -\frac{2}{\pi} Im \int \frac{d^2p}{(2\pi)^2} G_R(\overrightarrow{p},\varepsilon) \tag{4}$$

where, $G_R(\overrightarrow{p},\varepsilon)$ is the retarded Green's function. The DOS of a noninteractin electron gas moving in the random field of impurities has no essential singularities near the Fermi level. Inclusion of even short-range electron electron interactions in the 2d disordered metal gives rise to decreasing of DOS near the Fermi level as[6, 8, 9]:

$$\rho(\varepsilon) = \begin{cases} \rho_\circ^{2d} + \frac{\lambda_\nu}{(2\pi)^2 D^{(2)}} \ln\frac{|\varepsilon|\tau}{\hbar} & for\, 2D \\ \rho_\circ^{3d} + \frac{\lambda_\nu}{4\sqrt{2}\pi^2}\frac{\sqrt{|\varepsilon|}}{(\hbar D^{(3)})^{\frac{3}{2}}} & for\, 3D \\ \rho_\circ^{1d} - \frac{\lambda_\nu}{2\sqrt{2}\pi}\frac{1}{(\hbar|\varepsilon|D^{(1)})^{\frac{1}{2}}} & for\, 1D \end{cases} \tag{5}$$

where, $\lambda_\nu$is short-range interaction parameter and λ_ν=$U(\overrightarrow{q}=0)$; $D^{(d)}$ is the diffusion coefficient of D-dimensional electron gas and $D^{(d)} = V_F^2\frac{\tau}{d}$; (d=1,2,3) and τ is the relaxation time for electron-impurity collisions.

The DOS of a 2D disordered crystal with substitutional impurities turns out to have a singularity near the middle of the band even for the noninteracting electrons,[18] .In the processes of electron-impurity collisions, the electron can be scattered from the first Brillouin zone into the second zone. There exists strong Bragg reflection of a scattered electron wave in the half-filled band. Interference between the incident and reflected electronic waves results in singularity of DOS in the vicinity of the Fermi level..

The effect of randomness on the DOS can be studied in the weak localization limit when the condition $k_F l \gg 1$ (or $\varepsilon_F\tau \gg \hbar$) is satisfied. The new class of diagrams which

gives an essential contribution to the DOS is drawn in Fig.2a. A thin solid and dashed lines in Fig.2a correspond to the bare retarded Green's functions $G^{\circ}_{R}(\overrightarrow{p},\varepsilon)$ and $G^{\circ}_{R}(-\overrightarrow{p}+\overrightarrow{p}_{\circ},\varepsilon)$ for electrons the momentum of which lie in the first and second Brillouin zones correspondingly. The expression for $G^{\circ}_{R}(\overrightarrow{p},\varepsilon)$ is obtained from the following formula for bare Green's function by setting $\varepsilon > 0$:

$$G^{(\circ)}_{R}(\overrightarrow{p},\varepsilon) = [\varepsilon - (\varepsilon(\overrightarrow{p}) - \varepsilon_F) + \frac{isign\varepsilon}{2\tau_N}]^{-1} \tag{6}$$

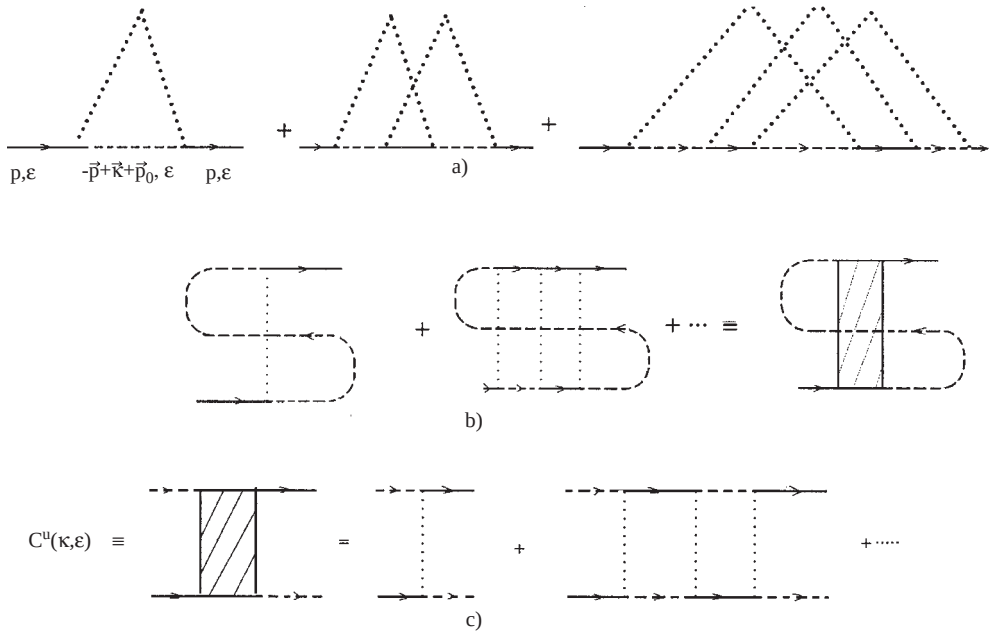

Figure 2.

