# Theory of a two-level system interacting with a degenerate electron gas. I. Partition function

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The problem of the two-level system (TLS) interacting with a free-electron gas is considered. In a previous work Yu and Anderson treated that problem by taking into account the screening by the conduction electrons described by an arbitrarily large phase shift. The present paper is devoted to a generalization of their result by including weak electron-assisted TLS transition processes. Generalizing the Yuval-Anderson technique, the partition function is derived, which has the form of the partition function of a one-dimensional Coulomb gas with logarithmic interactions. The charges introduced depend on the phase shifts and on the electron spin and orbital quantum numbers corresponding to the incoming and outgoing electrons in the related electron-TLS scattering processes. Additionally charged dipoles are introduced to describe those processes in which the scattered electrons do not change their quantum number. Special care is paid to the formal divergencies occurring in these processes if the long-time asymptotic expressions are used for the conduction-electron Green's functions. In this way, going beyond the charge-charge interaction, charge-dipole and dipole-dipole interactions are introduced. The next paper deals with the derivation of the scaling equations, which are derived by eliminating the short-time behavior.

## I. INTRODUCTION

In recent years two-level systems (TLS's) interacting with a fermionic heat bath have attracted considerable interest. This model was first applied to local excitations in the atomic motion of amorphous metals.[1] In these problems the transitions between the two levels are due to tunneling, thus they are very weak. Kondo proposed that such a model may show a strong similarity to the localized spin problem in metals known as the Kondo effect.[2,3] Anderson and Yu argued that such a model including the formation of the double-potential well for the atom representing the TLS's might contribute to the understanding of the behavior of the $A15$ compounds.[4] TLS's interacting with a heat bath also serves as a model system for quantum dissipation, which has been studied in great detail since the pioneering work by Caldeira and Leggett.[5,6] In these studies the dissipative heat bath is characterized by Bose degrees of freedom. The question has been raised as to what extent the fermionic and bosonic heat baths behave in a similar manner.[7–9] The problem under study is essentially a version of Anderson's orthogonality catastrophe.[10] In the present problem a particle with different positions is screened by a degenerate electron gas which has electron-hole excitations with very small energies. According to Anderson the screening clouds formed around the particle with different positions are orthogonal to each other. Thus, the hopping motion of a particle must be strongly influenced by the overlap matrix element of the related screening clouds. Problems of that kind have been well known since Kagan and Klinger studied the polaron problem in that context.[11] Kagan and Prokof'ev[12] have also studied the quantum diffusion of a particle coupled to different heat baths. The case of the fermionic heat bath was attacked also by Kondo, and since that time extensive study has been performed in that direction.[13] Possible applications are H or D or muon diffusion in metals, heavy ions in $He_3$ liquid, and maybe the dynamics of heavy fermions in metals. In those theories and overlap matrix elements of the screening clouds around particles with different positions play an important role in modifying the diffusion. The present study is concentrated on the problem of how electron-assisted transitions between the two positions of a TLS may change the dynamics of the TLS in an essential way. In that case a Kondo-like resonance or bound state may be formed by the particle and the heat bath, contrary to the case where the role of the electrons is only screening.[4,14,15] That problem has been extensively studied in the framework of perturbation theory using the multiplicative renormalization-group technique.[16] It has been always assumed that not only the assisted tunneling transitions are weak, but the screening is weak also. Recently, that problem has been attacked by the present authors with arbitrarily strong[7,8] screening. The subject of the present paper is to give an extensive description of the method and the results summarized in a previous Letter.[8]

The Hamiltonian of the electron TLS interaction can be given in general form[2,3] as

$$H_1 = \sum_{i=x,y,z} \sum_{\mathbf{k}\mathbf{k}'ss'} V^i_{\mathbf{k}\mathbf{k}'} a^\dagger_{\mathbf{k}s} a_{\mathbf{k}'s'} \sigma^i , \tag{1.1}$$

 

where the TLS is described in terms of Pauli operators $\sigma^i (i=x,y,z)$ and $\sigma^z=\pm 1$ represents the two positions of the tunneling atom or the two values of a collective coordinate corresponding to the two quasiequilibrium configurations of the atomic groups. The conduction-electron plane-wave states with momentum $\mathbf{k}$ and spin $s$ are created by the operator $a^\dagger_{\mathbf{k}s}$. The interaction $V^z_{kk'}$ gives the dependence of the electron scattering amplitude on the position of the TLS, which describes the screening of the TLS. The $V^x_{kk'}$ term represents the process in which the TLS changes its position due to the scattering of an electron. This term is due to the fluctuations in the density of the electrons which result in a fluctuating barrier for the tunneling states, thus the tunneling matrix element depends on the variables of the electrons. Such processes are called electron-assisted or incoherent tunneling, and their amplitude is proportional to the tunneling matrix element; therefore, $|V^x| \ll |V^z|$.[16] That process adds to the spontaneous coherent tunneling. In the physical Hamiltonian $V^y_{\mathbf{kk}'}$ can be taken as $V^y=0$.[17] In the case of the tunneling of a single atom $V^z$ was estimated by Kondo[2] and Black *et al.*,[18] while $V^x$ was evaluated by Vladár and Zawadowski.[16] In the perturbation theory $V^y_{\mathbf{kk}'}$ is generated to second order[2] and its amplitude at energy $\omega$ is proportional to $V^x V^z$

$$\sum_{\tilde{\mathbf{k}}} (V^z_{\mathbf{k}\tilde{\mathbf{k}}} V^x_{\tilde{\mathbf{k}}\mathbf{k}'} - V^x_{\mathbf{k}\tilde{\mathbf{k}}} V^z_{\tilde{\mathbf{k}}\mathbf{k}'}) \frac{1-n_F(\varepsilon_{\tilde{k}})}{\omega-\varepsilon_{\tilde{k}}} , \tag{1.2}$$

where $\varepsilon_{\tilde{k}}$ is the energy of the electron with momentum $\tilde{\mathbf{k}}$ in the intermediate state and $n_F$ is the Fermi distribution function. The summation over the momentum leads to a logarithmic function of the energy $\omega$.

Considering the momentum dependence of the couplings $V^i_{\mathbf{kk}'}$ two cases must be distinguished.

### A. Commutative case

When the commutator in the expression (1.2) vanishes then the coupling $V^y$ is not generated. The behavior of this model is similar to the special case where only $V^z$ is different from zero. The phenomenon is a time-dependent screening, thus it means repeated changes in a localized potential acting on the electrons, like a repeated x-ray absorption problem studied by Nozières and de Dominicis.[19] Scaling equations for the system were derived by applying the method of Yuval and Anderson[20] or the multiplicative renormalization-group technique,[16] where the short-time behavior or the electrons with large energies are eliminated, respectively. The similarity to the x-ray problem is that the coupling strength $V^2=V^{x\,2}+V^{z\,2}$ is not renormalized. That feature is shown also in the extended case where the electrons are coupled to a particle moving on an infinite lattice of arbitrary dimension.[13,21]

### B. Noncommutative case

In this case both the screening by the electrons and the assisted tunneling processes are considered and the perturbation theory generates logarithmic corrections like in the spin-Kondo problem. An Abrikosov-Suhl resonance is formed at the Fermi energy in the scattering amplitude,[3] and the temperature range below which the resonance occurs is characterized by the Kondo temperature $T_K$. Assuming that the couplings are important only in two spherical wave channels they can be given in terms of two dimensionless constants $v^x$ and $v^z$; furthermore, the Kondo temperature $T_K$ is a singular function of the coupling $v^z$ as

$$T_K = D(v^x v^z)^{1/2} \left[ \frac{v^x}{4v^z} \right]^{1/4v^z} \tag{1.3}$$

where $D$ is the energy cutoff. The factor $(v^x v^z)^{1/2}$ is the correction due to the second-order scaling to the result obtained in the framework of the multiplicative-renormalization-group method, where the two most relevant angular-momentum channels can be determined also. Further details can be found in Ref. 16. The second-order renormalization-group equations are derived in the limit $v^x, v^z \ll 1$. In the Kondo problem the first-order renormalization-group equations were derived by Anderson and Yuval and Hamann for the very anisotropic case $|J^x|, |J^y| \ll 1$ and $|J^z| \lesssim 1$.[20,22] The present work is devoted to the case, where the screening is described by an arbitrary phase shift $\delta$ and the assisted tunneling is given by a small parameter $v^x$.

Considering the large-phase-shift case, no method is known by the present authors which could provide a generalization of the multiplicative-renormalization-group technique. The only method which works for large $\delta$ is the functional integral method proposed by Anderson, Yuval, and Hamann.[22] This method provides a scaling equation for large $\delta$, which reproduces the first-order scaling in the weak-couping limit of the Kondo problem ($|J^x|, |J^y|, |J^z| \ll 1$). In this method path integrals with imaginary time $\tau$ are used and the partition function $Z$ is calculated.

The method is applied in two steps.

