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EFFECT OF THE VAN HOVE SINGULARITIES ON THE X-RAY ABSORPTION AND EMISSION IN METALS

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The process of relaxation to a suddenly created local potential is studied for a (quasi-) two-dimensinal metals with Van Hove points near the Fermi surface. The new intermediate time-asymptotic for the core hole Green's function is found. It turns out, that the problem can not be described in terms of creation of independent electron-hole pairs.

The consequences of the logarithmic singularity in the single electron density of states, caused by the Van Hove points [1] for (quasi-) two-dimensional metals, were extensively studied, mainly in connection with the effects of electron-electron interaction: charge-density-wave [2] and superconducting [3] instabilities. A more refined and mathematically elegant theory turned to be necessary for the model case, in which, in addition to the Van Hove points (always existing [4]), there is the nesting [5]. In this paper it is shown, that the local properties of metals in the presence of Van Hove singilarity are also peculiar. Such an investigation makes sence, of course, only in the metallic state, i.e. above the transition temperature to some nonmetallic phase (which can be very small or, in some cases, even zero [5]).

The only characteristic of the metal which is relevant for the local properties is the local electron Green's function

$$g_o(t) = -i \sum_{k,k'} \langle T a_k(t) a^+_{k'}(0) \rangle .$$

Due to the spectral representation

$$g_o = \int d\varepsilon \rho(\varepsilon) [\omega - \varepsilon + i\delta \mathrm{sign}\varepsilon]^{-1}$$

it is completly determined by the density of states, which, near the Van Hove singularity, has a shape: $\rho(\omega) = (1/W) \ln[W/\max(|\omega|, |\mu|)]$, where W is a constant of order of the conduction electrons bandwidth and μ is the chemical potential, accounted from the constant energy surface, which contains the Van Hove points.

One of the most interesting local processes in metals is the relaxation to a suddenly created potential (for simplicity, but without changing the qualitative results, the potential will be treated below as a point one). This process is the essence of the so-called X-ray problem [6], which was in principle solved (for the finite density of states at the Fermi surface) by Nozières and De Dominicis [7].

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They have introduced the transient electron Green's function, which obeys the Dyson equation

$$\varphi(\tau,\tau') = ig_o(\tau-\tau') + \lambda V \int_t^{t'} d\tau'' g_o(\tau-\tau'')\varphi(\tau'',\tau') \qquad (1)$$

and anables one to calculate all the quantities of physical interest (X-ray transition rate, etc.; for more details see [7]). The eq(1) is written for the case of absorption. The case of emission is completly analogous and does not require any special consideration. Here V is the interaction of the conduction electrons with the core hole, created by the absorption of X-ray quantum, $0 \leq \lambda \leq 1$ and for large τ the kernel of (1) has the form:

$$g_o(\tau) = -\frac{\ln \tau}{W\tau}, \quad \tau \gg 1/W, \qquad (2)$$

where μ is set equal to zero. In absence of the Van Hove singularity one would has $g_o(\tau) \sim 1/\tau$, instead of (2). Thus, in the present case, as it can be understood already from (2), it is more difficult for the electronic system to relax to an external potential (a nonzero μ will reduce the asymptotic (2) to $\sim 1/\tau$ for $\tau \gg 1/|\mu|$, so one has to demand $|\mu| \ll W$).

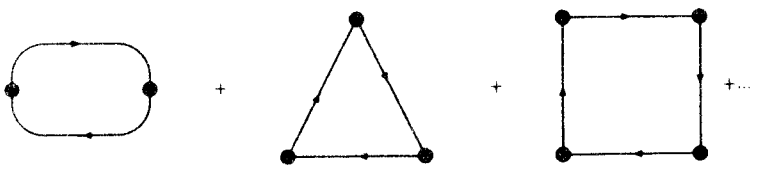

Fig.1. The linked cluster expansion for the closed loops contribution $C(t)$; lines represent electron Green's functions, points - interactions with the potential, which acts during the time interval $[t,t']$

The core hole Green's function $\mathcal{G}(t) = -i\langle Tb(t)b^+(0)\rangle$, which tells us how the core hole level broadens due to the interaction with electrons, using the linked clusters theorem, can be written as $\mathcal{G}(t) = -i\exp[C(t)]$, where $C(t)$ is the contribution of all single closed loops (Fig.1):

$$C(t) = -iV \int_0^1 d\lambda \int_t^{t'} d\tau \varphi(\tau,\tau).$$

The first and third graphs on the Fig.1 give:

$$\mathrm{Re}C(t) = -\frac{2}{3}g^2 \ln^3 t + \frac{4\pi^2}{15} g^4 \ln^5 t, \qquad (3)$$

where the coupling constant $g = V/W$ is introduced. The second graph vanishes for the case of electron-hole symmetry (one can show also, that in the absence of such a symmetry it would contribute a term: $\sim g^3 \ln^3 t$). The imaginary part of $C(t)$ is responsible for the energy shift of the core hole level, in which I am not

interested here. Note also, that the effect of electron spin is included in (3); it simply doubles the $C(t)$.

