Theory of the interaction between electrons and the two-level system in amorphous metals. II. Second-order scaling equations

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A general Hamiltonian for the interaction between conduction electrons and the two-level system is considered. Renormalization-group equations of second order are constructed with the use of the multiplicative renormalization-group technique. The mass renormalization is treated in detail to determine the effect of screening by conduction electrons on the energy splitting E. The crossover temperature $T_K = D(v^x v^z)^{1/2}(v^x/4v^z)^{1/4v^z}$ between the weak and strong coupling regions is determined, and it is reduced by 2 orders of magnitude compared to the expression obtained in first-order scaling. The scaled values of the couplings are calculated analytically. In the crossover region the off-diagonal couplings are $v^x \sim v^y \sim \frac{1}{8}$. The crossover temperature can be found in the region of physical interest ($T_K > 1$ K) if the initial diagonal coupling $v^z > 0.2$. In this case, the energy splitting calculated is reduced by more than 2 orders of magnitude. That reduction results in a large enhancement in the distribution of the energy splitting at the low-energy side. The position of the lower end of the scaling region is discussed where scaling in terms of temperature is hindered by the energy splitting.

I. INTRODUCTION

A general theory of the interaction between conduction electrons and two-level systems (TLS) has been presented in the preceding paper (paper I).[1] This theory treats the infrared divergencies at the Fermi surface which are due to the screening by conduction electrons. The relevant dimensionless variables are energies over the conduction-electron bandwidth cutoff and the logarithmic corrections depend on those variables. In the noncommutative model the first-order vertex corrections contain logarithmic terms, contrary to the commutative model[2] and to the Mahan–Nozières–De Dominicis (MND) x-ray absorption problem.[3] In the noncommutative case it has been demonstrated[1,4] by constructing a simple scaling equation in terms of the bandwidth cutoff D that a weak coupling problem scales to the strong coupling limit. In a more appropriate theory the scaling equation has the general form

$$\frac{dv^i}{d\ln D} = \beta(v) , \tag{1.1}$$

where the β function is a polynomial of the coupling v. In the first-order scaling, β is a quadratic function, and in the second-order scaling third powers appear as well. In the analytical formulation of scaling the difficulty is that the β function can be constructed only in the framework of perturbation theory. Disregarding the possibility of nonenhanced couplings, a fast convergence is expected only if there is a small parameter in the problem such as ϵ for phase transition in dimension 4-ϵ. Since in the present problem there is no small parameter, the fixed points are expected to be either infinite or of order of unity. Furthermore, considering the Kondo problem, Anderson[5] and Fowler[6] argued against the existence of a finite fixed point on the basis that the problem can be mapped on a one-dimensional problem, which cannot exhibit phase transition at finite temperature and, therefore, singularity cannot occur either for any finite coupling. Since there is a strong resemblance between the Kondo and the present problem, this argument must hold here also. Thus one can expect the fixed points in the infinity and a scaling to an isotropic problem as has been suggested in paper I.[1]

The crossover between the weak and strong coupling regions has already been treated using first-order scaling in paper I. In higher-order calculations the crossover temperature T_K is modified. That has been shown for the Kondo problem by Abrikosov and Migdal[7] and by Fowler and

Zawadowski[8] who applied the multiplicative renormalization-group technique developed by Gell-Mann and Low[9] for field theory. These works have been initiated by the scaling argument of Anderson, Yuval, and Hamann.[10] In the second-order scaling the modified Kondo temperature is

$$T_K = D(2J\rho_0)^{1/2}\exp(-1/2J\rho_0)\ , \tag{1.2}$$

where J is the exchange coupling between the conduction electrons and the localized impurity spin and, furthermore, ρ_0 is the conduction-electron density of states for one spin direction at the Fermi level. In this expression the square-root term is the correction to the Kondo temperature obtained in first-order scaling. Furthermore, it must be emphasized that the expression (1.2) is correct only in the case of weak initial coupling, since only the singular terms of the initial couplings are kept[11]:

$$T_K = D\exp\left[-\frac{1}{2J\rho_0}+\tfrac{1}{2}\ln(2J\rho_0)+P(J\rho_0)\right]\ , \tag{1.3}$$

where the correction to expression (1.2) is analytical since $P(J\rho_0)$ is a polynomial. This polynomial is of importance only if the initial coupling $J\rho_0$ is not weak, and that can be determined only by numerical methods. Since the second-order scaling equations provide correctly the singular contributions to T_K, there is no reason to perform higher-order scaling in analytical form.

The first aim of the present paper is to determine the crossover temperature similar to expression (1.2) for the present problem. The result of the present paper[12] is

$$T_K = D(v^x v^z)^{1/2}(v^x/4v^z)^{1/4v^z}\ , \tag{1.4}$$

where v^z and v^x are the diagonal and the electron-assisted dimensionless couplings, respectively. The correction to the first-order scaling expression is essential, because $(v^x v^z)^{1/2}\sim 10^{-2}$.

The second aim of introducing the second-order scaling is to find mass renormalization similar to those found by Black and the present authors[2] for the commutative model. It will be shown that in the present case, due to the screening by conduction electrons, the renormalization of the TLS energy splitting E can be a reduction even larger than 2 orders of magnitude. Since at a given temperature T only those TLS can be excited for which $E \lesssim k_B T$, in determining the number of active TLS the reduction plays a crucial role. As has been shown in other problems, the self-energy correction of present interest is connected with vertex corrections by Ward identities (see, e.g., Refs. 13 and 8). These vertex corrections of second order will be taken into account.

In the present paper, a simplified version of the Gell-Mann and Low[9] renormalization group is applied which has been proposed by Sólyom studying the problem of one-dimensional conductors with Menyhárd[14] (see also Ref. 15). The new feature of that method is that the existence of scaling is *a priori* assumed and later checked in the approximation used. The elimination of the unimportant part of the phase space is associated with introducing new couplings. The remaining differences are incorporated in the multiplicative renormalization constants which depend only on the ratio of the new and old cutoffs and on the couplings.

The commutative model has been first attacked, using the renormalization group, by Black and Gyorffy[16] applying a method suggested by Anderson, Yuval, and Hamann.[10] Later, Black and the present authors[2] applied the method of Sólyom in more detail and the technique for the mass renormalization has been worked out. The behavior of the commutative model is relatively simple, because the combination of the couplings $(v^x)^2+(v^z)^2$ is invariant under the scaling, which does not hold in the present case. The common feature, however, of these problems is that starting with a diagonal TLS Hamiltonian ($\Delta^x=\Delta^y=0$) the renormalization leads to off-diagonal self-energy terms. Thus in every step of the renormalization group the off-diagonal terms generated must be transformed out by a rotation in the quasispin space of the TLS.

The paper is organized as follows. In Sec. II the Hamiltonian is given in terms of some new notations introduced for convenience; furthermore, the basic schema of the renormalization-group transformation is presented. In Sec. III the second-order self-energy and vertex corrections are calculated and a set of renormalization-group equations is constructed. In order to determine the correct expression for the crossover temperature these equations for the couplings are solved analytically in Sec. IV. In Sec. V the scaling equations for the mass renormalization are discussed and solved for the energy splitting in two limiting cases; furthermore, the role of the energy splitting in the lower limit of the scaling region is discussed. The main results of the paper are discussed in Sec. VI. Some mathematical details are presented in the Appendix. The study of different measurable quantities is left for the third paper of this series (paper III).[17]

II. HAMILTONIAN AND GENERAL FORM OF THE MULTIPLICATIVE RENORMALIZATION-GROUP TRANSFORMATION

The general Hamiltonian for the conduction electron and TLS can be written as

$$H=H_e+H_{\rm TLS}+H_1 , \tag{2.1}$$

where the electron Hamiltonian

$$H_e=\sum_{k,\sigma}\epsilon_k a^\dagger_{k\sigma}a_{k\sigma} \tag{2.2}$$

is the expression (2.3) of paper I, with electron energy ϵ_k and with electron creation and annihilation operators $a^\dagger_{k\sigma}$ and $a_{k\sigma}$, respectively. The conduction-electron band is taken with uniform energy density ρ_0 (for one spin direction) and a sharp and symmetric bandwidth cutoff D is assumed. The Hamiltonian for the TLS is given by Eq. (2.1) of paper I as

$$H_{\rm TLS}=\lambda_{\rm ps}\sum_\alpha b^\dagger_\alpha b_\alpha+\tfrac{1}{2}\sum_{\substack{\alpha,\beta,\\ i=x,y,z}}\Delta^i b^\dagger_\alpha\sigma^i_{\alpha\beta}b_\beta , \tag{2.3}$$

where $b^\dagger_\alpha$ and b_α are the tunneling-atom creation and annihilation operators at position α (if there is more than one atom tunnel, then they are related to the relevant collective coordinates) and $\lambda_{\rm ps}$ is the fictitious chemical potential for which the limit $\lambda_{\rm ps}\to\infty$ must be taken in order to avoid the occupation of both sides with $\alpha=1,2$ simultaneously. Furthermore, Δ^z describes the energy splitting and Δ^x and Δ^y are the tunneling amplitudes between the two sites. This Hamiltonian (2.3) can be diagonalized, and the eigenvalues are $\lambda_{\rm ps}\pm\frac{1}{2}E$, where

$$E=[(\Delta^x)^2+(\Delta^y)^2+(\Delta^z)^2]^{1/2} . \tag{2.4}$$

If closed pseudofermion loops appear in the calculation, then the result must be normalized by $2\cosh(\frac{1}{2}E\beta)\exp(-\beta\lambda_{\rm ps})$, where β $(=1/k_BT)$ is the inverse temperature. It has been pointed out in Ref. 2 that this normalization factor is not associated with any further renormalization in the leading and in the next-to-leading logarithmic approximations.