(i) The $z$ component of the quasispin of the TLS is taken as a classical variable $\sigma(\tau)$ and a typical path is depicted in Fig. 1. For this problem the electronic response due to the interaction $V^z$ is calculated using Muskhelishvili's method for the long-time limit of the electron Green's function in a manner similar to the one developed by Nozières and de Dominicis.[19]

(ii) The effect of the assisted tunneling coupling $V^x$ is treated in perturbation theory. By applying the method developed by Yuval and Anderson[20] the contribution to the diagrams are given as products of determinants built from electron Green's functions with the same quantum numbers (spin and orbital momentum). In the Kondo problem the method is simpler to apply as the spin-flip of the localized spin is always associated with the opposite flip of the electron spin. This correlation has the consequence that the determinants for up- and down-spin electrons are of the same size. Such correlation between the quasispin of the TLS's and the orbital quantum numbers of the electrons does not exist.[16,7] In the case of two angular momentum channels such correla-

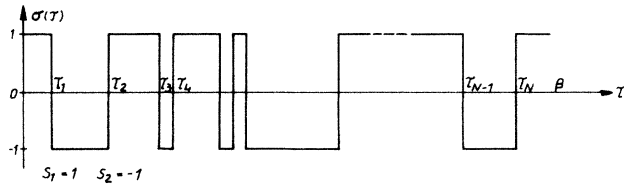


FIG. 1. A typical TLS path on the imaginary time axis is depicted with times of the transitions $\tau_1, \tau_2, \ldots, \tau_N$. The value of the TLS transition index $S_i = \pm 1$ is also indicated at the transitions.

tion would mean $V^x = V^y$ in contrast to the assumption $V^y = 0$. Applying the multiplicative renormalization group[16] or the Anderson-Yuval-Hamann method[7] it was shown that the very first part of the scaling region the coupling $V^y$ is so extensively generated that in the main part of the scaling region $V^x \sim V^y$. Zawadowski and Zimányi[7] derived the scaling equations by taking advantage of that observation. In the Anderson-Yuval-Hamann technique the short-time behavior is eliminated from the partition function by replacing the contribution of the pairs of the interaction processes with short-time difference by modified parameters of the theory. In the Kondo problem only spin-flip processes are eliminated which involve both the localized spin and the conduction electrons. A similar calculation was performed for the TLS problem by eliminating pairs of assisted tunnelings.[7] In an early work by Black *et al.*[18] the pairs of spontaneous tunnelings are eliminated in the framework of the commutative model. Later the present authors were successful in generalizing the Anderson-Yuval-Hamann technique to the case where the assisted and spontaneous tunnelings are treated on equal footing. The couplings are treated as matrixes in the angular momentum and spin variables of the electrons. The difficulty in this method is that in a given order of the perturbation theory the summation over all possible diagrams cannot be given by a determinant in a closed form. Therefore, in a given order of the perturbation theory for each vertex matrix the different matrix elements are considered separately. For such a vertex configuration the contribution of the electrons can be expressed as a product of determinants of the Green's functions with the same quantum numbers. The summations over the different configurations are not performed. Thus, the scaling must be derived for each configuration separately; furthermore, the assisted and spontaneous tunneling must be treated simultaneously without making the assumption $V^x = V^y$.

The present work is divided into two parts. In the first part the partition function is given in terms of charges associated with the particular matrix elements of the interaction. The interaction between changes depends logarithmically on the time difference $|\tau_i - \tau_j|$ of the corresponding interaction points ($\ln|\tau_i - \tau_j|$). The treatment of the Hartree-Fock diagrams results in further difficulties. Namely, if an interaction matrix elements is diagonal, then a Green's function may connect the same time point, and therefore the long-time approximation[19] cannot be applied for the Green's function. As the in- and out-going electron lines are associated with separate charges, in this case the corresponding interaction therefore cannot be treated as a logarithmic one. Both of these two charges, however, interact with another charge and these interactions can be treated as a dipole interaction, because for a diagonal interaction matrix element the in- and out-going electron lines with the same quantum number are associated with opposite charges. In this way the charge-charge interaction dipole-charge and dipole-dipole interactions occur. As the charge-charge interaction is logarithmic the latter ones are proportional to the inverse time difference and its square, respectively. A very elaborate study shows, however that the introduction of these interactions cannot be done in a formal way as some specific terms must be omitted in the expansion of the partition function expressed in terms of the charges and dipoles.

In the following paper the scaling equations are derived and solved, thus the related part of the introduction can be found there.

The paper is organized as follows. In Sec. II the Hamiltonian is given. Section III is devoted to the construction of the partition function and this consists of several parts. In Sec. III A the schema of the calculation is outlined. The results for the partition function $Z_1$ without assisted tunneling are summarized in Sec. III B. The contribution of the assisted tunnelings $Z_2$ is evaluated in detail in Sec. III C. The concept of the charges and dipoles are given at the very end of that section. A very brief summary is provided in Sec. V. The Appendix contains some detailed calculations related to the derivation of the dipole-dipole interaction.

## II. THE HAMILTONIAN

The Hamiltonian $H$ to be treated consists of three terms,

$$H = H_0 + H_1 + H_2 , \tag{2.1}$$

which will be explained in detail. The free-electron gas is described by

$$H_0 = \sum_{\mathbf{k},s} \varepsilon_{\mathbf{k}} a^{\dagger}_{\mathbf{k}s} a_{\mathbf{k}s} , \tag{2.2}$$

where $a^{\dagger}_{\mathbf{k}s}$ and $a_{\mathbf{k}s}$ are the creation and annihilation operators for the electrons with momentum vector $\mathbf{k}$ and spin $s$, and $\varepsilon_k$ is the band energy. A simplified electron band structure will be used which is spherical symmetric and in which the density of states $\rho(\varepsilon)$ for one spin value is constant, thus

$$\rho(\varepsilon) = \begin{cases} \rho & \text{for } -D < \varepsilon < D , \\ 0 & \text{otherwise} , \end{cases} \tag{2.3}$$

where a cutoff energy $D$ is applied for the band energy $\varepsilon$, which is of the order of the Fermi energy $E_F$.

The operators acting on the two states of the TLS's are given in form of Pauli operator as $\sigma^x$, $\sigma^y$, $\sigma^z$. The first part $H_1$ of the TLS-electron interaction describes the screening of the TLS by the electrons, and has a di-

agonal form in the TLS variables as

$$H_1=\sum_{\mathbf{k},\mathbf{k}',s} V^{z1}_{\mathbf{k}\mathbf{k}'}\sigma^z a^\dagger_{\mathbf{k}s}a_{\mathbf{k}'s}\ , \tag{2.4}$$

where $V^{z1}_{\mathbf{k}\mathbf{k}'}$ is the coupling.

All of the remaining terms are incorporated in $H_2$, which has six contributions

$$H_2=\sum_{\alpha=1}^{6} H_{2\alpha}\ . \tag{2.5}$$

The terms with $\alpha=1,2,3$ stand for the intrinsic dynamics of the TLS, which are

$$H_{21}=\Delta^-\sigma^+\ , \tag{2.6}$$

$$H_{22}=\Delta^+\sigma^-\ , \tag{2.7}$$

$$H_{23}=\Delta^z\sigma^z\ , \tag{2.8}$$

where $\sigma^\pm=\frac{1}{2}(\sigma^x\pm i\sigma^y)$, and $\Delta^z$ gives the energy splitting of the TLS and $\Delta^-=\Delta^+$ is responsible for the spontaneous transitions (tunneling) between the two states.

$H_{24}$ and $H_{25}$ correspond to the electron-induced transitions (electron assisted tunneling) between the two states of the TLS and they have the forms

$$H_{24}=\sum_{\mathbf{k},\mathbf{k}',s} V^-_{\mathbf{k}\mathbf{k}'}\sigma^+ a^\dagger_{\mathbf{k}s}a_{\mathbf{k}'s} \tag{2.9}$$

and

$$H_{25}=\sum_{\mathbf{k},\mathbf{k}',s} V^+_{\mathbf{k}\mathbf{k}'}\sigma^- a^\dagger_{\mathbf{k}s}a_{\mathbf{k}'s}\ . \tag{2.10}$$

Here $V^+_{\mathbf{k}\mathbf{k}'}=(V^-_{\mathbf{k}'\mathbf{k}})^*$ is the coupling.

Finally, in order to treat that part of the interaction of the form $H_1$, which is generated by the application of the renormalization group, $H_{26}$ is introduced as

$$H_{26}=\sum_{\mathbf{k},\mathbf{k}',s} V^{z2}_{\mathbf{k}\mathbf{k}'}\sigma^z a^\dagger_{\mathbf{k}s}a_{\mathbf{k}s} \tag{2.11}$$

with the value $V^{z2}=0$ before the application of the renormalization group.

Furthermore, the Hamiltonian may contain a potential scattering of the electrons by the TLS, which does not depend on the TLS variables. This term is not introduced since it can simply be taken into account as a renormalization of the electron wave functions in their spherical forms.

The interaction couplings $V^\pm_{\mathbf{k}\mathbf{k}'}$, $V^{z1}_{\mathbf{k}\mathbf{k}'}$, and $V^{z2}_{\mathbf{k}\mathbf{k}'}$ can be simplified by assuming that they depend only on the directions of the wave vectors but not on their lengths. As in the previous works[3,16,7,8] the spherical representation will be used for the electrons where the annihilation operator $a_{lms}$ is defined as

$$a^\dagger_{mls}=(2\pi^2)^{-1/2}\int d^3\mathbf{k}\ Y_l\left(\frac{\mathbf{k}}{|\mathbf{k}|}\right)a_{\mathbf{k}s}\ , \tag{2.12}$$

where the spherical quantum numbers are denoted by $l$ and $m$ and $y_{lm}$ is the spherical harmonic function. Following the previous works[16] it is more convenient to use such linear combinations of the spherical waves for which $V^{z1}$ is diagonal. In the following new indices $m$, which represent both the spherical indices in the new representation and the spin indices, will be introduced. In this representation the Hamiltonians given by Eqs. (2.4), (2.9), (2.10), and (2.11) have simpler forms:

$$H_1=\sum_{m,m'} V^{z1}_{mm'}\sigma^z a^\dagger_m a_{m'}\ , \tag{2.13}$$

$$H_{24}=\sum_{m,m'} V^-_{mm'}\sigma^+ a^\dagger_m a_{m'}\ , \tag{2.14}$$

$$H_{25}=\sum_{m,m'} V^\dagger_{mm'}\sigma^- a^\dagger_m a_{m'}\ , \tag{2.15}$$

and

$$H_{26}=\sum_{m,m'} V^{z2}_{mm'}\sigma^z a^\dagger_m a_{m'}\ , \tag{2.16}$$

where $V^{z1}_{mm'}$ is a diagonal matrix, and according to the previous studies[3,16] $V^{z1}$, $V^-$, and $V^+$ do not commute in a realistic model. The definite form of $V^z$, $V^x$, and $V^y$ can be given in a model where a pointlike tunneling atom is described by the TLS.[16,18] The notations of Ref. 16 and of this work are related as $V^\pm=V^x\pm iV^y$, $V^{z1}=V^z$, and $\Delta^\pm=(\Delta^x\pm i\Delta^y)/2$, and the present $\Delta^z$ is half of $\Delta^z$ in Ref. 16.

