PHYSICAL REVIEW B VOLUME 26, NUMBER 4 15 AUGUST 1982

Renormalization-group theory for the commutative model of tunneling states in metallic glasses

J. L. Black
*Department of Physics, Brandeis University, Waltham, Massachusetts 02254, Brookhaven National Laboratory, Upton, New York 11973, and Texas Instruments, Inc., P.O. Box 226015, N/S 238, Dallas, Texas 75266**

K. Vladár
Central Research Institute for Physics, Budapest 1525, P.O.B. 49, Hungary

A. Zawadowski†
*Department of Physics, University of California, Los Angeles, California 90024**
(Received 5 March 1982)

Using the multiplicative renormalization technique, we obtain the scaling behavior of a model for tunneling states interacting with conduction electrons in which the conduction-electron-assisted tunneling is not taken into account. There is a crossover temperature which characterizes the transition from the high-temperature region where the many-body effects are effective to a region where the dynamics is frozen in. This crossover temperature is given as an effective level splitting which is reduced from its bare value due to the interaction. The renormalized coupling constants do not scale into a strong-coupling regime. Implications for the electrical resistivity are discussed, and the conclusion is drawn that if there is any logarithmic temperature-dependent term at all, the amplitude is so small that it is very unlikely to be observable.

I. INTRODUCTION

An important development in the physics of glasses has been the recent discovery of tunneling states (TLS) in metallic glasses at low temperatures.[1] These states result from local rearrangements of atoms as the glass makes quantum-mechanical transitions among configurations near the highly degenerate ground state.[2] Metallic glasses differ from insulating glasses in that TLS are coupled not only to phonons but also to conduction electrons near the Fermi surface.[3,4] Strong evidence of this electron-TLS coupling has already been seen in various ultrasonic experiments,[5,6] and this raises the question of a new Kondo-type effect with possible implications for the electrical transport properties. With this question in mind, Kondo[4,7] introduced two models, which Zawadowski and Vladár[8] have called "commutative" and "noncommutative." The essential difference between these two models is that the commutative model has only one coupling, which is the difference between the scattering amplitudes corresponding to the two positions of the tunneling atoms. In contrast, the noncommutative model has an additional coupling describing the conduction-electron-assisted tunneling process. These two couplings show different dependence on the momentum of the electrons and, in fact, do not commute. In both models, however, the underlying physics is the divergent response of an electron gas to a local time-dependent potential, which is a feature these models share with the x-ray[9] and magnetic Kondo[10] problems.

At the present time one of the most important problems is to choose the appropriate model for a given glass, as these two metallic glass models behave in very different ways. In the commutative model, as we shall see, the rate for electrons scattering on TLS is not renormalized up to fourth order in perturbation theory. The noncommutative model, however, exhibits a logarithmic enhancement of the electronic elastic scattering rate of the form $\ln^2|D/T|$, where D is the electronic bandwidth cutoff and T is the temperature. This result, first obtained by Kondo,[7] has been confirmed and extended in the renormalization-group treatment of Zawadowski and Vladár[8] and of Zawadowski.[11] Even so, the relevance of this enhancement to actual electronic transport anomalies[12] in metallic

glasses is doubtful because of the broad distributions of coupling constants and of TLS energy splittings E, which cut off the singularities when $T < E$. Thus, if the electron-assisted coupling can be treated by simple perturbation theory, the amplitude of the aforementioned $\ln^2|D/T|$ contribution is negligible.[13] The noncommutative model can result in physically significant enhancement in the electronic scattering only if the couplings exceed some threshold value beyond which it is no longer valid to keep only the first terms in the perturbation series.[14]

Returning to the commutative model, the purpose of this paper is to clarify a controversial situation regarding its electronic scattering rate. We will present calculations which strongly suggest that all previously published scattering rates[15,16] are incorrect. The actual leading logarithmic corrections can at most[17] be of the form $\ln^2|E/T|$, which is much weaker than $\ln^2|D/T|$. In the following, we shall present a multiplicative-renormalization-group analysis of the logarithmic divergences in the commutative model at low temperatures. The main physical effect we find is a downward renormalization of the TLS energy splitting with decreasing D. This result is in accord with the scaling theory of Black and Gyorffy,[15] who exploited a connection between this model and an infinite sequence of x-ray problems. The same result for E had been conjectured on the basis of low-order perturbation theory by Kondo.[4] For the rotationally-invariant electron-TLS coupling, on the other hand, we find no renormalization at all.[17] This result has been obtained in both leading and next-leading order in the coupling constants, which leads us to expect no terms of the form $\ln^2|D/T|$ in the electrical resistivity.[18]

II. THE COMMUTATIVE MODEL

The general commutative or noncommutative Hamiltonian consists of a noninteraction part H_0 plus the electron-TLS interaction H_1. These are given by

$$H_0 = \sum_k \epsilon_k a_k^\dagger a_k + E S_z \ , \tag{1}$$

$$H_1 = \sum_{kk'} (V^z_{kk'} S_z + V^x_{kk'} S_x) a_k^\dagger a_{k'} \ , \tag{2}$$

where ϵ_k is the electronic energy, E is the TLS energy splitting, and $V^i_{kk'}$ ($i = x$ or z) is a momentum-dependent coupling constant. Since the concentration of TLS is very small,[1] we consider a single TLS embedded in the electron gas. As usual,[1-4] the atomic displacements of the TLS are described by spin-$\frac{1}{2}$ operators S_i ($i = x$ or y) and E is the result of both an asymmetry energy Δ and a tunneling splitting Δ_0 with $E^2 = \Delta^2 + \Delta_0^2$. It is often useful to view Eq. (1) as the result of a rotation around the y axis in spin space, which diagonalizes a TLS Hamiltonian of the form $S_z - \Delta_0 S_x$, and we shall insist on always performing such rotations to recover the form (1) in the course of the renormalization process.