The electron-hole symmetry relation given by Eq(2) can be used in the expression of $G^{\circ}_{R}(-\overrightarrow{p}+\overrightarrow{p_{\circ}},\varepsilon)$ to reduced it into the first Brillouin zone. The random potential has a δ-correlated Gaussian character and it is denoted in the diagrams by a dotted line with cross. It should be noticed that the scattering processes in the problem is described by two relaxation times τ_N=τ, and τ_u, which characterize Normal (τ_N) and Umklapp-scattering (τ_u) processes (Fig.3).We adopt τ_N and τ_u to be equal, $\tau = \tau_N = \tau_u$.,

$$\rho(\varepsilon) = -\frac{2}{\pi}\int \frac{d^2p}{(2\pi)^2} Im\left\{G^{\circ}_{R}(\overrightarrow{p},\varepsilon))^2 \sum(\overrightarrow{p},\varepsilon)\right\} \tag{7}$$

where $\sum(\overrightarrow{p},\varepsilon)$ is the self-energy part.

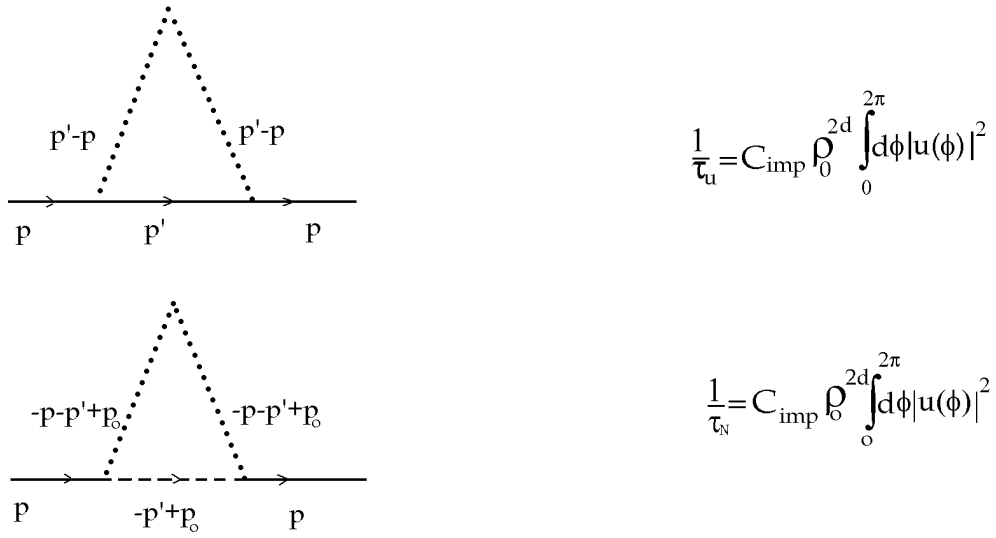

Figure 3.

Redrawing the new diagrams, given in Fig.2a as ladder type diagrams (Fig 2b), the self energy part $\sum(\overrightarrow{p}, \varepsilon)$ can be expressed by the correlation function $C^u(\overrightarrow{k}, \varepsilon)$ in the particle particle channel (or "Cooperon").

$$\sum(\varepsilon, \overrightarrow{p}) = \int \frac{d^2k}{(2\pi)^2} C^u(\overrightarrow{p}, \varepsilon) G_R(-\overrightarrow{p} + \overrightarrow{k} + \overrightarrow{P}_\circ, \varepsilon) \tag{8}$$

The diagram series for $C^u(\overrightarrow{k}, \varepsilon)$ is shown in Fig.2c. Summing up the series in Fig.2c in the limit of small ε and k ($\varepsilon\tau \ll 1$ and $kl \ll 1$) yields a diffusion pole for $C^u(\overrightarrow{k}, \varepsilon)$:

$$C^u(\overrightarrow{k}, \varepsilon) = \frac{1}{2\pi\rho_\circ\tau} \frac{1}{[-4i\varepsilon\tau + (kl)^2]} \tag{9}$$

