Theory of Hopping Motion of a Heavy Particle Interacting with a Degenerate Electron Gas

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A heavy particle moving by hopping on a lattice is considered. The screening and assisted hopping due to the electrons result in logarithmic contributions to the scattering amplitude. In the study of a one-dimensional model, scaling similar to the anisotropic antiferromagnetic Kondo problem is found. The large-scaled couplings reduce the width of the heavy-particle band essentially. The results obtained hold also for heavy particles forming a degenerate Fermi gas.

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Since the discovery of Anderson's orthogonality catastrophe and the realization of the importance of noncommutative couplings between a degenerate electron gas and other degrees of freedom, considerable interest has been attracted by problems exhibiting such features. The orthogonality catastrophe means that the electronic screening clouds formed around a particle with different positions are orthogonal.[1] Kondo pointed out[2] that in the Hamiltonian of a particle hopping between two sites and interacting with an electron gas the terms corresponding to screening and electron-assisted tunneling do not commute, and it became known that they scale to strong couplings.[3,4] Recently, Caldeira and Leggett[5] have studied the interaction of a heavy particle coupled to an environment described by bosonic variables.

If we consider the momentum dependence of the coupling and the energy density of the excitations in the heat bath, the marginal case separates the models with and without infrared divergencies. As regards the applications most of the models of interest belong to that marginal case and show "Ohmic behavior." The two-site problem with electron-assisted tunneling is one of the exceptions.[4] The hopping motion of a particle on a lattice and its coupling to bosonic[6,7] and fermionic[7-12] environments have been extensively studied also. In the latter case the screening results in a reduced hopping rate but not in renormalization of the screening coupling.[8,11,12] Kagan and Prokof'ev[10] emphasized that it is appropriate to solve the kinetic equation with the reduced hopping rate, as long as the coupling is not enhanced.

The model to be studied is a heavy particle (HP), and its interaction with electrons includes screening and assisted hopping (see Fig. 1). According to our knowledge this is the first noncommutative model on a lattice which scales to strong coupling. The applications of this problem may include the motion of hydrogen and muon in metals[8] and the dynamics of f electrons in heavy-fermion systems.[13] The following treatment is restricted to logarithmic approximation at low temperature.

The HP moves by hopping motion on a cubic lattice of dimension d with lattice vectors $\mathbf{R_n}=a\mathbf{n}=a(n_1, n_2, \ldots, n_d)$, where n_i $(i=1,2,\ldots,d)$ is an integer and the lattice constant is denoted by a. The annihilation operator of the HP on site $\mathbf{n}$ is $a_{\mathbf{n}}$. The unperturbed Hamiltonian is

$$H_0=t\sum_{\mathbf{n},\boldsymbol{\delta}} a^{\dagger}_{\mathbf{n}+\boldsymbol{\delta}}a_{\mathbf{n}}+\sum_{\mathbf{k},\sigma}\epsilon_k b^{\dagger}_{\mathbf{k}\sigma}b_{\mathbf{k}\sigma}, \tag{1}$$

where t stands for the overlap integral and $\boldsymbol{\delta}$ are the vectors pointing to the neighboring sites ($|\boldsymbol{\delta}|^2=1$). A conduction electron with momentum $\mathbf{k}$ and spin σ is created by the operator $b^{\dagger}_{\mathbf{k}\sigma}$ and the related energy is ϵ_k.

The screening of the HP by the conduction electrons is given by the Hamiltonian

$$H_V=V\sum_{\mathbf{n}} a^{\dagger}_{\mathbf{n}}a_{\mathbf{n}}\psi^{\dagger}_{\sigma}(\mathbf{n})\psi_{\sigma}(\mathbf{n}), \tag{2}$$

where $\psi_{\sigma}(\mathbf{n})$ is the electron field operator taken at site $\mathbf{n}$ which can be expressed by plane-wave annihilation operators $b_{\mathbf{k}\sigma}$ as

$$\psi_{\sigma}(\mathbf{n})=\Omega^{-1/2}\sum_{\mathbf{k}} e^{ia\mathbf{k}\cdot\mathbf{n}}b_{\mathbf{k}\sigma},$$

