Theory of the interaction between electrons and the two-level system in amorphous metals. I. Noncommutative model Hamiltonian and scaling of first order

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The general form of the interaction between tunneling two-level systems (TLS) and conduction electrons is discussed for metallic glasses. The particular form of the Hamiltonian is given in the case where only a single atom tunnels between two positions. There are two couplings corresponding to the two basic scattering processes: In the first one, the tunneling atom does not change position; the second process is the conduction-electron-assisted tunneling process. The two coupling parameters are estimated. The difference in the angular dependence of these couplings on the directions of the incoming and of the outgoing electrons is responsible for the appearance of logarithmic corrections in the scattering amplitude. Scaling equations are derived for the couplings in terms of changing the bandwidth cutoff. It is shown that the scaling equations lead to especially strong coupling in two conduction-electron scattering channels which are linear combinations of the s-, p-, and d-like spherical wave functions. The Hamiltonian scales to a spin $S=\frac{1}{2}$ antiferromagnetic Kondo Hamiltonian, which indicates the formation of a "bound state," where the motions of the tunneling atom and of the conduction-electron screening cloud around the TLS are strongly correlated; thus the Friedel oscillations follow the tunneling atom. The crossover temperature, below which the correlation becomes especially strong, is determined in the leading logarithmic approximation.

I. INTRODUCTION

Since great improvements have been achieved during the last ten years in understanding the anomalous features of insulating glasses,[1] the low-temperature behavior of metallic glasses has attracted considerable interest.[2,3] In understanding the low-temperature properties of glasses, the key step has proved to be the introduction of the two-level system (TLS) by Anderson, Halperin, and Varma[4] and independently by Phillips.[5] The TLS's are the typical excitations of a glass, which are associated with a larger atomic volume at some places where an atom or a group of atoms can be found in two different configurations with a small energy difference E between them ($E/k_B < 50$ K). If only one atom is involved, then a double potential well describes the two quasistable energy minima, and the atom oscillates between these minima by tunneling (see Fig. 1). If several atoms are involved, then the description is not so simple, but the actual situation is very similar to the case of a single tunneling atom.

Recently, the interaction between the TLS and the conduction electrons has been investigated experimentally and theoretically in great detail. The most striking experimental results concerning this interaction have been obtained by ultrasonic measurements as ultrasonic absorption and the change in the sound velocity.[1-3] In metallic glasses the giant ultrasonic power necessary to saturate the ultrasonic absorption has clearly indicated that the TLS's in metals have faster relaxation by several orders of magnitude than in insulating materials.[6,7] For this fast relaxation the generally accepted explanation[6] is that the TLS can create electron-hole pairs in the relaxation process, just as the nucleus spin does in the case of the Korringa relaxation. These experiments gave the first direct evidence for the crucial importance of the TLS-electron coupling in the TLS relaxation processes. Very recent experiments on superconducting metallic glasses show that the coupling between the TLS and electrons can be especially large.[8,9] Beyond the ultrasonic measurements there are also anomalies in the bulk electrical resistivity.[2,10] Namely, in a considerable number of cases resistivity minima occur in the temperature depen-

dence of the electrical resistivity, and at the low-temperature side the behavior shows some logarithmic temperature dependence. In spite of the fact that the resistivity minimum with logarithmic slope may be caused by magnetic impurities, there are speculations that such effects may be due to electron scattering by TLS's. It must be emphasized that the experimental situation is far from clear. Furthermore, there are several experimental data for glasses which can be explained by anomalously short inelastic scattering time τ_{in}. These measurements, which are related to the electron localization[11] or to the phase-slip centers in superconducting bridges,[12] have been carried out on samples of small size. The common nature of these experiments is that the inelastic relaxation times obtained were always shorter roughly by 2 orders of magnitude than expected on the basis that the electrons are inelastically scattered by the TLS's.[11,12] This controversy justifies further theoretical study of the interaction between electrons and TLS's.

Cochrane, Harris, Strom-Olsen, and Zuckerman[13] were the first to point out the possibility of logarithmic contributions in the electron-TLS scattering amplitude. This work contains a perturbation study of an appropriately chosen Hamiltonian, and a logarithmic correction $\ln(k_B T/D)$ has been obtained for the electron lifetime in third-order perturbation theory where D is the characteristic bandwidth cutoff for the electron gas and T is the temperature.

The idea has been raised also that an analogy may exist between the TLS-electron interaction and the magnetic Kondo problem in dilute alloys. This problem has also been attacked by Kondo[14,15] who suggested, surprisingly, that the first correction to the temperature dependence of the electrical resistivity is proportional to $(\ln T)^2$ and that occurs in the fourth order of the perturbation theory. In this paper the conclusion has been drawn that a new type of infrared catastrophe may occur in metallic glasses. The correction obtained by Kondo was, however, too small to observe experimentally. It has been well known since the work of Mahan[16] and of Nozières and De Dominicis[17] that a change in a localized potential acting on an electron gas is followed by a very slow buildup of the screening in the electron gas, and this slow formation of the screening is associated with Anderson's orthogonality catastrophe.[18] This catastrophe is based on the fact that the unperturbed and perturbed ground states are different in electron-hole excitations of very large numbers with very small energies where the number of excitations goes to infinity as the volume of the electron gas increases. This phenomenon is closely related to the formation of Friedel oscillation around the potential change. Yamada and Yoshida[19] also raised the idea that a particle oscillating between two positions in an electron gas may be involved in the orthogonality catastrophe due to the particle-electron interactions. The scaling technique was first applied by Black and Gyorffy[20] for metallic glasses.

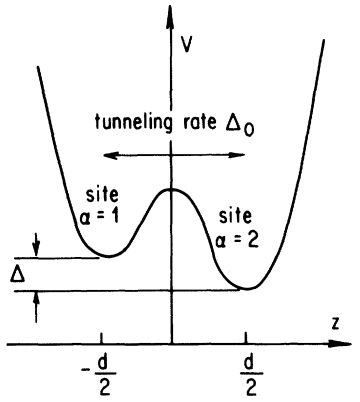

FIG. 1. Potential for single tunneling atom is shown, which has two minima with energy splitting Δ.

The situation remained somewhat unclarified from the point of view of the appearance of logarithmic corrections. It turned out that the differences between detailed features of the investigated models have been responsible for this unclear situation of whether logarithmic corrections occur, as suggested by Kondo,[14,15] or whether those with a considerable amplitude do not exist, as claimed by Black and Gyorffy.[20] In order to point out these differences, the two different electron-TLS scattering processes must first of all be introduced. Let us present the problem in the case where a single atom is tunneling and the generalization is rather obvious. The electron scattering is called diagonal (or V^z process) if the tunneling atom does not change position during the scattering. The scattering amplitude, however, does depend on the position of the tunneling atom even if the absolute value of the scattering amplitude remains the same. Furthermore, the scattering is called off-diagonal (or V^x process) if the atom changes position by tunneling during the scattering. In this case, that change in the tunneling amplitude is of interest which is due to the conduction electrons. This term is also called electron-assisted tunneling. Because in this process an atomic tunneling is involved, the off-diagonal scattering must be smaller than the diagonal scattering by at least 3 or 4 orders of magnitude.[15,21] Therefore, at first glance the assisted tunneling process is negligible. These two processes are shown in Fig. 2. The labels V^z and V^x for these processes have the following origin: If the operators in the two-dimensional

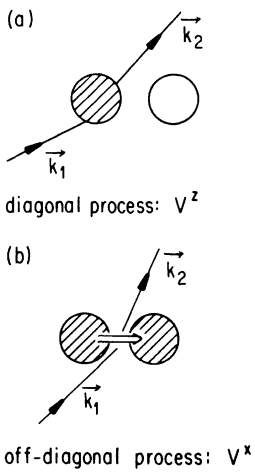

FIG. 2. Scattering of electron by TLS is shown: (a) the atom does not move (diagonal process), (b) the atom moves from one position to the other (off-diagonal process). The occupied postions of the atom are shaded.

space describing the TLS are written in terms of Pauli operators, then these scattering amplitudes are associated with the Pauli operators σ^z and σ^x, respectively.

Furthermore, it is very important to point out that the nonlocal nature of these electron-TLS couplings in the real space is of crucial importance. As has been emphasized by the present authors,[22] the occurrence of logarithmic vertex corrections in the scattering behavior depends on the existing differences between the nonlocal properties of the diagonal and off-diagonal scatterings. This difference appears as the different dependences of the scattering amplitudes on the incoming electron momentum k_1 and on the outgoing momentum k_2. The two fundamental processes contributing to the vertex corrections of first order are shown in Fig. 3. If the couplings depend on the momenta in a similar way (couplings commute in the momentum space if the electrons are on the Fermi sphere), then the contributions due to these two fundamental diagrams cancel each other, as in the case of simple potential scattering. The commutative case is realized, e.g., when both couplings have the form of a Dirac δ function. If the momentum dependence of the couplings, however, is essentially different (couplings do not commute), then there is a logarithmic vertex correction[22] as in the Kondo problem of magnetic impurities. In the latter case there are logarithmic contributions to the electrical resistivity in the leading logarithmic order (contributions of form $V^{n+2}\ln^n$ even if the term with $n=1$ is missing for some particular reason). The fact that the results obtained for metallic glasses are sensitive to the momentum dependence of the coupling was first pointed out by Kondo.[15]

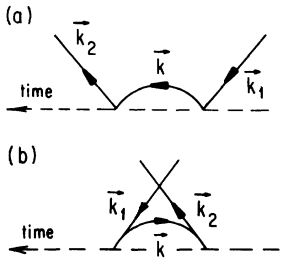

FIG. 3. Diagrams for electron-TLS scattering are depicted in second order. The solid lines represent the electron and the dotted lines stand for the TLS which also indicates the time flow. In diagram (a) an electron, in diagram (b) a hole is in the intermediate state.

