

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 in (quasi-) two-dimensional metals with van Hove points near the Fermi surface. The new intermediate time-asymptotic for the core hole Green's function is found. It was found that the problem cannot 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 points¹ for (quasi-) two-dimensional metals, were studied extensively, mainly in connection with the effects of electron-electron interaction: charge-density wave² and superconducting³ instabilities. A more refined and mathematically elegant theory turned out to be necessary for a model in which, in addition to the van Hove points (which always exist⁴), there is nesting.⁵ In this paper we show that the local properties of metals in the presence of van Hove singularity are also peculiar. Such an investigation makes sense only in the metallic state, i.e., above the temperature of the transition to a nonmetallic phase (which can be very small or even zero in some cases).⁵

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

$$g_0(t) = -i \sum_{k,k'} \langle T a_k(t) a_{k'}^+, (0) \rangle.$$

Because of the spectral representation

$$g_0 = \int d\varepsilon \rho(\varepsilon) [\omega - \varepsilon + i\delta \operatorname{sign} \varepsilon]^{-1},$$

it is completely determined by the density of states, which near the van Hove singularity has the shape: $\rho(\omega) = (1/W) \ln[W/\max(|\omega|, |\mu|)]$, where W is a constant on the order of the conduction electron bandwidth, and μ is the chemical potential, determined 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). This process is the essence of the so-called x-ray problem⁶ which was basically solved (for the finite density of states at the Fermi surface) by Nozières and de Dominicis.⁷ They have introduced the transient electron Green's function which obeys the Dyson equation

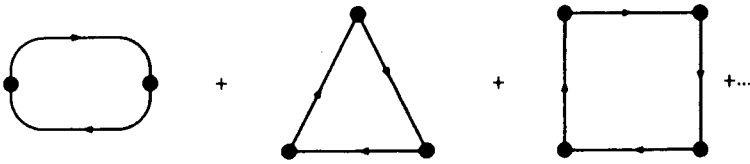


FIG. 1. The linked cluster expansion for the closed-loops contribution $C(t)$; the lines represent electron Green's functions; points—interactions with the potential which acts during the time interval $[t, t']$.

$$\varphi(\tau, \tau') = ig_0(\tau - \tau') + \lambda V \int_t^{\tau'} d\tau'' g_0(\tau - \tau'') \varphi(\tau'', \tau') \quad (1)$$

and enables one to calculate all the quantities of physical interest (x-ray transition rate, etc.; for more details see Ref. 7). Equation (1) is written for the case of absorption. The case of emission is completely analogous and does not require any special consideration. Here V is the interaction of the conduction electrons with the core hole, which is created by the absorption of an x-ray, $0 \leq \lambda \leq 1$, and for large τ the kernel in (1) has the form

$$g_0(\tau) = -\frac{\ln \tau}{W\tau}, \quad \tau \gg 1/W, \quad (2)$$

where μ is set equal to zero. In absence of the van Hove singularity one would have $g_0(\tau) \sim 1/\tau$, instead of (2). As is evident from (2), in our case it is thus more difficult for the electronic system to relax to an external potential [a nonzero μ reduces the asymptotic (2) to $\sim 1/\tau$ for $\tau \gg 1/|\mu|$, so the condition $|\mu| \ll W$ must be satisfied].

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):

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

The first and third graphs in Fig. 1 give

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

where the coupling constant $g = V/W$ is introduced. The second graph vanishes for the case of electron-hole symmetry (one can show that in the absence of such a symmetry it would contribute the 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 there is no interest here. Note also that the effect of electron spin is taken into account in (3); it simply doubles the $C(t)$.

The result (3) differs qualitatively from the standard asymptotic expression: $\text{Re } C(t) = -2[\delta(g)/\pi]^2 \ln t$, where $\delta(g)$ is the scattering phase. The point, however, is that the second nonvanishing term of the perturbation expansion is even more singular

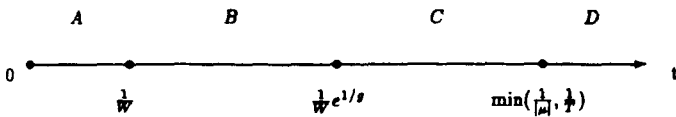


FIG. 2. Schematic time evolution of the core hole Green's function. The region *A* is governed by the relaxation of high-energy degrees of freedom. The region *B* corresponds to the intermediate asymptotics (4) and the region *C* corresponds to the potential-independent asymptotics (5), which breaks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

than the first one, which means that the perturbation theory never works for large enough t . It is also basically different from the usual case, in which the first term of the linked cluster expansion remains the main term for arbitrary large t (and, of course, for $g \ll 1$; see Refs. 7 and 8).

Equation (1) with kernel (2) cannot be solved exactly. Fortunately, for the particular problem involving the calculation of $C(t)$ one can adopt the Hamman's point of view⁹ of taking the limit $t=0, t' \rightarrow \infty$ in Eq. (1) from the beginning and then use the standard methods of solving singular integral equations.¹⁰ Not having space in this letter for mathematical details, we will present here only the results and leave the detailed justification for another, more comprehensive paper.¹¹ The exact asymptotic expression for the closed-loops contribution is

$$\text{Re } C(t) = -\frac{1}{2} \ln t, \quad t \rightarrow \infty, \quad g \neq 0. \quad (4)$$

This expression would coincide with the standard expression if we insert the scattering phase $\delta = \pi/2$. For the x-ray transition rate we have

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

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

Thus, the old x-ray problem acquires new features in the case of a metal with a van Hove singularity. The perturbation expansion leads to the unusual asymptotic $\text{Re}C(t) \sim \ln^3 t$, which serves as an intermediate one for $1/W \ll t \ll t_0 = (1/W) \exp(1/g)$ [as can be seen, for example, 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 excitations could be created independently. But it is not the case in the higher-order processes (because of the Pauli principle). As a result, for $t > t_0$ increasingly more singularities occur (with different signs). Finally, they can be summarized by the usual log-asymptotics (Fig. 2). For large enough t , therefore, the problem cannot be described, even qualitatively, in terms of independent electron-hole pairs.¹² Note that the pre-log factor is *potential independent*. This means that the limit $g \rightarrow 0$ can be reached not due to the decrease of the pre-log factor, as in the usual case, but through the shifting ($t_0 \rightarrow \infty$) of the region of applicability ($t \gg t_0$) of the result (4). The additional log factor survives in the transition rate, but with different powers of absorption and emission, which accounts for strongly asymmetric threshold. This result 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 the presence of the static potential is $\tilde{g}_0(\tau) \sim 1/\tau \ln \tau$].

Of course, expressions (3) and (4) give also the exponent for the orthogonality catastrophe¹³ (after substitution $t \rightarrow N = \text{number of particles}$). 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 is the exchange, and $J \ll W$).

An additional motivation for this work was the intention to build a simple, exactly solvable example, in which the singularity in the overlap integral is different from the usual log singularity, as is the case in the Luttinger liquid.¹⁴ We have seen that in the case of the van Hove singularity the asymptotic relation indeed changes, but only for the intermediate t , and the true limit $t \rightarrow \infty$ is governed by the usual log. Whether a similar scenario holds also for the Luttinger liquid remains unclear.

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