where Ω denotes the volume. Similarly,

$$a_{\mathbf{n}}=N^{-1/2}\sum_{\boldsymbol{\theta}} e^{i\boldsymbol{\theta}\cdot\mathbf{n}}a_{\boldsymbol{\theta}},$$

where $\boldsymbol{\theta}$ is the dimensionless momentum $(-\pi<\theta_i<\pi)$

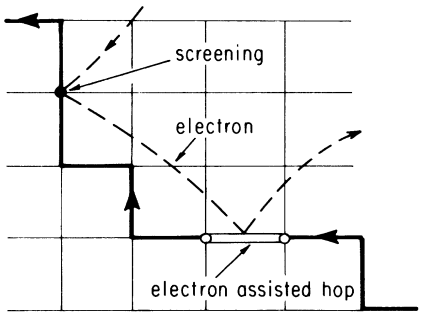

FIG. 1. Typical hopping path on a two-dimensional lattice. The solid line (dashed) represents the heavy particle (electrons). The solid circle is the screening interaction, and the double line connecting two sites shown by open circle is the assisted hopping.

and N is the number of sites.

The jump of the HP from site $\mathbf{n}$ to the neighboring site $\mathbf{n}+\boldsymbol{\delta}$ can be considered as a tunneling through a potential barrier V_B. The fluctuations of the electron density $\delta\rho$ in the barrier interact with the HP by a local coupling V' and that results in an effective barrier $V_{\text{eff}}=V_B+V'\delta\rho$. The change in the tunneling rate due to $\delta\rho$ is called assisted tunneling, and it can be expanded in terms of $\delta\rho$.[2,14,15] For the sake of simplicity, the electron density fluctuation is taken at the middle of the bound, $\tilde{\mathbf{n}}=\mathbf{n}+\frac{1}{2}\boldsymbol{\delta}$. The corresponding phenomenological Hamiltonian is

$$H_U=\tfrac{1}{2}U\sum_{\mathbf{n},\boldsymbol{\delta}}a^\dagger_{\mathbf{n}+\boldsymbol{\delta}}a_{\mathbf{n}}\psi^\dagger_\sigma(\tilde{\mathbf{n}})\psi_\sigma(\tilde{\mathbf{n}}), \tag{3}$$

which can be given in momentum representation as

$$H_U=\frac{1}{\Omega N}U\sum_{\mathbf{n}}\sum_{\boldsymbol{\theta}',\boldsymbol{\theta}''}\frac{1}{2}\sum_{\boldsymbol{\delta}}\exp[-\tfrac{1}{2}i(\boldsymbol{\theta}'+\boldsymbol{\theta}'')\cdot\boldsymbol{\delta}]a^\dagger_{\boldsymbol{\theta}''}a_{\boldsymbol{\theta}'}b^\dagger_{\mathbf{k}''}b_{\mathbf{k}'}\exp\{i[\boldsymbol{\theta}'-\boldsymbol{\theta}''+a(\mathbf{k}'-\mathbf{k}'')]\cdot\tilde{\mathbf{n}}\}. \tag{4}$$

The summation over $\tilde{\mathbf{n}}$ for a fixed value of $\boldsymbol{\delta}$ results in the conservation of momentum. The sum of the interactions given by Eqs. (2) and (3) can be given as

$$H_1=\frac{1}{\Omega}\sum_{\boldsymbol{\theta}'+a\mathbf{k}'=\boldsymbol{\theta}''+a\mathbf{k}''}\left[V+\frac{1}{2}U\sum_{\boldsymbol{\delta}}\cos\left(\frac{\boldsymbol{\theta}'+\boldsymbol{\theta}''}{2}\cdot\boldsymbol{\delta}\right)\right]a^\dagger_{\boldsymbol{\theta}''}a_{\boldsymbol{\theta}'}b^\dagger_{\mathbf{k}''\sigma}b_{\mathbf{k}'\sigma}. \tag{5}$$

The total Hamiltonian to be treated is $H=H_0+H_1$. The appearance of the dependence on $\boldsymbol{\theta}=\frac{1}{2}(\boldsymbol{\theta}'+\boldsymbol{\theta}'')$ is the key feature of the present model. In a more appropriate theory the shift of the barrier relative to the shifts of the two neighboring sites must be considered; thus $\psi^\dagger(\tilde{\mathbf{n}})\psi(\tilde{\mathbf{n}})$ must be replaced by

$$\psi^\dagger(\tilde{\mathbf{n}})\psi(\tilde{\mathbf{n}})-\tfrac{1}{2}[\psi^\dagger(\mathbf{n})\psi(\mathbf{n})+\psi^\dagger(\mathbf{n}+\boldsymbol{\delta})\psi(\mathbf{n}+\boldsymbol{\delta})].$$

That results in a form factor proportional to $\sin^2[(\mathbf{k}''-\mathbf{k}')\cdot\boldsymbol{\delta}a/4]$ in the interaction, which is not essential and will be disregarded.