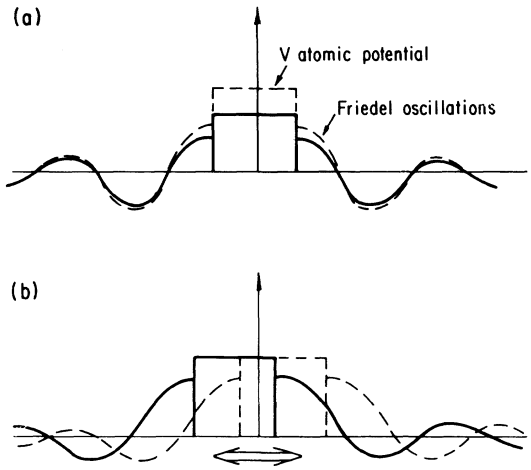

FIG. 4. Change of the potential due to the tunneling atom is shown. The solid and dotted lines represent the two potentials corresponding to the 2° of freedom of the TLS, and the associated Friedel oscillations are represented in the same way. Case (a) is where the height of the potential is oscillating (commutative model), case (b) corresponds to the tunneling atom oscillating between two positions (noncommutative model).

Let us turn to the explanation of the physical situation concerning the momentum dependence of the couplings, where two scattering amplitudes V^z and V^x, describing the couplings between the electrons and the TLS, must be considered. The difference between the commutative and noncommutative cases can be presented in the following way.

A. Commutative model

If the shapes and the positions of the potentials are independent of the internal degree of freedom of the TLS and only their amplitudes are affected, and, futhermore, if the assisted tunneling is described by a similar potential, then the model is obviously commutative. Thus in this case the two fundamental

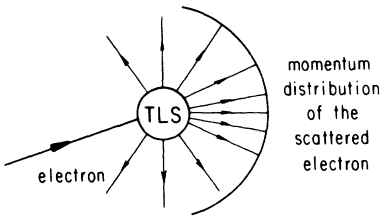

FIG. 5. Momentum distribution of the electron scattered by the TLS is shown. In higher-order processes this distribution depends on the order of the different (diagonal and off-diagonal) scattering processes.

vertex diagrams (see Fig. 3) cancel each other, and a recent careful study[23] shows that in the electrical resistivity no logarithmic term occurs in the leading or in the next-to-leading logarithmic approximations. In this case the Friedel oscillation does not change its position when the TLS tunnels; only the amplitude of the Friedel oscillation is modified [see Fig. 4(a)]. The case considered here is not the one which is believed to be realistic for a glass, because it is rather difficult to accept that the amplitude of the potential is modified by the TLS.

Finally, we mention that in the commutative model the combination of the couplings $(V^x)^2 + (V^z)^2$ is invariant if scaling transformation is performed to reduce the bandwidth cutoff D. The most likely realization of the commutative model is the trivial case, where the assisted tunneling is so weak that V^x can be ignored.

B. Noncommutative model

The simplest realization of the noncommutative case is when the potential moves with the tunneling atom; thus the two potentials are of the same shape but at different positions [see Fig. 5(b)]. The V^z term in the interaction describes the change in the potential; thus it is proportional to the difference of these potentials. Furthermore, the V^z term is odd under a reflection transformation through the symmetry plane of the two positions of the TLS. On the other hand, the assisted tunneling amplitude (V^x term) must behave like an even function under this transformation. Hence it is obvious that the scattering depends very much on the order of the different scatterings; in other words, the model is noncommutative. In this model the Friedel oscillation must also change position following the hopping of the tunneling atom. This model is very difficult to treat in general; therefore, a simplified model has been suggested where, considering the scattering processes, only two of the spherical harmonics have been kept.[21,22]

The appropriate method to treat that model is the bandwidth scaling where the less interesting part of the conduction-electron phase space is eliminated by changing the bandwidth cutoff from D to D'; but in order to keep the physical quantities unchanged the coupling constants and the parameters of the TLS are adjusted. The solution of this scaling equation shows that the couplings tend to infinity. The model formally scales to a Hamiltonian which has the form of the antiferromagnetic Kondo problem. This means a very strong resemblance to the Kondo problem, where at low temperature a highly correlated state (bound state) is formed in which the spin of the impurity is completely screened by the conduction-electron spin polarization and the ground state is a singlet. There is a crossover temperature below which the correlated state builds up. This phenomenon is very much based on the fact that in the scattering of electrons by the impurity, the electron scattering amplitude depends strongly on the order of the spin-flip and spin-conserving processes. This strong dependence can be traced in the spin part of the scattered wave function.

In the case of the TLS the scattering amplitude is sensitive on the order of the V^x and V^z processes, but the influence of the order is in the orbital part. Namely, the angular dependence of the scattered wave function is affected by the position and motion of the TLS (see Fig. 5). The detailed investigations show[21] that below an appropriate crossover temperature the motion of the TLS system and electron screening cloud exhibiting the Friedel oscillation move tightly together. Thus the noncommutative model behaves like an "orbital Kondo problem," where the impurity spin is replaced by the TLS, and instead of the conduction-electron polarization a spin-independent charge screening cloud is formed. It is worthwhile to emphasize that the formation of the correlated ground state is not obvious in the sense that while in the original spin Kondo problem the total spin is a conserving quantity, in the case of the TLS there is no similar quantity for the orbital motion. Several results concerning the noncommutative model have been indicated in a previous short communication[24] and summarized elsewhere.[25]

The aims of the first of the present three papers are the following. In Sec. II, the general form of the conduction-electron-TLS Hamiltonian is given, which is followed by a detailed description of the general properties of that Hamiltonian in Sec. II B. Section II B is devoted to the model of a single tunneling atom and the couplings V^z and V^x are derived and their ratio is estimated, where concerning V^z the line suggested by Black, Gyorffy, and Jäckle[26] is followed, and concerning V^x an idea that has previously been suggested[21] is elaborated. This estimation plays a crucial role in the different applications of the theory presented in paper II. In Sec. II C the an-

gular dependences of the couplings are worked out in great detail to demonstrate that the model studied is indeed noncommutative.

The scaling equation valid in leading logarithmic order is shortly derived in Sec. III. This is followed by a general discussion of the structure of the fixed point in Sec. III A. Section III B is devoted to proving that, concerning the spherical harmonics, there is justification for retaining a two-dimensional subspace, and a procedure is given to find that appropriate subspace. The application of this procedure to the model of the single tunneling atom is presented in Appendix A. In Sec. IV, the scaling equations are solved approximately, and the crossover temperature is determined for the case of the two-dimensional subspace where a simple version of the Hamiltonian is assumed. The case of a general Hamiltonian has already been briefly discussed elsewhere,[21] but in Appendix B a generally applicable method is given. In Appendix C the exact mathematical solution of the scaling is also given for comparison with the approximate method presented in the main body of the paper. The general features of the results achieved are discussed in Sec. V.

The present (first) paper is restricted to the leading logarthmic approximation and to the general concepts of the TLS's. In the second paper[27] (II) the scaling equations are generalized to the next order, and the correct form of the crossover temperature will be derived. That form will be the basis for further numerical estimations. Finally, the amplitude of different measurable quantities such as resistivity, electron inelastic relaxation time, and the relaxation rate of the TLS will be calculated in the third paper[28] (III).

II. THE MODEL

The physical phenomenon associated with the TLS is a particular part of lattice dynamics in amorphous materials. In amorphous materials at low temperature the bulk phonons play a negligible role; thus we restrict our considerations to the localized motion due the TLS's. This motion can be regarded as an oscillation between two configurations by tunneling. At low temperature no excited states around the two configurations of the TLS must be considered. Thus these two almost orthogonal configurations can be described by a pair of either boson or fermion creation and annihilation operators $b_\alpha^\dagger$ and b_α with $\alpha=1,2$. As these configurations are alternative, only one excitation can be present at a given time; therefore, the Fermion representation will be preferred. In the special case where the TLS means a single tunneling atom, the operators $b_\alpha^\dagger$ and b_α are the creation and annihilation operators of the atom at site $\alpha=1,2$. In the general case, however, these operators are, rather, related to collective variables describing the two configurations. In this formalism unphysical states occur when neither or both states are occupied. These unphysical states are not involved in any dynamical process, but they have an effect on the statistical weight. The usual way to cure this situation is to assign a very large chemical potential $\lambda_{\rm ps}$ to these fermions to prevent the system from double occupation and to correct the normalization[29] of the statistical weight by a factor of the probability of single occupation, which is proportional to $\exp(\beta\lambda_{\rm ps})$, where β is the inverse temperature. The operation in this two-component space can be described in terms of Pauli spin operators σ^i $(i=x,y,z)$ acting on the two states as $|\uparrow\rangle=b_1^\dagger|0\rangle$ and $|\downarrow\rangle=b_2^\dagger|0\rangle$, where $|0\rangle$ is the vacuum state, and in the case of a single tunneling atom the states $|\uparrow\rangle$ and $|\downarrow\rangle$ correspond to the atom sitting in the potential well on the left and on the right. In the spin representation the b_α operators are the Abrikosov's pseudofermion representation[30] of the spin. The general form of the TLS Hamiltonian can be written as

$$H'_{\rm TLS}=\lambda_{\rm ps}\sum_\alpha b_\alpha^\dagger b_\alpha+\tfrac{1}{2}\sum_{\substack{\alpha,\beta,\\ i}}\Delta^i b_\alpha^\dagger\sigma_{\alpha\beta}^i b_\beta\ , \tag{2.1}$$

where $i=x,y,z$. The term with Δ^z describes the energy splitting between the two states while Δ^x and Δ^y stand for the tunneling transition. If the two configurations of the TLS are described by a real wave function, then the overlap integral (tunneling matrix element) is real; thus $\Delta^y=0$ will be assumed without losing the generality. Thus $H_{\rm TLS}$ will be written as

$$H_{\rm TLS}=\lambda_{\rm ps}\sum_\alpha b_\alpha^\dagger b_\alpha+\tfrac{1}{2}\sum_{\alpha,\beta}(\Delta b_\alpha^\dagger\sigma_{\alpha\beta}^z b_\beta+\Delta_0 b_\alpha^\dagger\sigma_{\alpha\beta}^x b_\beta)\ , \tag{2.2}$$

where Δ is the energy splitting and Δ_0 is the tunneling matrix element which is proportional to the tunneling rate $e^{-\lambda}<1$. This Hamiltonian (2.2) can be diagonalized by a rotation around the y axis in the quasispin space. The energy splitting is $E=(\Delta^2+\Delta_0^2)^{1/2}$ in the diagonalized form.