## III. CONSTRUCTION OF THE PARTITION FUNCTION

### A. Outline of the calculation

The present paper is devoted to the calculation of the grand canonical partition function $Z$ for the Hamiltonian given in Sec. II by applying the path-integral method with imaginary time variables denoted by $\tau$. A given classical path will be considered for the $z$ component of the TLS spin $\sigma(\tau)$, where the path is steplike and $\sigma(\tau)=\pm1$ between the steps. The steps will be called hops (see Fig. 1) and they are kinks or antikinks depending on whether $\sigma$ decreases or increases. The paths are considered in the interval $0<\tau<\beta$ where $\beta$ is the inverse temperature and the boundary conditions are $\sigma(0)=\sigma(\beta)=\pm1$. The average over the paths will be taken in the last step of the calculation. In the first part of the present work the partition function $Z\{\sigma(\tau)\}$ is evaluated as a functional of the time-dependent external field represented by $\sigma(\tau)$.

The method formulated is described as follows. Considering $H_0$ as the unperturbed Hamiltonian of the system, the perturbative series of $Z$ is

$$Z=Z_0\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\int_0^{\beta}d\tau_N\cdots\int_0^{\tau_{i+1}}d\tau_i\cdots\int_0^{\tau_2}d\tau_1\langle H_{\alpha_N}(\tau_N)\cdots H_{\alpha_i}(\tau_i)\cdots H_{\alpha_1}(\tau_1)\rangle_0\ , \tag{3.1}$$

where $\{\alpha\}=\{\alpha_1,\ldots,\alpha_i,\ldots,\alpha_N\}$ and $\alpha_i=1,21,\ldots,26$ is a configuration of the indices corresponding to specific terms of the Hamiltonian. $Z_0$ is the partition function of the electron gas represented by $H_0$. The operators $H_\alpha(\tau)$ are given in the interaction representation with the unperturbed Hamiltonian $H_0$, and the average $\langle\ \rangle_0$ is taken with the unperturbed density matrix. This average is restricted to the states which are eigenstates of the TLS operator $\sigma_z$ with, e.g., $\sigma_z=1$. This restriction provides the boundary condition for the paths in the path integral. Considering the integrand on the right-hand side of Eq. (3.1) and taking a given configuration $\{\alpha\}$, the operators $\sigma^z$ can be substituted by their $c$ values, which are determined by the time variables $\tau_i$ of the tunneling processes associated with $H_{21}$, $H_{22}$, $H_{24}$, and $H_{25}$. These $c$ values $\sigma(\tau)$ determine the path depicted in Fig. 1. Considering a given path $H_1(\tau)$ is a functional of $\sigma(\tau)$ and $H_0+H_1(\tau)$ can be taken as the unperturbed Hamiltonian, then

$$Z=Z_0\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\int_0^{\beta}d\tau_N\cdots\int_0^{\tau_{i+1}}d\tau_i\cdots\int_0^{\tau_2}d\tau_1 Z_1\langle\tilde{H}_{2\alpha_N}(\tau_N)\cdots\tilde{H}_{2\alpha_i}(\tau_i)\cdots\tilde{H}_{2\alpha_1}(\tau_1)\rangle_1\ , \tag{3.2}$$

where $\{\alpha\}=\{\alpha_1,\ldots,\alpha_N\}$ with $\alpha_i=1,2,\ldots,6$ and the interaction representation is defined for an arbitrary operator $F$ as

$$\tilde{F}(\tau)=S_1^{-1}(\tau)e^{H_0\tau}F(\tau)e^{-H_0\tau}S_1(\tau) \tag{3.3}$$

with

$$S_1(\tau)=T_\tau\exp\left[-\int_0^{\tau}\tilde{H}_1(\tau')d\tau'\right]\ ,$$

where $T_\tau$ is the time-ordering operator. The thermal average $\langle\ \rangle_1$ and $Z_1$ are defined as

$$\langle\tilde{F}(\tau)\rangle_1=\mathrm{Tr}[e^{-\beta H_0}S_1(\beta)\tilde{F}(\tau)]/\mathrm{Tr}[e^{-\beta H_0}S_1(\beta)] \tag{3.4}$$

and

$$Z_1=\langle S_1(\beta)\rangle_0 \tag{3.5}$$

The expectation value in Eq. (3.2) will be denoted by $Z_2$ for a given path.

The main steps of the calculation are as follows.

(i) $Z_1$ is calculated by using the long-time limit of the electron Green's function in the presence of the external field $\sigma(\tau)$. The interaction is $H_1$ given by Eq. (2.4).

(ii) $Z_2$ is determined by applying perturbation theory in $H_2$.

(iii) The summation over all of the paths is a functional integral

$$Z=Z_0\int D[\sigma(\tau)]Z_1Z_2=Z_0Z_I\ , \tag{3.6}$$

where $Z_I=\int D[\sigma(\tau)]Z_1Z_2$. This functional integral cannot be evaluated explicitly; therefore, we apply the renormalization group to derive scaling equations. This procedure is equivalent to the summation of the diagrams with logarithmic accuracy in the weak-coupling case $V^{z1}\rho\ll 1$, but represents a generalization of the previous results[16] for arbitrarily strong $V^{z1}$.

### B. Calculation of $Z_1$ and the one-particle Green's function

The present calculation closely follows the method developed by Hamann[23] and applied for the Hamiltonian $H_1$ by Yu and Anderson;[4] therefore, only the main steps of the calculations will be repeated. The method is based on the observation that the partition function can be expressed by the one-particle Green's function.

The electrons move in the time-dependent classical field representing the TLS, and the corresponding Dyson equation can be solved by Muskhelishvili's method for the one-particle Green's function. This solution is described below.

Considering the $\sigma$ variable in the Hamiltonian $H_1$ given by Eq. (2.4) as a classical variable, it is convenient to introduce the classical external field $V_m(\tau)$ by the definition

$$V_m(\tau)=\sigma(\tau)V^{z1}_{mm}\ , \tag{3.7}$$

where the representation in which $V^{z1}$ is diagonal is used. The electrons move in this time-dependent external field. Using the definition (3.5), the function $Z_1$ has the form

$$Z_1=\left\langle T_\tau\exp\left[-\sum_m\int_0^{\beta}d\tau\,V_m(\tau)a_m^{\dagger}(\tau)a_m(\tau)\right]\right\rangle_0\ . \tag{3.8}$$

The definition of the one-particle Green's function is

$$G_m^{1g}(\tau,\tau')=-\langle T_\tau[a_m(\tau)a_m^{\dagger}(\tau')]\rangle_1\ , \tag{3.9}$$

which satisfies the Dyson equation

$$G_m^{1g}(\tau,\tau')=G_m^0(\tau-\tau')+g\int_0^{\beta}d\tau''\,G_m^0(\tau-\tau'')V_m(\tau'')\times G_m^{1g}(\tau'',\tau')\ , \tag{3.10}$$

where $g$ is introduced by Hamann[23] only for technical purposes. After replacing $V_m(\tau)$ by $gV_m(\tau)$ in Eq. (3.8), the quantity $\partial Z_1/\partial g$ is just an integral of the Green's function $G^{1g}$. Integrating the expression $\partial Z_1/\partial g$ with respect to $g$, Hamann obtained the following expression for $Z_1$:

$$Z_1=\exp\left[-\int_0^1 dg\int_0^\beta d\tau\sum_m [gV_m(\tau)G_m^{1g}(\tau,\tau^+)]\right] \tag{3.11}$$

where $\tau^\pm=\tau\pm\delta$ and $\delta\to+0$.