In any diagram the electron momentum summation for momenta parallel to a particular direction $\boldsymbol{\kappa}$ ($|\boldsymbol{\kappa}|^2=1$) can be performed separately. As the infrared behavior of a slowly moving HP is studied ($v_F/ta\gg 1$), at each vertex the momentum conservation can be approximated as $\boldsymbol{\theta}'+\boldsymbol{\kappa}'Q=\boldsymbol{\theta}''+\boldsymbol{\kappa}''Q$ where $Q=k_Fa$.[12]

A straightforward calculation shows that the first-order correction to the HP-electron vertex contains a logarithmic term $\ln(D/\max\{T,\omega,t\})$, where D is the electron bandwidth cutoff, T is the temperature, ω is an energy variable, and the bandwidth of the HP is proportional to t. The logarithmic term occurs as the two basic diagrams depicted in Fig. 2 do not cancel each other, in contrast to the case of simple potential scattering. That is due to the θ dependence of the vertex [see Eq. (5)]. In the present case θ plays the role of the localized spin in the Kondo effect. The results are presented for the 1D case, where $\boldsymbol{\kappa}$ is replaced by $\mu=\pm 1$ for the right- and left-going electrons. In the Hamiltonian (5) only the backscattering of the electron is retained as the normal forward scattering is irrelevant. The general dimensionless scattering coupling is denoted by $v_b(\theta)$, which has the starting form

$$v_b(\theta)=\rho_0(V+U\cos\theta)=v_b+u_b\cos\theta,$$

where $\rho_0=(2\pi v_F)^{-1}$ is the density of the conduction electrons at one side of the Fermi surface for one spin direction, and v_b and u_b are the dimensionless couplings. With that vertex for the vertex corrections depicted in Fig. 2, the intermediate momenta of the HP are $\theta'\pm Q\mu'$. The generated vertex is the anomalous forward scattering $v_f(\theta';\mu')$, which is odd both in variables θ' and μ'; thus it depends on whether the momenta of the electron and the HP are parallel or not. In the lowest order $v_f(\theta,\mu)$ has the form

$$v_f(\theta,\mu)=\mu v_f\sin\theta\sin Q$$

for the limit $v_b\gg|u_b|$, and then $v_f\sim v_bu_b$. The combination of the backward and the anomalous forward scatterings in the diagrams shown in Fig. 2 generates backscattering. The scaling equations in terms of the electron bandwidth D are given as functions of the scaled width D' and are obtained by taking the derivatives of the vertex corrections with respect to D and the results

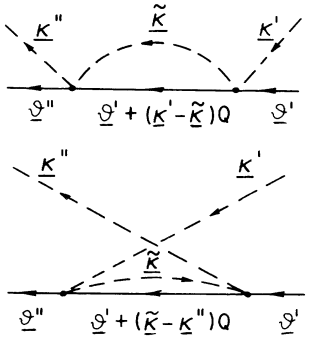

FIG. 2. The two lowest-order vertex corrections. The ingoing (outgoing) momentum of the HP and the direction of the ingoing electron momentum are $\boldsymbol{\theta}'$ and $\boldsymbol{\kappa}'$ ($\boldsymbol{\theta}''$ and $\boldsymbol{\kappa}''$), respectively, and $\boldsymbol{\kappa}$ corresponds to the intermediate state of the electron. The momenta of the HP in the intermediate states are different in these two diagrams.

are

$$dv_f(\theta,\mu)/d\ln D' = v_b^2(\theta+\mu Q) - v_b^2(\theta-\mu Q), \quad (6)$$

$$dv_b(\theta)/d\ln D' = -2v_b(\theta)\{v_f(\theta+\mu Q;\mu) - v_f(\theta-\mu Q;\mu)\}. \quad (7)$$