The conduction electrons will be taken as free electrons. This simplification is justified in treating the TLS system, as in this theory the electron density and not the wave function is of importance. In the particular model of single-atom tunneling the wave function is considered only at very short distances (smaller than atomic distance) at the center of the TLS. The use of spherical harmonics may help to visualize the dynamics in the conduction band

even if we are aware of the fact that the spherical wave functions do not have any resemblance to the real wave functions in amorphous materials.

Thus we can have the electron Hamiltonian as

$$H_e=\sum_{k,\sigma}\epsilon_k a^\dagger_{k\sigma}a_{k\sigma}\ , \tag{2.3}$$

where $a^\dagger_{k\sigma}$ and $a_{k\sigma}$ are the free-electron creation and annihilation operators with energy ϵ_k and with spin σ. The ϵ_k is measured from the chemical potential. The real electron spin will not play an essential role in most of the following considerations; thus σ will not be indicated in most of the formulas. The effect of the real spin will occur as a factor of 2 for closed electron loops.

The general form of the interaction between the electrons and the TLS is[21,22]

$$H'_1=\sum_{\substack{k_1,k_2,\sigma,\\ \alpha,\beta}} b^\dagger_\beta a^\dagger_{k_2\sigma}V^{\beta\alpha}_{k_1k_2}a_{k_1\sigma}b_\alpha\ . \tag{2.4}$$

In the Hamiltonian the inverse of the volume of the sample must appear in front, but for the sake of brevity it will be dropped. The matrix element $V^{\alpha\beta}_{k_1k_2}$ can be decomposed in terms of Pauli operators as

$$V^{\beta\alpha}_{k_2k_1}=\sum_i V^i_{k_2k_1}\sigma^i_{\beta\alpha}+V^0_{k_2k_1}\delta_{\beta\alpha}\ , \tag{2.5}$$

where $i=x,y,z$. The last term is due to that part of the potential scattering which is independent of the position of the TLS. This term can be eliminated by choosing the electron wave functions to be eigenfunctions in the presence of the potential $V^0_{k_2k_1}$.

Thus we can use the Hamiltonian in the following form[21,22]:

$$H_1=\sum_{\substack{k_1,k_2,\sigma,\\ \alpha,\beta,\\ i=x,y,z}} (a^\dagger_{k_2\sigma}V^i_{k_2k_1}a_{k_1\sigma})b^\dagger_\beta\sigma^i_{\beta\alpha}b_\alpha\ . \tag{2.6}$$

In the following the summation will not be indicated for the pair of indices.

The physical significance of the couplings V^x, V^y, and V^z are as follows. V^z describes the difference between the electron scattering amplitudes corresponding to the two positions of a rigid TLS. The terms V^x and V^y describe the processes where the electron scattering is associated with a tunneling process of the TLS. These processes will be called conduction-electron-assisted tunneling. In the case of a single tunneling atom these processes are shown in Fig. 2.

A. General properties of $V^i_{k_2k_1}$

It will be useful, for the following discussion, to list the general properties of the interaction given in form of the Hamiltonian (2.6):

(i) H_1 is Hermitian; thus

$$V^i_{k_2k_1}=(V^i_{k_1k_2})^*\ . \tag{2.7}$$

(ii) The time-reversal symmetry can be formulated easily because the real electron spin does not enter into this problem in an essential way. If the TLS is described by a real wave function, then for the matrix elements the following must hold:

$$(k_2\sigma\beta\,|\,H_1\,|\,k_1\sigma\alpha)=(-k_1\sigma\alpha\,|\,H_1\,|\,-k_2\sigma\beta)\ ,$$

where $|\,k\sigma\alpha)$ is the product of the wave functions of the TLS and of a single electron. By comparison with the form of Hamiltonian (2.6) one gets

$$V^z_{k_2k_1}=V^z_{-k_1-k_2}\ , \tag{2.8a}$$

$$V^x_{k_2k_1}=V^x_{-k_1-k_2}\ , \tag{2.8b}$$

$$V^y_{k_2k_1}=-V^y_{-k_1-k_2}\ . \tag{2.8c}$$

(iii) It is very reasonable to assume that in the electron-assisted tunneling the role of electrons appears in terms of electron density operator

$$\rho(\vec{r})=\sum_{k_1,k_2,\sigma}\exp[i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}]a^\dagger_{k_2\sigma}a_{k_1\sigma}\ , \tag{2.9}$$

because the fluctuations $\delta\rho$ in the electron density may result in the change of the tunneling barrier height due to the interaction between the tunneling atom and conduction-electron density at the atom. The tunneling rate being a functional of $\rho(r)$, which depends only on the difference $\vec{k}_1-\vec{k}_2$, the following notation can be introduced:

$$V^i_{k_2k_1}=V^i(\vec{k}_1-\vec{k}_2)\ . \tag{2.10}$$

It can be emphasized that only the property (iii) does imply a restriction on the Hamiltonian. By combining (ii) and (iii) it is easy to show that restriction (iii) has a strong effect on Hamiltonian (2.6), namely

$$V^y_{k_2k_1}=0 \tag{2.11}$$

holds. It is important to emphasize that this property does not sustain for the renormalized vertex, because the higher-order terms in $\delta\rho$ are not necessarily local, thus V^y can be generated by the interaction as if it has first been pointed out by Kondo.[15]

B. Estimation of V^x and V^z for the model of single tunneling atom

In the special model treated here, a single atom is tunneling in a double-well potential. The minima are separated by a vector $\vec{d}$ shown in Fig. 1. The es-

timation of V^z follows the works by Kondo[15] and by Black, Gyorffy, and Jäckle.[26] Furthermore, V^x is estimated in the way suggested by one of the present authors[21] which is more detailed than the original version given by Kondo[15]

Following Kondo let us assume that the single atomic wave functions ϕ_1 and ϕ_2 at the minima $\sigma=1,2$ are similar; thus only the variables of the functions are shifted as

$$\phi_1(\vec{R})=\phi\left[\vec{R}-\frac{\vec{d}}{2}\right], \tag{2.12a}$$

$$\phi_2(\vec{R})=\phi\left[\vec{R}+\frac{\vec{d}}{2}\right], \tag{2.12b}$$

where the wave function along the axis of the TLS is

$$\phi(R)=\frac{1}{r_0^{1/2}\pi^{1/2}}\exp\left[-\frac{R^2}{2r_0^2}\right], \tag{2.13}$$

which is the solution for a quadratic potential well; furthermore, r_0 is the averaged extension of the wave function in the minimum. The zero-point energy is $\frac{2}{3}\omega_0\hbar$, where ω_0 is related to R_0 as

$$r_0=(\hbar/M\omega_0)^{1/2}, \tag{2.14}$$

where M is the mass of the tunneling atom. Considering typical values as $\hbar\omega_0\sim 100$–500 K, $M\approx 50m_p$ (m_p is the proton mass), one obtains (in angstroms)

$$r_0\sim 0.1\text{–}0.03\ . \tag{2.15}$$

The off-diagonal term Δ_0 in Hamiltonian (2.2) can be simply estimated as

$$\Delta_0\sim\hbar\omega_0 e^{-\lambda}, \tag{2.16}$$

where λ is the Gamow factor. If our interest is focused on low-energy excitation, which can be thermally excited at $T\simeq 1$ K, then it must be assumed for the TLS energy that $E=(\Delta_0^2+\Delta^2)^{1/2}\leq 1$ K; thus $\Delta_0\leq 1$ K or $e^{-\lambda}\leq 10^{-2}$ ($\lambda\geq 5$). Furthermore, as $e^{-\lambda}\sim\exp(-d^2/4r_0^2)$, therefore $d/r_0>4.5$, and because of Eq. (2.15), $d>0.2$ Å for the TLS of present interest. On the other TLS, d cannot be larger than $d\sim 0.5$ Å, because then the tunneling rate would become very slow to consider the electron-assisted tunneling. Thus we can expect d to be (in angstroms)

$$0.5\geq d\geq 0.15, \tag{2.17}$$

for an atom with $M\sim 50m_p$. The value of d can be even larger by a factor of 2, if the potential between the minima is not so high as it is in the case where the potential is composed of two quadratic minima. For very light atoms such as hydrogen, r_0 and d can be considerably larger. For further estimates d can be related to the Fermi momentum $k_F\sim 1$ Å^{-1} as

$$k_F d\simeq 0.15\text{–}0.5\ . \tag{2.18}$$

Turning to the expression for V^z the electron-atom interaction must be considered which can be described by a pseudopotential U. The pseudopotential may be a nonlocal function in space. As V^z is the difference between the two potentials corresponding to the two atomic positions ($\alpha=1,2$), thus V^z has the form

$$V^z(\vec{r})=\int u(\vec{r}-\vec{R})\tfrac{1}{2}[\phi_1^2(\vec{R})-\phi_2^2(\vec{R})]d^3\vec{R}\ , \tag{2.19}$$

which has the Fourier transform

$$V^z_{k_2k_1}=U(\vec{k}_1-\vec{k}_2)\int d^3R\,\exp[i(\vec{k}_1-\vec{k}_2)\cdot\vec{R}]\times\tfrac{1}{2}[\phi_1^2(\vec{R})-\phi_2^2(\vec{R})]\ , \tag{2.20}$$

where the factor $\frac{1}{2}$ is due to the Pauli operator in the Hamiltonian (2.6). The typical value of this coupling can be obtained by assuming that the wave functions $\phi_\alpha(R)$ are well localized at $R\sim\pm d/2$ and, furthermore, that $|\vec{k}_1-\vec{k}_2|\sim k_F$, and by expanding with respect to the small parameter, we assume that $\frac{1}{2}k_F d\sim 0.15\ll 1$. Thus the following estimated value is obtained:

$$V^z_{k_2k_1}\simeq(d/2)(k_1^z-k_2^z)U(k_1-k_2)\ , \tag{2.21}$$

where d is directed in the z direction.