The coupling constants $V^i_{kk'}$ are derivable, in principle, on the same basis as the electron-phonon interaction,[1,4,8,20] and their magnitude has been estimated from ultrasonic experiments.[5] The crucial distinction between the commutative and the noncommutative model lies in the momentum dependence of these quantities.[7,8] The commutative model satisfies[8]

$$V^i_{k'\bar{k}} V^j_{\bar{k}k} - V^j_{k'\bar{k}} V^i_{\bar{k}k} = 0 \ , \tag{3}$$

for all $k', k, \bar{k}$ (no summation over $\bar{k}$), and this implies that V^x and V^z have the same momentum dependence. Otherwise the model is noncommutative.

If there is only one coupling, which describes the difference in the electron scattering amplitudes corresponding to the two positions of the tunneling atom,[1,19] then V^z and V^x are produced by rotation of this coupling around the y axis, implying that V^x and V^z must have the same dependence on the electron momenta. On the other hand, if the electron-assisted tunneling is considered as well, then these two couplings have different momentum dependence, and Eq. (3) is not fulfilled. In this way all terms violating (3) are smaller by an overlap factor than the commutative terms in (2).[7,8,13] Thus for TLS, with weak coupling[14] the commutative model appears to be a very good approximation.[13] If the couplings exceed some critical values,[14] the existence of divergences in the noncommutative model can render normally negligible terms quite important. Such effects have been discussed elsewhere[7,8,11,14,20] and will not be dealt with here. In what follows, we shall explore the consequences of satisfying (3) with the additional nonessential simplification that V^x and V^z are actually independent of momentum.

III. MULTIPLICATIVE RENORMALIZATION GROUP

In this section we apply the multiplicative-renormalization-group method to obtain the scaling

behavior of the commutative model. This method has been successfully applied to the x-ray, Kondo, and one-dimensional electron-gas problems, all of which (like the present problem) are characterized by logarithmic divergences in low-order perturbation theory.[21] Specifically we use the Gell-Mann–Low scheme as modified by Menyhárd and Sólyom[22] and generalize it to include the mass term ES_z. Our renormalization-group procedure consists of two distinct steps: (i) a reduction of the bandwidth cutoff from D to D' by an infinitesimal small amount which generates a new effective Hamiltonian with different coupling constants but with the same physics, and (ii) a rotation in spin space to put the new Hamiltonian into exactly the form of Eqs. (1) and (2). These steps are applied sequentially. The resulting changes in the parameters V^x, V^z, and E generate scaling trajectories which reflect the low-temperature behavior of the model.[23] The scaling equations we shall derive are the following:

$$\frac{dE}{dl}=\tfrac{1}{2}N_s(v^x)^2E\ , \tag{4}$$

$$\frac{dv^z}{dl}=-\tfrac{1}{2}N_s(v^x)^2v^z\ , \tag{5}$$

$$\frac{dv^x}{dl}=\tfrac{1}{2}N_s(v^z)^2v^x\ , \tag{6}$$

where $v^x=\rho V^x$, $v_z=\rho V^z$, $l=\ln D$, ρ is the electronic density of states (per spin) at the Fermi surface, and N_s is the spin degeneracy factor (equal to 2 for electrons).

The first step in deriving these results is to rewrite the TLS spin operators in Eqs. (1) and (2) in terms of creation and annihilation pseudofermion operators,[24] which are in fact the creation and annihilation operators of the tunneling atom if only one atom is associated with the tunneling:

$$H_0=\sum_k \epsilon_k a_k^\dagger a_k+\sum_\alpha \delta_\alpha b_\alpha^\dagger b_\alpha\ , \tag{7}$$

$$H_1=\sum_{\substack{\alpha\alpha'\\kk'}} V_{\alpha\alpha'}a_k^\dagger a_{k'}b_\alpha^\dagger b_{\alpha'}\ , \tag{8}$$

where $\alpha=\pm1$, $\delta_\alpha=\frac{1}{2}\alpha E+\lambda$, and

$$2V_{\alpha\alpha'}=V^x(1-\delta_{\alpha\alpha'})+\alpha V^z\delta_{\alpha\alpha'}$$

Following Abrikosov,[24] we have introduced the chemical potential λ, which goes to infinity at the end of the calculation to avoid simultaneous occupation of both pseudofermion states. We have verified that this procedure leads to no spurious divergences to the leading and next-leading logarithmic approximations discussed in this paper (see the Appendix).

Next we introduce the single-particle Green's functions G and $\mathcal{G}_\alpha=(\omega-\delta_\alpha)^{-1}$ (corresponding to conduction electrons and pseudofermions, respectively) and the vertex function Γ^i, $i=x,z$, corresponding to the interaction H_1. For convenience we also introduce the notation $\tilde{\Gamma}^i=\Gamma^i/V^i$ $(i=x,z)$. In the following, the energy ω will be measured from λ, thus δ_α will not contain λ.

(i) Reduction of the bandwidth. Under a change in the conduction-bandwidth cutoff from D to D', we shall verify that these quantities are multiplied by frequency-independent factors Z_1, Z_2, and Z_3:

$$G(\omega,D',V')=Z_1G(\omega,D,V)\ , \tag{9}$$

$$\mathcal{G}_\alpha(\omega/D',V')=Z_2\mathcal{G}_\alpha(\omega/D,V)\quad(\alpha=\pm1)\ , \tag{10}$$

$$\tilde{\Gamma}^i(\omega/D',V')=Z_3^{-1}\tilde{\Gamma}^i(\omega/D,V)\quad(i=x,z)\ , \tag{11}$$

$$V'^i=Z_1^{-1}Z_2^{-1}Z_3V^i\quad(i=x,z)\ , \tag{12}$$

where for the sake of simplicity the energy splitting δ_α is not indicated. Note that Z_2 and Z_3 depend on $V^x,V^z,D/D'$, but they are independent of α and i.