There are two regions in the scaling: (i) where $v_b(\theta)$ and $v_f(\theta,\mu)$ keep their functional form obtained in lowest order and $v_b \gg |u_b|, |v_f|$; (ii) where their functional forms change and their amplitudes are comparable and exceed the starting value of v_b. In region (i) the right-hand side of Eqs. (6) and (7) can be linearized in v_b and v_f, and the result is

$$dv_f/d\ln D' = -4v_b u_b, \quad (8)$$

$$du_b/d\ln D' = -4v_b v_f \sin Q, \quad (9)$$

with v_b = const. These scaling equations are equivalent to those of the anisotropic antiferromagnetic Kondo problem with the unrenormalized couplings $|J_z| \gg |J_x|$ and $J_y = 0$, which can be solved exactly.[14,16] The energy T_{cr} characterizing the crossover between the two regions is[14]

$$T_{cr} = D(u_b/2v_b \sin^{1/2} Q)^{1/4v_b \sin^{1/2} Q}. \quad (10)$$

In general, the Kondo energy T_K reflects the crossover to the strong-coupling limit. If $4v_b \sin^{1/2} Q \simeq 0.3-1$, then $T_K/T_{cr} < 10$.

The solution of the scaling equations (6) and (7) is schematically depicted in Fig. 3 for the two regions of the scaling ($Q \simeq \pi/2$). In the strong-coupling region (ii), the maximum values of the couplings scale to infinity and the θ dependences keep changing. For $0 < \theta < \pi$ the scaled couplings are always positive.

Concerning the applicability of the model presented, a few remarks must be made. The logarithmic corrections in the scattering amplitude occur in case of arbitrary dimension d. The assumption that there is only a single heavy fermion or boson particle (or hole) can be dropped. In 1D a straightforward calculation shows that the occupation factor for the HP drops out, but the logarithmic behavior remains. Similar behavior is found in second order independently of the dimensionality. Thus, the HP considered may have a Fermi surface. In the case where the HP is an f electron (or d electron), the s-f hybridization must be taken into account as a first step. In this case the on-site Coulomb interaction is very important[13] but that very likely does not block the renormalization described.

Thus, in a large class of HP problems, logarithmic terms of infrared origin can be expected in the scattering amplitude, in spite of the fact that the summation of the leading logarithmic terms is performed only in the case $d = 1$.

The strength of the assisted hopping U is of the order of the spontaneous hopping (tunneling) rate if the height

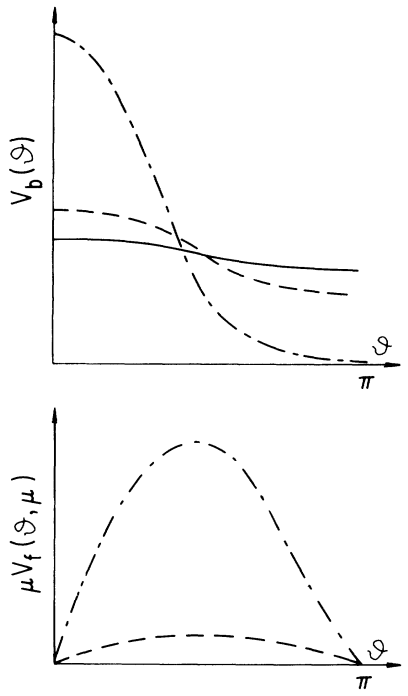

FIG. 3. The couplings of electron backscattering $v_b(\theta)$ and of anomalous forward scattering $v_f(\theta;\mu)$ are shown schematically: initial values by solid line, in regions (i) and (ii) by dashed and dashed-dotted lines, respectively.

of the potential barriers V_B is comparable with the screening strength V'. As for charged HP, $V' \simeq 1$ eV; therefore that condition is satisfied in most of the cases. A typical value of the hopping rate is $t \simeq 10^{-2}$ eV; thus

$$U/4V \sin^{1/2} Q \simeq 10^{-2}-10^{-3} \quad (V \simeq 1 \text{ eV}).$$

With use of $D \simeq 10$ eV, a reasonable value for the crossover energy T_{cr} is obtained if $3V\rho_0 \sin^{1/2} Q \sim 0.5-1$. Thus either the screening strength V or the density of states ρ_0 must be large. It is important that in case of s-f hybridization the HP bandwidth is larger, but that occurs only as the lower cutoff in the logarithmic integrals. As a consequence, the system may not scale to the real strong-coupling limit, and in that case the behavior of the system is only modified by consideration of the coupling U.