Concerning the electron-assisted tunneling, we follow the outline of Ref. 21, which takes into account the change in the barrier due to the interaction between the tunneling atom and the fluctuation $\delta\rho$ in the conduction-electron density. The effective height of the barrier at point z is

$$V_{B,\mathrm{eff}}(z)=V_B(z)+\delta V_B(z)\ , \tag{2.22}$$

where $V_B(z)$ is the height with the electron density in equilibrium $\delta\rho=0$ and δV_B is due to the fluctuation $\delta\rho$. The fluctuations in the height of the barrier must be measured from the averaged shifts of the potential at the minimum of the potential wells. Thus the density fluctuation of interest is

$$\delta\rho(\vec{r})=\rho(\vec{r})-\tfrac{1}{2}[\rho(\vec{d}/2)+\rho(-\vec{d}/2)]\ , \tag{2.23}$$

and then the fluctuation in the height of the barrier is expressed with the pseudopotential U as

$$\delta V_B(\vec{r})=U\delta\rho(\vec{r})\ , \tag{2.24}$$

where for the sake of simplicity a local pseudopotential is used (see Fig. 6).

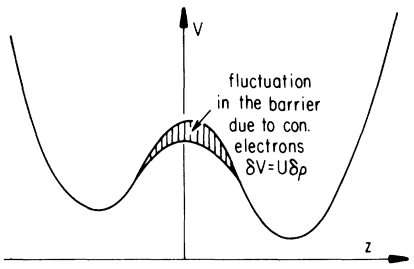

FIG. 6. Fluctuation in the double-well potential for the TLS is shown. These fluctuations are produced by the density fluctuations $\delta\rho$ in the conduction-electron band. The shift of the potential is proportional to the pseudopotential U for the electron-atom scattering.

The overlap integral between the two wave functions $\phi_\alpha(r)$ $(\alpha=1,2)$ can be calculated easily in the presence of the conduction-electron density fluctuations, and the result is

$$\hbar\omega_0 \exp\left[-\frac{1}{\hbar}\int_{z_1}^{z_2}[2MV_{B,\text{eff}}(z)]^{1/2}dz\right], \tag{2.25}$$

where dz covers the area of tunneling $z_1<z<z_2$. If $\delta\rho=0$, then the exponential factor is $e^{-\lambda}$ and an expansion is taken around this value; thus

$$\hbar\omega_0 e^{-\lambda}\left[1-\frac{1}{\hbar}\int_{z_1}^{z_2}\frac{M}{[2MV_B(z)]^{1/2}}U\delta\rho(z)dz\right]. \tag{2.26}$$

This expression has a simpler form if the barrier is taken as squarelike with width w and height V_B and with the Gamow integral

$$\lambda=\hbar^{-1}w(2MV_B)^{1/2}$$

being introduced; therefore one gets

$$\hbar\omega_0 e^{-\lambda}\left[1-\frac{\lambda U}{2wV_B}\int_{z_1}^{z_2}\delta\rho(z)dz\right], \tag{2.27}$$

where $\delta\rho(z)$ can be replaced by Eq. (2.23), thus

$$\hbar\omega_0 e^{-\lambda}\left[1-\frac{\lambda U}{2wV_B}\int_{z_1}^{z_2}\{\rho(z)-\tfrac{1}{2}[\rho(\vec{d}/2)+\rho(-\vec{d}/2)]\}dz\right]. \tag{2.28}$$

Finally, using the expression (2.9) for $\rho(r)$ one can make an expansion in the factor

$$\exp[i(\vec{k}_1-\vec{k}_2)\cdot r]a^\dagger_{k_2}a_{k_1}$$

assuming that $k_F w \leq k_F d \ll 1$. The result of this expansion is

$$\hbar\omega_0 e^{-\lambda}\left\{1-\frac{\lambda U}{wV_B}\sum_{k_1,k_2,\sigma}\int_{z_1}^{z_2}\left[\left[\frac{z\Delta k_z}{2}\right]^2-\frac{d^2}{8}(\Delta k_z)^2\right]dx\, a^\dagger_{k_2\sigma}a_{k_1\sigma}\right\}, \tag{2.29}$$

where the notation $\Delta k_z=k_1^z-k_2^z$ has been introduced.

This expression gives a good approximation for the electron-assisted tunneling rate as

$$V^x_{k_2k_1}\sim\Delta_0\frac{\lambda U}{16V_B}(\Delta k_z d)^2, \tag{2.30}$$

where the notation (2.16) has been used and $w\sim d$ has been replaced. In order to get an estimation for the amplitude of $v^x_{k_2k_1}$ one can use the average of $(\Delta k_z)^2_{\text{av}}\sim\frac{2}{3}k_F^2$; thus

$$V^x\sim\Delta_0\frac{\lambda U}{24V_B}(k_F d)^2. \tag{2.31}$$

By comparing expressions (2.21) and (2.31) an estimation for the ratio V^x/V^z is obtained:

$$\frac{V^x}{V^z}\sim\Delta_0\frac{\lambda(k_F d)}{24V_B}\sim\frac{e^{-\lambda}}{12\lambda}(k_F d)\frac{w^2}{r_0^2}, \tag{2.32}$$

where $\lambda=(2MV_B)^{1/2}$. w and Eqs. (2.14) and (2.16) are taken into account to make the result more transparent. To get a numerical value one can use $w\sim 3r_0$, $k_F d\sim 0.3$, and $\lambda\sim 5$, and then one gets

$$\frac{V^x}{V^z}\sim 10^{-4}-10^{-3}, \tag{2.33}$$

which is correct for TLS with $\Delta_0\sim 1$ K. This estimation means that for single-atom tunneling one can expect $V^x/V^z\lesssim 10^{-3}$ for a large number of those TLS which play the dominating role at temperature range $T\sim 1$ K.

C. The angular dependence of the couplings V^x and V^z

As it has been emphasized in the Introduction and as it has been pointed out earlier by one of the present authors,[21] the momentum dependence of the coupling V^x and V^z plays a crucial role in formation of the Kondo-type ground state. In order to give an explicit form for the momentum dependence, the nonlocal behavior of the pseudopotential must be specified. Taking the incoming and outgoing momenta at the Fermi sphere the angular dependence of the pseudopotential can be expressed in terms of differential partial waves as

$$U(\vec{k}_1-\vec{k}_2)=\sum_l a_l \sum_{m=-1}^{m=l} Y_l^{m*}(\hat{k}_2)Y_l^m(\hat{k}_1) = \sum_l \frac{2l+1}{4\pi} a_l P_l(\cos\theta_{k_1k_2}) , \quad (2.34)$$

where Y_l^m are the spherical functions with quantum number l and m, and a_l is the scattering length for the different partial waves. Finally, $\hat{k}_1$ and $\hat{k}_2$ are unit vectors.

The coupling can be expressed in partial waves as well. Let us first have the coupling expanded in terms of a complete set of orthogonal functions $f_\alpha(\hat{k})$, which depends only on the direction $\hat{k}$ as

$$V^i_{\vec{k}_2\vec{k}_1} \sim V^i_{\hat{k}_2\hat{k}_1} = \sum_{\alpha,\beta} f^*_\beta(\hat{k}_2)V^i_{\beta\alpha} f_\alpha(\hat{k}_1) , \quad (2.35)$$

where it is assumed that the coupling also is sensitive only on the direction of $\vec{k}_1$ and of $\vec{k}_2$, but not on their absolute values. It turns out that the most convenient choice is

$$f_\alpha(\hat{k}) \simeq i^l\sqrt{4\pi}Y_l^m(\hat{k}) , \quad (2.36)$$

and then the matrix elements of $V^i_{\hat{k}_2\hat{k}_1}$ are

$$V^i_{l_2l_1}(m)=\frac{i^{l_1-l_2}}{4\pi}\int Y^{m*}_{l_2}(\hat{k}_2)V^i_{\hat{k}_2\hat{k}_1}Y^m_{l_1}(\hat{k}_1)d\Omega_1 d\Omega_2 . \quad (2.37)$$