The quantities Z_1, Z_2, and Z_3 are calculated by perturbation theory in V. For example, a lowest-order logarithmic contribution to the vertex renormalization constant Z_3 is obtained from the parquet diagram shown in Fig. 1(a), which yields

$$\Gamma^{(a)}_{\alpha\alpha'}=\rho\sum_{\alpha_1=\pm1}V_{\alpha\alpha_1}V_{\alpha_1\alpha'}\ln|D/\omega|\ , \tag{13}$$

where ω is the frequency on the external lines. In Eq. (13) and in what follows we have consistently replaced expressions like $\ln|\omega-\delta_{\alpha_1}|$ by $\ln|\omega|$ under the assumption that the TLS splittings are

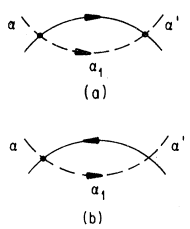

FIG. 1. Two lowest-order logarithmic contributions to the electron-TLS vertex function. The solid line represents the electron propagator, and the broken line represents the pseudofermion (TLS) propagator. These two diagrams are leading-logarithmic or "parquet" diagrams.

negligible compared to the frequency or temperature variables. The other lowest-order contribution, shown in Fig. 1(b), is the same as Eq. (13) but has the opposite sign. Thus $\tilde{\Gamma}$ is independent of D and D' to this order,[22] which means that

$$Z_3 = 1 + O(V^2 \ln |D/D'|) .$$

Furthermore,

$$Z_2 = 1 + O(V^2 \ln |D/D'|) ,$$

since its leading contribution comes from Fig. 2(d), and $Z_1 = 1$ to all orders because there can be no closed pseudofermion loops.[9,21,24] Thus there are no parquet-type leading logarithmic divergences in the commutative model, in sharp contrast with both the noncommutative model[8] and the Kondo problem.[21]

Nontrivial renormalization does occur, however, in the next order of logarithmic perturbation theory. Consider the vertex corrections shown schematically in Figs. 2(a)–2(c). The first two of these are parquet-type and can be shown to cancel against each other as was the case with the contributions in Fig. 1. The diagram in Fig. 2(c), however, survives and leads to

$$Z_3 = 1 + \tfrac{1}{4} N_s [(v^z)^2 + (v^x)^2] \ln |D/D'| , \quad (14)$$

where Z_3 is independent of α and includes the spin-degeneracy (true electron spin) factor N_s because of the closed electron loop.

Finally, consider the pseudofermion self-energy diagram shown in Fig. 2(d). This yields, using the notation $\mathcal{G} = (\mathcal{G}^{(0)-1} - \Pi)^{-1}$,

$$\Pi_{\alpha\alpha'} = -\rho^2 N_s \sum_{\alpha_1} V_{\alpha\alpha_1} V_{\alpha_1\alpha'} (\omega - \delta_{\alpha_1}) \ln |D/\omega| . \quad (15)$$

The part of Eq. (15) proportional to ω leads to "wave-function renormalization" given by

$$Z_2 = 1 + \tfrac{1}{4} N_s [(v^z)^2 + (v^x)^2] \ln |D/D'| , \quad (16)$$

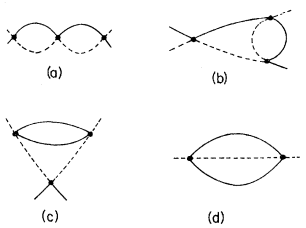

FIG. 2. Various contributions of order V^3. Diagrams (a) and (b) are leading-logarithmic (parquet) terms as in Fig. 1. Diagrams (c) and (d) are next-leading-logarithmic contributions.

from which Z_2 is now seen to be independent of α and to be precisely equal to Z_3 and hence able to cancel it completely. Thus the net effect of Z_2 and Z_3 in Eq. (12) is seen to be

$$V'_{\alpha\alpha'} = V_{\alpha\alpha'} . \quad (17)$$

This means that step (i) of our renormalization group leads to a new Hamiltonian with exactly the same values of v^x and v^z. Nontrivial effects must come from the mass renormalization terms which we now discuss. The terms in Eq. (15) which are proportional to δ_{α_1} lead to "mass renormalization" for the pseudofermions. This possibility has not yet been taken into account in Eq. (10), which must be generalized to read

$$\mathcal{G}(\omega/D', V', E', \Delta'_0) = Z_2 \mathcal{G}'(\omega/D, V, E, 0) . \quad (18)$$

In Eq. (18) it is now explicitly recognized that lowering the cutoff from D to D' will generate an off-diagonal mass term Δ'_0 [corresponding to adding $\Delta'_0 S_x$ to Eq. (1)], even though the starting Hamiltonian contains only the diagonal splitting E. In particular, Eqs. (15) and (18) yield

$$E' = E[1 - \tfrac{1}{2} N_s (v^x)^2 \ln |D/D'|] , \quad (19)$$

$$\Delta'_0 = -\tfrac{1}{2} N_s E v^x v^z \ln |D/D'| . \quad (20)$$

(ii) Rotation around y axis to eliminate Δ'_0. We now implement step (ii) by rotating the pseudospin axes so as to eliminate Δ'_0 and recover a Hamiltonian in the form of Eq. (1). This rotation[1,2] leads to new coupling constants (doubled primed) given by

$$E'' = [(E')^2 + (\Delta'_0)^2]^{1/2} \cong E' , \quad (21)$$

$$(v^z)'' = (E'')^{-1} [E' v^z - \Delta'_0 v^x] \cong v^z - (\Delta'_0/E) v^x , \quad (22)$$

$$(v^x)'' = (E'')^{-1} [\Delta'_0 v^z + E' v^x] \cong (\Delta'_0/E) v^z + v^x , \quad (23)$$

where the second equality ($\cong$) neglects terms of higher than first order in the infinitesimal $\ln |D/D'|$. The final results presented in Eqs. (4)–(6) are now easily obtained from Eqs. (21)–(23) by making use of Eqs. (19) and (20) (in the limit that $E'' - E = dE$, $\ln D' - \ln D = dl$, etc.).