If the problem scales to strong coupling, then the large scaled couplings occur in the scaling equation of the HP Green's functions, and the right-hand side of that equation is quadratic in the couplings. The calculation is similar to the case with only screening.[11,12,17] At zero temperature and large enough initial coupling, the bandwidth D' can be scaled to zero. For smaller couplings the scaling is terminated when D' becomes comparable with the renormalized HP bandwidth. The increase of the couplings has two consequences: (i) The bandwidth of the HP is narrowed, and thus the coherent motion of

the HP slows down; (ii) the incoherent contribution due to the assisted transition is, however, enhanced. The band narrowing may be responsible for anomalous low-temperature muon diffusion observed in several metals.[18] Finally, it is worthwhile to mention that in a realistic model for heavy fermions instead of the assisted f-f transition the assisted hopping between d and f levels on neighboring sites must be considered. Such models are the subject of further studies.

Summarizing, the present results with assisted hopping strongly suggest that different physical systems with strong enough screening may scale to strong coupling at low temperature in a manner similar to the antiferromagnetic Kondo problem. The similarity is based on the fact that the electron screening cloud far from the particle (Friedel oscillation) depends on the previous path of the HP, just as the spin polarization of the electrons depends on the history of localized spin in the Kondo problem. This behavior is different from the one shown by HP moving in bosonic environment.

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[1]P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967).

[2]J. Kondo, Physica (Amsterdam) **84B&C**, 40 (1976).

[3]A. Zawadowski, Phys. Rev. Lett. **45**, 211 (1980).

[4]K. Vladár, G. T. Zimányi, and A. Zawadowski, Phys. Rev. Lett. **56**, 286 (1986); A. Muramatsu and F. Guinea, Phys. Rev. Lett. **57**, 2337 (1986).

[5]See, for a review, A. I. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).

[6]See, e.g., A. Schmid, Phys. Rev. Lett. **54**, 1506 (1986); U. Weiss and H. Grabert, Phys. Lett. **108A**, 63 (1985); V. Hakim and V. Ambegaokar, Phys. Rev. A **32**, 423 (1985); M. P. A. Fisher and W. Zwerger, Phys. Rev. B **32**, 6190 (1985).

[7]K. Itai, Phys. Rev. Lett. **58**, 602 (1987).

[8]See, for review, J. Kondo, Physica (Amsterdam) **126B**, 377 (1984).

[9]F. Guinea, Phys. Rev. Lett. **53**, 1268 (1984); F. Sols and F. Guinea, to be published; P. Hedegård and A. O. Caldeira, Phys. Rev. B **35**, 106 (1987).

[10]Yu. Kagan and N. Y. Prokof'ev, Zh. Eksp. Teor. Fiz. **90**, 2176 (1986) [Sov. Phys. JETP **63**, 1276 (1986)].

[11]K. Yamada, A. Sakurai, and N. Takeshige, Prog. Theor. Phys. **70**, 73 (1983); K. Yamada, A. Sakurai, and S. Miyazima, Prog. Theor. Phys. **73**, 1342 (1985); K. Yamada, to be published.

[12]G. T. Zimányi, V. Vladár, and A. Zawadowski, Phys. Rev. B (to be published).

[13]P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Comments Condens. Matter Phys. **12**, 99 (1986).

[14]K. Vladár and A. Zawadowski, Phys. Rev. B **28**, 1564 (1983).

[15]R. Bruinsma and Per Bak, Phys. Rev. Lett. **56**, 420 (1986).

[16]H. Shiba, Prog. Theor. Phys. **43**, 601 (1970).

[17]J. Kondo, Physica (Amsterdam) **123B**, 175 (1984).

[18]See, for a review, J. Kondo, Hyperfine Interact. **31**, 117 (1986), where the anomalous low-temperature behavior is accounted for by an unexplained inhomogeneous level broadening of the muon sites.