This expression is diagonal in the quantum number m as the axis of the TLS is directed in the z direction and, therefore, z is a rotational axis. In order to perform a concrete calculation we can simplify our formulas by neglecting the extension of the TLS in the directions perpendicular to the z axis. In this case only $m=0$ plays a role. The forms (2.30) and (2.31) obtained for V^x and for V^z show that V^x is even and V^z is odd with respect to the inversion symmetry where the symmetry plane is perpendicular to the z axis and goes through the center of the TLS. This is rather obvious because the scattering amplitude difference in V^z must be odd, while the tunneling matrix element must be even. Thus one obtains that

$$V^x_{l_2l_1}(m)=0 \text{ for } l_1+l_2=\text{ odd} , \quad (2.38a)$$

$$V^z_{l_2l_1}(m)=0 \text{ for } l_1+l_2=\text{ even}. \quad (2.38b)$$

With the use of expressions (2.30) and (2.31) for the angular dependence of the couplings and the form (2.34) of the pseudopotential,

$$V^z_{\hat{k}_2\hat{k}_1}=\frac{i}{2}(k_Fd)\frac{1}{4\pi}(a_0+3a_1\cos\theta_{k_2k_1})(\hat{k}^z_1-\hat{k}^z_2) \quad (2.39)$$

and

$$V^x_{\hat{k}_2\hat{k}_1}=\tfrac{1}{16}(k_Fd)^2\frac{\Delta_0\lambda}{V_B}\frac{1}{4\pi}(a_0+3a_1\cos\theta_{k_2k_1}) \times(\hat{k}^z_1-\hat{k}^z_2)^2, \quad (2.40)$$

where only a_0 and a_1 are kept (this is an adequate approximation except for transition-metal impurities). The matrix forms of the interaction in channels $l=0,1,2,3$ are

$$[\underline{V}^z(m=0)_{l_2l_1}]=\frac{k_Fd}{2}\begin{bmatrix} 0 & (a_0-a_1)\sqrt{3} & 0 & 0 \\ (a_0-a_1)/\sqrt{3} & 0 & 2a_1/\sqrt{15} & 0 \\ 0 & 2a_1/\sqrt{15} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (2.41a)$$

and

$$[\underline{V}^x(m=0)]_{l_2 l_2}=\frac{(k_F d)^2}{16}\frac{\Delta_0 u\lambda}{V_B}\begin{vmatrix} \frac{2}{3}a_0-\frac{2}{9}a_1 & 0 & \frac{2}{3\sqrt{5}}a_0-\frac{4}{3\sqrt{5}}a_1 & 0 \\ 0 & -\frac{2}{3}a_0+\frac{6}{5}a_1 a_1 & 0 & \frac{2\sqrt{3}}{5\sqrt{7}}a_1 \\ \frac{2}{3\sqrt{5}}a_0-\frac{4}{3\sqrt{5}}a_1 & 0 & -\frac{8}{15}a_1 & 0 \\ 0 & \frac{2\sqrt{3}}{5\sqrt{7}}a_1 & 0 & 0 \end{vmatrix} . \tag{2.41b}$$

It is interesting to note that the zeros necessarily appear in the even and odd positions (alternately), respectively.

In the following we will use extensively dimensionless quantities. It is easy to check that the couplings multiplied by the conduction-electron density ρ_0 taken at the Fermi energy for one spin direction are dimensionless. In the following the dimensionless coupling is defined as

$$v^i=V^i\rho_0 \tag{2.42}$$

for an arbitrary representation.

III. SCALING

This section is devoted to the scaling equations in the leading orders. As we have discussed in the Introduction, the perturbation theory leads to logarithmically divergent contributions as the electron energy tends to the Fermi energy and the temperature approaches zero. The two simplest vertex corrections are shown in Fig. 3, where the solid lines stand for the electrons and the dotted lines for the pseudofermions. As the pseudofermion has a very large fictitious energy λ_{ps}, the interaction points on the dotted lines are therefore time ordered as indicated in Fig. 3. With the use of the Hamiltonian (2.6), the contributions of these diagrams can be calculated easily if a constant electron density ρ_0 is assumed near the Fermi surface and a symmetric sharp bandwidth cutoff is applied. Beyond the sign the essential differences in the contributions of diagrams (a) and (b) in Fig. 3 are in the factors due to the interaction, which are

$$(\vec{V}_{\hat{k}_2\hat{k}}\cdot\vec{\sigma})(\vec{V}_{\hat{k}\hat{k}_1}\cdot\vec{\sigma})$$

and

$$(\vec{V}_{\hat{k}\hat{k}_1}\cdot\vec{\sigma})(\vec{V}_{\hat{k}_2\hat{k}}\cdot\vec{\sigma}),$$

respectively. In diagram (a) in the intermediate state there is an electron while in (b) there is a hole.

The vertex can be calculated easily up to the second order [see Eq. (5), Ref. 22] and it has the form for $T=0$

$$V^s_{\hat{k}_2\hat{k}_1}-2i\rho_0\sum_{i,j}\int\frac{dS_F}{S_F}(V^i_{\hat{k}_2\hat{k}}V^j_{\hat{k}\hat{k}_1})\epsilon^{ijs}\ln\left[\frac{D}{\hbar\omega}\right], \tag{3.1}$$

where ω is the ingoing energy, the Levi-Cività symbol ϵ^{ijs} is due to the commutation relations for the Pauli operators, dS_k is a surface element, and S_F is the total area of the Fermi surface ($S_F=4\pi k_F^2$). It is important to emphasize that the self-energy does not contribute to the leading order.

A. Scaling equations

The idea of scaling is to reduce the cutoff and at the same time to correct the bare couplings in order to keep the scattering amplitude nearby the Fermi energy unchanged. The scaling equation can be constructed in the "poor-men's" style suggested by Anderson,[31] and it has the form

$$\frac{\partial V^s(D)}{\partial\ln D}=2i\rho_0\sum_{i,j}\epsilon^{ijs}\int V^i_{\hat{k}_2\hat{k}}(D)V^j_{\hat{k}\hat{k}_1}(D)\frac{dS_k}{S_F}, \tag{3.2}$$

which leaves the scattering amplitude given by the vertex (3.1) invariant. One can write this equation in a more convenient form by using the matrix representation $V^S_{\beta\alpha}$ given by Eq. (2.35) for the couplings and by introducing the dimensionless variable $x=\ln(D_0/D)$ with the original physical value of the coupling D_0 and with the scaled value D as

$$\frac{\partial V^s_{\alpha\beta}(x)}{\partial x}=-2i\sum_{i,j}\epsilon^{ijs}\sum_{\gamma}V^i_{\alpha\gamma}(x)V^j_{\gamma\beta}(x) . \tag{3.3}$$

The boundary condition for the scaling equation is that at the original physical value of the cutoff $D=D_0(x=0)$, the scaled coupling matches the unrenormalized bare coupling $V^s(0)$; thus $V^s(x=0)=V^s(0)$. It is important to emphasize that all of the equations quoted in this section are valid

only if D/k_B and $\hbar\omega/k_B$ are larger than the temperature T and the parameters of the TLS as Δ and Δ_0. In the other case the $\ln(D/\hbar\omega)$ term in Eq. (3.1) should be replaced by

$$\ln[D/\max(\hbar\omega,k_BT,\Delta,\Delta_0)],$$

and thus the scaling equation given by Eq. (3.3) cannot be applied for $D<k_BT,\Delta,\Delta_0$.

The solution of these scaling equations for the coupling is equivalent to the summation of the parquet diagrams for the vertices. (The parquet diagrams are those which can be cut into two pieces by cutting one electron and one pseudofermion line in such a way that the diagrams produced are also parquet diagrams.)

It is interesting to note that if two of the couplings differ from zero and if they do not commute, then the third coupling is generated by the scaling equation (3.3). The behavior of the system essentially depends on whether or not the couplings commute. In the commutative case the vertex is not renormalized in the leading order nor is the "invariant coupling" enhanced in the next-to-leading logarithmic approximation. However, we have seen that in the physical model of a single tunneling atom the couplings given by Eqs. (2.41a) and (2.41b) do not commute. Considering the noncommutative model the scaling equation (3.3) cannot be solved for arbitrary couplings $V^i_{\alpha\beta}$; therefore, we have to restrict the calculation to some subspace. In Ref. 21, a two-component subspace was used without physical justification; however, the scaling was discussed in considerable detail. The following two sections, III B and III C, are devoted to giving physical justification for using a two-component subspace and to providing a procedure for how this subspace can be found. Here a detailed analysis will be given for those results which are quoted in Ref. 24.

B. The general features of the fixed point

The problem treated in the present work is not a real three-dimensional one from the point of view of phase transition. There is a single TLS and the electron states of interest can be characterized by the absolute value of the wave vector k of the spherical waves and by a few quantum numbers such as $l=0,1,2$ and the corresponding m values. Wilson[32] has shown that such an electron gas can be mapped on a single chain of fermions decorated by the discrete quantum numbers and the chain is semi-infinite with the TLS at the end. If a finite number of l,m are kept, then the problem is a real one-dimensional problem without phase transition; furthermore, according to Anderson's argument[31,33] there is no finite singular point on the scaling trajectories. Thus fixed points may occur only at zero or at infinity. However, using the model with two spherical modes, it has been pointed out in Ref. 21 that only the finite fixed point is stable.

In order to explore the consequences of the ideas mentioned above, attention must be focused on the matrix structure of the scaling equation (3.3). In a certain approximation near the fixed point, the vector space in which the matrices operate can be divided into invariant subspaces, and the scaling equations can be separately studied. More precisely, in a well-established approximation scheme at the fixed point, there is at least one subspace which can be treated independently of the others. In the treatment of Sec. III C, that subspace is of two dimensions.

Let us consider one subspace labeled by μ. After eliminating a large part of the phase space by scaling, it can be generally expected that the matrix character of the coupling $v^i_{\alpha\beta}$ does not change with further scaling. Thus in the neighborhood of the fixed point the matrices $v^i_{\alpha\beta}$ can be factored as

$$v^i_{\alpha\beta}(x)\rightarrow v^i(x)V^{*i}_{\alpha\beta}\ , \tag{3.4}$$

where the unitary matrix $V^*_{\alpha\beta}$ describes the matrix structure near the fixed point and $v^i(x)\geq 0$ is the amplitude. In this case the scaling equation (3.3) falls into two parts,

$$\frac{\partial v^s_\mu(x)}{\partial x}=2\sum_\mu v^i_\mu(x)v^j_\mu(x),\quad i\neq js \tag{3.5}$$

and

$$iV^{*s}_{\alpha\beta}(\mu)=\sum_{i,j}\sum_\gamma V^{*i}_{\alpha\beta}(\mu)V^{*j}_{\gamma\beta}(\mu)\epsilon^{ijs}. \tag{3.6}$$

As a consequence of the last equation, the $V^{*i}_{\alpha\beta}(\mu)$ must be the infinitesimal generators of an irreducible unitary representation of the rotational group characterized by a spin S_μ. The dimension of the subspace is $2S_\mu+1$.