The electron-TLS interaction has been given by Eq. (2.6) of paper I as

$$H_1=\sum_{\substack{k_1,k_2,\sigma,\\ i=x,y,z}}(a^\dagger_{k_2\sigma}V^i_{k_2k_1}a_{k_1\sigma})b^\dagger_\beta\sigma^i_{\beta\alpha}b_\alpha , \tag{2.5}$$

where $V_{k_2k_1}$ is the interaction matrix element coupled to the Pauli operator $\sigma^i_{\beta\alpha}$ describing the TLS. Following paper I, it is assumed that $V^i_{k_2k_1}$ depends only on the directions of vectors $\vec{k}_1$ and $\vec{k}_2$; thus $V^i_{k_2k_1}$ can be expanded in terms of an orthogonal set of wave functions $f_\alpha(\hat{k})$ of spherical type ($\hat{k}$ is a unit vector), and following Eq. (3.5) of paper I one can have the form

$$V^i_{k_2k_1}=V^i_{\hat{k}_2\hat{k}_1}=\sum_{\alpha,\beta}f^*_\alpha(\hat{k}_2)V^i_{\alpha\beta}f_\beta(\hat{k}_1) , \tag{2.6}$$

where the coupling $V^i_{\alpha\beta}$ is given in matrix form.

In the following calculation the thermodynamical Green's-function technique is applied. The discrete fermion energy values are labeled by ω_n. The electron and pseudofermion or tunneling-atom Green's functions are

$$G_e=\frac{1}{\omega-\epsilon_k-\Sigma_e} \tag{2.7}$$

and

$$\mathcal{G}=\frac{1}{\omega-\lambda_{\rm ps}-\frac{1}{2}\sum_i\Delta^i\sigma^i-\Sigma(\omega)} , \tag{2.8}$$

respectively, where instead of $i\omega_n$ the energy variable ω is used, which results as an analytical continuation of $i\omega_n$ and, finally, it is taken to be real with a small imaginary part. Σ_e and Σ are the self-energies for the electrons and TLS, respectively. The denominators of $\mathcal{G}$ and Σ are matrices.

The renormalized electron-tunneling-atom vertex function $\Gamma^i_{\alpha\beta}\sigma^i$ with four branches is given by $\Gamma^i_{\alpha\beta}$ which can be written as a product,

$$\Gamma^i_{\alpha\beta}=V^i_{\alpha\beta}\tilde{\Gamma}^{(i)}_{(\alpha\beta)} , \tag{2.9}$$

where at least two of $\tilde{\Gamma}^{(i)}_{(\alpha\beta)}$ start with unity in the perturbation theory, and the indices of $\tilde{\Gamma}$ are in parentheses to avoid summation with respect to them. For the time being let us assume that $V^i_{\alpha\beta}\neq 0$, which assumption will be dropped later. The vertex part proportional to $\delta_{\alpha\beta}$ is not considered here because that part is not renormalized (see, e.g., Ref. 8).

The construction of scaling equations is very similar to the method applied in Ref. 2, and they are constructed in the framework of the simplified version of the multiplicative renormalization group developed by Sólyom.[14,15] The basic idea is the following. It is assumed that the system at small energies behaves with a reduced cutoff D' in a similar way as it does with the original cutoff D, but the couplings $V^i_{\alpha\beta}$ and the TLS energies Δ^i must be appropriately changed as well. The difference between the original and scaled Green's and vertex functions can be given by multiplicative factors Z_1, Z_2, and $Z^{(i)}_{(\alpha\beta)}$, respectively, which are called renormalization constants. The multiplicative renormalization-group transformation can be given as

$$G_e\left[\frac{\omega}{D'},V',\Delta'\right]=Z_1\left[\frac{D'}{D},V\right]G_e\left[\frac{\omega}{D},V,\Delta\right], \tag{2.10a}$$

$$\mathcal{G}_{\alpha\beta}\left[\frac{\omega}{D'},V',\Delta'\right]=Z_2\left[\frac{D'}{D},V\right]\mathcal{G}_{\alpha\beta}\left[\frac{\omega}{D},V,\Delta\right], \tag{2.10b}$$

and

$$\tilde{\Gamma}^{(i)}_{\alpha\beta}\left[\frac{\omega}{D'},V'\right]=(Z^{(i)}_{(\alpha\beta)})^{-1}\left[\frac{D'}{D},V\right]\tilde{\Gamma}^{(i)}_{(\alpha\beta)}\left[\frac{\omega}{D},V,\Delta\right], \tag{2.10c}$$

$$V'^{i}_{\alpha\beta}=Z_1^{-1}Z_2^{-1}Z^{(i)}_{(\alpha\beta)}V^{i}_{\alpha\beta}, \tag{2.10d}$$

where for the sake of simplicity only one energy variable of the vertex is indicated. The new scaled couplings $V'^{i}_{\alpha\beta}$ and parameters Δ'^{i} are labeled by prime. The $\Delta^i\rightarrow\Delta'^i$ mapping is not simply multiplicative; therefore, it will be given only along the detailed calculation. It is important to point out that the renormalization constants depend only on the relative change of the cutoff D'/D and on the coupling V^i. The aim of the renormalization-group transformation is to eliminate the irrelevant part of the phase space for the conduction electrons, but the procedure can be applied only as far as $D'>k_BT,E'$, where

$$E'^2=(\Delta'^x)^2+(\Delta'^y)^2+(\Delta'^z)^2 .$$

The electron Green's-function renormalization does not play any role, as the electron self-energy contains a closed pseudofermion loop; therefore, the self-energy tends to zero as $\lambda_{ps}\rightarrow\infty$. In this way $Z_1=1$ holds.

There is an essential simplification if Δ^z is different from zero only, and $\Delta^x=\Delta^y=0$. In this case the tunneling-atom Green's function $\mathcal{G}_{\alpha\beta}$ is diagonal if the self-energy term is dropped in Eq. (2.8). Δ^x and Δ^y can always be eliminated by a rotation around the y axis and x axis in the fictitious spin space of the TLS.

The scheme of the renormalization-group transformation consists of two separate steps. At the start it is assumed that Δ^x and Δ^y have already been eliminated by appropriate rotations. Then the steps are the following:

(i) Reducing the cutoff by a multiplicative renormalization-group transformation given by Eqs. (2.10a)–(2.10d). It will be shown, however, that the transformation $\Delta^i\rightarrow\Delta'^i$ is such that Δ'^x and Δ'^y are generated even if Δ^x and Δ^y were zero before the transformation.

(ii) By a pair of appropriate rotations Δ'^x and Δ'^y are eliminated. These rotations are associated with the transformation of the couplings $V'^{i}_{\alpha\beta}$ with respect to their upper indexes. The new set of the parameters Δ^i and of the coupling $V^{i}_{\alpha\beta}$ are labeled as Δ''^i and $V''^{i}_{\alpha\beta}$, where $\Delta''^x=\Delta''^y=0$.

