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THE METAL INSULATOR TRANSITION IN DISORDERED ELECTRON SYSTEMS

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Abstract: The selfconsistent current relaxation theory for the motion of fermions in a random potential is generalized by taking into account Coulomb interaction effects. In particular the influence of various local field corrections to the random phase approximation on the metal insulator transition point are examined. The conductivity and the static dielectric constant near the mobility edge are calculated.

The Coulomb force acting between the particles in a charged Fermi liquid or between the particles and a regular array of ions can yield a metal insulator transition (MIT) if for example the particle density n is varied /1/. If non-interacting fermions move in a random potential, provided for example by a random array of scattering centres there can occur also a phase transition from a state where the particle wave functions are extended to one where they are localized. This disorder induced MIT was discussed first by Anderson /2/. In this note we want to contemplate the questions of the interplay of the two mentioned mechanisms driving the MIT. The answer to this question would be of relevance to understand the conductivity in some disordered electron systems like e.g. in doped semiconductors or in liquid metals. To proceed we will generalize the selfconsistent current relaxation theory (SCCR), proposed as an approximation approach towards the motions of non-interacting particles in strongly disordered systems /3/, such, that the Coulomb interaction is taken into account within the random phase approximation (RPA) including local field corrections (LFC) /4/.

The model to be discussed is specified by the Hamiltonian $H = H_0 + H_D + H_I$. Here H_0 is the free particle part $H_0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} a^*_{\vec{k}\sigma} a_{\vec{k}\sigma}$ expressed as usual by creation and annihilation operators for fermion states with momentum $\vec{k}$ and degeneracy index σ running from 1 to 2 g_v, g_v is the valley degeneracy. For the kinetic energy a parabolic band approximation with mass $m = m^* m_e$ is used: $\varepsilon_k = k^2/2m$. The interactions due to the electron charge then reads: $H_I = \frac{1}{2}\sum_{\vec{q}} \rho^*(\vec{q})\, V(\vec{q})\, \rho(\vec{q})$ where $V(q) = 4\pi e^2/q^2 \varepsilon_L$. Here ε_L denotes the lattice dielectric constant and $\rho(\vec{q})$ abbreviates the electron

density fluctuations for wave vector $\vec{q}$. The disorder is specified by $H_D = \sum_{\vec{q}} \rho^*(\vec{q})U(\vec{q})$ with $U(\vec{q})$ denoting the random potential Fourier transform. The average of the random potential we assume to be absorbed in the chemical potential so that $\langle U(\vec{q})\rangle = 0$. The fluctuations are parametrised in the form

$$\langle |U(\vec{q})|^2 \rangle = n_i \left(\frac{4\pi e^2}{\varepsilon_L}\frac{1}{q^2}\right)^2 Z^2(q) S(q) \quad . \tag{1}$$

So we imagine the disorder to be caused by scatterers of density n_i, scatterer structure factor $S(q)$, and charge form factor $Z(q)$. $Z(q=0)=Z$ is the impurity valency. The q-variation of $Z(q)$ describes the deviation of the electron impurity pseudopotential from a Coulomb law due to core screening, exclusion principle and various polarization effects.

The generalized SCCR is based on two equations. One connects the current relaxation kernel $M(\omega)$, a causal function of frequency ω, with the Kubo relaxation function /5/ $\phi(q,\omega)$ for the density fluctuations of wave vector q /3/, which holds approximatively also for the interacting system

$$M(\omega) = \frac{1}{3nm}\sum_{\vec{q}} q^2 \langle |U(\vec{q})|^2 \rangle \phi(q,\omega) \quad . \tag{2a}$$

The other expresses $\phi(q,\omega)$ in terms of the electron compressibility $g(q)$ and a reference function $\phi^R(q,\omega)$ as

$$\phi(q,\omega) = \frac{\phi^R(q,\omega+M(\omega))}{1+M(\omega)\phi^R(q,\omega+M(\omega))/g(q)} \quad . \tag{2b}$$

In the preceeding work /6/ the compressibility was approximated by the one of the non-interacting Fermi gas $g^\circ(q)$ and for $\phi^R(q,\omega)$ the corresponding free gas function $\phi^\circ(q,\omega)$ was used. We now generalize by using as reference susceptibility the RPA result with a local field correction $G(q)$ /4/:

$$\chi^R(q,\omega) = \frac{\chi^\circ(q,\omega)}{1+V(q)(1-G(q)/g_V)\chi^\circ(q,\omega)} \quad . \tag{2c}$$