The unperturbed Green's function is given by considering Eqs. (2.12) and (3.9) as

$$G_m^0(\tau)=\rho\int_{-D}^{D} e^{-\varepsilon\tau}\left[\frac{1}{e^{\beta\varepsilon}-1}-\Theta(\tau)\right]d\varepsilon\ , \tag{3.12}$$

where $\Theta$ is the Heaviside function. This formula is just a consequence of the simplified band structure introduced in Sec. II. This Green's function can be approximated as

$$G_m^{(0)}(\tau)=\begin{cases}-\rho/\tau & \text{for } \tau_0<|\tau|<\beta\ ,\\ \pm\rho/\tau_0 & \text{for } 0<\pm\tau<\tau_0\ ,\end{cases} \tag{3.13}$$

where $\tau_0=1/D$ is a short-time cutoff. This approximation provides the correct results both in the $|\tau|\ll\tau_0$ and $\tau_0<|\tau|<\beta$ limits that are the relevant regions in the present calculation.[23]

The Dyson equation (3.10) can be solved by the method of Muskhelishvili applied first by Nozières and de Dominicis[19] for a similar problem. The asymptotic solution of Yu and Anderson[4] for $|\tau-\tau'|\gg\tau_0$ can be written in a symmetric form

$$G_m^{1g}(\tau,\tau')=-\rho\frac{P}{\tau-\tau'}\cos[\delta_m(\tau)]\cos[\delta_m(\tau')]\frac{X_m^0(\tau')}{X_m^0(\tau)}$$
$$+\rho\pi\sin[\delta_m(\tau)]\cos[\delta_m(\tau)]\delta(\tau-\tau')\ , \tag{3.14}$$

where

$$\delta_m(\tau)=-\arctan[g\pi\rho V_m(\tau)] \tag{3.15}$$

with $g=1$ the time-dependent phase shift corresponding to the TLS position-dependent part of the scattering and

$$X_m^0(\tau)=\exp\left[\frac{1}{\pi}\mathrm{P}\int_0^\beta\frac{\delta_m(\tau'')}{\tau''-\tau}d\tau''\right]\ , \tag{3.16}$$

where P stands for the principal value. Using the identity (3.11), Yu and Anderson[4] obtained the final result

$$Z_1=Z_{11}Z_{12}Z_{13}$$
$$=\exp\left[\sum_m\left\{\int_0^\beta\frac{d\tau}{\tau_0}\left[\ln[1+\gamma_m^2(\tau)]+\frac{1}{\pi}\delta_m(\tau)\Big|_{g=1}\right]\right.\right.$$
$$\left.\left.+\int_0^\beta d\tau\int_0^\beta d\tau'\frac{1}{\pi^2}\ln(|\tau-\tau'|)\frac{d\gamma_m(\tau')}{d\tau'}\frac{d}{d\tau}\left[\frac{\gamma_m}{\gamma_m^2(\tau)-\gamma_m^2(\tau')}\ln\left[\frac{1+\gamma_m^2(\tau)}{1+\gamma_m^2(\tau')}\right]\right]\right\}\right]\ , \tag{3.17}$$

where

$$\gamma_m=\pi\rho V_m^{z1} \tag{3.18}$$

and

$$\gamma_m(\tau)=\sigma(\tau)\gamma_m \tag{3.19}$$

and $Z_{11}$, $Z_{12}$, and $Z_{13}$ are defined in the following.

The first logarithmic term in Eq. (3.17) is independent of the path, and this contributes to the partition function by

$$Z_{11}=\prod_m(1+\gamma_m^2)^{\beta\tau_0^{-1}}\ , \tag{3.20}$$

which gives an uninteresting additive constant to the thermodynamic potential. The remaining product $Z_{12}Z_{13}$ depends on the path which is labeled in Fig. 1, where $\tau_i$ with odd (even) index corresponds to a kink (antikink). An index $S_i$ for the hops is introduced[8] as

$$S_i=\tfrac{1}{2}[\sigma(\tau_i-0)-\sigma(\tau_i+o)]\ , \tag{3.21}$$

which is $+1$ $(-1)$ for kinks (antikinks). Using this index the remaining path of $Z_i$ can be easily evaluated, and for a path with $N$ hops the results are

$$Z_{12}=\exp\left[\sum_m 2\frac{\delta_m}{\pi\tau_0}\left[\sum_i S_i\tau_i+\tfrac{1}{2}\beta\right]\right] \tag{3.22}$$

and

$$Z_{13}=\exp\left[\sum_m\left[\frac{2\delta_m}{\pi}\right]^2\sum_{i<j}S_iS_j\ln\left[\frac{|\tau_i-\tau_j|}{\tau_0}\right]\right]\ , \tag{3.23}$$

where the phase shift $\delta_m$ is the amplitude of $\delta_m(\tau)$ defined by Eq. (3.15) for $g=1$, thus

$$\delta_m=-\arctan\gamma_m\ , \tag{3.24}$$

where the notation (3.18) is used. The second part in the exponent of the expression (3.22) of $Z_{12}$ is a constant, thus that gives only an additive constant to the thermodynamic potential, and therefore will be dropped. $Z_{13}$ has been calculated by Hamann[23] using the long-time asymptotic expression (3.14) for the Green's function, thus Eq. (3.23) is valid only if the distances between the hops are large enough

$$\tau_{i+1}-\tau_i\gg\tau_0,\quad i=1,2,\ldots \tag{3.25}$$

[see formulas (4.15)–(4.18) in Ref. 23]. In the opposite

case $\tau_{i+1}-\tau_i<\tau_0$ the logarithmic singularity in Eq. (3.23) must be replaced by a smooth function, just as has been done in the case of $G^{(0)}$ given by Eq. (3.13).

In the calculation of $Z$ the explicit form of the Green's function (3.14) with $g=1$ will be needed, which can be expressed by the hop indices defined by Eq. (3.21) as

$$G_m^1(\tau,\tau')=-\frac{\rho}{\tau-\tau'}\cos^2\delta_m \times\exp\left[2\frac{\delta_m}{\pi}\sum_i S_i\ln\left(\frac{|\tau_i-\tau'|}{|\tau_i-\tau|}\right)\right] \quad (3.26)$$

which is valid if $|\tau_i-\tau|\gg\tau_0$, $|\tau_i-\tau'|\gg\tau_0$, and $|\tau-\tau'|\gg\tau_0$. As in the later applications the variables $\tau$ and $\tau'$ will be the times of hoppings; therefore, the limit $|\tau-\tau'|<\tau_0$ will be required also. In that limit the exponent in Eq. (3.26) is expanded in the variable $\tau-\tau'$. The zero-order term is singular as $(\tau-\tau')^{-1}$, which must be smoothed as in Eq. (3.13). Keeping only the zero- and first-order terms, the Green's function has the limiting form

$$G_m^1(\tau,\tau')=\frac{\rho}{\tau_0}\cos^2\delta_m+2\rho\frac{\delta_m}{\pi}\cos^2\delta_m\sum_i\frac{S_i}{\tau-\tau_i} \quad (3.27)$$

for $-\tau_0<\tau-\tau'<0$ and $|\tau_i-\tau|\gg\tau_0$. As $\delta_m(\tau)$ changes sign when $\tau$ passes through a hop, $\cos[\delta_m(\tau)]$ is well defined for $\tau$ taken at a hop, but $\sin[\delta_m(\tau)]$ is not, that changes its sign around the hop. The latter one has a zero average around the hop, thus the second term in the expression (3.14) for $G_m^1$ is just omitted.

Finally, it is interesting to note that the results given here can be generalized for an arbitrary spherical wave representation in which $V^{z1}$ is not diagonal. As all the quantities used, such as $\delta(\tau)$, $\gamma$, and $\delta$, are expressed by $V^{z1}$, if $V^{z1}$ is a matrix then all of our results hold in matrix form because the corresponding matrices commute with each other.

### C. Perturbative expansion of $Z_2$

A complete perturbative expansion is constructed for $Z_2$ by generalizing the method of Yuval and Anderson[20] developed for the Kondo problem. In the latter case, considering the spin-flip interaction as perturbation the spin-up and spin-down unperturbed electron Green's functions form two separate but identical determinants. In the present problem the index $m$ covers orbital and spin indices, thus $m$ has at least four different values and the numbers of the Green's function with different indices may be different in the same term of the expansion. The Green's functions with the same indices $\mu=m$ also form, however, determinants denoted by $\det_\mu$. The perturbative series for $Z_I$ is constructed using the perturbed Green's functions calculated before. Special care is necessary in the case of Hartree-Fock (HF) diagrams, where for the closed electron loops the asymptotic solution of the Green's function cannot be used; therefore, those must be considered in a separate manner. Finally, there is an additional difficulty as the summation over the indices $m$ cannot be performed explicitly, contrary to the Kondo problem, where the spin indices are treated automatically. Thus, the summations over indices $m$ are only indicated in front of the different terms.

According to Eqs. (3.2) and (3.6) the function $Z_2$ for a given path $\sigma(\tau)$ is

$$Z_2=\langle\tilde H_{2\alpha_N}(\tau_N)\cdots\tilde H_{2\alpha_1}(\tau_1)\rangle_1 . \quad (3.28)$$

In each interaction point $\tilde H_2(\tau)$ those terms of $H_2=\sum_{\alpha=1}^6 H_{2\alpha}$ must be considered which are topologically allowed for a given path, thus the terms proportional to $\sigma^+$, $\sigma^-$, and $\sigma^z$ must be taken at antikinks, at kinks, and between hops, respectively. The expansion for $Z_I$ can be written as

$$Z_I=\sum_{N=0}^{\infty}(-1)^N\sum_{\{\sigma\}}\int_0^\beta d\tau_N\cdots\int_0^{\tau_{i+1}}d\tau_i\cdots\int_0^{\tau_2}d\tau_1 Z_1[\sigma(\tau)]\langle\tilde H_{2\alpha_N}(\tau_N)\tilde H_{2\alpha_{N-1}}(\tau_{N-1})\cdots\tilde H_{2\alpha_1}(\tau_1)\rangle_1 , \quad (3.29)$$

where $\{\alpha\}=\alpha_1,\alpha_2,\ldots,\alpha_N$ stand for a given configuration of the $\alpha_i=1,\ldots,6$ indices in the product of Hamiltonians $H_2$. The integrals and the summation over the configurations $\{\alpha\}$ also play the role of the summation over all the paths $\sigma(\tau)$. The Hamiltonians $H_2$ are given in the interaction representation [see Eq. (3.3)]. After using the expression for $H_{2\alpha}$ given by Eqs. (2.6)–(2.11) the spontaneous and electron assisted processes can be written separately in Eq. (3.29), and then $Z_I$ has the following form:

$$Z_I=\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\sum_{\{m;n\}}\left[\prod_{j=1}^N{}^{(s)}\Delta^{(\alpha_j)}\right]\mathrm{Tr}\left[\prod_{k=1}^N\sigma^{(\alpha_k)}\right] \times\int_0^\beta d\tau_n\cdots\int_0^{\tau_{i+1}}d\tau_i\cdots\int_0^{\tau_2}d\tau_1 Z_1[\sigma(\tau)]\left\langle T_\tau\left[\prod_{\alpha=1}^N{}^{(a)}V_{m_in_i}^{(\alpha_i)}a_{m_i}^\dagger(\tau_i)a_{n_i}(\tau_i)\right]\right\rangle_1 , \quad (3.30)$$

where the superscripts $(\alpha_i)=\pm z$ correspond to the superscripts in $H_2$'s given by Eqs. (2.15), (2.14), and (2.16). In the products $\prod_{i=1}^{N}{}^{(a)}$ ($\prod_{i=1}^{N}{}^{(s)}$) for a given configuration $\{\alpha_i\}$ the index $i$ runs over only those values which are associated with assisted (spontaneous) processes. The summation over the index pairs $(m_i,n_i)$ of the assisted processes is indicated as the summation over the configuration $\{m;n\}$. In the calculation of the expectation value all possible pairings must be taken. In the following a single term is considered which corresponds to a given $\{m;n\}$ configuration. Following Yuval and Anderson,[20] the Green's functions with the same index $\mu$ can be written in the form of a determinant

$$\det_\mu[G^1_\mu(\tau_i,\tau_j)]_{ij} , \tag{3.31}$$

where only those rows and columns of the determinant are kept for which $m_j=n_i=\mu$. The dimension of the determinant is $p_\mu\times p_\mu$. Using this notation the following identity is obtained:

$$\left\langle T_\tau\left[\prod_{i=1}^{N}{}^{(a)} a^\dagger_{m_i}(\tau_i)a_{n_i}(\tau_i)\right]\right\rangle_1 = R\prod_\mu R_\mu \det_\mu[G^1_\mu(\tau_i,\tau_j)]_{ij} , \tag{3.32}$$

where the Wick's theorem is applied for a rearranged sequence of the annihilation and creation operators labeled by $i$ and $j$ respectively; furthermore, $R=(-1)^P$ and $R_\mu=(-1)^{P_\mu}$ are combinational factors related to the rearranged sequence. $P$ is the number of the necessary neighbor exchanges of operators only with different $m_i=\mu$ and $n_i=\mu'$ indices to obtain such a sequence where the indices $\mu$ form a nondecreasing set, thus the operators are grouped with respect to their indices $\mu$. $P_\mu$ denotes the number of the necessary further neighbor exchanges of a creation operator and of an annihilation operator with the same indices $\mu$ to arrive at the sequence alternating in the creation and annihilation operators (starting with an creation operator on the left), but keeping the original time ordering among the creation and annihilation operators with the same index $\mu$, separately ($\tau_j>\tau_{j'}$ if $j>j'$ for two creation operators and $\tau_i>\tau_{i'}$ if $i>i'$ for two annihilation operators with index $\mu$).

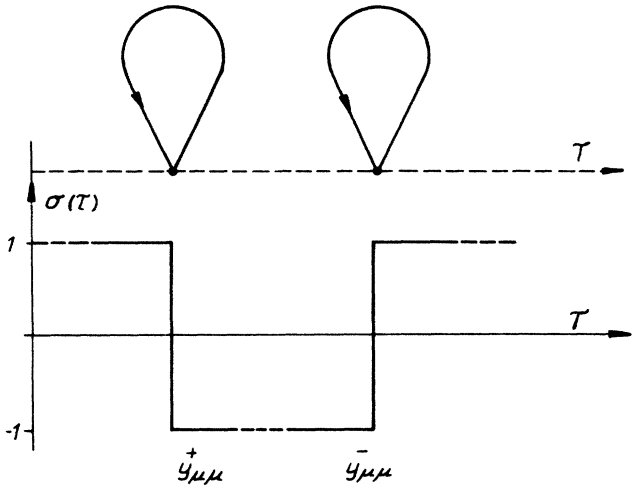


FIG. 2. The HF electron loop diagrams are shown by solid lines, and the dotted line is the time axis or TLS line with time order. In the lower part the TLS path with a kink and an antikink is depicted, which is associated with the HF contributions with fugacities $y^+_{\mu\mu}$ and $y^-_{\mu\mu}$, respectively.

At the evaluation of the determinant $\det_\mu$ two cases must be distinguished: (i) where there is no such $i$ and $j$ index pair for which $m_i=n_j$ and $\tau_i=\tau_j$ holds simultaneously and (ii) where that situation occurs at least once. The typical Hartree-Fock loop diagrams (see Fig. 2) appear only in the second case, where for the Green's functions in the Hartree-Fock diagrams the short-range expression (3.27) must be used instead of the asymptotic form (3.26).

### 1. *Nondiagonal interaction*

In the first case the determinant $\det_\mu$ must be calculated using Eq. (3.26) for the Green's functions. The exponential terms occur as a multiplicative factor of the determinant formed by the unperturbed Green's functions given by Eq. (3.13) as

$$\det_\mu[G_{m_i n_j}(\tau_i,\tau_j)]_{ij}=(\cos\delta_\mu)^{2p_\mu}\left[\prod_{\substack{i=1\\(n_i=\mu)}}^{N}\prod_{\substack{i'=1\\(i'\neq i)}}^{N}|\tau_i-\tau_{i'}|^{-2S_{i'}\delta_\mu/\pi}\right]\left[\prod_{\substack{j=1\\(m_j=\mu)}}^{N}\prod_{\substack{i'=1\\(i'\neq j)}}^{N}|\tau_j-\tau_{i'}|^{2S_{i'}\delta_\mu/\pi}\right]\det_\mu\left[\frac{\rho}{\tau_j-\tau_i}\right]_{ij} . \tag{3.33}$$

The determinant occurring on the right-hand side of Eq. (3.33) is known as the Cauchy determinant, and can be given by a simple expression[24]

$$\det(\tau_j-\tau_i)_{ij}=\frac{\prod_{\substack{i,i'\\i<i'}}(\tau_i-\tau_{i'})\prod_{\substack{j,j'\\j>j'}}(\tau_j-\tau_{j'})}{\prod_{i,j}(\tau_j-\tau_i)} , \tag{3.34}$$

where $i$ and $i'$ ($j$ and $j'$) stand for the first (second) indices of the determinant. Using this identity the following result can be obtained:

$$\det_\mu\left[\frac{\rho}{\tau_j-\tau_i}\right]_{ij}=R_\mu(\rho\tau_0^{-1})^{p_\mu}\prod_{\substack{i,j\\i<j}}\left|\frac{\tau_i-\tau_j}{\tau_0}\right|^{T_i^\mu T_j^\mu} \tag{3.35}$$

with the notation

$$T_i^{\mu}=\begin{cases}\delta_{m_i\mu}-\delta_{n_i\mu} & \text{if } \alpha=4,5,6\ ,\\ 0 & \text{if } \alpha=1,2,3\ ,\end{cases} \tag{3.36}$$

where $\delta$ stands for the Kronecker symbol and the matrix $T$ is defined for assisted and nonassisted processes as well. At the moment, only the nondiagonal part of the interaction is considered ($n_i\neq m_i$), but later this definition will be generalized also for $n_i=m_i$. The advantage of this definition is that the projection on the subspace $\mu$ and the Cauchy's expression (3.34) can be simultaneously cast into a compact form. The appearance of the factor $R_{\mu}=(-1)^{P_{\mu}}$ is caused by taking the absolute values of $\tau_i-\tau_j$. The proof of the sign can be given by considering the definition of $R_{\mu}$ where the number of neighbor exchanges of the creation and annihilation operators were $P_{\mu}$ in order to get their alternative sequence. This alternative sequence can be obtained in two steps in a different way. In the first step the annihilation operators are collected on the right, and in the second step the alternative sequence is achieved. The parity of the exchanges in the first step is equal with the sign of $\prod_{i,j}(\tau_j-\tau_i)$ in Eq. (3.34), and the parity of exchanges in the second step is $(-1)^{(1/2)p_{\mu}(p_{\mu}-1)}$. Finally, for the product $\prod_{j,j'/j>j'}(\tau_j-\tau_{j'})>0$ holds. $\tau_0$ is introduced only for convenience.

The expression of $Z_I$ can be obtained by inserting Eqs. (3.32), (3.33), and (3.35) into (3.30), and the result

$$\begin{aligned}Z_I=\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\sum_{\{m;n\}}&\left[\prod_{j=1}^{N}{}^{(s)}\Delta^{(\alpha_j)}\right]\left[\prod_{i=1}^{N}{}^{(a)}V_{m_in_i}^{(\alpha_i)}\right]\mathrm{Tr}\left[\prod_{k=1}^{N}\sigma^{(\alpha_k)}\right]\\ &\times\int_0^{\beta}d\tau_n\cdots\int_0^{\tau_{i+1}-\tau_0}d\tau_i\cdots\int_0^{\tau_2-\tau_0}d\tau_1 R\rho^N\tau_0^{-N}Z_{12}\prod_{\mu}(\cos\delta_{\mu})^{2p_{\mu}}\prod_{\substack{i,j\\ i<j}}\left|\frac{\tau_i-\tau_j}{\tau_0}\right|^{T_i^{\mu}T_j^{\mu}}\\ &\times\left|\frac{\tau_i-\tau_j}{\tau_0}\right|^{S_jT_i^{\mu}4\delta_{\mu}/\pi}\left|\frac{\tau_i-\tau_j}{\tau_0}\right|^{S_iS_j(2\delta_{\mu}/\pi)^2}+(\text{diagonal})\ ,\end{aligned} \tag{3.37}$$

where the definition (3.36) and the identity $(R_{\mu})^2=1$ are also used and the last bracket indicates the contribution of second type (ii) which contains diagonal matrix elements. Furthermore, the intervals defined by the inequalities $\tau_i-\tau_{i-1}<\tau_0$ are excluded, which is due to the short-time cutoff $\tau_0$ used in, e.g., Ref. 22.