The present definition of the renormalized vertex with the renormalization constants $Z^{(i)}_{(\alpha\beta)}$ contains an assumption that $V^{i}_{\alpha\beta}\neq 0$, which does not hold in the general case. In order to avoid the introduction of $Z^{(i)}_{(\alpha\beta)}$ by Eqs. (2.10c) and (2.10d) it is better not to use the notation $\tilde{\Gamma}^{(i)}_{(\alpha\beta)}$ [see Eq. (2.9)]. As an alternative we can get a more compact scaling equation for the vertex by multiplying Eq. (2.10c) by $V'^{i}_{\alpha\beta}$ and by inserting the definition (2.10d) for $V'^{i}_{\alpha\beta}$ into the right-hand side of the equation that has been obtained. Thus the following general scaling equation can be derived:

$$\Gamma^{i}_{\alpha\beta}\left[\frac{\omega}{D'},V'\right]=Z_2^{-1}\left[\frac{D'}{D},V\right]\Gamma^{i}_{\alpha\beta}\left[\frac{\omega}{D},V\right], \tag{2.11}$$

where Eq. (2.9) and $Z_1=1$ have been taken into account. This set of equations can be considered as a new definition for the renormalized coupling $V'^{i}_{\alpha\beta}$ which can be applied even in the case where some of the couplings $V^{i}_{\alpha\beta}$ are initially zero.

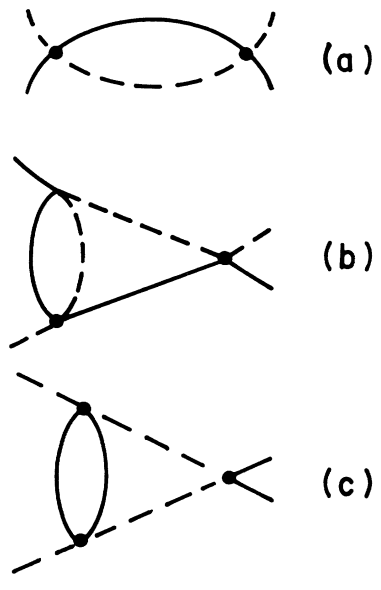

FIG. 1. Vertex corrections: (a) first-order correction; (b) second-order correction of parquet type; (c) non-parquet-type second-order correction. The diagrams (a) and (c) contribute to the β function of the renormalization-group equation for the couplings.

III. CONSTRUCTION OF THE RENORMALIZATION-GROUP EQUATIONS

In order to construct the renormalization-group transformations given by Eqs. (2.10a)—(2.10d) and (2.11) the perturbation theory must be applied; therefore, the result to be derived is not valid in the region of strong coupling. The vertex corrections of first and second order are shown in Figs. 1(a)—1(c). The diagrams of type (a) are those which have been taken into account in the first-order calculation developed in paper I. Furthermore, the diagrams of type (b) will not be calculated because they belong to the class of parquet diagrams and their contributions are exactly generated from the first-order diagrams by the scaling equations (2.10a)—(2.10d) and (2.11). The only second-order diagram of nonparquet-type is shown in Fig. 1(c). The analytical part of this diagram gives a simple logarithmic contribution (see, e.g., Refs. 2, 8, and 13) and one should deal with care only concerning the coupling part. If the couplings do not have any angular dependence, then the results agree with those given in Ref. 2. The calculation will be presented only for the self-energy in more detail. In this way the vertex correction can be given as

$$\Gamma^i_{\alpha\beta}\sigma^i = V^i_{\alpha\beta}\sigma^i - \sum_{j,k} 2\rho_0(\sigma^j\sigma^k - \delta_{jk}) \sum_{\gamma} (V^j_{\alpha\gamma}V^k_{\gamma\beta}) \ln\left[\frac{D}{|\omega|}\right] + \sum_{j,k,l} 2\rho_0^2(\sigma^k\sigma^j\sigma^l - i\epsilon^{kjl})V^j_{\alpha\beta} \sum_{\gamma}\sum_{\delta} (V^k_{\gamma\delta}V^l_{\sigma\gamma}) \ln\left[\frac{D}{|\omega|}\right] + \cdots , \tag{3.1}$$

where the ellipsis stands for the contributions of second-order parquet diagrams and the typical energy variable is ω, δ_{ij} is the Kronecker symbol, and ϵ^{ijk} is the Lévi-Cività symbol. Carrying out the spin algebra for the Pauli operators a simpler form is obtained:

$$\Gamma^i_{\alpha\beta} = V^i_{\alpha\beta} - \sum_{j,k} 2i\rho_0 \sum_{\gamma} (V^j_{\alpha\gamma}V^k_{\gamma\beta})\epsilon^{ijk} \ln\left[\frac{D}{|\omega|}\right] + \sum_{j} 2\rho_0^2[2V^j_{\alpha\beta}\,\mathrm{Tr}(\underline{V}^i\underline{V}^j) - V^i_{\alpha\beta}\,\mathrm{Tr}(\underline{V}^j\underline{V}^j)] \ln\left[\frac{D}{|\omega|}\right] , \tag{3.2}$$

where the trace is taken in the matrix space of the couplings. It is important to point out that here it has been assumed that $D > |\omega|$, $|\omega| \gtrsim E$, and, furthermore, $|\omega| > k_B T$; in the opposite case ($k_B T > |\omega|$), the energy ω must be replaced by $k_B T$ under the logarithm symbols in Eqs. (3.1) and (3.2).

The self-energy diagram is shown in Fig. 2, and its contribution is given in a detailed form as

$$\Sigma(\omega) = -2\int \frac{d^3k_1}{(2\pi)^3} \int \frac{d^3k_2}{(2\pi)^3} (V^i_{k_1k_2}\sigma^i) \frac{1}{\omega + \epsilon_{k_1} - \epsilon_{k_2} - \frac{1}{2}\Delta^z\sigma^z - \lambda_{\mathrm{ps}} + i\delta} (V^j_{k_2k_1}\sigma^j) n_F(\epsilon_{k_1})[1 - n_F(\epsilon_{k_2})] , \tag{3.3}$$

where the energy denominator corresponds to the intermediate state of the self-energy and depends on the direction of quasispin in the intermediate state and the prefactor of 2 is due to the electron spin.

The integral with respect to the electron momentum is performed as an electron energy integral and an integral with respect to the solid angle $d\Omega_k$; thus

$$\int \frac{d^3k}{(2\pi)^3} \to \rho_0 \int d\epsilon \int \frac{d\Omega_k}{4\pi} . \tag{3.4}$$

It has been shown in many papers (see, e.g., Ref. 2) that the integral in Eq. (3.3) vanishes if $\omega - \frac{1}{2}\Delta^z\sigma^z - \lambda_{\mathrm{ps}}$ is zero. This expression is small because it is zero on the energy shell. We can expand this integral in terms of this quantity, and the result is well known as

$$\Sigma(\omega) = -\sum_{i,j} 2\rho_0^2 \sum_{\sigma}\sum_{\beta} (V^i_{\alpha\beta}V^j_{\beta\alpha})\sigma^i[(\omega - \lambda)\underline{I} - \tfrac{1}{2}\Delta^z\sigma^z]\sigma^j \ln\left[\frac{D}{|\omega|}\right] , \tag{3.5}$$

which after performing the spin algebra has the detailed form

$$\Sigma(\omega)=-\sum_i 2\rho_0^2 \ln\left|\frac{D}{\omega}\right|[(\omega-\lambda)\,\mathrm{Tr}(\underline{V}^i\underline{V}^i)\underline{I}-\Delta^z\sigma^z\,\mathrm{Tr}(\underline{V}^z\underline{V}^z-\underline{V}^x\underline{V}^x-\underline{V}^y\underline{V}^y)$$

$$-2\Delta^z\sigma^x\,\mathrm{Tr}(\underline{V}^x\underline{V}^z)-2\Delta^z\sigma^y\,\mathrm{Tr}(\underline{V}^y\underline{V}^z)]\,, \tag{3.6}$$

where $\underline{I}$ is the unit matrix. We can see that the self-energy contains off-diagonal terms proportional to $\underline{\sigma}^x$ and $\underline{\sigma}^y$.

A. Reduction of the cutoff

First let us perform the first step (i) of the scaling. We perform this step in the second order of perturbation theory.

Let us start with the self-energy correction which is of second order; therefore, $V'\approx V$ can be inserted in the scaling Eq. (2.10b). If

$$\Delta^z=0\,, \tag{3.7}$$

using the correction (3.6), Z_2 can be easily determined from Eq. (2.10b) and one gets

$$Z_2\left[\frac{D'}{D},V'\right]=1-\sum_i 2\rho_0^2\ln\left[\frac{D'}{D}\right]\mathrm{Tr}(\underline{V}^i\underline{V}^i)\,, \tag{3.8}$$

which is real and gives back the special result obtained earlier for the commutative model [see Eq. (16) in Ref. 2], where a factor-of-4 difference is due to using the Pauli operators in the Hamiltonian (2.5) instead of spin operators.