Turning to the amplitude equation (3.5) the solution can be looked for in the following form:

$$v^i_\mu(x)^2=\psi^2_\mu(x)+v^i_\mu(x_0)^2\ , \tag{3.7}$$

where ψ satisfies the following equation:

$$\frac{\partial\psi^2}{\partial x}=4v^x(x)v^y(x)v^z(x)\ , \tag{3.8}$$

with the boundary condition $\psi_\mu(x_0)=0$ at an appropriately chosen x_0. For the infinite fixed point $|\psi_\mu|\rightarrow\infty$; thus $v^i_\mu(x)$ must tend to a uniform amplitude function $v_\mu(x)>0$ which is independent of the index i. The ψ_μ functions will be different in the different invariant subspaces; thus, disregarding the possibility of accidental degeneracy, one of the ψ_μ's

must be larger than the others. Let us call that subspace μ_m, and for our purposes only that subspace is considered. Summarizing the results obtained, the scaled Hamiltonian H_{μ_m} for $x \to \infty$ for subspace μ_m can be written in the following form:

$$H_{\mu_m} = \frac{1}{\rho_0} v_{\mu_m}(x)\vec{\sigma} \times \int (A^{\dagger}_{\mu_m k_2 \beta} \vec{S}_{\mu_m \beta\alpha} A_{\mu_m k_1 \alpha}) dk_2 dk_1 , \quad (3.9)$$

where $a_{k\alpha}$'s are annihilation operators for properly normalized spherical waves with momentum k (k is scalar) and with index α. The result (3.9) shows that keeping only the dominant subspace μ_m the scaled Hamiltonian is equivalent with the Kondo Hamiltonian for a single magnetic impurity with spin $S=\frac{1}{2}$; however, the electrons have generalized spin S_{μ_m}. The first spin $S=\frac{1}{2}$ corresponds to the TLS and the second S_{μ_1} corresponds to the different spherical orbitals. The coupling is isotropic in space and its strength $v(x)$ tends to infinity as $x \to \infty$.

It will be shown in Sec. III C that the dominant subspace μ_m is two dimensional. This result may be conjectured on the basis that the TLS with two positions is mainly coupled to two different spherical waves. The positive sign of the coupling $V_{\mu_m}(x) > 0$ corresponds to the antiferromagnetic Kondo problem which scales to the infinite strong coupling region also. Thus the present problem scales to the $S=\frac{1}{2}$ antiferromagnetic Kondo Hamiltonian. It is interesting to note that our starting Hamiltonian does not exhibit any conservation law, but for the scaled Hamiltonian there is a conserving quantity, namely, the fictitious total spin

$$\vec{S}_{\mu_m} + \tfrac{1}{2}\vec{\sigma} . \quad (3.10)$$

The appearance of a conserving quantity indicates that the ground state is highly correlated (Kondo-type ground state) in contrast with the high-temperature behavior.

Finally, we may mention that at very low temperature, if several invariant subspaces exist, the coupling can be very large in more than one subspace. In this case the single TLS spin is coupled simultaneously to several electron quasispins representing the electron orbitals. Thus the scaled Hamiltonian is the sum of the Kondo Hamiltonian

$$H = \frac{1}{\rho_0} \sum_{\mu} v_{\mu}(x)\vec{\sigma} \times \int \sum_{\alpha,\beta} (A^{\dagger}_{\mu k_2 \beta} \vec{S}_{\mu,\beta\alpha} A_{\mu k_1 \alpha}) dk_1 dk_2 , \quad (3.11)$$

but here the single impurity spin produces a strong coupling between different subspaces. The ground state for this Hamiltonian must be a very highly correlated state. We assume, however, that the temperature range of interest is not low enough for formation of this ground state of a new kind; thus it is sufficient to retain only one subspace and to consider the single Hamiltonian (3.9). It must be pointed out that, at very low temperatures, the dimensionality of the dominant subspace may change by lowering the temperature. The next section is devoted to showing that the subspace of interest is two dimensional and to giving a practical procedure to find that subspace.

C. Search for the relevant two-dimensional subspace

It will be shown that according to the scaling equation (3.3) the rate of increase is different for different α,β components of the coupling $v^i_{\alpha\beta}$ representing the angular behavior of the electron wave function. This consideration is based on the fact that it is assumed that in the first region of scaling the electron-assisted tunneling for the TLS is rather weak, thus $v^x, v^y \ll v^z$ ($v^x, v^y \sim e^{-\lambda}$). In this case we can expand the right-hand side of the scaling equation (3.3) with respect to the small parameter $e^{-\lambda}$; actually we linearize in v^x and v^y. This procedure becomes transparent if we choose a representation where v^z is diagonal. With the use of the matrix form of the couplings, $\underline{v}^z$ can be diagonalized by a unitary transformation $\underline{U}$; thus the new representation is given as

$$\tilde{\underline{v}}^i(x) = \underline{U}^{\dagger} \underline{v}^i(x) \underline{U} , \quad (3.12)$$

where $\tilde{\underline{v}}^z(x=0)$ is diagonal as

$$[\tilde{\underline{v}}^z(0)]_{\alpha\beta} = v^z_{\alpha}(0)\delta_{\alpha\beta} . \quad (3.13)$$

The result of the transformation of this kind is presented for the model of single-atom tunneling in Appendix A. The linearized version of the scaling equation for the coupling matrices is given as

$$\frac{\partial v^z(x)}{\partial x} = 0 , \quad (3.14a)$$

$$\frac{\partial v^x(x)}{\partial x} = -2i[v^x(x), v^z(x)]_- , \quad (3.14b)$$

$$\frac{\partial v^y(x)}{\partial z} = 2i[v^x(x), v^z(x)]_- , \quad (3.14c)$$

which are valid in the region of x where $v^x(x)$, $v^y(x) \ll v^z(0)$ and the square brackets with subscript $-$ is the commutator. The variables can be separated by considering the differential equations for

second order for the couplings. From Eqs. (3.14a)–(3.14c) it follows that

$$\frac{\partial^2 v^i(x)}{\partial x^2}=4[(v^i,v^z)_-,v^z]_- , \tag{3.15}$$

which has a simpler form in the new representation as

$$\frac{\partial^2 \tilde{v}^i_{\alpha\beta}(x)}{\partial x^2}=\tilde{v}^i_{\alpha\beta}(x)[\tilde{v}^z_\alpha(0)-\tilde{v}^z_\beta(0)]^2, \quad i=x,y \tag{3.16}$$

where the correct boundary condition is $v^y(0)=0$. The solutions of these equations can be given as

$$\tilde{v}^z_{\alpha\beta}(x)=\delta_{\alpha\beta}\tilde{v}^{(z)}_\alpha(0), \tag{3.17a}$$

$$\tilde{v}^x_{\alpha\beta}(x)=\tilde{v}^x_{\alpha\beta}(0)\cosh\{2[\tilde{v}^z_\beta(0)-\tilde{v}^z_\alpha(0)]x\} , \tag{3.17b}$$

$$\tilde{v}^y_{\alpha\beta}(x)=i\tilde{v}^x_{\alpha\beta}(0)\sinh\{2[\tilde{v}^z_\beta(0)-\tilde{v}^z_\alpha(0)]x\} . \tag{3.17c}$$

The components $\tilde{v}^x_{\alpha\beta}$ and $\tilde{v}^y_{\alpha\beta}$ with those indices α,β increase in the fastest way, for which

$$|\tilde{v}^z_\beta(0)-\tilde{v}^z_\alpha(0)| \tag{3.18}$$

is the largest. If the other differences of this type are somewhat smaller, then the corresponding matrix elements are negligible during scaling. Only components α,β associated with the largest difference are kept. In this way we have a procedure for finding the dominant representation which is two dimensional. In the concrete model of the single tunneling atom the subspace consists of two linear combinations of spherical functions $l=0$, $l=1$, and $l=2$ with $m=0$. (See Appendix A.)

IV. SOLUTION OF THE SCALING EQUATIONS

Making use of the results of the preceding section we retain only two components in the scaling equations (3.3). In this limited case we can write $v^i_{\alpha\beta}$ $(\alpha,\beta=1,2)$ as a linear combination of the Pauli operators $(\sigma^j_{\alpha\beta})_e$ and of the unit operators $(I_{\alpha\beta})_e$; thus

$$V^i_{\alpha\beta}=v^i_0(I_{\alpha\beta})_e+\sum_j v^i_j(\sigma^i_{\alpha\beta})_e \tag{4.1}$$

as has been done in Ref. 21, where the subscript e refers to the fact that the matrices act in the space describing the spherical part of the electron wave functions. The term proportional to $(I_{\alpha\beta})_e$ can be dropped, because the term v^i_0 is not enhanced due to scaling and does not effect the other coefficients as v^i_j. The coupling v^i_j $(i,j=x,y,z)$ has nine components. The scaling equations (3.3) become significantly simpler if v^i_j are diagonal; thus $v^i_j=v^i\delta_{ij}$ and

$$v^i_{\alpha\beta}=v^i(\sigma^i_{\alpha\beta})_e, \tag{4.2}$$

with no summation on index i. According to the results [(A5) and (A6)] derived in Appendix A this is actually the case for the model of single-atom tunneling, and this will be assumed in the following part of the paper. The general case with nine couplings v^i_j has already been discussed in Ref. 21 and a more general method is suggested in Appendix B, where it has been shown that by performing different rotations in the quasispin (upper index) and electron wave-function space (lower index), v^i_j can always be diagonalized. Thus the assumption (4.2) only means that the correct representation has been chosen. The diagonal case is similar to an anisotropic x-y-z Kondo problem, which was first discussed by Shiba.[34] In the major part of this paper we present a method to solve the scaling equation, which can also generalize to the more complicated case of more than two components and to the case of the second-order scaling to be treated in the following paper.[27] For completeness the exact solution of the scaling equation will be represented for the diagonal case in the Appendix C.