The result (3) differs qualitatively from the usual asymptotical expression: $\mathrm{Re}C(t) = -2[\delta(g)/\pi]^2 \ln t$, where $\delta(g)$ is the scattering phase. But the point is that the second nonvanishing term of the perturbation expansion is even more singular than the first one, what means that the perturbation theory never works for large enough t. It is also essentially unlike the usual case, in which the first term of linked cluster expantion remains the main one for arbitrary large t (and, of course, for $g \ll 1$; see [7,8]).

The eq(1) with kernel (2) can not be solved exactly, but, fortunately, for the particular problem of calculation $C(t)$ one can adopt the Hamman's point of view [9] of taking the limit $t = 0, t' \to \infty$ in eq(1) from the very beginning and then use the standart methods of solving singular integral equations [10]. Not having place in this letter for more mathematical details I am forced here only to quote the results and leave its detailed justification for an extended paper [11]. The exact asymptotic for the closed loops contribution is:

$$\mathrm{Re}C(t) = -\frac{1}{2} \ln t, \quad t \to \infty, \quad g \neq 0, \tag{4}$$

what would coinside with the standard expression if one inserts the scattering phase $\delta = \pi/2$. For the X-ray transition rate one has:

$$F(\nu) \sim (W/\nu)^{-1/2+\mathrm{sign}g} ln^{-1}(W/\nu), \quad \nu = \omega - \omega^{th} \text{ (absorption)}$$
$$F(\nu) \sim (W/\nu)^{-1/2+\mathrm{sign}g} \ln(W/\nu), \quad \nu = \omega^{th} - \omega \text{ (emission)}$$

Thus, the old X-ray problem acquires new colors for the case of a metal with Van Hove singularity. The perturbation expansion leads to the unusual asymptotic $\mathrm{Re}C(t) \sim \ln^3 t$, which serves as *intermediate* one for $1/W \ll t \ll t_o = (1/W)\exp(1/g)$ (as it can be seen e.g. from comparison of the terms in (3)). This result reflects the enhanced density of states of the electron-hole excitations (which is $\rho_{ph} \sim \omega \ln^2(W/\omega)$) and it would be exact if these exsitations could be created independently. But it is not the case in higher order processes (because of the Pauli principle) and, as a result, for $t > t_o$ more and more singularities occur (with different signs) and finally they sum up in the usual log-asymptotic (Fig.2). So, for large enough t the problem can not be described, even qualitatively, in terms of independent electron-hole pairs [12]. Note, that the pre-log factor is *potential independent*. It means, that the limit $g \to 0$ can be reached not due to the diminishing of the pre-log factor, as in usual case, but through the shifting ($t_o \to \infty$) of the region of applicability ($t \gg t_o$) of the result (4). The additional log factor survives in the transition rate, but in a different powers for absorption and emission, what makes the threshold strongly asymmetrical. It is natural, since the transition rate reflects the "local" density of states in the *final* state, which is enhanced for emission and suppressed for absorption (the electron Green's function in presence of the static potential is $\tilde{g}_o(\tau) \sim 1/\tau \ln \tau$).

Of course, the expressions (3),(4) give also the exponent for the Orthogonality Catastrophe [13] (after substitution $t \to N$ =number of particles). It is noteworthy that, for a magnetic impurity the parquet problem should be of $\log^2$-type and the Kondo temperature is given by $T_K \sim W \exp(-\sqrt{W/J})$ (J - exchange, and $J \ll W$).

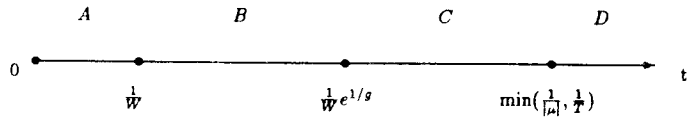

Fig.2. The schematic time "evolution" of the core hole Green's function. The region A is governed by the relaxation of high-energy degrees of freedom. The region B corresponds to the intermediate asymptotics (4) and the region C - to the potential independent asymptotics (5), which breaks down in the region D.

An additional motivation for this work was the intention to build a simple, exactly solvable, example in which the type of the singularity in the overlap integral is different from the usual log-one, as it happens in the Luttinger Liquid [14]. We have seen that in the case of the Van Hove singularity the asymptotic indeed changes, but only for the intermediate t and the true limit $t \to \infty$ is governed by the usual log. Whether or not a similar scenario holds also for the Luttinger Liquid case remaines yet unclear.

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