In the case when $\Delta^z\neq 0$, we use the following procedure. We choose the renormalization factor Z_2 to be independent of Δ^z; thus Z_2 is given by Eq. (3.8). In order to satisfy the scaling Eq. (2.10b) with Green's function (2.8) and self-energy (3.7) a new set of parameters Δ^i is introduced:

$$\Delta'^z=\Delta^z\left[1+4\rho_0^2\ln\left[\frac{D'}{D}\right]\mathrm{Tr}(\underline{V}^x\underline{V}^x+\underline{V}^y\underline{V}^y)\right]$$

$$+O(V^3)\,, \tag{3.9a}$$

$$\Delta'^x=-\Delta^z 4\rho_0^2\ln\left[\frac{D'}{D}\right]\mathrm{Tr}(\underline{V}^z\underline{V}^z)+O(V^3)\,, \tag{3.9b}$$

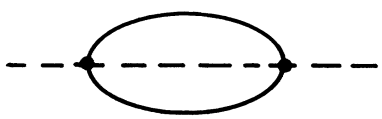

FIG. 2. Second-order self-energy correction for the pseudofermion Green's function.

and

$$\Delta'^y=-\Delta^z 4\rho_0^2\ln\left[\frac{D'}{D}\right]\mathrm{Tr}(\underline{V}^y\underline{V}^z)+O(V^3)\,. \tag{3.9c}$$

The absolute value of the splitting E given by Eq. (2.3) changes as

$$E'=[(\Delta'^x)^2+(\Delta'^y)^2+(\Delta'^z)^2]^{1/2}\approx\Delta'^z$$

$$=E\left[1+4\rho_0^2\ln\left[\frac{D'}{D}\right]\mathrm{Tr}(\underline{V}^x\underline{V}^x+\underline{V}^y\underline{V}^y)\right]$$

$$+O(V^3)\,, \tag{3.10}$$

where $E=\Delta^z$. This result shows that the effect of TLS-electron interaction is a screening for E; thus $E'<E$, as $\mathrm{Tr}(\underline{V}^x\underline{V}^x+\underline{V}^y\underline{V}^y)>0$, because for the interaction matrices $V^*_{\alpha\beta}=V_{\beta\alpha}$ holds [see Eq. (2.7) of paper I].

The renormalized coupling $V'^i_{\alpha\beta}$ can be obtained from Eq. (2.11) after inserting the perturbational results given by Eqs. (3.2) and (3.8). It will be assumed that $\ln(D'/D)\sim 1$; thus the renormalization-group transformation is carried out in small steps. In this case the first-order correction to $V^i_{\alpha\beta}$ itself satisfies that part of the scaling equation which is due to the parquet diagrams. The correction of second order arises from the non-parquet-type vertex correction given by diagram (c) in Fig. 1 and from the self-energy diagram (see Fig. 2). For the scaled coupling the final result of a straightforward calculation is the following form:

$$V'^i_{\alpha\beta}=\sum_{i,k}\left[V^i_{\alpha\beta}+2i\rho_0\sum_\gamma(V^j_{\alpha\gamma}V^k_{\gamma\beta})\epsilon^{ijk}\ln\left[\frac{D'}{D}\right]\right.$$

$$+4\rho_0^2[V^i_{\alpha\beta}\,\mathrm{Tr}(\underline{V}^j\underline{V}^j)$$

$$\left.-V^j_{\alpha\beta}\,\mathrm{Tr}(\underline{V}^j\underline{V}^i)]\ln\left[\frac{D'}{D}\right]\right]\,. \tag{3.11}$$

B. Rotation around the x and y axes

It has been shown that the renormalization-group transformation generates the parameters Δ'^x and Δ'^y even if they were equal to zero before the transfor-

mation [see Eqs. (3.10b) and (3.10c)]. In this step a rotation is carried out around the x and y axes to eliminate the small parameters Δ'^x and Δ'^y. The angles of the rotations are

$$\alpha_x = 4\rho_0^2 \ln(D'/D)\,\mathrm{Tr}(\underline{V}^y\underline{V}^z) \tag{3.12a}$$

and

$$\alpha_y = -4\rho_0^2 \ln(D'/D)\,\mathrm{Tr}(\underline{V}^x\underline{V}^z)\ . \tag{3.12b}$$

The new couplings obtained by rotation of the coupling V' given by Eq. (3.11) are labeled as V''^i and their values are

$$V''^z_{\alpha\beta} = V'^z_{\alpha\beta} - [4\rho_0^2\,\mathrm{Tr}(\underline{V}^x\underline{V}^z)V^x_{\alpha\beta} + 4\rho_0^2\,\mathrm{Tr}(\underline{V}^y\underline{V}^z)V^y_{\alpha\beta}]\ln\left[\frac{D'}{D}\right] + O(V^3) \tag{3.13}$$

and

$$V''^i_{\alpha\beta} = V'^i_{\alpha\beta} + 4\rho_0^2\,\mathrm{Tr}(\underline{V}^i\underline{V}^z)V^z_{\alpha\beta}\ln\left[\frac{D'}{D}\right] + O(V^3) \tag{3.14}$$

for $i=x,y$. Furthermore, the transformed values of Δ''^js are

$$\Delta''^z = \Delta'^z = \Delta^z\left[1 + 4\rho_0^2\ln\left[\frac{D'}{D}\right]\mathrm{Tr}(\underline{V}^x\underline{V}^x + \underline{V}^y\underline{V}^y)\right] + O(V^3) \tag{3.15}$$

and

$$\Delta''^x = \Delta''^y = 0\ . \tag{3.16}$$

Finally, after elimination of the intermediate coupling V'', the scaling equations (3.11) and (3.13)–(3.16) can be written in a differential form:

$$\frac{dV^z_{\alpha\beta}}{dx} = -\sum_{j,k} 2i\rho_0\epsilon^{zjk}\sum_\gamma (V^j_{\alpha\gamma}V^k_{\gamma\beta}) - 4\rho_0^2\,\mathrm{Tr}(\underline{V}^j\underline{V}^j)V^z_{\alpha\beta} + 4\rho_0^2\,\mathrm{Tr}(\underline{V}^z\underline{V}^j)V^j_{\alpha\beta} + 4\rho_0^2[\,\mathrm{Tr}(\underline{V}^x\underline{V}^z)V^x_{\alpha\beta} + \mathrm{Tr}(\underline{V}^y\underline{V}^z)V^y_{\alpha\beta}] \tag{3.17}$$

and

$$\frac{dV^z_{\alpha\beta}}{dx} = \sum_i\left[-\sum_{j,k} 2i\rho_0\epsilon^{ijk}\sum_\gamma (V^j_{\alpha\gamma}V^k_{\gamma\beta} - 4\rho_0^2\,\mathrm{Tr}(\underline{V}^j\underline{V}^j)V^i_{\alpha\beta} + 4\rho_0^2\,\mathrm{Tr}(\underline{V}^i\underline{V}^j)V^j_{\alpha\beta} - 4\rho_0^2\,\mathrm{Tr}(\underline{V}^i\underline{V}^z)V^z_{\alpha\beta}\right] \tag{3.18}$$

for $i=x,y$; furthermore,

$$\frac{d\Delta^z}{dx} = -4\Delta^z\,\mathrm{Tr}(\underline{V}^x\underline{V}^x + \underline{V}^y\underline{V}^y) \tag{3.19}$$

and

$$\Delta^x = \Delta^y = 0\ . \tag{3.20}$$

The equation clearly shows that the splitting Δ^z is reduced by the scaling due to the screening by the conduction electrons. In the present considerations the particular properties of the couplings have not been exploited. As discussed in paper I, the starting Hamiltonian shows time-reversal symmetry, and so the scaled Hamiltonian must also. The important consequence of this symmetry is that $V^y_{k_2k_1} = -V^y_{-k_1-k_2}$ and $V^i_{k_2k_1} = V^i_{-k_1-k_2}$ for $i=x,z$ [see Eqs. (2.8a)–(2.8c) of paper I]. Thus the rotation is always in the x-z plane as $\mathrm{Tr}(\underline{V}^y\underline{V}^z)\equiv 0$ and, therefore, $\alpha^x \equiv 0$ according to Eq. (3.12).

It is interesting to note that the rotation does not appear if $V^i_{\alpha\beta} = \underline{V}^i\bar{\sigma}^i_{\alpha\beta}$ where $\bar{\sigma}^i$ is a representation of the Pauli operators. This situation will be realized in two limiting cases to be discussed in Sec. V. This is not, however, the case when the bare couplings show these properties but instead $\Delta^z, \Delta^x \neq 0$, because then a rotation must first be performed to diagonalize H_{TLS}, which modifies that structure of the couplings. This behavior shows a strong resemblance to the commutative model discussed in Ref. 2, which is actually a particular limit of the general model studied here. Furthermore, as the rotation cannot be larger than $\pi/2$, the rotation must saturate as the strong coupling region is approached by scaling. Thus the scaled strong coupling Hamiltonian must not lead to any rotation, as that really follows from the fixed-point structure of the coupling $V^{i*}_{\alpha\beta} = V\bar{\sigma}^i_{\alpha\beta}$ (see Sec. III B in paper I).

