Theory of a Two-Level System Strongly Interacting with a Degenerate Fermi Gas

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A two-level system is treated which interacts with a degenerate fermionic heat bath. Arbitrarily strong screening by fermions is taken into account. The hopping of the two-level system may be spontaneous or assisted by the fermionic bath. By derivation of scaling equations it is shown for the spin-$\frac{1}{2}$ case that because of the assisted hops the two-level system cannot be localized in one of the states.

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Since the pioneering work of Caldeira and Leggett[1] the problem of the tunneling particle coupled to a heat bath has attracted great interest and the condition for self-localization in one of the potential wells has been studied in detail.[2] In these approaches the heat bath is characterized by Bose degrees of freedom. The question can be raised to what extent are the results modified when the tunneling particle is coupled to a degenerate Fermi gas instead of a Bose one. A possible realization of this problem is a two-level system (TLS) coupled to electrons in metallic glasses[3] or in A-15 compounds.[4] Recently, Yu and Anderson (YA) have examined the screening by electrons.[4] In their theory the scaling of the partition function in terms of the electron bandwidth leads to decreasing coupling. The similarity between that model and the bosonic case is obvious, because that fermionic Hamiltonian can be expressed in terms of Bose variables.[5] However, dealing with metallic glasses, Vladár and Zawadowski showed in the weak-coupling limit that the assisted tunneling processes may lead to strong coupling.[6] Later Zawadowski and Zimányi demonstrated the increase of the scattering phase shift even for its large values, assuming that the assisted tunneling processes dominate the tunneling processes but both are weak.[7] That result was obtained for spinless fermions. In this Letter a method is presented for the first time to our knowledge which is capable of treating the spontaneous and electron-assisted tunnelings without restricting their ratio in a unified framework and which is also applicable for arbitrary spin degeneracy N_s.

We make use of the electron Hamiltonian

$$H_0 = v_F \sum_{\mathbf{k}s} (k - k_F) a^\dagger_{\mathbf{k}s} a_{\mathbf{k}s}, \tag{1}$$

where $v_F|k-k_F| < D$ and $2D$ is the electron bandwidth. The v_F and k_F are the Fermi velocity and momentum, $a_{\mathbf{k}s}$ and $a^\dagger_{\mathbf{k}s}$ are the annihilation and creation operators of an electron with momentum $\mathbf{k}$ and spin s, and the density of states for one spin direction is constant, ρ.

The tunneling atom is placed in a double-well potential. If we consider an imaginary time variable τ, at low enough temperatures for most of the time the atom stays in one of the wells and the tunneling transitions are rare and short. In this case we can apply the TLS Hamiltonian

$$H_{21} = \Delta^- \boldsymbol{\sigma}^+, \quad H_{22} = \Delta^+ \boldsymbol{\sigma}^-, \quad H_{23} = \Delta^z \boldsymbol{\sigma}^z. \tag{2}$$

Here the $\boldsymbol{\sigma}^i$ Pauli matrices act on the two possible states of the atom. $\Delta^\pm$ are the transition amplitudes and Δ^z represents the energy difference of the left and right states. The TLS-electron interaction is described in an adequate spherical wave representation ($l = 0, 1, 2, \ldots$; $m = 0$).[6] The interaction Hamiltonian consists of the following terms:

$$\begin{aligned} H_1 &= \sum_m V^{z1}_{mm} \sigma^z a^\dagger_m a_m, \quad H_{24} = \sum_{mn} V^-_{mn} \sigma^+ a^\dagger_m a_n, \\ H_{25} &= \sum_{mn} V^+_{mn} \sigma^+ a^\dagger_m a_n, \quad H_{26} = \sum_{mn} V^{z2}_{mn} \sigma^z a^\dagger_m a_n. \end{aligned} \tag{3}$$

The indices m and n refer to a combination of spherical waves and to the spin simultaneously. The notation $a_m \sim \sum a_{km}$ is introduced, where the summation goes over the wave number k of the spherical wave and $v_F|k-k_F| < D$ holds. The doubling of the V^z term is only a technical trick. $H_1 + H_{26}$ represents the difference of the two atomic states in the scattering amplitude, while H_{24} and H_{25} describe the electron-assisted tunnelings. These terms arise from the fluctuation of the potential barrier due to the electron density.[6] In the following we use a basis set for the spherical waves such that V^{z1} is diagonal.