In order to arrive at a more-compact form the following notations are introduced. In similar problems[22,4] fugacities are introduced for the interactions which are defined as

$$y_j=\begin{cases}\Delta^{(\alpha_j)}\tau_0 & \text{for } \alpha_j=1,2,3\\ V_{m_jn_j}^{(\alpha_j)}\rho\cos\delta_{m_i}\cos\delta_{n_j} & \text{for } \alpha_j=4,5,6\end{cases} \tag{3.38}$$

where in the case of assisted process $y_j$ stands for a given matrix element $V_{m_jn_j}^{(\alpha_j)}$.

The charge associated with the interaction points introduced in Ref. 7 was generalized in Ref. 8 as

$$C_i^{\mu}=T_i^{\mu}+S_i2\delta_{\mu}/\pi\ . \tag{3.39}$$

For each interaction point $i$ a set of charges ($\mu=1,2,\ldots$) are defined, and in the interaction between interaction points $i$ and $j$ will be expressed by $\sum_{\mu}C_i^{\mu}C_j^{\mu}$. $C_i^{\mu}$ looks formally like a vector charge. The necessity of the introduction of the index $\mu$ is due to the fact, that the summation with respect to $\{m;n\}$ cannot be explicitly performed in expression (3.37) for $Z_I$ in contrast to the treatment of the second part of the scaling region considered in Ref. 7. Furthermore, in an arbitrary representation where the phase shift $\delta$ is a nondiagonal matrix, $C_i$ stands for a matrix which also can be obtained by a rotation from the diagonal form given by Eq. (3.39). In the latter case the interaction is expressed by $\mathrm{Tr}(C_iC_j)$.

Using the notation given by Eqs. (3.38) and (3.39), the expression (3.37) for $Z_I$ can be rewritten as

$$\begin{aligned}Z_I=\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\sum_{\{m;n\}}&\left[\prod_{j=1}^{N}y_j\right]\mathrm{Tr}\left[\prod_{i=1}^{N}\sigma^{(\alpha_i)}\right]\tau_0^{-N}\\ &\times\int_0^{\beta}d\tau_N\cdots\int_0^{\tau_{i+1}-\tau_0}d\tau_i\cdots\int_0^{\tau_2-\tau_0}d\tau_1 Z_{12}R\left[\sum_{i<j}\sum_{\mu}C_i^{\mu}C_j^{\mu}\ln\left[\frac{|\tau_i-\tau_j|}{\tau_0}\right]\right]+(\text{diagonal})\ .\end{aligned} \tag{3.40}$$

In the special case where $\sum_m \delta_m = 0$ this expression corresponds to a statistical physics model [$Z_{12} \equiv I$; see Eq. (3.22)]. In that model a one-dimensional Coulomb gas with matrix charges interacts by logarithmic interaction. The chemical potential of the charged particles is $\beta^{-1} \ln y^{(\alpha)}$.

### 2. *Contribution of the diagonal interaction to the Hartree-Fock terms*

The diagonal parts of the interaction contribute to the Hartree-Fock (HF) diagrams depicted in Fig. 2. The Green's function given by Eq. (3.27) stands for the closed loop, which is singular in the variable $\tau_0$ as $\tau_0 \to 0$; therefore, the large HF contributions will be treated separately. The HF terms with the interactions $V^+$ and $V^-$ occur as the renormalization of the spontaneous transitions $\Delta^+$ and $\Delta^-$ of the TLS. The $V^Z$ interaction has been treated exactly and their contribution $Z_1$ is given by Eqs. (3.17), (3.20), (3.22), and (3.23). It will be shown that the term $Z_{12}$ has the same structure as the contribution of the Hamiltonian $H_{23}$ given by Eq. (2.8) in terms of $y^z = \Delta^z \tau_0$; thus $Z_{12}$ is considered as the HF term due to the phase shift $\delta_\mu$.

The interaction $H_{23}$ acts at any arbitrary time $\tau$ and contributes as

$$-\frac{1}{\tau_0} y^z \sigma(\tau) \ . \tag{3.41}$$

The factor $-1$ is due to the factor $(-1)^N$ in the perturbation series. This must be integrated over the interval $(0,\beta)$ with respect to $\tau$, and the following expression is obtained:

$$Z_{21} = \exp\left[ -2y^z \tau_0^{-1} \left[ \sum_i S_i \tau_i + \tfrac{1}{2}\beta \right] \right] , \tag{3.42}$$

which depends on the hops like the expression $Z_{12}$ given by Eq. (3.22). Thus $Z_{12}$ and $Z_{21}$ can be given by a single expression

$$Z_3 = Z_{21} Z_{12} = \exp\left[ -2y^z_{\rm HF} \tau_0^{-1} \left[ \sum_i S_i \tau_i + \tfrac{1}{2}\beta \right] \right] , \tag{3.43}$$

where the renormalized splitting interaction is given as

$$y^z_{\rm HF} = y^z - \sum_\mu \frac{\delta_\mu}{\pi} \ , \tag{3.44}$$

and the irrelevant term $\beta/2\tau_0$ will be dropped.

The case of the interactions $V^\pm$ and $y^\pm$ is more simple as $V^+$ ($V^-$) can be placed just at the kinks with $S_i = 1$ (antikinks with $S_i = -1$), thus using the singular part of the Green's function (3.27) the renormalization of the fugacity $y^+$ is obtained as

$$y^\pm_{\rm HF} = y^\pm + \sum_\mu y^\pm_{\mu\mu} \ , \tag{3.45}$$

and the notation

$$y^\pm_{\mu\mu'} = V^\pm_{\mu\mu'} \rho \cos\delta_\mu \cos\delta_{\mu'} \tag{3.46}$$

is a modification of Eq. (3.38) for $\alpha_j = 4,5$.

The HF diagram calculated with the nonsingular correction to the Green's function given by (3.27) can be considered as a fugacity correction at time, e.g., $\tau_k$ in the same configuration $\{m;n\}$ with $y^\pm$ instead of $y^\pm_{\mu\mu}$ for the hop $k$ at time $\tau = \tau_k$. This correction

$$+2 \sum_\mu y^\pm_{\mu\mu} \frac{\delta_\mu}{\pi} \sum_{i\,(\neq k)} \frac{\tau_0 S_i}{\tau_k - \tau_i} \tag{3.47}$$

to the fugacity $y^\pm$ will be considered in the construction of the dipole interaction later in this section.

### 3. *Intermediate expression for $Z_I$*

The diagonal interaction can be taken into account in two steps.

(i) The HF corrections provide the renormalization of the fugacities $y^z$ and $y^\pm$ given by Eqs. (3.45) and (3.44).

(ii) The remaining contributions of the diagonal interactions are nonsingular in the variable $\tau_0$, thus the long-time expression of the Green's functions given by Eq. (3.26) and the expression (3.32) given in terms of determinants can be used. The HF terms are eliminated by a projection operator

$$p_{ij} = \begin{cases} 1 & \text{if } \tau_i \neq \tau_j \ , \\ 0 & \text{if } \tau_i \neq \tau_j \ , \end{cases} \tag{3.48}$$

in the determinants $\det_\mu$. Using Eq. (3.30), where $Z_1 = Z_{12} Z_{13}$ is given by Eqs. (3.22) and (3.23), incorporating $Z_{12}$ in $Z_3$ given by Eq. (3.43), and taking into account that the HF terms are substracted from the expectation value (3.32) given by the determinants, the partition function $Z_I$ can be given as

$$\begin{aligned} Z_I = \sum_{N=0}^{\infty} (-1)^N \sum_{\{\alpha\}} \sum_{\{m;n\}} \prod_{j=1}^{N} y_{j\rm HF} {\rm Tr} \left[ \prod_{i=1}^{N} \sigma^{(\alpha_i)} \right] \tau_0^{-N} \int_0^\beta d\tau_n \cdots \int_0^{\tau_{i+1}-\tau_0} d\tau_i \cdots \int_0^{\tau_2-\tau_0} d\tau_1 R \\ \times \exp\left[ -2y^z_{\rm HF} \sum_i \frac{S_i \tau_i}{\tau_0} \right] \prod_\mu \left\{ R_\mu \left[ \prod_{i'} \prod_{\substack{i(\neq i') \\ (n_i = \mu)}} |\tau_i - \tau_{i'}|^{-S_{i'} 2\delta_\mu/\pi} \right] \left[ \prod_{i'} \prod_{\substack{j \neq i' \\ (m_j = \mu)}} |\tau_j - \tau_{i'}|^{S_{i'} 2\delta_\mu/\pi} \right] \right. \\ \left. \times \left[ \exp\left[ 2\frac{\delta_\mu}{\pi} \right]^2 \sum_{i<j} S_i S_j \ln\left[ \frac{|\tau_i - \tau_j|}{\tau_0} \right] \right] \det_\mu \left[ \frac{\tau_0}{\tau_j - \tau_i} p_{ij} \right] \right\} , \end{aligned} \tag{3.49}$$

where $y_{j\mathrm{HF}}$ stands for the spontaneous fugacities renormalized by the HF processes and for the assisted fugacities. In this formula all of the corrections except the one given by Eq. (3.47) are incorporated. Due to the presence of the projection operator $p_{ij}$ the Cauchy formula (3.34) cannot be applied for the determinants $\det_\mu$.

The diagonal assisted fugacities with index $\mu$ at the hop $k$ contribute to the off-diagonal elements of the determinant $\det_\mu$. For the sake of simplicity it is assumed that the diagonal interaction appears only once; furthermore, the hop at $\tau_k$ is associated with the row and column of the determinant, which are labeled by $k$. As a formal trick the annihilation and the creation operators are taken at times $\tau_k$ and $\tau_k+\delta$, respectively, where $\delta\to 0$.