One then gets $\phi^R(q,\omega) = (\chi^R(q,\omega)-g(q))/\omega$ and $g(q) = \chi^R(q,0)$. The preceeding equations are a closed system to determine $M(\omega)$ and hence the dynamical conductivity in the standard form /7/.

$$\sigma(\omega) = \frac{ne^2}{m}\frac{i}{\omega+M(\omega)} \quad . \tag{3}$$

The electronic contribution to the polarizability is given as $\chi(\omega) = i\sigma(\omega)/\omega$ and thus the dielectric function reads $\varepsilon(\omega)=\varepsilon_L+4\pi\chi(\omega)$.

The discussion of the MIT described by the selfconsistency equations (2) can follow the preceeding work /3/ /6/. There are two relevant length scales involved: one is given by the Fermi wavevector $k_F \propto n^{1/3}$ the other one by the Thomas-Fermi screening vector $q_s \propto \sqrt{\rho_F/\varepsilon_L}$. Here $\rho_F \propto m k_F$ is the Fermi liquid density of states at the Fermi energy ε_F. The ratio $\xi = 2k_F/q_s$ measures the effective potential range relative to the particle wavelength: $1/\xi^2$ is proportional to the electron liquid parameter r_s. The implicite equation for the MIT reads A=1, where the dimensionless coupling parameter A, depending on n_i, and the other quantities like Z, g_v specifying the model, is given by

$$A = \frac{Zn_i}{n} \frac{4Z}{g_v \xi^2} \frac{1}{q_s} \int_0^\infty dq \; q^2 \frac{g^\circ(q)}{(\rho_F^2 q^2 + (1-G(q)/g_v) g^\circ(q))^2} \quad . \tag{4}$$

For A>1 the system is an insulator characterized by a finite static polarisability χ. For A<1 the system is a conductor with a non-vanishing dc conductivity σ. If one approaches the MIT from the conductor side e.g. by decreasing the electron density n to the critical one n_c, the conductivity tends to zero according to

$$\sigma = g_v \sigma_M q_s \sqrt{\xi^3} \, F_\sigma \sqrt{\frac{n-n_c}{n_c}} \, . \tag{5a}$$

Here $\sigma_M = e^2/4\pi\hbar$. The numerical factor F_σ depends on the path the system is driven towards n_c as well as on the approximation used for the LFC. For uncompensated systems ($Zn_i = n$) and the RPA one gets $F_\sigma = 0.22$ or 0.16 for $\xi_c \ll 1$ or for $\xi_c \gg 1$. If the MIT is approached from the insulator side by increasing n one finds a divergence given asymptotically as

$$\chi = \frac{\varepsilon_L}{12\pi} F_\chi \frac{n_c}{n_c - n} \quad . \tag{5b}$$

For the specified model $F_\chi = 1.25$ and 0.38 if $\xi_c \ll 1$ and $\xi_c \gg 1$. So the critical exponents are the same as predicted originally for the model of non-interacting particles /3/. The subtleties of the theory are hidden in n_c and in the scales for σ and χ. Most remarkable is the universality exhibited by the result for χ.

At the critical point the kernel $M(\omega)$ diverges like $|\omega|^{-1/3}$ /6/ and the conductivity is nonanalytical in ω:

$$\sigma = g_v \sigma_M \, q_s \, \xi^{4/3} F_\sigma^c |\omega|^{1/3} \tag{5c}$$

with $F_\sigma^c = 0.16$ or 0.085 for $\xi_c \ll 1$ or for $\xi_c \gg 1$.

In the following we restrict ourselves to the model $Zn_i=n$, $Z(q)=Z$, $S(q)=1$. The only parameter then is the electron or the impurity density. The phase transition criterion $A=1$ can be rewritten in the form

$$n_c^{1/3}\, a_H^* = f, \tag{6}$$

where $a_H^*=\hbar\varepsilon_L/me^2$ is an effective Bohr radius and f is a number of order 0.1. Within the RPA one finds

$$f = \begin{cases} 0.039\ Z^{4/3} & \xi_c<<1 \\ 0.22(Z/g_v)^{2/3} & \xi_c>>1\ . \end{cases} \tag{7}$$

In Table 1 the f values for various Z and g_v are reported for the RPA, and for the LFC according to the view of Hubbard /8/, G_H, Sham and Brosens et al. /9/ G_{SB}, Utsumi and Ichimaru /10/ G_{UJ}, and Ichimaru and Utsumi /11/ G_{JU}.

