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Theory of tunneling of an atom interacting with a degenerate electron gas

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The tunneling of an atom in a double potential well is treated in the presence of interaction with conduction electrons. Screening and assisted tunneling processes are considered as well. In the spinless electron case the partition function is calculated and logarithmic interactions between tunneling processes are derived and expressed by a phase shift which scales to $\pi/2$ as the bandwidth is reduced.

Since the pioneering work of Caldeira and Leggett[1] the tunneling particles coupled to a heat bath attracted considerable interest. The heat bath is characterized by Bose degrees of freedom.[2] A considerable part of the technique applied was developed by Anderson and his co-workers[3,4] for the Kondo problem where a spin flip triggers a screening process in the conduction band. Recently, Yu and Anderson[5] have treated the tunneling of an atom screened by electrons, but the possibility of electron assisted tunneling has not been considered. Scaling in terms of the conduction-electron bandwidth leads to a decreasing coupling. Dealing with two-level systems in metallic glasses Vladár and Zawadowski[6] showed in a weak coupling theory that the assisted tunneling may lead to scaling to strong coupling. The aim of the present work is to show the importance of the assisted tunnelings for an arbitrary strong coupling by using Anderson's[4] real-time technique and considering the partition function to derive the interaction between different tunneling processes (direct, assisted).

The present Rapid Communication deals with the strong assisted tunneling case, while Yu and Anderson[5] treated the opposite limit where the assisted processes are negligible.

The tunneling atom with coordinate Q ($Q=Q^z$, $Q^x=Q^y=0$) moves along the z axis in a double-well potential $V(Q)$. Thus the atomic Hamiltonian is

$$H_{\rm at}=\tfrac{1}{2}MQ^2+V(Q) \ , \tag{1}$$

where M is the mass of the atom. The equilibrium positions are $\pm Q_0$. A point interaction of strength U is assumed between the atom and the conduction electrons. Thus, the scattering matrix element between two single-electron states with momentum k and k' is $U\exp[i(k_z-k_z')Q]$. Expanding this result with respect to Q ($|Qk_F|<1$, where k_F is the Fermi momentum) and introducing spherical waves with $l=0,1$ ($m=0$) for the conduction electrons, we write the interaction Hamiltonian[6] as

$$H=U\sum_{k,k',l,l',s} a^{\dagger}_{sk'l'}(\lambda^x_Q\sigma^x_{l'l}+\lambda^z_Q\sigma^z_{l'l})a_{skl} \ , \tag{2}$$

where $\lambda^x_Q=\frac{1}{2}k_FQ/\sqrt{3}$, $\lambda^z_Q=-\frac{1}{3}(k_FQ)^2$, σ^i ($i=x,y,z$) are Pauli matrices, a_{skl} is the destruction operator for a spherical electron wave with momentum $k>0$, and the spin s takes N_s different values (in reality, $N_s=2$). In this Hamiltonian all the terms proportional to the unit matrix are dropped. The corresponding electron Hamiltonian is

$$H_0=v_F\sum_{k,l,s}(k-k_F)a^{\dagger}_{skl}a_{skl} \ , \tag{3}$$

where v_F is the Fermi velocity and a cutoff of order the Fermi energy E_F will be introduced.

We shall see that the second term of Hamiltonian (2) will be associated with electron assisted tunneling. Therefore, it is useful to separate out a term $-\frac{1}{3}U(k_FQ_0)^2\sigma^z$ which is constant in time and can be taken into account by a time-independent renormalization of the spherical waves. The remaining part of the Hamiltonian is given in a new representation $a_{sk\pm}=(a_{sk0}\pm a_{sk1})/\sqrt{2}$ as $H'=H_1+H_2$ where $H_1=E_1(Q)\sigma^z$ and $H_2=E_2(Q)\sigma^x$. Here $E_1\sim Q$ and $E_2\sim Q^2-Q_0^2$. The off-diagonal terms act only when the atom is out of the equilibrium positions $\pm Q_0$; thus, the contributions come from the tunneling processes.