Now the determinant without the projection operator $p_{ij}$ is considered; therefore, the Cauchy formula (3.34) can be applied. The additional factors in that formula due to the hop $k$ are

$$\frac{\tau_0}{(\tau_k+\delta)-\tau_k}\frac{\prod_{i(>k)}(\tau_k-\tau_i)\prod_{i(<k)}(\tau_i-\tau_k)\prod_{j(<k)}(\tau_k+\delta-\tau_j)\prod_{j(>k)}[\tau_j-(\tau_k+\delta)]}{\prod_{i(\neq k)}(\tau_k+\delta-\tau_i)\prod_{j(\neq k)}(\tau_j-\tau_k)}$$

$$=(-1)^{N_{\mu k}}\frac{1}{\delta}\frac{\prod_{i(\neq k)}(\tau_k-\tau_i)\prod_{j(\neq k)}[\tau_j-(\tau_k+\delta)]}{\prod_{i(\neq k)}(\tau_k+\delta-\tau_i)\prod_{j(\neq k)}(\tau_j-\tau_k)}$$

$$=(-1)^{N_{\mu k}}\left[\frac{\tau_0}{\delta}-\sum_{j(\neq k)}\frac{\tau_0}{\tau_j-\tau_k}-\sum_{i(\neq k)}\frac{\tau_0}{\tau_k-\tau_i}\right] \quad (3.50)$$

for small $\delta$. The first term is singular in $\delta$ and is the term which is projected out by $p_{ij}$. The remaining terms are independent of $\delta$. Thus the hop labeled by $k$ with diagonal interaction and without the HF contributions results in an additional correction factor to the same configuration $\{m;n\}$ but with a nonassisted fugacity $y^{\pm}$ at time $\tau=\tau_k$. Thus, that correction to the fugacity can be written in a compact form

$$+\sum_{i(\neq k)}\sum_{\mu}y^{\pm}_{\mu\mu}\frac{\tau_0 T_i^\mu}{\tau_k-\tau_i}\ , \quad (3.51)$$

where the summation over $\mu$ is performed also and the notation (3.36) is used; furthermore, index $i$ runs over all the hops.

Our results can be summarized in a form of $Z_I$ similar to the one given [Eq. (3.40)], where the diagonal interaction is excluded. The diagonal interactions contribute by the HF corrections ($y_{j\mathrm{HF}}$) and by the extra factor (3.51) in Eq. (3.49). The $|\tau_j-\tau_{i'}|^{\pm S_{i'}2\delta_\mu/\pi}$-type factors can be taken into account in formula (3.40) by generalizing the charge $C_i^\mu$ for the diagonal interaction with $T_i^\mu$ defined by Eq. (3.36) for arbitrary interaction ($T_i^\mu=0$ for the diagonal term). Thus

$$Z_I=\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\sum_{\{m;n\}}\left[\prod_{j=1}^{N}y_{j\mathrm{HF}}\right]\left[\prod_{i=1}^{N}\sigma^{(\alpha_i)}\right]\tau_0^{-N}$$
$$\times\int_0^\beta d\tau_n\cdots\int_0^{\tau_{i+1}-\tau_0}d\tau_i\cdots\int_0^{\tau_2-\tau_0}d\tau_1 R\left[\exp-2y^z_{\mathrm{HF}}\sum_i\frac{S_i\tau_i}{\tau_0}\right]$$
$$\times\exp\left[\sum_{i<j}\sum_{\mu}C_i^\mu C_j^\mu\ln\left[\frac{|\tau_i-\tau_j|}{\tau_0}\right]\right]+c\ , \quad (3.52)$$

where $c$ stands for corrections of type (3.47) and (3.51).

Both of these two corrections have been considered as corrections to the nonassisted fugacity $y^{\pm}$ in the same configuration $\{m;n\}$ but in which $y^{\pm}_{\mu\mu}$ is replaced by $y^{\pm}$. Considering this procedure at the hop at time $\tau=\tau_k$, the connection factors determined by Eqs. (3.47) and (3.51) can be given in terms of the charge $C_i^\mu$ defined by Eq. (3.39) in a concise form like

$$1+\sum_{\mu}\frac{y^{\pm}_{\mu\mu}}{y^{\pm}_{\mathrm{HF}}}\sum_{i(\neq k)}C_i^\mu\frac{\tau_0}{\tau_k-\tau_i} \quad (3.53)$$

for $|\tau_k-\tau_i|\gg\tau_0$. This correction will be interpreted as a dipole-charge interaction in the next subsection.

#### 4. $Z_I$ in terms of charges and dipoles

The interaction term in expression (3.52) for $Z_I$ has the form of Coulomb interaction in a one-dimensional Coulomb gas with logarithmic interaction.[4,22] The orbital and spin indices of the electrons are incorporated in a color index $\mu$. The interaction occurs as the sum of the interactions of the same colors. Considering only the electrons with a given color $\mu$ an arbitrary hop can be

associated with the following: no electron, a single electron which may be created or annihilated ($T_\mu=-1$ or $T_\mu=1$), or a pair of electrons where one is created and the other is annihilated with the same color. The hop with a single-electron process is considered as a charged hop. In the last case the assisted interaction must be diagonal ($y^{\pm}_{\mu\mu}$ and $y^{z}_{\mu\mu}$ have already been considered in Hamiltonian $H_1$) and the creation and annihilation operators have been split by $\delta$ on the time scale ($\delta\rightarrow+0$). Following the concept that the single electron is associated with charge, the pair is considered as dipole. In general, the interaction between a dipole and charge is given as the derivative of the charge-charge interaction and the dipole-dipole interaction with the second derivative. Thus the dipole-charge (dipole-dipole) interaction must behave like $(\tau_i-\tau_j)^{-1}$, $[(\tau_i-\tau_j)^{-2}]$. The non-HF part of diagonal interaction occurring as a correction to the fugacities $y^{\pm}_{\rm HF}$ with a time-dependent structure fits in the concept of dipoles. Considering the form (3.53) the dipole-charge interaction can be defined as

$$\sum_{i\neq j,\mu} C_i^\mu P_j^\mu \frac{\tau_0}{\tau_j-\tau_i} \tag{3.54}$$

where $|\tau_i-\tau_j|\gg\tau_0$ and the dipole moment may be defined as

$$P_j^\mu=\begin{cases} y^{+}_{\mu\mu}/y^{+}_{\rm HF} & \text{for } \alpha_j=5\ , \\ y^{-}_{\mu\mu}/y^{-}_{\rm HF} & \text{for } \alpha_j=4\ , \end{cases}$$

for a given $\{\alpha_i\}$ configuration. It is important to note that the splitting $\delta$ does not enter in this definition. In the following the interaction $y^{\pm}_{\mu\mu'}$ will stand only for the off-diagonal terms and the charge-dipole interaction will be associated with the interaction of a renormalized spontaneous diagonal transition with another hop. Thus $P^j_\mu$ is interpreted as

$$P_j^\mu=\begin{cases} y^{+}_{\mu\mu}/y^{+}_{\rm HF} & \text{for } \alpha_j=2\ , \\ y^{-}_{\mu\mu}/y^{-}_{\rm HF} & \text{for } \alpha_j=3\ . \end{cases} \tag{3.55}$$

In this way the renormalized spontaneous fugacity $y^{\pm}_{\rm HF}$ occurs with the correction factor

$$\exp\left[\sum_{i\neq j}\sum_{\mu} C_i^\mu P_j^\mu \frac{\tau_0}{\tau_j-\tau_i}\right], \tag{3.56}$$

where the expression (3.54) is exponentiated as $|\tau_i-\tau_j|\gg\tau_0$.

The dipole-dipole terms arise from the interaction of two diagonal assisted transitions with the same color. As it is shown in the Appendix the dipole-dipole term is

$$\sum_{i>j}\sum_{\mu} P_i^\mu P_j^\mu \frac{\tau_0^2}{(\tau_i-\tau_j)^2}\ , \tag{3.57}$$

which can be exponentiated as the dipole-charge term has been. This term is due to loop diagram shown in Fig. 2.

The final result is obtained by adding to Eq. (3.52) the corrections (3.56) and (3.57), and the result is

$$\begin{aligned} Z_I=\sum_{N=0}^{\infty}(-1)^N\sum_{\{\alpha\}}\sum_{\{m;n\}}&\left[\prod_{j=1}^{N} y_{j\rm HF}\right]{\rm Tr}\left[\prod_{i=1}^{N}\sigma^{(\alpha_i)}\right]\tau_0^{-N} \\ &\times\int_0^{\beta} d\tau_n\cdots\int_0^{\tau_{i+1}-\tau_0} d\tau_i\cdots\int_0^{\tau_2-\tau_0} d\tau_1 R\exp\left[-2y^{z}_{\rm HF}\sum_i\frac{S_i\tau_i}{\tau_0}\right] \\ &\times\exp\left[\sum_{i<j}\sum_{\mu} C_i^\mu C_j^\mu\ln\left[\frac{|\tau_i-\tau_j|}{\tau_0}\right]+\sum_{i\neq j}\sum_{\mu} C_i^\mu P_j^\mu\frac{\tau_0}{\tau_i-\tau_j}+\sum_{i<j}\sum_{\mu} P_i^\mu P_j^\mu\frac{\tau_0^2}{(\tau_i-\tau_j)^2}\right]. \end{aligned} \tag{3.58}$$

This form can be compared with the final result of the Appendix given by Eq. (A7). This comparison shows that $Z_I$ must be expanded with respect to $P_j$ and only the terms linear in any $P_i$ for a given hop $i$ must be kept, thus terms proportional to $P_i^2$ must be dropped but those proportional to $P_iP_j$ ($i\neq j$) must be kept. This is due to the fact that, e.g., $D_i^2$ does not occur in the expression (A7) for the determinant $\tilde{A}$. In this way all the denominators $y_{\rm HF}$ of the dipole moments defined by Eq. (3.53) are canceled by the former fugacity factors in Eq. (3.58).