(Z/g_v)	(4/1)	(3/1)	(2/1)	(1/1)	(1/2)	(1/4)	(1/6)
RPA	0.25	0.18	0.12	0.049	0.047	0.043	0.041
$G=G_H$	0.31	0.24	0.16	0.082	0.065	0.052	0.048
$G=G_{SB}$	0.35	0.29	0.22	0.14	0.124	0.072	0.055
$G=G_{UJ}$	0.33	0.26	0.19	0.11	0.086	0.060	0.051
$G=G_{JU}$	0.34	0.27	0.20	0.12	0.088	0.067	0.056

Table 1: f values entering the criterion (6), see text.

LFC increases the electron gas compressibility g(q) above the RPA value /4/ and according to equ. (4) this implies an increase of the dimensionless coupling A. Hence the LFC increases the tendency to localization and therefore the f values are too small if the RPA theory is used. Naturally, the LFC are less important if the degeneracy factor g_v for the electrons increases. Hubbard's approximation seems to underestimate the LFC but the differences of the f values obtained from the other quoted theories are not big enough to be significant for our purposes.

The phase transition criterion given by equ. (6) with f=0.25 was proposed originally by Mott /12/ /1/ for the correlation induced MIT. There is indeed a great variaty of alloys whose data for the transition point support the Mott criterion /13/. The result $f\propto g_v^{2/3}$ obtained in equ. (7) for $\xi_c>>1$ agrees also with earlier findings /14/. So, as far as the position of the MIT point is concerned, our theory is in accord with previous discussions. To emphasize the relevance of our result we compare in Table 2 critical densities for rare gas alloys with experiments for Ar:Hg /15/, Ar:La /16/

and Xn:Sn /17/. The LFC are taken from Ichimaru and Utsumi /11/. Notice, that no fit parameter enters the evaluation of n_c.

Z	2	3	4
alloy	Hg:Xe	La:Ar	Sn:Xe
$c^{atomic}_{Hg,La,Sn}$	0.80	0.31	0.31
ε_L	1.25	1.45	1.85
$n_c^{exp}/10^{22}cm^{-3}$	5.9	2.5	2.8
$n_c/10^{22}cm^{-3}$	2.8	4.4	4.2

Table 2: Critical densities for the MIT according to the present theory in comparison with experiment.

More relevant than the evaluation of the critical point within a first principle theory is of course the discussion of measurable quantities like σ and χ as functions of n/n_c. Such work is in progress. In Fig. 1 we demonstrate the influence of LFC on σ and χ.

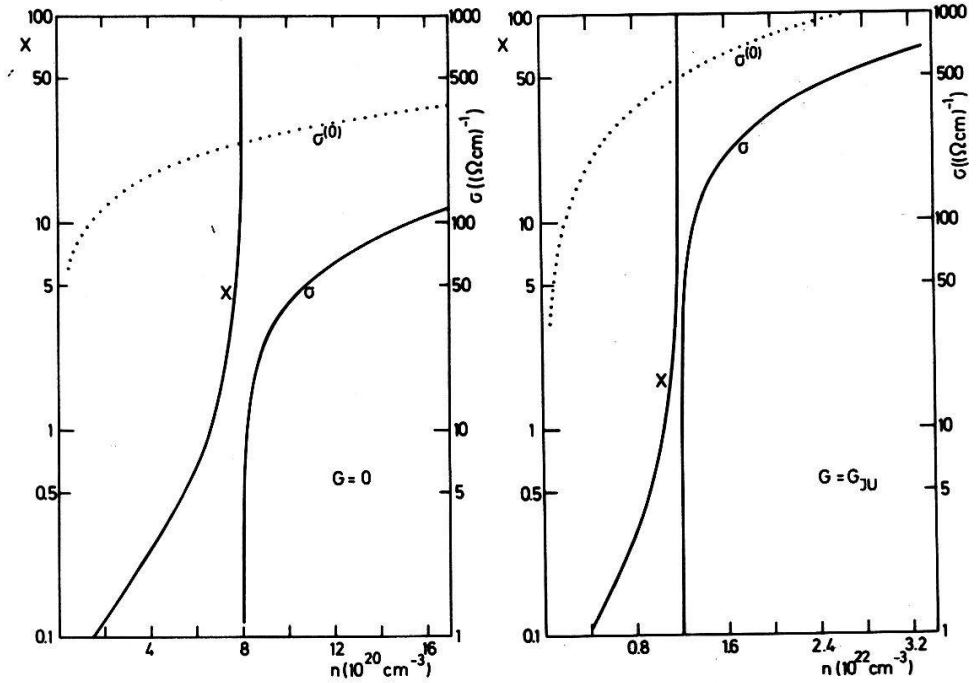

Fig. 1: Polarisability and conductivity as function of density.