Following Yu and Anderson[5] we treat the motion of the atom by a path-integral method, the partition function $Z\{Q\}$ is calculated for the Hamiltonian $\sum_{i=0}^{2}H_i$ as a functional of the classical path of the atom $Q(\tau)$ where τ is the complex time variable in the interval $(0,\beta)$ with β the inverse temperature. We shall take the limit $\beta\to\infty$. $Z\{Q\}$ can be written as $Z\{Q\}=Z_0Z_1Z_2$ where Z_0 is the partition function of the atom without interaction with the electrons and

$$Z_i=\left\langle T_\tau\exp\left[-\int_0^\beta d\tau\, H_i(\tau)\right]\right\rangle_i \quad (i=1,2) \ , \tag{4}$$

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

Yu and Anderson[5] have first determined Z_1 for a general path $Q(\tau)$, and then they considered a hopping path depicted in Fig. 1(a), where the atom is always in one of the equilibrium positions $\pm Q_0$ except during the tunneling. The tunneling path has been taken as a straight line in a time interval whose length $\tau_{\rm tun}$ is determined by minimalizing the contribution to the free energy. Using the Nozières–De Dominicis technique[7] they determined first the electron Green's function for a general path and for a longer time scale than the short time cutoff τ_F inversely proportional to the bandwidth. The Green's function is[5]

$$G_{s\pm}(\tau,\tau')=-\frac{N(0)}{\tau-\tau'}\cos[\delta(\tau)]\cos[\delta(\tau')]e^{\mp S(\tau)\pm S(\tau')} \ , \tag{5}$$

where $N(0)$ is the density of states for one spin direction

$$\delta(\tau) = -\tan^{-1}[\gamma(\tau)] \ ,$$

where

$$\gamma(\tau) = \pi N(0)(2\sqrt{3})^{-1} k_F Q(\tau)$$

and

$$S(\tau) = \frac{1}{\pi} \mathrm{P} \int_0^\beta \frac{\delta(\tau'')}{\tau'' - \tau} d\tau'' \ . \tag{6}$$

Considering hopping paths, with $2n$ hoppings at times τ_i $(i = 1, \ldots, 2n)$ they obtain the final result for Z_1 as

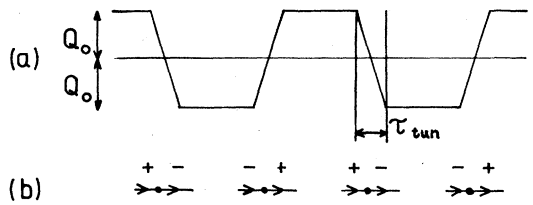

FIG. 1. (a) Tunneling path with straight lines during the tunnelings with time τ_{tun}. (b) The kink (antikink) is correlated with the change of the electron orbital index $+ \rightarrow -$ $(- \rightarrow +)$.

$$Z_1 = e^{-\beta \Delta V(Q_0)} \sum_{n=0} \left(\frac{y}{\tau_0} \right)^{2n} \int_0^\beta d\tau_{2n} \int_0^{\tau_{2n} - \tau_0} d\tau_{2n-1} \cdots \int_0^{\tau_2 - \tau_0} d\tau_1 \exp\left[N_s 8 \left(\frac{\delta}{\pi} \right)^2 \sum_{i>j} (-1)^{i-j} \ln \frac{|\tau_i - \tau_j|}{\tau_0} \right] \ , \tag{7}$$

where the phase shift is $\delta = -\tan^{-1}\gamma_0$ for the equilibrium position $Q = Q_0$ and $\Delta V(Q_0)$ is a hopping independent renormalization of the potential $V(Q)$. Also, $\tau_0 = \max(\tau_{tun}, \tau_F)$ and y is the hopping fugacity

$$y = \frac{\tau_0}{\tau_{tun}} \frac{1}{\gamma_0} (2e)^{-4\delta^2/\pi^2} \exp(-4Q_0^2 M/\tau_{tun}) \ .$$

The effect of the $\cos\delta$ terms appearing in the Green's function can be incorporated into y.