IV. RESULTS AND DISCUSSION

The low-temperature behavior of the commutative model can be inferred via scaling argu-

ments[21,23] from the solution to Eqs. (4)–(6) as $D=e^{l}D'$ decreases toward zero. The first thing to notice is that Eqs. (5) and (6) imply that

$$\frac{dg}{dl}=0 \tag{24}$$

and

$$\frac{d\ln(v^x/v^z)}{dl}=\tfrac{1}{2}N_s g^2 , \tag{25}$$

where $g^2=(v^x)^2+(v^z)^2$ is the rotationally invariant coupling constant. Then, using the fact that $d(Ev^z)/dl=0$, we obtain the solution

$$g^2=(v^x)^2+(v^z)^2 =(v_0^x)^2+(v_0^z)^2 , \tag{26}$$

$$v^x/v^z=(v_0^x/v_0^z)(D/D_0)^{(1/2)N_s g^2} , \tag{27}$$

$$\left[\frac{E}{E_0}\right]^2=\frac{1+(v^x/v^z)^2}{1+(v_0^x/v_0^z)^2} , \tag{28}$$

whose main features are illustrated in Fig. 3. The subscripts (D_0, E^0, etc.) refer to the initial values of the parameters. Note that if we could follow the trajectories to arbitrarily small D, the effective Hamiltonian would approach a fixed-point Hamiltonian with $v^x=0$, $v^z=g$, and

$$E/E_0=[1+(v_0^x/v_0^y)^2]^{-1} ,$$

whose properties are trivial to obtain because there

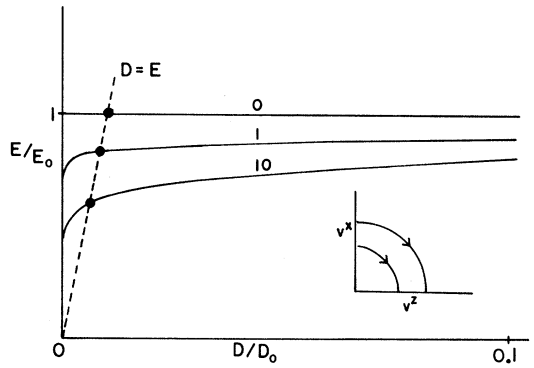

FIG. 3. Plot of the renormalized energy splitting E vs the cutoff D for three different values of the ratio v_0^x/v_0^x. The value of this ratio is shown above each curve. The dashed line represents $E=D$ for the case in which $D_0/E_0=100$. (In actual cases $D_0/E_0=10^4$ and the dashed line is almost vertical.) The intersections (solid dots) determine the crossover temperature T_0^*. These curves were obtained with $N_s g^2=0.2$. The inset shows the trajectories followed by v^x and v^y.

are no longer any off-diagonal terms which can flip spins.

In actuality we never reach this fixed point because a key element in our renormalization-group analysis breaks down as D decreases. This element is our neglect of E compared with ω (or temperature) in deriving our scaling equations. What eventually happens, as illustrated in Fig. 3, is that the cutoff D becomes comparative to the effective TLS splitting E as soon as $D=k_B T^*$, where T^* is given by

$$k_B T^*=\begin{cases} E_0(E_0/D_0)^{(1/2)N_s g^2}, & v_0^x \gg v_0^z \\ E_0\{1-\frac{1}{2}(v_0^x/v_0^z)^2[1-(E_0/D_0)^{N_s g^2}]\}, & v_0^x \ll v_0^z , \end{cases} \tag{29}$$

For temperatures less than the crossover temperature T^*, the behavior of the metallic-glass system changes markedly, just as in the case of magnetic systems at low temperature where the magnetic moments are quenched by an external magnetic field. The physics of T^* is easy to understand. For a noninteracting system ($g^2=0$), T^* is simply the temperature at which the TLS freezes into its ground state in the presence of the splitting E_0. It is only when $T<T^*$ that the TLS notices a preferred direction in spin space. For $g^2\neq 0$, the interpretation is still spin freezing, but now the splitting is reduced due to Anderson's overlap catastrophe.[26] It is clear that Eq. (29) generalizes the conclusions of Kondo[4] and of Black and Gyorffy,[15] which were derived in the special case $v_0^z=0$.

Aside from this result for T^*, the main conclusion to be drawn from our analysis is that the rotationally invariant coupling g^2 neither increases nor decreases as the temperature is lowered toward T^*. This result [Eq. (24)] is valid up to order g^3 assuming that $E \ll D$.[18] The implication is that a weak-coupling commutative model ($g \ll 1$) scales to a weak-coupling commutative model, in qualitative agreement with Ref. 14. This behavior is in clear contrast with the Kondo problem[23] and with the noncommutative model,[8,11] both of which scale into a strong-coupling regime where the analytic renormalization-group equations are no longer valid.

Turning finally to the electronic scattering rate, our analysis indicates that divergent terms of the form $(v_0^x)^2(v_0^z)^2\ln^2|D_0/T|$ should *not* be present despite two published perturbation calculations[15,16] reporting such terms in the inelastic channel.[17] First of all, in the case $E \ll k_B T$, we find no loga-

rithmic terms because g^2 is invariant[27] and the normalization does not provide any logarithmic contribution (cf. the Appendix). In the other case, $E \gg k_B T$, the inelastic channel cannot contribute, and thus the elastic rate proportional to v_z^2 dominates. In this case the coupling v_z can depend on E via a logarithmic term $\log(D/E)$ due to scaling given by Eq. (5). This term is proportional to $(v^x)^2(v^z)^2\log(D/E)$, but taking an average over the constant distribution of TLS energy $E > k_B T$ results in a term like $\Upsilon(v^x)^2(v^z)^2\log(D/T)$, which is monotonically decreasing with decreasing temperature. We do not believe that the small correction of this type is observable.