Substituting Eq. (7) and (8) into (6) we obtain the following expression for the correction to the DOS

$$\delta\rho^{2d}(\varepsilon) = \frac{1}{4\pi^2 D^{(2)}} \ln(\frac{\hbar}{4\tau\,|\varepsilon|}) \tag{10}$$

It should be noticed that the correction is valid only for the half-filling and DOS increases logarithmically in the vicinity of the Fermi level (Fig.4). A small offset from the middle of the band gives rise to disappearance of the correction $\delta\rho^{2d}(\varepsilon)$. Although the functional dependence of the disorder induced singularity in $\delta\rho^{2d}(\varepsilon)$ is similar to that for the van Hove singularity, the correction (9) should vanish with $\tau \to \infty$.

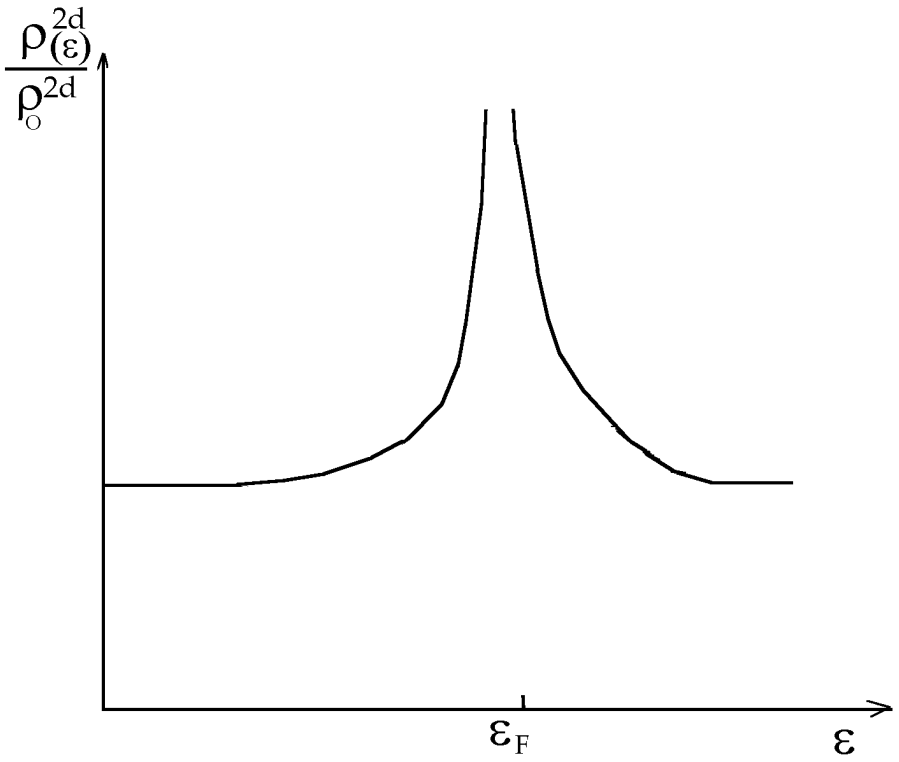

Figure 4.

Calculation of the quantum corrections to the DOS of 1D and 3D weakly disordered crystals by summing the diagrams in Fig.2a in one- and three- dimensions gives:

$$\delta\rho = \begin{cases} \frac{1}{4\pi}\frac{1}{(\hbar D^{(1)}|\varepsilon|)^{\frac{1}{2}}} & for 1D \\ -\frac{\sqrt{|\varepsilon|}}{4\pi^2(\hbar D^{(3)})^{\frac{3}{2}}} & for 3D \end{cases} \tag{11}$$

The problem for a 1D weakly disordered crystal has been studied in[11] by using the Berezinskii diagrammatic technique which gives an exact result. The obtained correction in[11] has a form

$$\delta\rho^{(1d)}(\varepsilon) \sim \frac{1}{|\varepsilon| \ln^3 |\varepsilon|} \tag{12}$$

which differs from that obtained by us in the framework of the diffusion approximation. Indeed, as it is well known the diffusion approximation can not be applicable to the 1D problems, since the interference effects in 1D disordered systems are strong.