In order to calculate Z_2 the expression (4) must be considered. It corresponds to the sum of all possible products of closed ring diagrams where the interaction is H_2 and the Green's functions are given by Eq. (5). A vertex with orbital index going $+ \rightarrow -$ or $- \rightarrow +$ at time τ is associated with the factor $\exp[-2S(\tau)]$ and $\exp[+2S(\tau)]$, respectively. The factor $\exp[S(\tau]$ can be evaluated for a hopping path starting and ending with, e.g., $+Q_0$:

$$e^{S(\tau)} = \left[\left(\frac{\beta - \tau}{\tau} \right)^{1/2} \prod_{i=1}^{n} \left| \frac{\tau_{2i} - \tau}{\tau_{2i-1} - \tau} \right| \right]^{2\delta/\pi} \ . \tag{8}$$

Here, if τ is near any hop τ_i and $|\tau - \tau_i| < \tau_0$ then $\tau - \tau_i$ must be replaced by τ_0.

Furthermore, H_2 acts only during a hop and gives a correcting factor to the fugacity. The fugacity of the electron assisted hopping[8] is $y_a \sim yU(k_F Q_0)^2 \tau_{tun}$. The numerical factor is the order of unity and depends on the shape of the barrier. In the following we treat the case where $y_a >> y$.

The observation on which Anderson's approach[4] is based for this kind of problem is that the subsequent hops are attractive; thus, the hops form pairs in the complex time interval. The main contribution to the free energy is due to such pairs. The final step of Anderson's approach is a renormalization-group consideration where the close pairs are transformed out and new parameters (couplings, fugacities) are introduced to replace the effects of the eliminated pairs.

Consider a close neighboring assisted tunneling pair $(\tau_i; \tau_{i+1})$ with time difference $\tau_{pair} = |\tau_i - \tau_{i+1}|$ small compared with the distances $\bar{\tau}$ of the other hops measured from the pair. For simplicity we take, e.g., $\delta > 0$. Two different limits are of special interest.

(i) $\delta = 0$ case. The part of a diagram with the pair is shown in Fig. 2 with two different time orders. If $|\tau_{pair}| << |\bar{\tau}|$, then the Green's functions connecting the pair with the other parts of the diagram are approximately the same for the two time orderings. The Green's functions connecting the pairs have opposite signs; thus, the two time-ordered diagrams cancel each other with accuracy $\tau_{pair}/\bar{\tau}$.

(ii) $\delta \neq 0$ case and $(\tau_{pair}/\tau_0)^{8\delta/\pi} >> 1$. The two time orderings considered above are different also in the factors $\exp[2S(\tau_i) - 2S(\tau_{i+1})]$ and $\exp[-2S(\tau_i) + 2S(\tau_{i+1})]$ where the S functions are taken at the two different hops. Depending on whether the hop is a kink or antikink the above quantities contain a very large or very small factor with order of magnitude $(\tau_{pair}/\tau_0)^{8\delta/\pi}$ or $(\tau_0/\tau_{pair})^{8\delta/\pi}$. The other factors appearing in these quantities for the two time orderings are approximately the same. Thus, in this limit only one of the two terms with the large factor should be kept. This approximation introduces a strict correlation between the orbital index changes $(+ \rightarrow -$ or $- \rightarrow +)$ and the kink or antikink. [See Fig. 1(b).]

Using these results we find an almost complete cancellation of the two time-ordered diagrams if $(\tau_{pair}/\tau_0)^{8\delta/\pi} << 1$ [region (i)]. One term is dominant if $(\tau_{pair}/\tau_0)^{8\delta/\pi} >> 1$ [region (ii)]. The conclusion is that the very close pairs do not contribute to the free energy. This region is the smaller the larger is δ. If the kink and antikink are represented symbolically by spin transition operators S^- and S^+, and the orbital transition $- \rightarrow +$ and $+ \rightarrow -$ by σ^+ and σ^-, then the region where the orbital transition is not correlated with a kink or antikink corresponds to $S^x\sigma^x = (S^+ + S^-) \times (\sigma^+ + \sigma^-)$ and the correlated region to $S^x\sigma^x + S^y\sigma^y = 2(S^+\sigma^- + S^-\sigma^+)$.