The results show that the scale for χ and σ is the one observed in certain semiconductors. The elementary formula of Mott and Jones for the conductivity $\sigma^{(o)}$, which is obtained as lowest order approximation for the present theory if the RPA density correlation $\phi(q,\omega)=\phi^R(q,\omega)$ are substituted on the r.h.s. of equ. (2a) /7/, is shown also by the dotted line for $G(q)=0$. The

dotted line for G_{JU} represents the zero order result including local field effects. In Fig. 2 the scaling laws for the polarisability and the conductivity are shown for $G=G_{JU}$. The dashed line represents the exponents 1 and 1/2 according equation (5a) and (5b). Note that the scaling laws hold only until $|\frac{n-n_c}{n_c}|<0.1$.

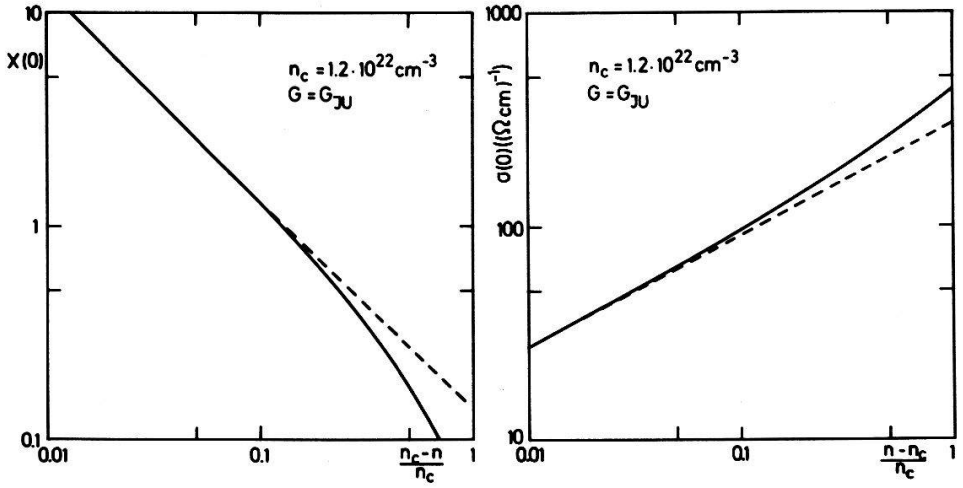

Fig. 2: Scaling laws for polarisability and conductivity

The preceeding results we consider as encouraging indication, that our theory provides an approximation scheme for the evaluation of the conductivity, of current and density spectra and the like in strongly disordered electron systems. In particular the theory is able to describe the metal insulator transition be it driven by disorder or by Coulomb interactions. The most interesting new physical feature in interacting electron systems as opposed to non-interacting ones is the existence of plasmon excitations. The present theory provides a frame to evaluate plasma damping in strongly disordered two and three dimensional conductors. In particular anomalies are obtained since the dynamical aspects of screening are taken into account. Details will be published shortly.

Altshuler and Aronov /18/ have predicted interesting anomalies of the conductivity due to the combined influence of disorder and Coulomb interactions. MacMillan /19/ and Oppermann /20/ have used renormalization group techniques to extend the original perturbation results /18/ into the regime of strong disorder. The present theory does not incorporate the Altshuler-Aronov anomalies and we do not understand the connection of our descriptions of a mobility edge with the other work /19 /20/. Exchange correlations,which

are taken into account in our work, imply the existence of a Coulomb gap in the density of states /21/ /22/. A theory of the dielectric constant near the MIT based on the Coulomb gap physics has not been worked out yet. In our work the implications of interaction on the density of state are not considered. Therefore the connection of the present approximations with the approximations studied for the Coulomb gap remain unclear.

We want to mention that the critical exponents of the scaling law depend somehow on the approximations. In a generalized hydrodynamic version like that done for the non-interacting system /23/ the exponents 1/2, 1 and 1/3 in equations (5a,b,c) would change to 1,2,1/2 respectively. We do not know which approximations describe the physical situation most adequately.

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