IV. CROSSOVER TEMPERATURE

The next part of the calculations is to determine the crossover temperature T_K. If the cutoff is in the range of the crossover temperature then, the first- and second-order corrections on the right-hand side of the scaling Eqs. (3.13) and (3.14) are of magnitudes of the same order. As we have seen in the

preceding paragraph, the renormalization of Δ affects the couplings as a rotation, which must leave the crossover temperature unchanged. Thus the crossover temperature T_K can be determined in the absence of Δ. In this case the scaling equations are somewhat simpler as the last terms can be dropped in Eqs. (3.17) and (3.18). Furthermore, at the start of the calculation, the rotation of the initial coupling parameters does not occur either; thus we can assume for the initial values of the couplings that $V^z \gg V^x$ and $V^z \gg V^y$ hold. The main steps of the calculation follow closely the earlier one focused on the leading logarithmic order and presented in Sec. IV of paper I. The scaling interval can be divided into two parts as before, namely, (i) where $V^y \lesssim V^x \ll V^z$, and (ii) where $V^x \sim V^y \lesssim V^z$ (these inequalities have only qualitative meaning, because V^i is a matrix). The solutions of these two regions are matched at a point $x = x_1$.

Let us consider the two regions separately:

(i) Region $V^y(x) \lesssim V^x(x) \ll V^z(0)$. In Sec. III C of paper I, the relevant two-dimensional subspace has been determined where the increase of the couplings is the fastest. First, the right-hand side of the scaling equation has been linearized in terms of V^x and V^y. The equations (3.17) and (3.18) have the following form for the dimensionless coupling matrices $v^i_{\alpha\beta} = V^i_{\alpha\beta}\rho_0$:

$$dv^i_{\alpha\beta}/dx = -\sum_{j,k} 2i\epsilon^{ijk} v^j_{\alpha\beta} v^k_{\gamma\beta} - \sum_j 4v^i_{\alpha\beta}\mathrm{Tr}[v^j v^j(1-\delta_{ij})] , \tag{4.1}$$

where the terms due to the rotations are dropped. This equation has the linearized forms

$$\frac{dv^x}{dx} = -2i(v^y v^z) - 4v^x \mathrm{Tr}(v^z v^z) , \tag{4.2a}$$

$$\frac{dv^y}{dx} = -2i(v^x v^z) - 4v^x \mathrm{Tr}(v^z v^z) , \tag{4.2b}$$

and

$$\frac{dv^z}{dx} = 0 , \tag{4.2c}$$

where the matrix notation is used for the coupling v^i.

In the following it is assumed that a representation is used in which v^z is diagonal; thus $v^z_{\alpha\beta} = v^z_{\alpha\beta}\delta_{\alpha\beta}$. The initial conditions for the couplings are $v^x_{\alpha\beta}(x=0) = v^x_\alpha(0)\delta_{\alpha\beta}$, $v^y_{\alpha\beta}(x=0) = 0$, and $v^z_{\alpha\beta}(x=0) = v^z_\alpha(0)\delta_{\alpha\beta}$. The solutions of the equations [(4.2a)–(4.2c)] satisfying the initial condition given above are

$$v^x_{\alpha\beta}(x) = v^x_{\alpha\beta}(0)\cosh\{2[v^z_\beta(0) - v^z_\alpha(0)]x\} \times \exp[-4\,\mathrm{Tr}(v^z v^z)x] , \tag{4.3a}$$

$$v^y_{\alpha\beta}(x) = iv^x_{\alpha\beta}(0)\sinh\{2[v^z_\beta(0) - v^z_\alpha(0)]x\} \times \exp[-4\,\mathrm{Tr}(v^z v^z)x] , \tag{4.3b}$$

$$v^z_\alpha(x) = v^z_\alpha(0) , \tag{4.3c}$$

which are similar to Eqs. (3.17a)–(3.17c) of paper I. In a similar way as in paper I only a pair of indices α and β are kept for which

$$|v^z_\beta(0) - v^z_\alpha(0)|$$

is the largest. Furthermore, it will be assumed here also that $v^i_{\alpha\beta} = v^i\sigma^j_{\alpha\beta}$ (no summation for index i) and $v^z > 0$. As we have discussed in paper I, this assumption does not mean any restriction on the general applicability of these results.

The matching point x_1 must be chosen in that way, so that the cosh and sinh functions can be replaced by exponentials; furthermore, $v^x \ll v^z$ holds. Thus

$$x_1 \gg \frac{1}{4v^z(x_1)}$$

and

$$\frac{1}{4v^z(0)[1-2v^z(0)]}\ln\frac{2v^z(0)}{v^x(0)} \gg x_1 .$$

The solution (4.3a)–(4.3c) at the point x_1 is

$$v^x(x_1) = \tfrac{1}{2}v^x(0)\exp\{4v^z(0)[1-2v^z(0)]x_1\} , \tag{4.4a}$$

$$v^x(x_1) \approx v^y(x_1) , \tag{4.4b}$$

$$v^z(x_1) \approx v^z(0) . \tag{4.4c}$$

(ii) Region $V^x(x) \sim V^y(x) \lesssim V^z(0)$. In this region there are only two quantities to be dealt with, v^x and v^z (since $v^x = v^y$). The scaling equation (4.1) has the form

$$\frac{d}{dx}v^z = 4(v^x)^2 - 16v^z(v^x)^2 , \tag{4.5}$$

$$\frac{d}{dx}v^x = 4v^x v^z - 8v^x[(v^x)^2 + (v^y)^2] , \tag{4.6}$$

with the boundary condition given by Eqs. (4.4a)–(4.4c). The solution of this system of equations will be given in the Appendix. The nontrivial fixed point of Eqs. (4.5) and (4.6) is $v^x = v^z = \frac{1}{4}$.

A. Crossover temperature

The next step is to match the solutions of regions (i) and (ii). Keeping only the terms singular in the

coupling, x_1 can be expressed from Eq. (4.4a) as

$$x_1=\frac{1}{4v^z(0)[1-2v^z(0)]}\ln\left[\frac{2v^x(x_1)}{v^x(0)}\right]$$
$$\approx\left[\frac{1}{4v^z(0)}+\frac{1}{2}\right]\ln\left[\frac{2v^x(x_1)}{v^x(0)}\right], \tag{4.7}$$

for $v^2(0)\approx v^z(x_1)\ll 1$. The singular part of the solution of Eqs. (4.5) and (4.6) can be given by using the exact solution (A5) derived in the Appendix; thus one obtains

$$x-x_1=\frac{1}{4}\frac{1}{v^z(0)}\ln[2v^z(0)]-\frac{1}{4v^z(0)}\ln[v^x(x_1)]$$
$$-\tfrac{1}{2}\ln[v^z(0)]-\tfrac{1}{2}\ln[v^x(x_1)]$$
$$+\frac{1}{8v^z(0)}\ln\left[\frac{v^z(x)-v^z(0)}{v^z(x)+v^z(0)}\right]. \tag{4.8}$$

By adding the results (4.7) and (4.8) the following result is obtained:

$$x=\frac{1}{4v^z(0)}\ln\left[\frac{4v^z(0)}{v^x(0)}\right]-\tfrac{1}{2}\ln[v^x(0)v^z(0)]$$
$$+\frac{1}{8v^z(0)}\ln\left[\frac{v^z(x)-v^z(0)}{v^z(x)+v^z(0)}\right], \tag{4.9}$$

which is an implicit equation for $v^x(x)$ as a function of x. With the use of equations (A1) and (A2), v^x can also be expressed by $v^z(x)$ as

$$v^x(x)=\left\{[v^z(x)]^2-\{[v^z(0)]^2-[v^x(0)]^2\}\frac{1-4v^z(x)}{1-4v^z(0)}\right\}^{1/2}. \tag{4.10}$$

It is important to note that $v^x(x_1)$ drops out from the final result; thus this result is independent of the actual value of the matching point x_1. It is important to note that the dropping out of x_1 is independent of the approximation $v^x(0)\ll 1$, as can be seen by adding Eqs. (A5) and (4.7).

The crossover region is characterized as the region where the renormalized coupling is not small anymore. Thus in this region the second term on the right-hand side of Eq. (4.9) can be ignored. The crossover temperature is defined as $x=\ln(D/k_BT_K)$, typical of the crossover region.