It is important to note that we considered only electronic scattering terms involving $\ln|D_0/T|$ and not, for example, much weaker terms involving $\ln|E_0/T|$. Terms of the latter form could arise after the crossover into the region $D < k_B T^*$, where the rotational symmetry is broken and where the present analysis is no longer valid. It is quite possible that corrected perturbation calculations will reveal such enhancements of the inelastic scattering rate.[17] Because of the recent conjectures[28] that TLS-induced inelastic processes may influence the experimental observation of electronic localization effects in amorphous metals, this question warrants further scrutiny.

In summary, we have derived renormalization-group equations valid up to order V^3 for the commutative model of tunneling states in metallic glasses. We find a crossover temperature T^*, which agrees with and generalizes previous calculations on this model. We also find, however, that published calculations for the electronic scattering rates are undoubtedly incorrect. Unlike the Kondo problem and the noncommutative model of metallic glasses, this model does not scale into a strong-coupling regime and the electrical resistivity is not enhanced at low temperature. These conclusions point to the need for more careful perturbative calculations of the scattering rate. The noncommutative model will be discussed elsewhere.[14,20]

ACKNOWLEDGMENTS

We would like to thank V. J. Emery, G. Grinstein, B. Gyorffy, and P. Nozières for helpful discussion. One of us (A.Z.) is also grateful to J. Sólyom and I. Tüttó for discussion on the consideration presented in the Appendix; furthermore, to the Department of Physics of UCLA for kind hospitality, and to the National Science Foundation (Grant No. DMR 78-10312) for partial financial support. The work at Brookhaven was supported by the Division of Basic Energy Sciences, U.S. DOE, under Contract No. EY-76-C-02-0016.

APPENDIX

In the main part of the paper we have referred to electrical resistivity several times, but no detail has been given. The validity of calculation of electrical resistivity depends very much on the applicability of Abrikosov's pseudofermion technique.[24] Therefore, the main part of this appendix deals with the normalization procedure in this technique. The normalization consideration given below is valid in both the magnetic impurity and TLS problem.

For the sake of simplicity, s-wave scattering is assumed, implying that the electron lifetime τ_e and the transport lifetime $\tau_{\rm tr}$ are the same. The lifetime in the leading and next-to-leading logarithmic order will be determined, keeping terms proportional to $V^n\log^{n-2}$ and $V^n\log^{n-3}$, where V stands for the coupling. In the pseudofermion technique the electron lifetime is

$$\tau_e^{-1} = 2\lim_{\lambda\to\infty}\frac{\mathrm{Im}\Sigma_e}{\langle N_{\rm ps}\rangle}\ , \tag{A1}$$

where Σ_e is the electron self-energy and $\langle N_{\rm ps}\rangle$ is the average number of pseudofermions at temperature T and at fictitious pseudofermion energy λ. The limit $\lambda\to\infty$ is taken to avoid double occupation of pseudofermions. Abrikosov[24] has shown that in the leading logarithmic order

$$\langle N_{\rm ps}\rangle = (2S+1)e^{-\beta\lambda}\ , \tag{A2}$$

where S is the spin of the pseudofermion. Thus in case of TLS, we have

$$\langle N_{\rm ps}\rangle = 2\exp(-\beta\lambda)\ .$$

If the calculations are carried out beyond the leading logarithmic order, then special care is required to show that $\langle N_{\rm ps}\rangle$ does not contain logarithmic corrections. In what follows we shall establish that such logarithmic corrections are absent in both the leading and the next-to-leading orders. In a previous calculation by Fazekas and Zawadowski[29] the normalization factor was incorrectly determined, resulting in an incorrect coefficient in the expansion of the magnetic susceptibility, as has been pointed out by Sólyom[30] [a renormalization factor Z is missing in the expression (53) of Ref. 29]. In the present calculation the numerator and the

denominator of Eq. (A1) will be studied separately to establish the absence of $\ln|D/T|$ corrections in the electrical resistivity for the commutative model.

It is important to point out the validity of any calculation using pseudofermion representation, for the spin relies on the correctness of the normalization. As we can prove the normalization procedure only in the framework of leading and of next-to-leading logarithmic approximations the validity of calculation (e.g., that be Abrikosov and Migdal[31] for the Kondo effect) beyond these orders is in doubt.

(i) The study of $Im\Sigma_e$. The diagram providing contributions to $\mathrm{Im}\Sigma_e(k_BT)$ $(\omega < k_BT)$ of the form $V^n\log^{n-2}$ and $V^n\log^{n-3}$ is shown in Fig. 4. In general the diagram of order n contains $n-1$ electron lines, and the integration with respect to the corresponding kinetic energy variables may result in logarithmic terms. However, taking the imaginary part at the cut indicated in Fig. 4, one of the electron energy integrals is limited to the region of Fermi energy. Thus not more than $n-2$ logarithmic integrals remain. If a cut with three electron lines is considered, then three energy integrals are limited and $n-4$ logarithmic integrals may occur, yielding a negligible term. The diagram in Fig. 4 contains two vertices and two pseudofermion lines and thus transforms like the square of the renormalized couplings in the renormalization-group transformation. In the case of TLS, performing simple spin algebra shows that the contribution is proportional to $(V^x)^2+(V^z)^2 = g^2$, which is an invariant. Thus, $\mathrm{Im}\Sigma_e$ does not contain any logarithmic correction in the order considered here. This statement does not hold in the case of the noncommutative model and of the Kondo problem, because the strengths of the couplings scale to infinity.