It is obvious that electron-electron correlation should also give an additional correction to the DOS. Such corrections for a correlated electron gas, moving in the field of random potential,decrease the DOS near the Fermi level. The problem of electron-electron correlation in the weakly disordered crystals is under investigation

Conductivity

The conductivity averaged over the random field of impurities is calculated at T=0 according to the following formula[19]

$$\sigma_{\alpha\beta}(\omega) = i\frac{ne^2}{m}\omega\delta_{\alpha\beta} + \frac{2e^2}{\omega}\int\frac{d^2P}{(2\pi)^2}\int\frac{d^2p'}{(2\pi)^2}\int\frac{d\varepsilon}{2\pi}v_\alpha v_\beta\langle G(\overrightarrow{p},\overrightarrow{p'};\varepsilon+\omega)G(\overrightarrow{p'},\overrightarrow{p};\omega)\rangle \tag{13}$$

where, n and v are the electron concentration and velocity,the bracket $\langle.....\rangle$ denotes averaging over the impurity distrubution. The diagram series for the conductivity is shown in Fig.5. The new diagram series are appeared (see Fig.5c-5g),due to the existence of perfect nesting in the half-filled band[20]. The diagrams 5a and 5b characterize the Normal scattering processes. As it is well known Drude's expression for $\sigma(\omega)$ is determined by the diagram in Fig.5a, calculation of which cancels the imaginary part of the conductivity in the Kubo formula (12) and result in $\sigma_\circ = \frac{ne^2\tau}{m}\frac{1}{1-i\omega\tau}$. The maximally crossed diagrams in Fig.5b are responsible for the electron localization in the system,[4]. The localization correction to the conductivity can be obtained by redrawing the "fan" diagrams as ladder type diagrams in the particle-particle channel and by summation of these series,[4]:

$$\delta\sigma^{loc}(\omega) = -\frac{e^2}{2\pi^2\hbar}\ln(-\frac{1}{2i\omega\tau}) \tag{14}$$

Notice that for a nonzero temperature (T$\neq$ 0) and small values of external frequency, such that $\omega < \frac{1}{\tau_{in}(T)}$ where τ_{in}(T) is the inalestic relaxation time, -iω in eq[13] should be replaced by $\frac{1}{\tau_{in}(T)}$.

Effect of periodicity gives rise to appearance new class of diagrams given in Fig.5c-5g. In the process of electron scattering on the random impurities, the electron can be found in the second Brillouin zone due to the Umklapp process. There exists strong Bragg reflection of electronic waves for a half-filled band. The diagrams in Fig 5c-5g represent the interference of multiple backward scattered and reflected electronic wave. The quantum correction to $\sigma(\omega)$ from the diagram series in Fig.5c turns out to be negative:

$$\delta\sigma_\nu(\omega) = -\frac{e^2}{4\pi^2\hbar}\ln(-\frac{1}{2i\omega\tau}) \tag{15}$$

The diagram series in Fig.5d have a destructive effect on the localization and summation of these diagrams gives:

$$\delta\sigma_\nu(\omega) = \frac{e^2}{4\pi^2\hbar}\ln(-\frac{1}{2i\omega\tau}) + i\frac{e^2}{4\pi^2\omega\tau} \tag{16}$$