In this way the crossover temperature T_K is obtained from Eq. (4.9) as

$$T_K=\frac{D}{k_B}\left[\frac{v^x(0)}{4v^z(0)}\right]^{1/4v^z(0)}[v^x(0)v^z(0)]^{1/2}. \tag{4.11}$$

The last term is a correction to the result of first order given by Eq. (4.11) in paper I, and that has a strong resemblance to the similar expression (1.2) in the spin Kondo problem.[7,11]

B. Discussion of the results obtained

In our discussion of regions (i) and (ii), in Sec. IV A, and in the Appendix, the scaling equations for the couplings have been integrated in the different regions. In order to plot the couplings as functions of x the different regions must be considered separately.

In the region $v^y(x)\lesssim v^x(x)\ll v^z(0)$, which holds for $0<x<x_1$, the couplings are given in an explicit form by Eqs. (4.3a)–(4.3c). The difference between $v^x(x)$ and $v^y(x)$ is so small for $v^x(0)\ll 1$ and $v^y(0)=0$ that it cannot be presented on a reasonable scale. According to these equations $v^x(x)\approx v^y(x)$ holds for $x\gtrsim 2/v^z(0)$. The upper boundary of this region is in the range

$$\frac{2}{v^z(0)}<x<\left[\frac{1}{4v^z(0)}+\frac{1}{2}\right]\ln\left[\frac{4v^z(0)}{v^x(0)}\right],$$

and it can be chosen as an arbitrary point x_1.

For the region $x>x_1$, Eqs. (4.5) and (4.6) have been analytically integrated in the Appendix. Combining Eqs. (A5) and (4.7), x can be given as a function $v^z(x)$. We have already pointed out that the matching points x_1 and $v^x(x_1)$ do not appear in this solution. Furthermore, if for a given x, $v^z(x)$ is known, then dv^z/dx can be calculated by Eq. (A3) and, finally, v^x is obtained in terms of $v^z(x)$ and dv^z/dx by Eq. (A1).

The results of these analytical integrations are shown in Figs. 3 and 4 for different initial values of the couplings. The crossover temperature T_K calculated in the limit $v^z(0)\ll 1$ and given by Eq. (4.11) is also indicated.

With the use of the scaling equations of first order, it has been found in paper I that the scaled couplings diverge as the crossover temperature or energy is approached. In the present case there is a stable fixed point $(v^x)^*=(v^y)^*=(v^z)^*=\frac{1}{4}$. In the region $v^x(x)=v^y(y)\sim\frac{1}{8}$ the first- and second-order terms on the right-hand side of the scaling equations become the same order of magnitude (region of crossover temperature); thus the perturbation theory cannot be applied for lower temperatures. The appearance of a finite fixed point is an artifact as has been discussed by Anderson[6] and by Fowler[7] in the case of the spin Kondo problem; thus a correct calculation valid for arbitrary strong couplings should give the infinite strong coupling fixed point. It has been shown by Wilson,[11] however, that the second-

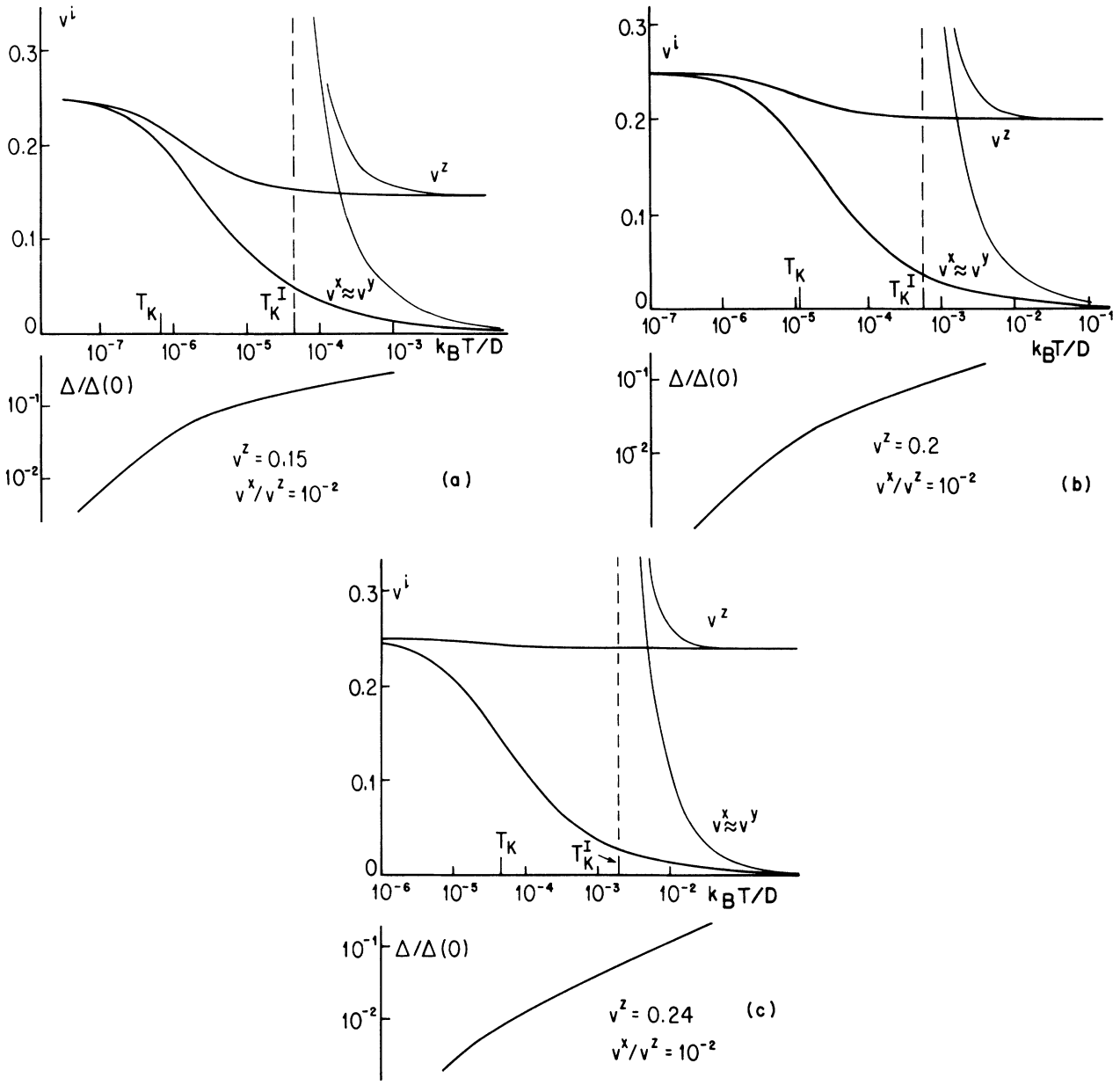

FIG. 3. Scaled couplings v^i $(i=x,y,z)$ and energy splitting Δ as a function of k_BT/D. The initial v^z coupling is 0.15, 0.2, and 0.24, respectively. The initial ratio is $v^x/v^z=10^{-2}$. The narrow (heavy) lines represent the result of first- (second-) order scaling. T_K^I and T_K are the crossover temperature in the first- and second-order scaling, respectively. The dotted line $T=T_K$ is the asymptote of the coupling in the first-order scaling. The narrow lines represent the analytical solutions of Eqs. (4.9) and (4.7) of paper I. The heavy lines for v^i are obtained analytically in a way discussed in Sec. IV B. The region where $v^x\approx v^y$ does not hold is not represented. The ratio of the scaled and initial energy splitting $\Delta/\Delta(0)$ is calculated for the symmetric TLS by using Eq. (5.6). (The index x of Δ^x is dropped.)

order scaling provides the value of the crossover temperature correctly, assuming that the initial couplings are small. Furthermore, keeping the singular terms only in the solution of the scaling equations is justified only if $v^z(0)\ll\frac{1}{4}$; thus in the region $v^z(0)\sim\frac{1}{4}$, represented also in the figure, this procedure is rather questionable. It is interesting to point out that the analytical formula (4.11) of the crossover temperature calculated by keeping only the singular terms describes very well the position of T_K, even if $v^z(0)\sim\frac{1}{8}$ or somewhat larger.

The value of the crossover temperature can be easily estimated on basis of Eq. (4.11). The typical value of the bandwidth cutoff is $D=10$ eV $\sim(10^5$ K$)k_B$. The ratio $v^x(0)/4v^z(0)$ has been estimated as $v^x(0)/4v^z(0)\sim10^{-4}$ [see Eq. (2.33) in paper I].