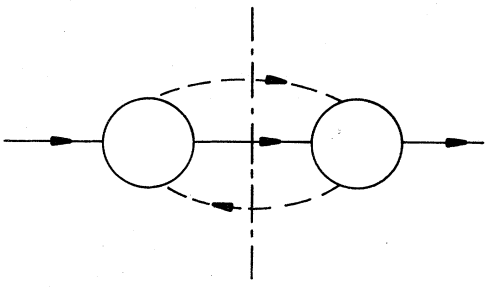

FIG. 4. Electron self-energy diagram with intermediate state represented by —·— line. There is only one electron in the intermediate state.

(ii) The study of $\langle N_{ps}\rangle$. The following treatment is valid for general spin S. The spectral function of pseudospin is introduced as

$$\rho_{\lambda\alpha}(\omega) = -\frac{1}{\pi}\mathrm{Im}\mathcal{G}(\omega+i\delta) = \frac{1}{\pi}\frac{|Im\Sigma_\alpha|}{(\tilde{\omega}_\alpha-\mathrm{Re}\Sigma'_\alpha)^2+(\mathrm{Im}\Sigma'_\alpha)^2}\ , \tag{A3}$$

where $\mathcal{G}$ stands for the pseudofermion Green's function and

$$\tilde{\omega}_\alpha=\omega-\tilde{\delta}_\alpha=\omega-\lambda-\tfrac{1}{2}\alpha-\mathrm{Re}\Sigma_\alpha(\tilde{\omega}_\alpha=0)\ ,$$

where H_{eff} is the effective magnetic field acting on the spin α (in case of TLS H_{eff} is the renormalized energy splitting). Furthermore, a subtraction

$$\mathrm{Re}\Sigma'_\alpha(\omega_\alpha)=\mathrm{Re}\Sigma_\alpha(\omega_\alpha)-\mathrm{Re}\Sigma_\alpha(\tilde{\omega}_\alpha=0)$$

has been applied. The quantity $\tilde{\delta}_\alpha$ is the renormalized version of δ_α introduced by Eq. (7). Using the definition of the spectral function (A3), the averaged occupation number of pseudofermions is

$$\langle N_{\mathrm{ps}}\rangle=\sum_\alpha\int d\omega\, n_F(\omega)\rho_\alpha(\omega)\ , \tag{A4}$$

where $n_F(\omega)$ is the Fermi function.

In addition, the spectral function $\rho_\alpha(\tilde{\omega})$ obeys the sum rule

$$\int\rho_\alpha(\omega)\,d\omega=1\ . \tag{A5}$$

If the width of the pseudofermion spectral function at the resonance is small compared with k_BT, then it is useful to divide the range of integration with respect to $\tilde{\omega}_\alpha$ as

$$\int_{-D}^{D}d\tilde{\omega}_\alpha\cdots=\int_{-D}^{-k_BT}d\tilde{\omega}_\alpha\cdots+\int_{-k_BT}^{k_BT}d\tilde{\omega}_\alpha\cdots+\int_{k_BT}^{D}d\tilde{\omega}_\alpha\cdots\ . \tag{A6}$$

In the first and in the last integral $\mathrm{Im}\Sigma$ and $\mathrm{Re}\Sigma/\tilde{\omega}_\alpha$ are functions of $\tilde{\omega}_\alpha$, while in the middle region they are functions of k_BT. [$\mathrm{Re}\Sigma$ is proportional to $\tilde{\omega}_\alpha$ as can be seen from Eq. (15) and from Eqs. (20) and (21), in Ref. 29.] In case $|\tilde{\omega}_\alpha|\ll k_BT, \mathrm{Re}\Sigma=-\tilde{\omega}_\alpha\alpha_\Sigma$ holds where α_Σ is a polynomial of the coupling and of $\log k_BT$. The contribution of the middle region to the sum rule given by Eq. (34) can be calculated easily, and by making use of $|\mathrm{Im}\Sigma|<k_BT$ it gives

$$\int_{-k_BT}^{k_BT}d\tilde{\omega}_\alpha\rho_\alpha(\tilde{\omega}_\alpha)=Z=\frac{1}{1+\alpha_\Sigma}\sim 1-\alpha_\Sigma\ , \tag{A7}$$

where Z is the strength of the pole and has the

form

$$Z=1+\cdots V^2\log\cdots+\cdots V^3\log\cdots .$$

Furthermore, for the other two regions the spectral function (34) can be approximated as

$$\rho_\alpha(\tilde{\omega}_\alpha)\approx\frac{1}{\pi}\frac{\mathrm{Im}\Sigma_\alpha(\tilde{\omega}_\alpha)}{\tilde{\omega}_\alpha^2} , \tag{A8}$$

where the terms beyond the leading and next-to-leading approximations are dropped.

For the forthcoming considerations the identity

$$\mathrm{Im}\Sigma_\alpha(-\tilde{\omega}_\alpha)=\mathrm{Im}\Sigma(\tilde{\omega}_\alpha)\exp(-\beta\tilde{\omega}_\alpha) \tag{A9}$$

will be used. This is valid for $\beta H_{\mathrm{eff}}\ll 1$ and will be proved at the end of this appendix. It is obvious from this identity that the first region does not contribute to the sum rule in the leading and next-leading logarithmic order. The last integral provides typical logarithmic contributions as $\mathrm{Im}\Sigma_\alpha\sim\tilde{\omega}_\alpha$ holds for $\tilde{\omega}_\alpha>k_BT$. It is straightforward to check for both the TLS and the Kondo problem that this integral combined with (A7) satisfies the sum rule, thus

$$\int_{k_BT}^{D}\rho_\alpha(\tilde{\omega}_\alpha)d\tilde{\omega}_\alpha=\alpha_\Sigma . \tag{A10}$$

See Ref. 29 for detailed calculation.