In the following only region (ii) is considered. Only the dominant terms are kept. The situation is very similar to a uniaxial Kondo problem. In evaluating Z_2, the method of Yuval and Anderson[2] is closely followed. Take a classical path for the atom and consider the order $2p$ in Hamiltonian H_2. Associate the $p+ \rightarrow -$ and $p- \rightarrow +$ transition with p arbitrarily chosen kinks and antikinks, respectively. Consid-

FIG. 2. Two diagrams with close pairs of tunnelings $(i, i+1)$ are shown.

er all diagrams with the unrenormalized Green's function $G^{(0)}(\tau-\tau')=-N(0)/\tau-\tau'$ first. It can be shown that the factor containing S given by Eq. (8) contributes by a multiplying factor depending only on the atomic motion. The sum of the products of Green's functions $G^{(0)}$ in any order $2p$ can be cast into a form which is a product of Cauchy determinants D.[3] These determinants consist of Green's functions with only the plus or minus orbital index. They can be evaluated, and the contributing factor to Z_2 is

$$D^2=\tau_0^{2p}\left[\prod_{\substack{i>i'\\(K)}}(\tau_i-\tau_{i'})\prod_{\substack{j>j'\\(A)}}(\tau_j-\tau_{j'})\prod_{\substack{i(K)\\j(A)}}(\tau_i-\tau_j)^{-1}\right]^2 , \tag{9}$$

where K (A) stands for a kink (antikink). It is easy to show that the factors $\exp[\pm S(\tau_i)]$ and $\exp[\pm S(\tau_j)]$ together contribute $D^{-8\delta/\pi}$ in the case where τ_i and τ_j are both assisted hops. When only one of τ_i,τ_j is assisted, the factor $\tau_i-\tau_j$ appears with half of the previous exponent.

The total contribution to Z_1Z_2 of a classical path with $2n(i=1\ldots 2n)$ hopping amongst which p kinks and p antikinks are assisted, is

$$e^{-\beta\Delta V(Q_0)}\left(\frac{y}{\tau_0}\right)^{2(n-p)}\left(\frac{y_a}{\tau_0}\right)^{2p}\int_0^\beta d\tau_{2n}\int_0^{\tau_{2n}-\tau_0}d\tau_{2n-1}\cdots\int_0^{\tau_2-\tau_0}d\tau_1\exp\left[\sum_{i>j}\alpha_{ij}(-1)^{i-j}\ln\frac{|\tau_i-\tau_j|}{\tau_0}\right] , \tag{10}$$

where i and j run over all of the hops. The coefficients α_{ij} are

$$\alpha_{ij}=2\epsilon_i\epsilon_j , \tag{11}$$

where $\epsilon_i=1-2\delta/\pi=\epsilon_a$ for assisted and $\epsilon_i=-2\delta/\pi=\epsilon_n$ for nonassisted hops. Since we have not included contributions of electron spin, this result is valid only for $N_s=1$.

We follow the method of Anderson and co-workers[4,5] to derive the scaling equations. The elimination of a closed pair of assisted tunnelings with pair distance $\tau_0<\tau_{\text{pair}}<\tau_0+d\tau_0$ permits the relation

$$Z(y,y_a,\alpha_{ij})=\exp(y_a^2\beta\,d\tau)\,\bar{Z}(\bar{y},\bar{y}_a,\bar{\alpha}_{ij}) ,$$

where $\bar{Z}$ is the scaled partition function which has the form of the original one but with the scaled parameters which are obtained from the following equations.