The scaling equations (3.3) to be solved in the special two-dimensional diagonal case have the simple form

$$\frac{\partial v^x}{\partial x}=4v^yv^z, \tag{4.3a}$$

$$\frac{\partial v^y}{\partial x}=4v^zv^x, \tag{4.3b}$$

$$\frac{\partial v^z}{\partial x}=4v^xv^y. \tag{4.3c}$$

These equations will be integrated in two intervals where (i) $v^y\lesssim v^x\ll v^z$ and (ii) $v^y\sim v^x\lesssim v^z$, and the solutions will be matched at some arbitrary points x_1 in the region between (i) and (ii). The final result will be independent of the choice of x_1. The main purpose of solving the scaling equations (4.3a)–(4.3c) is to find the crossover temperature T_K (frequently called Kondo temperature) which corresponds to that small value of the cutoff where the scaled couplings approach the order of unity. At this region the scaling treatment in the present form loses its applicability because the right-hand side of the scaling equation has been determined in the framework of perturbation theory. Thus the crossover temperature or energy separates the weak and strong coupling regions where the behavior of the system is essentially different.

Let us consider the two regions separately:

(i) Region $v^y(x) \lesssim v^x(x) \ll v^z(0)$. The solution for this region has already been presented. With the use of the notation (4.2) the result given by Eqs. (3.17b)—(3.17c) can be written in the form

$$v^x = v^x(0)\cosh[4v^z(0)x] , \tag{4.4a}$$

$$v^y = v^x(0)\sinh[4v^z(0)x] . \tag{4.4b}$$

Let us choose x_1 so that $4v^z(0)x_1 \gg 1$; thus

$$v^x(x_1) \sim v^y(x_1) \sim v^x(0)\tfrac{1}{2}\exp[4v^z(0)x_1] .$$

Furthermore, $v^x(x_1) \sim v^y(x_1) \ll v^z(0)$. One can express x_1 from the equation above as

$$x_1 = \frac{1}{4v^z(0)} \ln\left[\frac{2v^x(x_1)}{v^x(0)}\right] . \tag{4.5}$$

(ii) Region $v^y(x) \sim v^x(x) \lesssim v^z(x)$. In this region we have only two equations to be considered as $v^x \sim v^y$, thus

$$\frac{\partial v^z}{\partial x} = 4v^{x2} \tag{4.6a}$$

and

$$\frac{\partial v^x}{\partial x} = 4v^x v^z . \tag{4.6b}$$

In this region there is a scaling invariant, namely

$$[v^z(x)]^2 - [v^x(x)]^2 = C^2 . \tag{4.7}$$

The first equation can be integrated after eliminating $(v^x)^2$ with the aid of Eq. (4.7). The result can be obtained in a straightforward way; thus

$$x - x_1 = \frac{1}{8C}\left[\ln\left[\frac{v^z - C}{v^z + C}\right]\right]_{v^z(x_1)}^{v^z}$$
$$= \frac{1}{8C}\left[\ln\left[\frac{v^z - C}{v^z + C}\right] - 2\ln\left[\frac{v^x(x_1)}{v^z(x_1) + C}\right]\right] , \tag{4.8}$$

where, using Eq. (4.7), $v(x)$ has been inserted with $x = x_1$. Making use of $v^x(x_1) \ll v^z(x_1)$ one obtains that $C \simeq v^z(x_1) \simeq v^z(0)$, and then the above result has a simpler form for $v^z \gg v^z(0)$ as follows:

$$x - x_1 \simeq \frac{1}{4v^z(0)}\left[-\frac{v^z(0)}{v^z} - \ln\left[\frac{v^x(x_1)}{2v^z(0)}\right]\right] . \tag{4.9}$$

Finally, by adding Eqs. (4.5) and (4.9) one gets

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

It is important to notice that $v^x(x_1)$ does not appear in this equation, and that makes the method proposed here applicable.

Let us define the crossover temperature as[35]

$$k_B T_K = D_0 \left[\frac{v^x(0)}{4v^z(0)}\right]^{1/4v^z(0)} , \tag{4.11}$$

which has a singular point of $v^z = 0$. With the use of this expression for T_K, Eq. (4.10) can be written as

$$x = \frac{1}{4v^z(x)} + \ln\left[\frac{D_0}{k_B T_K}\right] . \tag{4.12}$$

The numerical solution of the scaling equations for v^x and v^z as a function of $D/D_0[x = \ln(D_0/D)]$ is shown in Fig. 7. If $v^z \gtrsim 1$, then D is proportional to T_K and the proportionality factor depends only on v^z, and that is the order of unity. Thus T_K indeed indicates the crossover from the weak to the strong coupling region. It is interesting to note that $v_z \to \infty$ as $D \to k_B T_K$, but this result has no physical significance because it occurs where the scaling Eqs. (4.3a)—(4.3c) of first order are not applicable. In Fig. 7 the scaling of v^x and v^z is also shown. As we have earlier discussed in this section, the initial value of coupling v^y is $v^y(0) = 0$, but that increases faster than v^x does; thus for $D < D_0 \exp[-1/4v^z(0)]$ the couplings v^x and v^y are approximately the same. The region where $v^y \ll v^x$ is so short that it cannot be seen clearly in Fig. 7. In the next region, where $v^x \sim v^y \ll v^z$, the coupling v^z is almost constant and that is approached by the increasing v^x and v^y. If D is in the order of magnitude of the crossover temperature T_K, then $v^x \sim v^y \sim v^z$.

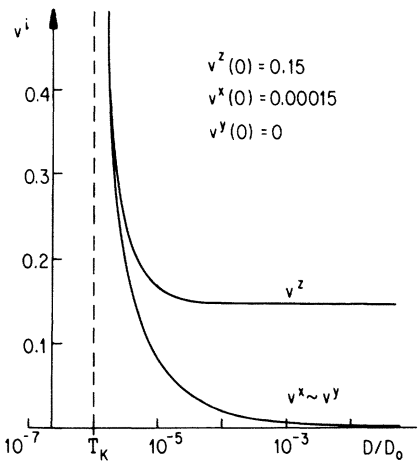

FIG. 7. Scaling of the couplings v^x, v^y, and v^z are calculated using Eqs. (4.3a)—(4.3c) with initial values $v^z(0) = 1.5 \times 10^{-1}$, $v^x(0) = 1.5 \times 10^{-4}$, and $v^z(0) = 0$. The crossover temperature given by Eq. (4.11) is indicated by the dotted line.

The crossover temperature given by Eq. (4.11) has a singular point at $v^z(0)=0$; therefore, if $v^z(0)$ decreases, then T_K is approaching zero. Using the typical values $v^x/4v^z \sim 10^{-3}$ [see Eq. (2.33)] and $D_0 \sim 10$ eV $\sim(10^5\ \mathrm{K})k_B$, we can conclude that v^z has a lower bound $v^z > 0.2$ in order to get $T_K > 1$ K.

V. DISCUSSION

The present paper is based on the previous observation[22] that the commutative and the noncommutative models behave in very different ways. Treating the noncommutative model in the first order of the perturbation theory, the electron-TLS scattering results in different angular distributions for the momenta of the outgoing electrons depending on whether the diagonal or the off-diagonal term in the interaction has been taken into account. Furthermore, it has previously been emphasized that in the higher order of the perturbation theory the angular distribution of the scattered electrons keeps some memory of the subsequent order of the different scattering processes (v^x and v^z processes). This behavior is somewhat similar to the problem of magnetic impurity where a similar memory is built in the spin polarization of the scattered wave function of the conduction electrons. Studying a simplified model with two spherical wave functions, it has been shown also[21] that the scaling in the cutoff drives the system into the strong coupling region. The present paper has been focused to show that this conclusion is independent of the special details of the model. On the other hand, all of the general features have been demonstrated using a simple physical model for the TLS where only a single atom is tunneling.

The general structure of the Hamiltonian considered here is completely independent of the special features of the model studied here (see Sec. II A); thus the structure of the scaling equations derived in Sec. III and their solution presented in Sec. IV hold for the general case. The scaling equation (3.4) has been constructed by using elementary consideration; thus on the right-hand side of this equation only the first term of a polynomial has been kept. As the problems studied here are scaled to the strong coupling region, the application of the first-order scaling equations is, therefore, limited to the high-temperature region $T > T_K$. With the use of the general structure of the scaling equation (3.4) it has been concluded in Secs. III A and III B that, in the space of the angular distributions of the incoming and outgoing momenta for the electrons, it is sufficient to keep only two angular functions f_α ($\alpha=1,2$) and, furthermore, a procedure is suggested to determine these functions. With the use of a general argument (see Sec. III A) supported by the detailed calculations of Sec. IV, the conclusion has been drawn that in the relevant subspace for the spherical harmonics the problem scales to a strong coupling Hamiltonian with a form which coincides formally with the *s-d* Kondo Hamiltonian with impurity spin $S=\frac{1}{2}$. In this correspondence the quasispin of the TLS and the magnetic impurity spin are related and furthermore, the angular dependence of the scattered electron wave functions and the conduction-electron spins are related. The ground state of this scaled Hamiltonian is a highly correlated state, where the TLS and the screening conduction-electron cloud move together. It is an interesting feature of the theory that the original electron-TLS Hamiltonian given by Eq. (2.6) does not contain any conserving quantity, but for the scaled Hamiltonian there exists a fictitious total spin [see Eq. (3.10)] which is conserved. This is a strong indication that at low temperature there is a strong correlation between the quasispin of the TLS and the angular distribution of the electron momenta.