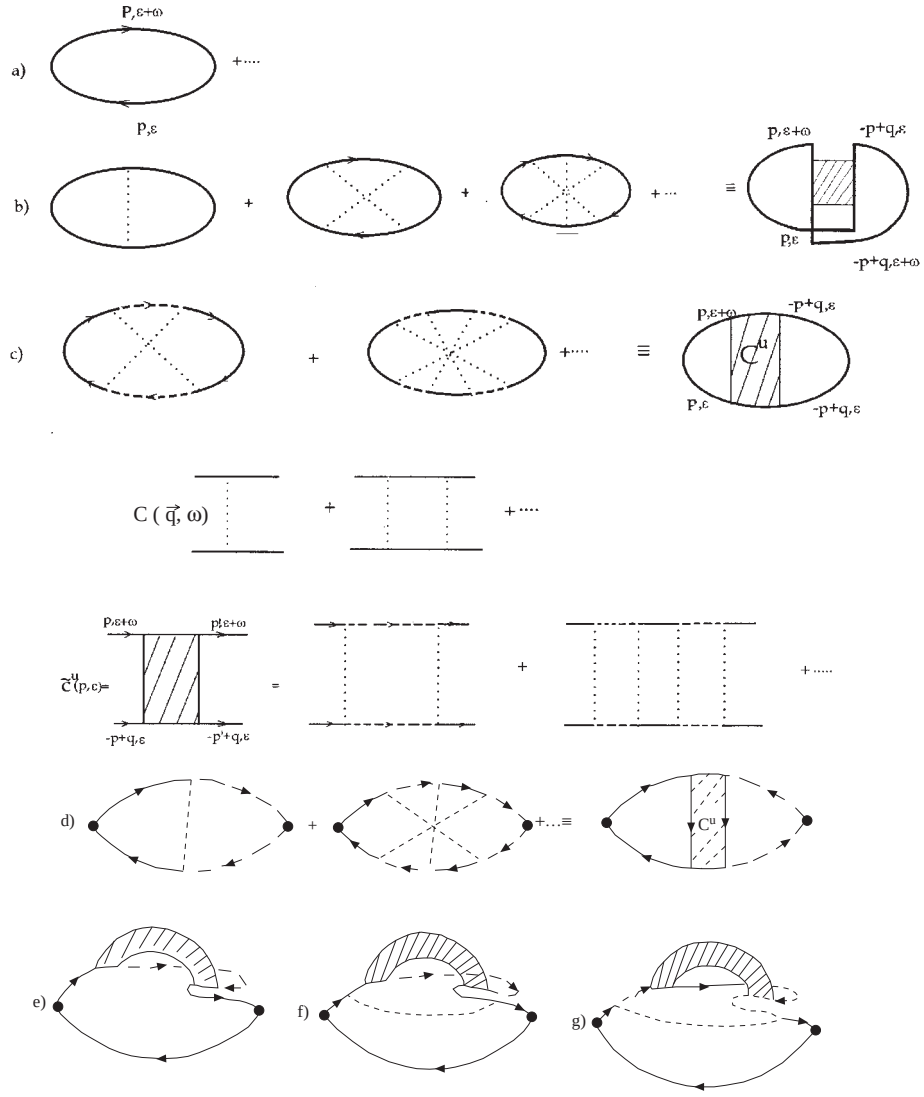

Figure 5.

However there exists the compensating diagram given in Fig.5c-5g. These diagrams similar to that in Fig.5b-5d correspondingly with one additional U-scattering. These diagrams give exactly the same contributions to $\sigma(\omega)$ as Eq.(13)-(15) but with opposite signs, i.e. the only last U-scattering is sufficient to destroy the localization effects. However, in this process electron does not lose its memory and, therefor,the localization contributions

are exactly cancelled. As a result,the residual expression for $\sigma(\omega)$ is obtained as

$$\sigma(\omega) = \sigma_\circ + i\frac{e^2}{2\pi^2\omega\tau} \tag{17}$$

It should be noticed that a small offset from the middle of the band gives rise to disappearance of contributions from the diagrams in Fig.5c-5g and the conductivity should decreases.

Conclusion

In this paper the effects of periodicity on the DOS and the conductivity are studied for a 2D weakly disordered crystal with half-filled band.

For small values of the band filling the effective mass approximation can be applied,as a result of which the problem is reduced the motion of free electron gas in the field of randomly distributed impurities. In this limiting case the DOS has not a singularity. The existence of electron-electron interaction in the weakly disordered system gives rise to logarithmically decrease of DOS near the Fermi level. Notice that the correlation problem for the strongly disordered systems has been exactly solved. The inclusion of long-range Coulomb repulsion in the strongly disordered systems results in vanishing of the DOS at the Fermi level, which is called the Coulomb gab[21].

We have shown that the DOS of a 2D weakly disordered crystal should increases logaritmically with approaching the middle of the band, (see, Eqs (9)-(10)). Notice that such enhancement of DOS in the 2D disordered square lattice should exist at all "rational" point of the electron band, when the electron energy ε satisfy the condition: $\mathrm{P}_{x,y}(\varepsilon) = \frac{m\pi}{na}$, ..m=$\pm1, \pm2, \pm3, ..., \pm$n; (n=2,3.....). However the maximum effect take place in the case of the minimum value of n, i.e. n=2, corresponding to the half-filling.

The behavior of the system with small band filling is defined by the localization effects, valid for the motion of free electron gas in the random potential of impurities. For low temperatures, satisfying the condition $\mathrm{K}_B\mathrm{T} \ll \frac{h}{\tau}$, the conductivity of 2D disordered crystal should decreases logarithmically with temperature. However, with approaching the middle of the band the quantum localization corrections to the conductivity vanish and Re $\sigma(\tau) = \frac{e^2 n\tau}{m^*}$, i.e. the electronic states are delocalized in the middle of the band.

The problem is interesting with regard to the quantum Hall effect. Since according to the theorem of Aoki and Ando[22] ,if all the states are localized, Hall conductivity σ_{xy} vanishes identically for any ε_F Delocalization of the electronic states in the middle of the band due to Umklapp-processes may be the another possibility to explain the Quantum Hall effect.

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