$$d\alpha_{ij}=-2y_a^2(\alpha_{ia}+\alpha_{ja})\,d\ln\tau_0 , \tag{12}$$

where the index a stands for assisted tunneling. The last step is to change $\tau_0\rightarrow\tau_0=\tau_0+d\tau_0$ in $\ln|\tau_i-\tau_j|/\tau_0$. It is easy to show that the number of $\ln\tau_0$ terms in the exponent of Eq. (10) is proportional to the number of the assisted pairs p and to half of the number of nonassisted tunneling steps $n-p$, but it is independent of the number of assisted-nonassisted pairs. Thus,

$$dy_\alpha=-y_\alpha(\epsilon_\alpha^2-1)\,d\ln\tau_0 \quad(\alpha=a,n) , \tag{13}$$

where $y_n=y$ and the tunneling rates are $\Delta_a=y_a/\tau$ and $\Delta=y/\tau$.

The scaling Eqs. (12) can be satisfied in the form (11) by a scaled phase shift obtained from the equation

$$\frac{1}{\pi}\frac{\partial\delta(\tau_0)}{\partial\ln\tau_0}=y_a^2\left[1-\frac{2}{\pi}\delta(\tau_0)\right] . \tag{14}$$

The phase shift has a fixed point at the resonance $\delta=\pi/2$.

The scaling procedure given above works if the nearest-neighbor pairs are assisted tunnelings and no normal tunneling enters to separate them $(y<y_a)$. Thus, two cases must be distinguished: (i) $y\ll y_a$ holds during the scaling and therefore normal tunneling does not play any role; (ii) $y=y_a$ is reached before $y_a\rightarrow 1$, beyond which our scaling procedure cannot be applied.

If the electron spin is included with value $N_s=2$ the assisted pair can be of parallel and of antiparallel spins and in this case until now we were not able to prove rigorously the scaling equations for the couplings.

The results obtained here are in agreement with the scaling theory[6] derived for the two level system interacting with electrons in the weak coupling region $\delta/\pi\ll 1$. In that theory there are phenomenologically introduced couplings between the electrons and the two level system $v^z=\delta/\pi$, $v^x=\frac{1}{2}y_a$, and $v^y=0$ which occur in an anisotropic Kondo Hamiltonian. In the first region of scaling in that problem v^y is generated until $v^x\approx v^y$. That corresponds to our region, where $(\tau/\tau_0)^{8\delta/\pi}\gg 1$ does not hold and we are not able to establish scaling rules for an arbitrary δ. Following that region the uniaxial Kondo region takes place $(v^x=v^y)$, where in our problem the kinks and antikinks are tied to $-\rightarrow+$ or $+\rightarrow-$ orbital index changes and scaling works.

In the present theory the renormalization by the electrons is taken into account by the renormalized phase shift δ and by the renormalized values of the assisted and nonassisted tunneling rates proportional to y and y_a. In the case $y_a\gg y$ the renormalization means the elimination of the close assisted tunneling pairs and δ scales to the strong coupling. In the opposite case $y\gg y_a$ the elimination of the nonassisted tunneling pairs leads to a decrease in δ. In the latter case Eq. (13) holds and the index a must be replaced by n in Eq. (13); finally, the right-hand side of Eq. (14) becomes $-2y^2\delta/\pi$, in agreement with the results of Anderson and Yu.[5] Furthermore, the present theory holds only in the dilute tunneling case $y_a,y\ll 1$ where the asymptotic solution (5) of the Green's function holds but there is no restriction on δ. The end of the scaling region is determined by $y_a=1(y=1)$ or by $y_a=y$. In the strong coupling case $\delta/\pi>\frac{1}{4}$ we have found, however, that the scaling is never stopped by $y=y_a$ as can be seen from Eq. (13) and, therefore, self-localization in one of the potential wells does not occur as y and y_a do not go to zero.

Summarizing, we have shown that the inclusion of the interaction leading to assisted tunneling may introduce new strong coupling features in the present problem where the heat bath is a degenerate fermion gas.

The essential difference between the model without and

with assisted tunneling is that in the first case the fermion part of the Hamiltonian can be linearized in terms of boson operators, but that cannot be done in the model treated here.[9] The treatment of fermions with spins are of physical interest, but that appears to be a rather sophisticated problem.

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