The main steps of our method are the following:

(i) We apply the path-integral method of YA[8] for a given TLS path $\sigma^z(\tau)$ $[|\sigma^z(\tau)| = 1]$ and obtain the partition function and the electron Green's function of the $H_0 + H_1$ problem for long times.

(ii) Using that electron Green's function we obtain the perturbative series in $H_2 = \sum_{i=1}^6 H_{2i}$ for the partition function as the functional integral

$$Z = Z_0 \int D\sigma^z(\tau) Z_1 Z_2 = Z_0 Z_I, \tag{4}$$

where Z_i is a functional of the TLS path:

$$Z_i=\left\langle T_\tau \exp\left[-\int_0^\beta d\tau\, H_i(\tau)\right]\right\rangle_i \quad (i=1,2). \tag{5}$$

Here T_τ is the time ordering operator, $H_i(\tau)$ is given in the interaction representation with the unperturbed Hamiltonian $H^{(i-1)}=\sum_{j=0}^{i-1}H_j$, and $\langle\ \rangle_i$ means thermal average also with $H^{(i-1)}$.

(iii) We sum up the perturbative series with logarithmic accuracy at high temperatures by means of electron bandwidth scaling.

Step (i).—After introducing the matrix notation $\boldsymbol{\delta}=-\arctan(\pi\rho\mathbf{V}^{z1})$ let us modify the parameters $\Delta^\pm$ and Δ^z in Eq. (2) in such a manner that

$$\mathrm{Tr}(\mathbf{V}^{z1})=\mathrm{Tr}(\mathbf{V}^+\cos^2\boldsymbol{\delta})=\mathrm{Tr}(\mathbf{V}^-\cos^2\boldsymbol{\delta})=0$$

and we define $\mathbf{V}^{z1}(\tau)=\sigma^z(\tau)\mathbf{V}^{z1}$. In the next section we extend the method of YA, outlined in Ref. 8, by using the fact that $V^{z1}(\tau)$ and $V^{z1}(\tau')$ commute and their trace is zero. We obtain for the partition function and the electron Green's function[7] for a given TLS path

$$Z_1=\prod_m(1+\gamma_{mm}^2)^{\beta/\tau_0}\exp\left[\sum_m\left(\frac{2\delta_m}{\pi}\right)^2\sum_{i<j}S_iS_j\ln\frac{|\tau_i-\tau_j|}{\tau_0}\right] \tag{6}$$

and

$$\mathbf{G}(\tau,\tau')=-\rho\frac{\mathrm{P}}{\tau-\tau'}\cos^2\boldsymbol{\delta}\exp\left[\frac{2}{\pi}\boldsymbol{\delta}\sum_i S_i\ln\left|\frac{\tau_i-\tau}{\tau_i-\tau'}\right|\right]. \tag{7}$$

Here τ_i denotes the time of the ith hop, $\boldsymbol{\gamma}=\pi\rho\mathbf{V}^{z1}$, $\beta=1/kT$, P denotes principal part, $S_i=\frac{1}{2}[\sigma^z(\tau_i-0)-\sigma^z(\tau_i+0)]$ is the index of "spontaneous tunneling," and we have arranged the τ_i variables in increasing order. Finally, $\tau_0\sim 1/D$ is a cutoff and our expressions are valid provided $|\tau_i-\tau_j|\gg\tau_0$.