Turning to the averaged occupation number given by Eq. (A4) we consider

$$\langle N_{\mathrm{ps},\alpha}\rangle=\int d\tilde{\omega}_\alpha n_F(\tilde{\omega}_\alpha+\delta_\alpha)\rho_\alpha(\tilde{\omega}_\alpha) . \tag{A11}$$

Let us divide the integral into three parts again, like (A6), and use the approximation

$$n_F(\omega_\alpha\lambda+\delta_\alpha)\sim\exp[-\beta(\omega_\alpha\lambda+\delta_\alpha)] .$$

The middle integral has the value $\exp(-\beta\delta_\alpha)(1-\alpha_\Sigma)$. Furthermore, as a consequence of identity (A9) and Eq. (A10), the first integral gives $\alpha_\Sigma\exp(-\beta\delta_\alpha)$ and the last one is negligible. It is interesting to note that, in case of sum rule (A5), the low-energy tail (and in case of occupation number the high-energy tail) does not contribute. Thus the nonlogarithmic normalization factor (31) has been verified in weak external fields (H_{eff}) and weak-coupling ($\beta\,\mathrm{Im}\Sigma\ll 1$) regions.

(iii) The proof of identity (38). The imaginary part of the self-energy Σ can be calculated from the following expression:

$$\mathrm{Im}\Sigma_\alpha(\tilde{\omega}_\alpha)=2\pi\sum_\beta\int d\xi_1 d\xi_2\,|\,\Gamma_{\alpha\beta}(\tilde{\omega}_\alpha,0,\xi_1\xi_2)\,|^2 \times[1-n_F(\xi_2)]n_F(\xi_1) \times\delta(\tilde{\omega}_\alpha+\delta_\alpha-\delta_\beta-(\xi_2-\xi_1)) , \tag{A12}$$

where there is one electron and one hole in the intermediate state with energies ξ_1 and ξ_2, respectively; furthermore, there is one pseudoparticle with $\tilde{\omega}_\beta=0$. In case of magnetic impurities the electron spin variables must be indicated, as well. The vertex Γ has two pseudofermion and two electron legs, and it includes the coupling. In order to prove identity (A9) let us change the signs of variables $\tilde{\omega}_\alpha$, ξ_1, and ξ_2 in expression (A12). The identity holds at

$$|\,\Gamma(\tilde{\omega}_\alpha,0,\xi_1,\xi_2)\,|^2=|\,\Gamma(-\tilde{\omega}_\alpha,0,-\xi_1,\xi_2)\,|^2 .$$

In order to prove (A9) for $\mathrm{Im}\Sigma$, up to terms like $V^{n+2}\log^n$, one should use the expression for Γ in the leading logarithmic order, where Γ is real and depends only on the absolute values of combinations of the variables. Hence the result is proved.

Finally, one can make the following remark. If H_{eff} is large, then the above proof fails at several points, but the normalization factor can be nevertheless generalized:

$$\langle N_{\mathrm{ps}}\rangle_\lambda=\sum_\alpha\exp(-\beta\delta_\alpha) , \tag{A13}$$

which holds instead of (A2). The proof is similar, but one should consider the non-spin-flip and spin-flip parts of $\mathrm{Im}\Sigma$ separately. Thus one can write

$$\mathrm{Im}\Sigma_\alpha(\tilde{\omega}_\alpha)=\sum_{\alpha_1}\mathrm{Im}\Sigma_\alpha^{\alpha_1}(\tilde{\omega}_\alpha) , \tag{A14}$$

where α_1 is the pseudospin in the intermediate state considered in Eq. (A12). Then one can derive the following generalization of identity (A9)

$$\mathrm{Im}\Sigma_{-\alpha}(-\tilde{\omega}_\alpha)=e^{-\tilde{\omega}\beta}\{\mathrm{Im}\Sigma_\alpha^\alpha(\tilde{\omega}_\alpha)+\exp[-\beta(\delta_\alpha-\delta_{-\alpha})]\mathrm{Im}\Sigma_\alpha^{-\alpha}(\tilde{\omega}_\alpha)\} , \tag{A15}$$

in a similar manner as (A12) has been proved. Using this identity instead of (A9) one can prove Eq. (A13).

In this limit ($E\beta>1$) the electrical resistivity is influenced by E as well, because the non-spin-flip and spin-flip contributions have different thermal weights, thus the resistivity is not simply proportional to the invariant $(V^x)^2+(V^z)^2$. The resistivi-

ty is found to be proportional,

$$(v^z)^2+(v^x)^2\frac{\min[exp(-\beta\delta_\alpha)+\exp(-\beta\delta_{-\alpha})]}{\exp(-\beta\delta_\alpha)+\exp(-\beta\delta_{-\alpha})}$$
$$\approx(v^z)^2+(v^x)^2\exp[-\beta(\delta_\alpha-\delta_{-\alpha})]\ , \quad \text{(A16)}$$

where the last approximation is valid if $(\delta_\alpha-\delta_{-\alpha})\beta\simeq E\beta\gg 1$. This result means that the off-diagonal scattering is frozen in. In this case we can have logarithmic correction of type $\log(D/E)$ for the following reason. The scaling given by Eqs. (5) and (6) results in a rotation in the coupling constant plane v^x-v^z, but this rotation does not leave expression (A16) invariant. The contribution is of type $(v^z)^2(v^x)^2\log(D/E)$. In order to estimate the resistivity we must integrate over the variable E with a uniform weight factor. This may result in a correction term as $T(v^z)^2(v^x)^2\log(D/T)$ which is decreasing with decreasing temperature.