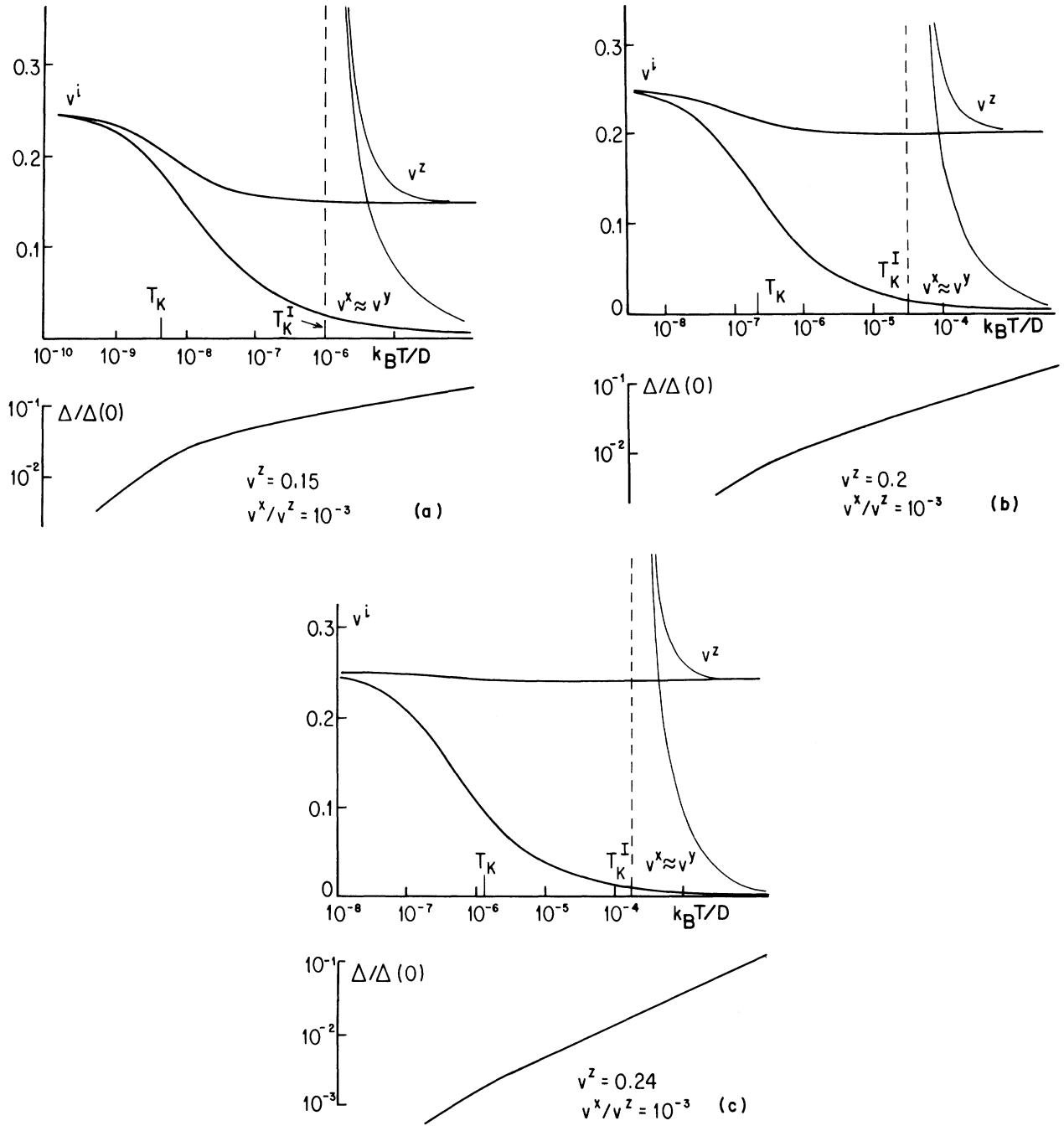

FIG. 4. As for Fig. 3, but with the ratio $v^x/v^z = 10^{-3}$.

Furthermore,

$$[v^x(0)v^z(0)]^{1/2} \sim 2 \times 10^{-2} v^z(0) .$$

In order to get the crossover temperature in a temperature region easily available by experiments, $k_B T_K \gtrsim 1$ K and $v^z(0) \geq 0.25$ must be satisfied. Thus a reasonable value of the coupling is $v^z(0) \sim 0.3$. It has been seen that even in this region the expression (4.11) works fairly well; thus it does give the crossover region correctly. Finally, it may be mentioned that the initial Hamiltonian does not show the invariance with respect to rotation in the quasispin space, but the scaled Hamiltonian is isotropic below T_K.

V. RENORMALIZATION OF THE ENERGY SPLITTING

From the point of view of determining the number of TLS which can be excited at a given tempera-

ture T, the renormalization of the energy splitting E is of crucial importance. The main question to be answered is how much reduction is expected in the energy splitting when the system is cooled down to the crossover temperature. The basic scaling equation for the energy splitting is given by (3.19), but it is hard to solve for the general case. An important step of the renormalization procedure developed is that at each step a rotation is carried out to bring the splitting Δ^i into a diagonal form ($\Delta^x=\Delta^y=0$), and it has been seen that this transformation must be carried out at the beginning of scaling transformation as well. The scaling will be discussed for two cases in great detail. The initial values of the splittings are the following in these cases: (i) $\Delta^z\neq 0$ and $\Delta^x=\Delta^y=0$; (ii) $\Delta^x\neq 0$ and $\Delta^y=\Delta^z=0$. It will be assumed as well that $V^i_{\alpha\beta}=V^i\sigma^i_{\alpha\beta}$ (no summation for i) and this assumption makes these two cases solvable. The later assumption does mean a serious restriction for the system, but it does hold for the case where only a single atom tunnels [see Eq. (4.2) in paper I]. The treatment of these two limiting cases provides an insight into the general behavior of screening.

A. Case (i): $\Delta^z\neq 0$, $\Delta^x=\Delta^y=0$

In this case there is no need for rotation at the first step. The scaling equations (3.17)–(3.19) show that $v^i_{\alpha\beta}=v^i\sigma^i_{\alpha\beta}$ holds at the beginning, then this form maintains during the whole scaling procedure; furthermore, the rotations (3.12a) and (3.12b) do not occur either. Thus in order to get the renormalized Δ^z, Eq. (3.19) must be integrated in a similar way as it has been performed in the preceding section.

In order to estimate the renormalization of Δ an upper limit will be given. With the use of the fact that $v^y(0)=0$, which has been generally accepted, thus $(v^y)^2\lesssim(v^x)^2$, and using scaling Eq. (3.19) one gets

$$-\frac{\partial\ln\Delta^z}{\partial x}\leq 8\,\mathrm{Tr}(v^xv^x)=16(v^x)^2\,. \tag{5.1}$$

This equation can be integrated easily by replacing $(v^x)^2$ from Eq. (A1). Thus one gets

$$\ln\left[\frac{\Delta^z(0)}{\Delta^z(x)}\right]\leq\ln\left[\frac{1-4v^z(0)}{1-4v^z(x)}\right]\,. \tag{5.2}$$

This expression can never be large even for $v^z(x)\sim\frac{1}{8}$; therefore, in this case the renormalization cannot reduce Δ^z more than by a factor of 2.