Step (ii).—The construction of the complete perturbative series for Z_I leads to

$$Z_i=\sum_{N=0}^\infty(-1)^N\sum_{\{\alpha\}}\int_0^\beta d\tau_N\cdots\int_0^{\tau_i<\tau_{i+1}-\tau_0}d\tau_i\cdots d\tau_1 \times Z_1\,\mathrm{Tr}\langle T_\tau\{H_{2\alpha_N}(\tau_N)\cdots H_{2\alpha_i}(\tau_i)\cdots H_{2\alpha_1}(\tau_1)S(\beta,0)\}\rangle, \tag{8}$$

where $\{\alpha\}=\alpha_1,\ldots,\alpha_N$ stands for a given configuration of the indices $\alpha_i=1,\ldots,6$ in the product of H_2's and $S(\beta,0)$ corresponds to the S matrix and Tr acts on the TLS spin matrices. When we introduce $a_m(\tau)$ and $a_m^\dagger(\tau)$ as the interaction representation of a_m and $a_m^\dagger$ the following form is obtained:

$$Z_I=\sum_{N=0}^\infty(-1)^N\sum_{\{\alpha\}}\sum_{\{mn\}}\left[\prod_{j=1}^{N}{}^{(s)}\Delta^{(\alpha_j)}\right]\mathrm{Tr}\left[\prod_{l=1}^N\sigma^{(\alpha_l)}\right] \times\int_0^\beta d\tau_N\cdots\int_0^{\tau_k<\tau_{k+1}-\tau_0}d\tau_k\cdots d\tau_1\,Z_1\left\langle T_\tau\left[\prod_{i=1}^{N}{}^{(a)}V_{m_in_i}^{(\alpha_i)}a_{m_i}^\dagger(\tau_i)a_{n_i}(\tau_i)\right]\right\rangle. \tag{9}$$

In the product $\prod_i^{(a)}$ ($\prod_i^{(s)}$) for a given $\{\alpha_i\}$ the index runs over only those values which are associated with assisted (spontaneous) tunnelings. Calculating the expectation value in Eq. (9) we have to sum up all possible pairings of the operators where each pairing is associated with a $\mathbf{G}(\tau,\tau')$. Now we consider a single term of the sum in Eq. (9) corresponding to a configuration $\{mn\}$ with given matrix elements $V_{m_in_i}^{(\alpha_i)}$ at each interaction point with assisted tunneling. The $\{mn\}$ configurations are restricted to those which contribute in Eq. (9). The products of Green's function with same index μ form determinants.[8] The exponential part of $\mathbf{G}(\tau,\tau')$ can be treated separately and the remaining terms form a Cauchy determinant. The absolute value of this determinant is[9]

$$\tau_0^{-p_\mu}\prod_{i=1}^{N}{}^{(a)}\prod_{j=i+1}^{N}{}^{(a)}\left|\frac{\tau_i-\tau_j}{\tau_0}\right|^{T_{i\mu}T_{j\mu}}, \tag{10}$$

where electrons interact with the TLS p_μ times at the moments τ_i. The "assisted tunneling charge" vector $\mathbf{T}_i$ is defined for given $\{mn\}$ at site i by the components $T_{i\mu}=\delta_{n_i\mu}-\delta_{m_i\mu}$ and $\mathbf{T}_i=0$ for spontaneous tunneling. Here δ_{ij} means the Kronecker symbol. Now with use of Eqs. (6)–(9) the complete partition function is

$$Z_I\sim\sum_{N=0}^\infty(-1)^N\sum_{\{\alpha\}}\sum_{\{mn\}}\left[\prod_{j=1}^N y^{(\alpha_j)}\right]\mathrm{Tr}\left[\prod_{l=1}^N\sigma^{(\alpha_l)}\right]R \times\int_0^\beta d\tau_N\cdots\int_0^{\tau_k<\tau_{k+1}-\tau_0}d\tau_k\cdots d\tau_1\,\tau_0^{-N}\exp\left[\sum_{i<j}(\mathbf{C}_i\cdot\mathbf{C}_j)\ln\frac{|\tau_i-\tau_j|}{\tau_0}\right]. \tag{11}$$