In the present result all of the diagonal assisted terms ($y^{+}_{\mu\mu}$ and $y^{-}_{\mu\mu}$) are incorporated in the fugacities or in the dipole terms provided that $y^{z}_{\mu\mu}=0$, thus the Hamiltonian $H_{26}$ is absent before the application of the renormalization group. Finally, it can be easily shown, that signs due to the Pauli operators and to the factor $R$ are not changed because a pair of a creation and annihilation operators with the same color is always considered and $y^{z}_{\mu\mu}=0$. In any other representation of the spherical waves $P_i$ is also a tensor like $C_i$ with respect to the indices $\mu$, and then Tr replaces the sums in Eq. (3.58).

In the present formulation the contribution of the diagonal fugacities contains the sum of the independent charge-dipole part and the pair correlation between dipoles in the form of dipole-dipole interaction. Correlations of higher orders are beyond our approximation scheme. The main guideline in the present approximation is that the fugacities are small, and therefore the distances between hops are large $|\tau_i-\tau_j|\gg\tau_0$.

## IV. CONCLUSION

In paper I of these two papers[25] an expression for the partition function is derived for the general electron TLS

interaction where the electron-assisted TLS transitions are included as well. This expression is achieved by generalizing the Yuval-Anderson[20] method worked out for the Kondo problem. There the long-time asymptotic solution is used for the electron Green's function and the electronic contribution is calculated in a closed form, thus the partition function depends only on the positions of the spin-flip processes on the imaginary time axis, and the scattering diagonal in the spin variables is taken into account by phase shift without perturbation series. The interaction occurs in the partition function as a pair potential of logarithmic type between two scattering events. The relative simplicity of the Kondo case means that in a spin-flip scattering process the incoming and outgoing electrons are always in different spin subspaces. The complexity of the TLS problem is the consequence of the existence of more than two orbital channels and that an electron scattered on the TLS by a TLS quasi-spin-flip process may stay in the same orbital subspace. Therefore, using the long-time approximation for the Green's functions of the electrons, divergences occur due to electron creation and annihilation with short-time differences in the partition function obtained by a brute-force generalization of Yuval and Anderson's[20] expression. The adequate treatment of that problem results in an expression for the electronic contribution of a particular color (angular momentum and spin) subspace which is not a single Cauchy determinant, thus which cannot be written as a single product. The additional terms are derived in a careful way and the results are summarized in Secs. III C 3 and III C 4. In order to correctly treat the singularities which appear and obtain finite final expressions, the concept of dipoles is introduced, which enters in a natural way.

In the case of the Kondo problem the strength of the logarithmic pair potential depends only on the phase shifts and their sign depends on whether the spin-flip processes are in the same spin directions or not. In the present case, due to the greater variety of the scattering processes, the amplitude of the logarithmic pair potential depends not only on the type of transition of the TLS (spin turn up or down) but also on the colors describing the electronic orbital momentum and spin subspaces in which the electrons are scattered in or out. This additional dependence occurs formally as the charges depend not only on the phase shift but also on the transition index $T^{\mu}$, defined by (3.36).

The attempt by the authors to eliminate the color indices of the electrons from the partition function was not successful; therefore, the different color combinations remained as the sum over the $\{m;n\}$ configuration, e.g., in Eqs. (3.40) and (3.68). Such a sum is not contained in the expression of Yuval and Anderson for the Kondo problem. This complication resulted also in the generalization of the charges given by Eq. (3.39). The concept of the dipoles mentioned above is discussed in detail in Sec. III C 4. Formally, the dipoles can be interpreted as a creation and annihilation of an electron with a very-short-time difference, thus the corresponding two charges in the same color subspace form a dipole. The partition function given by Eq. (3.58) contains charge-dipole and dipole-dipole interactions as well, which fit with the logarithmic charge-charge interaction in a one-dimensional Coulomb gas. The details are given in Secs. III C 3 and III C 4 and in the Appendix, and they are also summarized in Sec. II of paper II.

Finally we have to emphasize that the results presented are based on the long-time approximation, and that the Coulomb gas must be very dilute (fugacities are small). The phase shifts describing the screening of the TLS by the conduction electron can be, however, arbitrarily large. In the long-time approximation poles of higher orders and potentials additional to the pair potential are not required. It will be demonstrated in paper II, however, that in the scaling equation derived in terms of the short-time cutoff the charges and dipoles enter on the same footing.

The results for the TLS, which have been previously obtained by Black and Gyorffy[14] and by Yu and Anderson,[4] are reflected by the present result as a special case where the electron assisted TLS transitions are dropped. The results for the Kondo problem derived by Yuval and Anderson[20] can be recovered also as a special case by interchanging the spin and orbital subspaces of the electronic system.

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## APPENDIX

In Sec. III the contributions of the diagonal fugacities to the partition function $Z_I$ are discussed. As $y^{\pm}_{\mu\mu}$ is associated with a pair of creation and of annihilation operators, therefore, the hop interacts with the charges of the other hops by dipole forces proportional to $|\tau_i-\tau_j|^{-1}$. The subject of this appendix is to derive the dipole-dipole interaction. In the following a term is considered in which the diagonal fugacities occur twice. This contribution will be determined when it occurs in addition to the contribution of two independent diagonal transitions. The calculation is similar to the one presented in Sec. III C 3, which is based on expression (3.49). The main part of the derivation is restricted to evaluate the determinant $A=\det_{\mu}[p_{ij}\tau_0/(\tau_i-\tau_j)]$ which is not a Cauchy determinant. In order to use the value (3.34) of the Cauchy determinant the determinant $\tilde{A}$ must be expressed by Cauchy determinants, which contain singularities if $\tau_i=\tau_j$. To avoid those singularities the time arguments of the creation operators are shifted by $\delta>0$ and then the limit $\delta\to+0$ is taken as in Sec. III C 3. The final result for $\tilde{A}$ must be independent of $\delta$. In the present case the Cauchy determinant $A=\det_{\mu}(1/\tau_i-\tau_j)$ contains two elements for which $\tau_i=\tau_j$ holds.

For the sake of simplicity those will be taken to be at diagonal positions and they are labeled by $k$ and $l$, thus $\tau_k+\delta$ and $\tau_l+\delta$ are the time arguments of the creation operators and $\tau_k$ and $\tau_l$ are the arguments of the annihilation operators.

The singularities like $1/\delta^2$ and $1/\delta$ must be canceled in the final expression for $\tilde{A}$.

The determinant $\tilde{A}$ can be expressed by the Cauchy determinant $A$ and by its subdeterminants. $A_i$ denotes the subdeterminant obtained by omitting the row and column labeled by $i$, and $A_{ij}$ corresponds to that one in which those are dropped which are labeled either by $i$ or $j$. It can be shown by simple algebra that

$$\tilde{A}=A-A_{\text{sing}} , \tag{A1}$$

where

$$A_{\text{sing}}=\frac{\tau_0}{\delta}(A_l+A_k)-\frac{\tau_0^2}{\delta^2}A_{kl} . \tag{A2}$$

$A_{\text{sing}}$ contains the HF terms singular in $\delta$, which have been substracted from $A$ to define $\tilde{A}$. By using the result given by Eqs. (3.50) and (3.51), $A_k$ and $A_l$ can be expressed as

$$A_\alpha=\left[\frac{\tau_0}{\delta}+D_\alpha\right]A_{kl} \quad (\alpha=k,l) , \tag{A3}$$

where

$$D_\alpha=\sum_{i\,(\neq\alpha)}\frac{\tau_0}{\tau_\alpha-\tau_i}T_i^\mu \quad (\alpha=k,l) . \tag{A4}$$

The determinant $A$ can be expressed by $A_{kl}$, and the remaining factors can be easily obtained by considering Eq. (3.34). The results can be written for small $\delta$ as

$$A=A_{kl}\frac{A_k}{(\tau_0/\delta)A_{kl}}\frac{A_l}{(\tau_0/\delta)A_{kl}}\left[\frac{\tau_0}{\delta}\right]^2\frac{(\tau_k-\tau_l)^2}{(\tau_k-\tau_l)^2-\delta^2}$$
$$=\frac{A_kA_l}{A_{kl}}+A_{kl}\left[\frac{\tau_0}{\tau_k-\tau_l}\right]^2 , \tag{A5}$$

where in the last term the singular part of $A_\alpha$ given by Eq. (A3) is used. The determinant $\tilde{A}$ given by Eq. (A1) can be expressed by using Eqs. (A2) and (A5), and then one gets

$$\tilde{A}=\frac{1}{A_{kl}}\left[A_k-\frac{\tau_0}{\delta}A_{kl}\right]\left[A_l-\frac{\tau_0}{\delta}A_{kl}\right]$$
$$+A_{kl}\left[\frac{\tau_0}{\tau_k-\tau_l}\right]^2 , \tag{A6}$$

and using Eq. (A3) again the final results are obtained

$$\tilde{A}=A_{kl}\left[\left[\frac{\tau_0}{\tau_k-\tau_l}\right]^2+D_kD_l\right] . \tag{A7}$$

The first term is the dipole-dipole term in Eq. (3.68) and the second term is the second-order correction in the expansion in the charge-dipole interaction, where only the products $D_kD_l$ due to different dipoles ($k\neq l$) occur.

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