B. Case (ii): $\Delta^x\neq 0$, $\Delta^y=\Delta^z=0$ (symmetrical case)

In this case one must start with a rotation around the y axis by $\pi/2$. In the rotated frame, instead of $v^i_{\alpha\beta}=v^i\sigma^i_{\alpha\beta}$ we have $\tilde{v}^x_{\alpha\beta}=-v^z\sigma^z_{\alpha\beta}$, $\tilde{v}^y_{\alpha\beta}=v^y\sigma^y_{\alpha\beta}$, and $\tilde{v}^z_{\alpha\beta}=v^xv^x_{\alpha\beta}$. The matrices $(-\sigma^z,\sigma^y,\sigma^x)$ can be considered as another representation of the Pauli operators $(\tilde{\sigma}^x,\tilde{\sigma}^y,\tilde{\sigma}^z)$ with the same commutation relations. Thus $v^i_{\alpha\beta}=\tilde{v}^i\tilde{\sigma}^i_{\alpha\beta}$, where $\tilde{v}^x=v^z$ and $\tilde{v}^z=v^x$ ($\tilde{v}^y=v^y$) and $\tilde{\Delta}^z=\Delta^x$, $\tilde{\Delta}^y=\tilde{\Delta}^x=0$. It holds again that the matrix structure does not change and there is no further rotation due to the scaling. The scaling equation (3.19) can be written as

$$-\frac{\partial\ln\Delta^x}{\partial x}=-\frac{\partial\ln\tilde{\Delta}^z}{\partial x}=4\,\mathrm{Tr}(\tilde{v}^x\tilde{v}^x+\tilde{v}^y\tilde{v}^y)$$

$$=8[(v^y)^2+(v^z)^2]\,. \tag{5.3}$$

The scaling equations for v^y and v^z have been given in Sec. IV. It has been used in case (i) that $(v^y)^2\leq(v^x)^2$ and it has been shown that even for the upper bound for v^y there is no essential renormalization. Thus we can approximate Eq. (5.3) as

$$-\frac{\partial\ln\Delta^x}{\partial x}=8(v^z)^2\,, \tag{5.4}$$

which can be rewritten by inserting Eq. (A3) as

$$-\frac{\partial\ln\Delta^x}{\partial x}=8\left[\frac{1}{4}\frac{\partial v^z(x)/\partial x}{4v^z(x)-1}-C^2[4v^z(x)-1]\right]\,. \tag{5.5}$$

Straightforward integration and making use of expression (A4) for C gives

$$\Delta^x(x)=\Delta^x(0)\left[\frac{1-4v(z)}{1-4v(0)}\right]\left[[1-4v^z(0)]^2\left[\frac{v^x(0)}{4v^z(0)[1-2v^z(0)]}\right]^2\frac{v^z(x)+v^z(0)/[1-4v^z(0)]}{v^z(x)-v^z(0)}\right]^{v_z(0)/[1-2v^z(0)]}\,, \tag{5.6}$$

which can be approximated in the region where $v^x(0)\ll v^z(0)\ll 1$ and $v^z(x)\gg v^z(0)$ as

$$\Delta^x(x)=\Delta^x(0)\left[\frac{v^x(0)}{4v^z(0)}\right]^{2v^z(0)}\,, \tag{5.7}$$

where only the terms singular in the initial couplings are kept.

This result shows that the screening of the direct tunneling rate Δ^x can be reduced essentially, because $v^x(0)/4v^z(0)\sim 10^{-4}$ is a typical value. The results

given by Eq. (5.6) are also shown in Figs. 3 and 4. It is interesting to note that the simple expression (5.7) gives the correct order of reduction due to screening even in the region where $v^z(0)\approx 0.15$, but Eq. (5.6) gives smaller reduction by an order of magnitude for $v^z(0)=0.25$.

The conclusion can be drawn that the reduction of the energy splitting is the larger the more symmetric the potential well is. The renormalization for the symmetric case can be a reduction of order 10^2 in E.

VI. DISCUSSION

The multiplicative renormalization-group method has been applied to the noncommutative model. The scaling equations (3.17) and (3.18) are derived for the couplings in the second-order approximation, which is equivalent to summing up the leading and next-to-leading logarithmically divergent diagrams. These scaling equations provide the correct range of crossover between the weak and strong coupling regions. The crossover temperature T_K is given by Eq. (4.11), which is very sensitive to the initial coupling values. The estimations show that only for $v^z>0.2$ can one expect to have $T_K>1$ K. In the crossover range $v^x\sim v^y\sim\frac{1}{8}$ and in this case the terms due to the first- and second-order scalings are of the same magnitude in the β function. Thus in this region the perturbation theory breaks down. The spurious divergence in the couplings at a finite temperature does not occur contrary to the first-order scaling. Below T_K the couplings approach a fixed point $(v^i)^*=\frac{1}{4}$, which is an artifact of the second-order scaling. In an exact theory the couplings must asymptotically approach the axis $T=0$ and must tend to infinity as $T\to 0$. The scaled values of the couplings are calculated analytically and results are shown in Figs. 2 and 3.

The derivation of the scaling for the energy splitting E is the most significant result of the present paper. In the general case, the mass renormalization is somewhat complex, because a rotation in the quasispin space of the TLS has been applied continuously. That rotation corresponds to a TLS wave-function renormalization. However, the shape of the wave function is not so interesting, since the structure of the TLS itself is not specified except in the case of the model of the single tunneling atom. The essential result is that the TLS energy splitting E can be substantially renormalized due to the screening. Two special cases have been treated in Sec. V, where $\Delta^x=\Delta^y=0$ and $\Delta^z=0$, respectively. The first case is rather obscure as the electron-assisted tunneling is taken into account by having $v^z\neq 0$, but the intrinsic tunneling (Δ^x,Δ^y) is ignored. Thus for a strong coupling TLS the second case is more realistic where E can be reduced roughly by 2 orders of magnitude. This will be important to determine the amount of the thermally activated TLS at a given temperature.

It must be emphasized that the temperature is the relevant scaling variable as far as $T>E$. Since the decrease in E is slow, by lowering the temperature a crossover can be expected below which $E>T$ and the TLS is frozen by E. This freezing is significant if it occurs at $T>T_K$, since in the opposite case the TLS has already been scaled into the strong coupling region; thus E has a smaller effect. In this way, only those TLS scale into the strong coupling region for which the splitting E is smaller than a critical value E_c. For TLS with $E=E_c$ the crossover $E(T)\sim T$ occurs at $T\approx T_K$. Taking the renormalization $E(T)/E(0)$ from Figs. 3 and 4 the E_c can be given as

$$E_c=T_K\left[\left|\frac{E(T)}{E(0)}\right|^{-1}\right]_{T=T_K}. \tag{6.1}$$

Furthermore, since a uniform distribution of $E(0)$ is usually assumed, the TLS near this critical value $(E\lesssim E_c)$ plays the dominant role in the strong coupling region.

Finally, it is worth mentioning that an interesting theoretical problem remained without an answer. In the case $E=0$ scaling can be continued to zero temperature as the exact ground state is formed. In the present work only the two dominant conduction-electron channels are considered, although, at very low temperature the couplings for the other channels increase as well (for a discussion, see paper I). Thus the real ground state must show a more complicated structure, which cannot be studied by the method applied here. The structure of the ground state, however, could likely be attacked by the Bethe ansatz method developed independently by Andrei[18] and by Wiegmann[19] for the spin Kondo problem. The application of that method for the present problem would be interesting in order to learn how the couplings for the other channels develop at low temperatures. The application of the presented results for observable physical quantities is the subject of the third paper.[17]

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APPENDIX

This appendix is devoted to the solution of the system of equations given by (4.5) and by (4.16). First v^x is eliminated. From Eq. (4.5) it follows that

$$(v^x)^2=-\frac{dv^z/dx}{4(4v^z-1)}\ , \tag{A1}$$

and then this is inserted into Eq. (4.6) which is multiplied by V^x. Then both sides of Eq. (4.6) are a total derivative; thus

$$-\frac{1}{8}\frac{d}{dx}\left[\frac{dv^z/dx}{(4v^z-1)^2}\right]=\frac{1}{2}\frac{d}{dx}\left[\frac{(v^z)^2}{4v^z-1}\right]\ , \tag{A2}$$

or by integrating one gets

$$-\frac{1}{4}\frac{dv^z/dx}{(4v^z-1)^2}=\frac{(v^z)^2}{4v^z-1}+C^2\ , \tag{A3}$$

where C^2 is given by the initial values taken at x_1 as $v^z(x_1)$, $v^z(x)_1$, and $(dv^z/dx)_{x_1}$, which is expressed by $v^x(x_1)$ using Eq. (A1). Finally, C^2 has the value

$$C^2=\frac{v^z(x_1)^2-v^x(x_1)^2}{1-4v^z(x_1)}\ . \tag{A4}$$

In order to obtain v^z, Eq. (A3) must be integrated; thus one gets

$$\begin{aligned}x-x_1=-\frac{1-4v^z}{2v^z(1-2v^z)}\Bigg[&-\frac{2v^z(1-2v^z)}{1-4v^z}\ln\left[\frac{1-4v^z(x)}{1-4v^z}\right]\\&-\tfrac{1}{4}(1-4v^z)\ln\left[\frac{[v^z(x)+v^z/1-4v^z](1-4v^z)}{2v^z(1-2v^z)}\right]\\&+\frac{1}{4(1-4v^z)}\ln\left[\frac{[v^z(x)-v^z](1-2v^z)2v^z}{v^x(x_1)^2(1-4v^z)}\right]\Bigg]\ ,\end{aligned} \tag{A5}$$

where $v^z=v^z(x_1)\approx v^z(0)$ according to Eq. (4.4c). Assuming that $v^z(0),v^x(x_1)\ll 1$ one can keep only the singular terms in the result (A5); thus one obtains Eq. (4.8).

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