Here the "total charge vector" of the hop at τ_i is

$$\mathbf{C}_i=\mathbf{T}_i+S_i\frac{2}{\pi}\boldsymbol{\delta}, \tag{12}$$

where $(\boldsymbol{\delta})_\mu=\delta_{\mu\mu}$ and in Eq. (11) $\mathbf{C}_i$ and $y^{(\alpha_i)}$ depend on α_i and in case of assisted tunneling also on m_in_i. R is a combinatorial factor with the values ± 1 or 0 and we introduced the hopping fugacities for $\alpha=1,2,3$ as $y^{(\alpha)}=\Delta^{(\alpha)}\tau_0$ and for $\alpha=4,5,6$ as

$$y_{mn}^{(\alpha)}=V_{mn}^{(\alpha)}\rho\cos\delta_{mn}\cos\delta_{nn}. \tag{13}$$

It is worth mentioning that here the total charge vector may depend on the incoming and outgoing electron indices in contrast to Ref. 7 where the charge is introduced only after the summation over the electron indices was performed.[10]

Step (iii).—Turning to the scaling we apply the scaling procedure of Anderson, Yuval, and Hamann.[11] We change simultaneously the scaling parameters τ_0 and the fugacities and charges to leave Z_I unmodified. τ_0 occurs essentially in two different ways in Z_I: explicitly in the integrand and in the boundaries of the integration. We choose $\mathbf{V}^{z2}=0$ as the initial value.

Collecting terms of τ_0 explicitly appearing in the exponent and in the prefactor one sees by making use $\sum_i\mathbf{C}_i=0$ that the changes are compensated, if

$$dy^{(\alpha_i)}/d\ln\tau_0=y^{(\alpha_i)}(1-\tfrac{1}{2}|\mathbf{C}_i|^2). \tag{14}$$

On the other hand, the change of τ_0 in the integration boundaries means that we have to perform a small part of the integration explicitly for a "closed pair," viz. when $\tau_0<\tau_{i+1}-\tau_i<\tau_0+d\tau_0$.[11] We distinguish two cases: when $\mathbf{C}_i+\mathbf{C}_{i+1}=0$ and when $\mathbf{C}_i+\mathbf{C}_{i+1}\neq 0$. In the first case we follow step by step Ref. 11. The integration over τ_i yields a $d\tau_0$ factor only; then we expand the integrand with respect to $\tau_0/\bar{\tau}\ll 1$ ($\bar{\tau}$ is the average distance of neighboring hops) and perform the integration over τ_{i+1}; finally, we exponentiate back the obtained expression using the smallness of $d\tau_0$. This way we arrive at the same form as Z_I but with scaled parameters and with a multiplicative factor. The scaled charges can be reproduced by scaling the phase shift $\boldsymbol{\delta}$ in Eq. (12) as

$$[d(\boldsymbol{\delta}/\pi)/d\ln\tau_0]=[\mathbf{y}^+,\mathbf{y}^-]_- -(2\boldsymbol{\delta}/\pi)[\mathrm{Tr}(\mathbf{y}^+,\mathbf{y}^-)+y^+y^-], \tag{15}$$

where $y^+=y^{(2)}$, $y^-=y^{(3)}$, $\mathbf{y}^+=y^{(4)}$, and $\mathbf{y}^-=y^{(5)}$. When the total charge of a closed pair is not zero, then the expression of the integrand with respect to $\tau_0/\bar{\tau}$ cannot be performed, and so we integrate over τ_i and generate a new charge $\mathbf{C}=\mathbf{C}_i+\mathbf{C}_{i+1}$ at τ_{i+1}. These charges, except one, correspond to scatterings independent of the TLS state, which are of no importance. The only exception generates V_{mn}^{z2} with $m\neq n$ which must be added to V_{mn}^{z1} and occurs as the off-diagonal part of the commutator in Eq. (15).