---

*Present address.
†Permanent address: Central Research Institute for Physics, Budapest 1525 P.O.B. 49, Hungary.

[1]J. L. Black, in *Metallic Glasses,* edited by H. J. Güntherodt (Springer, New York, 1981), p. 167.
[2]W. A. Phillips, J. Low Temp. Phys. 7, 351 (1972); P. W. Anderson, B. I. Halperin, and C. M. Varma, Philos. Mag. 25, 1 (1972).
[3]R. Cochrane, R. Harris, J. Ström-Olson, and M. Zuckerman, Phys. Rev. Lett. 35, 676 (1975).
[4]J. Kondo, Physica (Utrecht) 84B, 40 (1976).
[5]B. Golding, J. E. Graebner, A. B. Kane, and J. L. Black, Phys. Rev. Lett. 41, 1487 (1978); P. Doussineau, J. Phys. (Paris) Lett. 42, L83 (1981); W. Arnold, P. Doussineau, Ch. Frenois, and A. Levelut, *ibid.* 42, L289 (1981); G. Weiss, S. Hunklinger, and H. v. Löhneysen, in *Proceedings of the 16th International Conference on Low Temperature Physics LT-16, Los Angeles, 1981,* edited by W. G. Clark, [Physica (Utrecht) 108B-C, Part III (1982)].
[6]G. Weiss, W. Arnold, K. Dransfeld, and H. J. Guntherodt, Solid State Commun. 33, 111 (1980).
[7]J. Kondo, Physica (Utrecht) 84B, 207 (1976).
[8]A. Zawadowski and K. Vladár, Solid State Commun. 35, 217 (1980).
[9]P. Nozières and C. T. DeDominicis, Phys. Rev. 178, 1097 (1969); S. Doniach and M. Sunjic, J. Phys. C 3, 285 (1970).
[10]P. W. Anderson, C. Yuval, and D. R. Hamann, Phys. Rev. B 1, 4464 (1970).
[11]A. Zawadowski, Phys. Rev. Lett. 45, 211 (1980).
[12]S. Kobe and A. R. Ferchin, J. Mater. Sci. 12, 1713 (1977); R. Hasegawa and C. C. Tsuei, Phys. Rev. B 2, 1631 (1970); R. W. Cochrane and J. O. Stron-Ölsen, J. Phys. F 7, 1799 (1977).
[13]Noncommutative coupling terms can be shown (see Refs. 1, 4, and 7) to be proportional to Δ_0/ω_0, where Δ_0 is the tunneling energy and ω_0 is the zero-point energy. This means that logarithmically divergent terms acquire a factor of $(\Delta_0/\omega_0)^2$, which leads to an overall contribution of the form $T^3\ln^2 T$ after integrating over a constant TLS density of states up to $E\simeq k_BT$. Such a factor of T^3 would completely mask the logarithmic divergence.
[14]K. Vladár and A. Zawadowski, Solid State Commun. 41, 649 (1982); A. Zawadowski, in *Proceedings of the Conference on Trends in Physics* (European Physical Society, Istanbul, 1982).
[15]J. L. Black and B. L. Gyorffy, Phys. Rev. Lett. 41, 1595 (1978).
[16]H. Keiter and G. Morandi, Phys. Rev. B 22, 5004 (1980).
[17]A reexamination of the perturbation theory indicates that the logarithmic terms occur only in the inelastic channel and have a $\mathrm{sech}^2(E/T)$ prefactor, in agreement with Ref. 16. Additional cancellations not previously noted, however, preclude the possibility of $\ln^2(D/T)$ terms, leaving at most the possibility of $\ln^2(E/T)$ terms, in disagreement with Ref. 16. Details of this analysis will be published elsewhere.
[18]The apparent disagreement with Ref. 15 on this point reflects the fact that they retained terms of the form $(E/D)^2\ln D$, which we systematically discard. Such terms represent very weak corrections and are probably nonuniversal.
[19]J. L. Black, B. L. Gyorffy, and J. Jäckle, Philos. Mag. B40, 331 (1979).
[20]K. Vladár and A. Zawadowski (unpublished).
[21]A. Zawadowski, in *Proceedings of Nobel Symposium XXIV, Uppsala, 1973* (Almquist and Wiksell, Uppsala, Sweden, 1973), p. 76, J. Sólyom, J. Phys. F 4, 2269 (1974); M. Fowler and A. Zawadowski, Solid State Commun. 9, 471 (1971).
[22]N. Menyhárd and J. Sólyom, J. Low Temp. Phys. 12, 529 (1973).
[23]P. Nozières, J. Phys. (Paris) 37, C-271 (1976); K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975); H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B 21, 1003 (1980).
[24]A. A. Abrikosov, Physics 2, 5 (1965).
[25]This statement is true regardless of whether we assume $|\delta_\alpha| \ll \omega$.
[26]P. W. Anderson, Phys. Rev. Lett. 18, 1049 (1964).
[27]Our argument relies on the observation that any logarithmic rate contribution of the form $\ln^n|D/T|$ must be unchanged as $E\to 0$ as long as $T\gg E$. In the limit of vanishing E, the Hamiltonian becomes isotropic in spin space, implying that the only dependence of the

rate upon the coupling constant is via g^2 (see the Appendix).

[28]D. J. Thouless, Solid State Commun. 34, 683 (1980); N. Giordano, W. Gilson, and D. E. Prober, Phys. Rev. Lett. 43, 725 (1979); P. Chaudhuri and H. U. Habermeier, Solid State Commun. 34, 687 (1980).

[29]A. Zawadowski and P. Fazekas, Z. Phys. 226, 235 (1969).

[30]J. Sólyom (private communication).

[31]A. A. Abrikosov and A. A. Migdal, J. Low Temp. Phys. 3, 519 (1970).