Solving the scaling equations (4.3a)—(4.3c) of the first order, the crossover temperature T_K given by Eq. (4.11) has been determined which is between the weak and strong coupling regions. For the correct value of the crossover temperature T_K the scaling equation of the second order must be used with quadratic correction on the right-hand side of Eq. (4.3a)—(4.3c). The construction of these scaling equations is more sophisticated; therefore, those will be discussed in the following paper (paper II). As the crossover temperature T_K is very sensitive on the coupling v^z, the detailed discussion of the order of magnitude will be presented in the following paper (paper II), where the correct expression for T_K will be derived. The main feature found in Sec. IV, however, remains valid, namely, that v^z must exceed some critical value to obtain a crossover temperature in the observable temperature range. If the coupling v^z is too small, then the coupling v^x remains negligible in the whole range of scaling; thus the commutative model is appreciable.[23]

The scaling argument presented here can be applied to temperatures which are large compared to the energy splitting E. Below this temperature region there is no essential temperature dependence because the TLS cannot be excited by thermal excitations. It is to be noted that the splitting E itself is also renormalized in an essential way, as will be discussed in the following paper (paper II).

In addition to the general treatment, the model of the single tunneling atom has been treated in considerable detail. It has been found that the two angular modes for the momentum dependence of the electron wave functions are linear combinations of the

s-, p-, and d-like harmonics. Expressions (2.21) and (2.30) have been derived for the two bare couplings and the ratio v^x/v^z given by Eq. (2.32) has been estimated, and it has been found in the order of magnitude $v^x/v^z \sim 10^{-4}$. This ratio apppears in the expression (4.11) of the crossover temperature; thus that plays a role of crucial importance. Even if this value has been obtained in the particular model treated here, we are going to accept it as a rough estimation for the general case.

Finally, we mention that we have used a free-electron-like wave function for the conduction electrons, which is not realistic in the case of metallic glasses. We may note, also, that the actual dimension of the sample in real space does not enter in this problem, because that affects not the energy density of states but only the energy spacing of the levels. The spacing of the levels does not play any significant role, unless it becomes larger than the scaled value of the cutoff D. The latter case does not look interesting for real physical systems. Furthermore, the main results obtained here are certainly valid in the case where the TLS excitations are at the surface of the sample.

It is interesting to point out concerning the Hamiltonian suggested by Cochrane *et al.*,[13] that the exact form of that Hamiltonian has been recovered in the scaling region (ii) (Sec. IV) where $v^y(x) \sim v^x(x) \lesssim v^z$, and an interpretation has been given for the orbital indices $\alpha = 1,2$ assigned by them to the conduction electrons. Thus the suggested Hamiltonian appears in the present theory as the scaled Hamiltonian with the scaled couplings in region (ii) (Sec. IV).

In the following paper (II) the scaling equations of the second order are constructed in order to obtain the correct expression at the crossover temperature T_K and the scaling of the energy splitting E. Applying these results and the scaling, different physical quantities such as electrical conductivity, TLS relaxation time, and inelastic electron lifetime are calculated and compared with the available experimental results in a separate paper (III).

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APPENDIX A

For the model of single-atom tunneling the transformation which diagonalizes the matrix v^z given by Eq. (2.41a) can be constructed easily. The basic wave functions for the diagonalized form are

$$\overline{f_1} = \frac{1}{\sqrt{2}}[(\cos\theta\, Y_0^0 - \sin\theta\, Y_2^0) + iY_1{}^0], \tag{A1}$$

$$\overline{f_2} = \frac{1}{\sqrt{2}}[-(\cos\theta\, Y_0^0 - \sin\theta\, Y_2^0) + iY_0^0], \tag{A2}$$

$$\overline{f_3} = -\cos\theta\, Y_2^0 - \sin\theta\, Y_0^0, \tag{A3}$$

$$\overline{f_4} = -iY_3^0, \tag{A4}$$

with

$$\theta = \arctan[\sqrt{4/5}a_1/(a_0 - a_1)].$$

Furthermore, the coupling matrices (2.41a) and (2.41b) have the new forms

$$[\underline{v}^z(0)]_{\alpha\beta} \sim v^z(0) \begin{bmatrix} 1 & 0 & \\ & & \underline{0} \\ 0 & -1 & \\ 0\ \underline{0} & & \underline{0} \end{bmatrix} \tag{A5}$$

and

$$[\underline{v}^x(0)]_{\alpha\beta} \sim v^x(0) \begin{bmatrix} 0 & 1 & \\ & & \underline{X} \\ 1 & 0 & \\ \underline{X} & & \underline{X} \end{bmatrix}, \tag{A6}$$

where for the sake of simplicity the components of no importance are indicated by X. In the form above, both $v^z(0)$ and $v^x(0)$ are positive and

$$v^z(0) = \rho_0 \tfrac{1}{2} dk_F \left[\left[\frac{a_0 - a_1}{3} \right]^2 + \tfrac{4}{15} a_1^2 \right]^{1/2}. \tag{A7}$$

One can work out the channels with $m \neq 0$ also, but it turns out that they are not the dominant channels.

APPENDIX B

We have mentioned in Sec. IV that, after restricting the space of spherical harmonics to a two-component subspace, the general form of the coupling matrices decomposed in terms of Pauli operators [see Eq. (4.1)],

$$v_{\alpha\beta}^i = \sum_j v_j^i (\sigma_{\alpha\beta}^j)_e, \tag{B1}$$

where the term of unit matrix is dropped; thus the corresponding term in the interaction is

$$\sum_j v_j^i \sigma^i (\sigma_{\alpha\beta}^u)_e \ , \tag{B2}$$

where σ^i acts on the states of the TLS and $(\sigma_{\alpha\beta}^i)_e$ on the spherical harmonics for the conduction electrons.

First it should be pointed out that rotations can be performed separately in the TLS pseudospin space and in the space of the spherical harmonics. The rotations correspond to the introduction of a new set of basic functions for the TLS or for the spherical harmonics, respectively. We show here that one can always find a representation where the coupling matrix v_j^i is diagonal.

Let us consider the appropriate transformation to diagonalize the matrix $\underline{\hat{V}}$ with real (ij) component v_j^i. These transformations are associated with rotations of the spin operators [σ^i and $(\underline{\sigma}^j)_e$] or with the introduction of new basic vectors, but the latter will not be discussed in detail. The main steps are the following:

(i) $\underline{\hat{V}}^T\underline{\hat{V}}$ is symmetric matrix and real; thus $(\underline{\hat{V}}^T\underline{\hat{V}})^{-1/2}$ exists; furthermore the matrix $\underline{\hat{O}}_1 = (\underline{\hat{V}}^T\underline{\hat{V}})^{-1/2}\underline{\hat{V}}^T$ is orthogonal, where $\underline{V}^T$ is the transposed of $\underline{V}$.

(ii) Let us transform the upper index of v_j^i by the orthogonal matrix $\underline{\hat{O}}_1$ as $\underline{\hat{O}}_1\underline{\hat{V}} = (\underline{\hat{V}}^T\underline{\hat{V}})^{1/2}$, which is also symmetric. This transformation means a rotation in the spin space representing the TLS.

(iii) An orthogonal matrix $\underline{\hat{O}}$ must exist which diagonalizes the symmetric matrix $\underline{\hat{O}}_1\underline{\hat{V}}$. This transformation leads to the diagonalized matrix $\underline{\hat{O}}\,\underline{\hat{O}}_1\underline{\hat{V}}\,\underline{\hat{O}}^+$ and the transformation means a rotation in the TLS-spin space and in the electron-spin space (describing the spherical harmonics) simultaneously.

APPENDIX C

The integration of the scaling Eqs. (4.3a)–(4.3c) can be carried out exactly. First we note that the solution of the scaling equation can be written as given by Eq. (3.7) in terms of the function ψ; if in the right-hand side of (3.8) $v^i(x)$'s are expressed by ψ and by their initial values $v^i(0)$, then in Eqs. (3.4) and (3.8) the matrix part of the coupling has been given by spin operators instead of Pauli matrices. With the use of Pauli matrices an extra factor 2 appears on the right-hand side of Eqs. (3.4) and (3.8). Then the differential Eq. (3.8),

$$\frac{\partial\psi}{\partial x} = 4\{\psi^2+[v^x(0)]^2\}^{1/2}\{\psi^2+[v^z(0)]^2\}^{1/2} \ , \tag{C1}$$

can be easily integrated as

$$\tfrac{1}{4}\int_0^{\psi} d\frac{\psi}{\{\psi^2+[v^x(0)]^2\}^{1/2}\{\psi^2+[v^y(0)]^2\}^{1/2}} = x \ , \tag{C2}$$

where we used the fact that $v^y(0)=0$. By using the integral on p. 245 of Ref. 36,

$$x = \tfrac{1}{4}\frac{1}{v^z}F\left[\arctan\left[\frac{\psi}{v^x(0)}\right], \frac{\{[v^z(0)]^2-[v^x(0)]^2\}^{1/2}}{v^z(0)}\right], \tag{C3}$$

where F is an elliptical integral of the first kind. In the interesting region, $\psi \gg v^x(0)$ holds; thus $\arctan[\psi/v^x(0)] \sim \pi/2$ and $F(\pi/2,y)=K(y)$, and

$$x = \tfrac{1}{4}\frac{1}{v^z(0)}K\left[\frac{\{[v^z(0)]^2-[v^x(0)]^2\}^{1/2}}{v^z(0)}\right] . \tag{C4}$$

Furthermore, by approximating the complete elliptic integral of the first kind K,

$$K(m) \simeq \tfrac{1}{2}\ln\left[\frac{16}{1-m^2}\right] \text{ for } m \sim 1 \ . \tag{C5}$$

Thus in the limit $v^z(0) \gg v^x(0)$,

$$x = \frac{1}{4v^z(0)}\ln\left[\frac{4v^z(0)}{v^x(0)}\right] . \tag{C6}$$

It is interesting to note that the integral calculated very slightly depends on ψ in region $\psi \gg v^x(0)$, and the result given by Eq. (C6) is equivalent to that obtained for the crossover temperature T_K by the approximation given in Sec. IV [compare with Eq. (4.11) for $x = \ln(D_o/k_B T_K)$].

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