When we add the two contributions in the final result, Eq. (15) is combined with

$$\frac{d\mathbf{y}^\pm}{d\ln\tau_0}=\pm 2\left[\frac{\boldsymbol{\delta}}{\pi},\mathbf{y}^\pm\right]_- -2\mathbf{y}^\pm\,\mathrm{Tr}\left[\left(\frac{\boldsymbol{\delta}}{\pi}\right)^2\right], \tag{16}$$

$$dy^\pm/d\ln\tau_0=y^\pm\{1-2\,\mathrm{Tr}[(\boldsymbol{\delta}/\pi)^2]\}, \tag{17}$$

$$dy^z/d\ln\tau_0=y^z. \tag{18}$$

These equations are consistent for 2×2 matrices with Ref. 7 if the assisted tunnelings dominate and with Ref. 6 in the limit $2\delta/\pi\ll 1$.[12] These equations are exact in the scattering phase shift $\boldsymbol{\delta}$ and are valid to lowest nonvanishing order in the fugacities $y^{(\alpha)}$, since our assumption of rare hoppings requires $y^{(\alpha)}\ll 1$ for all α. Furthermore, it can be shown that the other generated new charges remain negligible ($\sim y^2$) during the scaling.[13]

When one solves Eqs. (15) and (16), $2N_s$-dimensional subspace (a direct product of two spherical waves and N_s spin states) plays the important role, whose parameters increasingly dominate the others.[6] In this subspace $\boldsymbol{\delta}/\pi=z\sigma^z$, $\mathbf{y}^\pm=y_a\sigma^\pm$, where y_a is the strength of assisted tunneling; furthermore, δ and $y^\pm$ are diagonal in the spin states. The σ^i operators act on the spherical wave states. With use of the notation $y=(y^+y^-)^{1/2}$ the scaling equations in the reduced subspace take the form

$$dz/d\ln\tau_0=y_a^2(1-2N_sz)-2zy^2, \tag{19}$$

$$dy_a/d\ln\tau_0=4zy_a(1-N_sz), \tag{20}$$

$$dy/d\ln\tau_0=y(1-4N_sz^2). \tag{21}$$

These equations have a repelling fixed line at $y=y_a=0$. They are valid if $y,y_a\ll 1$, and this condition limits our scaling region. The temperature dependences of our effective parameters can be obtained by inserting $\tau_0=T^{-1}$, which show the following features in case $N_s=2$:

The value of y_a always increases with decreasing temperature.

y decreases if $z>z_c=2^{-3/2}$ and increases if $z<z_c$. Some of the trajectories may pass this value of z_c; thus $y(T)$ is not necessarily monotonic. Furthermore, y never reaches zero in our scaling region since the increasing value of y_a stops the scaling.

The behavior of z is governed by the surface S defined by $dz/d\ln\tau_0=0$, which separates the parameter space into two parts. Trajectories starting with $dz/d\ln\tau_0<0$ approach S, but never intersect it, yielding monotonic temperature dependence of $z(T)$ with $dz/dT>0$. Trajectories starting from the other side and far enough from S also approach it, but the condition $y, y_a \ll 1$ stops the scaling before they reach S which behaves like an attractive surface. Finally, the trajectories which start close to S may be nonmonotonic in $z(T)$.

The conclusions can be summarized as follows. The existence of scaling has been demonstrated in the simultaneous presence of normal and assisted tunnelings for an arbitrary value of the phase shift δ. In the case of absence of assisted tunneling the system behaves like a bosonic heat bath where self-localization may occur for a large enough phase shift $(N_s > 1)$. In the present model, self-localization does not occur for $N_s = 2$ if the starting value of the assisted tunneling fugacity y_a is different from zero as y_a increases as a result of the scaling, but that may occur for $N_s > 2$. These statements do not depend on the approximations made, because the present theory is exact in the limit $y, y_a \ll 1$. In the limit $y_a \gg y$ the phase-shift renormalization is toward the value $\delta = \frac{1}{2}\pi / N_s$.

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[10]In Ref. 7 the summation could be performed only because the first region of the scaling was excluded and, therefore, considering assisted tunnelings the kinks and antikinks in the tunneling path were associated with uniquely given spherical index changes.

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[12]The last term $y^+ y^-$ in Eq. (15) does not occur in Ref. 6, since the logarithmic terms with coefficient $(\Delta/D)^2$ were dropped there.

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