Spin-polarized tunneling between strongly correlated systems

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Application of the saddle-point approximation of the slave-boson approach to tunneling between two strongly correlated systems is shown to result in a Bardeen-like formula with renormalized tunneling matrix elements, which generally contain additional angular dependences due to the vector boson field.

Spin-polarized tunneling between two weakly coupled, magnetically ordered systems of noninteracting electrons is described by a Bardeen-like formula,[1] which can be written as[2,3]

$$I=\frac{2\pi e}{\hbar}\int d\varepsilon\ \mathrm{Tr}\{\hat{T}_{RL}\hat{\rho}_L(\varepsilon)\hat{T}_{LR}\hat{\rho}_R(\varepsilon)\}[f_L(\varepsilon)-f_R(\varepsilon)],\tag{1}$$

where $\hat{\rho}_{L,R}(\varepsilon)$ is the local density of states in the left (L) and right (R) systems, $\hat{T}_{RL,LR}$ is the tunneling matrix element between these systems, and $f_{R,L}(\varepsilon)$ are the Fermi distribution functions with the chemical potentials μ_L and μ_R chosen in such a way that $\mu_L-\mu_R=eV$, where V is the applied voltage. The local densities of states for free spin-polarized electrons can be written as follows:[3]

$$\hat{\rho}_{L,R}=\rho_{0L,R}\hat{I}+\rho_{sL,R}\hat{\sigma}\cdot\mathbf{M}_{L,R},\tag{2}$$

where $\rho_{0L,R}$ and $\rho_{sL,R}$ are the spin-independent and spin-dependent parts of the density of states, respectively, and $\mathbf{M}_{L,R}$ is the local magnetization vector. The tunneling matrix element $\hat{T}_{LR,RL}$ is a one-particle hopping integral, which is assumed to be diagonal in spin. Calculation of the trace over the spin indices in Eq. (1) yields[2,3]

$$I=I_0+I_s\mathbf{M}_L\cdot\mathbf{M}_R,\tag{3}$$

$$I_{0,s}=\frac{2\pi e}{\hbar}\int d\varepsilon|T_{RL}|^2\rho_{0L,sL}(\varepsilon)\rho_{0R,sR}(\varepsilon)[f_L(\varepsilon)-f_R(\varepsilon)].\tag{4}$$

The second term in Eq. (3) describes the spin-dependent contribution to the tunneling current, which is sensitive to the relative orientation of the electron spins in the left and right systems. Higher orders of the perturbation theory in the tunneling matrix elements give rise to the terms in the tunneling current which are biquadratic in magnetization.[4]

Equations (2) and (3) contain the equilibrium magnetizations of noninteracting left and right systems, although the tunnel coupling may perturb their values. For example, $\delta\mathbf{M}_L$ is of the order $\propto T_{LR}^2\mathbf{M}_R$, since $T_{LR}^2\mathbf{M}_R$ plays the role of a weak, external, magnetic field that shifts the equilibrium magnetization. The tunnel current is proportional to T_{LR}^2 so that the corrections to the current induced by changes in the magnetization due to tunnel coupling are proportional to T_{LR}^4 and, therefore, are of the next order in small parameter T_{LR}. Thus, for weak tunnel coupling the current has the same structure as in Eq. (3), which contains the equilibrium magnetization of the isolated systems.

Equation (2) was obtained under the assumption that electrons in each system are described by single-particle Hamiltonians. The magnetic ordering, however, arises as a result of the electron-electron interaction; therefore, applicability of Eq. (2) to real interacting systems is questionable. For example, Coulomb interaction can result in separation of the charge and spin degrees of freedom. In the latter case the spinons and holons can be considered as "good" quasiparticles.[5] At the same time, tunneling between two weakly coupled systems involves transfer of a real particle (an electron with its spin and charge), which is a superposition of "good" quasiparticles, rather than an eigenstate of the interacting system.

The goal of this study was to consider the tunneling between two magnetically ordered, strongly correlated systems in the saddle-point approximation of the slave-boson approach.[6]

We assume that the electrons in the L and R systems are described by the Hubbard Hamiltonian[7] (we omit subscripts L and R whenever possible):

$$\hat{H}=\sum_{ij\sigma}t_{ij}\hat{f}^+_{i\sigma}\hat{f}_{j\sigma}+U\sum_i\hat{f}^+_{i\sigma}\hat{f}_{i\sigma}\hat{f}^+_{i-\sigma}\hat{f}_{i-\sigma},\tag{5}$$

where t_{ij} is the hopping integral, $\hat{f}^+_{i\sigma}$ is the electron creation operator, and U is the Coulomb repulsion.

To describe the four atomic states $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$, additional boson fields $\hat{e}$, $\hat{p}_\sigma$, and $\hat{d}$ must be introduced.[6] The physical states in the extended space are obtained by applying new fermionic $\hat{c}^+$ and bosonic $\hat{e}^+$, $\hat{p}^+_\sigma$, $\hat{d}^+$ creation operators to the vacuum state. To preserve the operator equivalence between the original Hamiltonian and the new one that act in the extended space, additional constraints on the Bose and Fermi operators are introduced. The site states are obtained as

$$|0\rangle=\hat{e}^+|\mathrm{vac}\rangle,$$
$$|\sigma\rangle=\hat{c}^+_\sigma(\hat{p}^+_0\hat{I}+\hat{\mathbf{p}}^+\cdot\hat{\sigma})|\mathrm{vac}\rangle,$$
$$|\uparrow\downarrow\rangle=\hat{d}^+\hat{c}^+_\uparrow\hat{c}^+_\downarrow|\mathrm{vac}\rangle.\tag{6}$$

The singly occupied states $|\sigma\rangle$ possess spin-1/2, which results from the addition of the vector boson (spin-1) $\hat{\mathbf{p}}^+$, and a new spin-1/2 fermion $\hat{c}_\sigma^+$. Equation (6) for a singly occupied site follows from the angular momentum addition formula (see, e.g., Ref. 8):

$$\left|\frac{1}{2},M\right\rangle=\sqrt{\frac{3/2-M}{3}}\left|\frac{1}{2}\right\rangle\left|M-\frac{1}{2}\right\rangle+\sqrt{\frac{3/2+M}{3}}\left|-\frac{1}{2}\right\rangle\left|M+\frac{1}{2}\right\rangle, \qquad (7)$$

where $|\pm 1/2\rangle$ are the fermion states with spin projections $\pm 1/2$, and $|M\pm 1/2\rangle$ are the boson states with spin projections $0,\pm 1$. The original fermionic operators $\hat{f}_{\uparrow\downarrow}^+$ can be represented by combinations of new fermionic and bosonic operators with the moment projection $M=0,\pm 1$ ($\hat{p}_0^+$, $\hat{p}_{\pm 1}^+$, respectively):

$$\hat{f}_\uparrow^+=-\hat{c}_\uparrow^+\hat{p}_0^++\sqrt{2}\hat{c}_\downarrow^+\hat{p}_{+1}^+,$$
$$\hat{f}_\downarrow^+=\hat{c}_\downarrow^+\hat{p}_0^+-\sqrt{2}\hat{c}_\uparrow^+\hat{p}_{-1}^+. \qquad (8)$$

Expressing the operators with definite moment projections in terms of their Cartesian counterparts,[9] we obtain

$$\hat{p}_{+1}^+=-\frac{1}{\sqrt{2}}(\hat{p}_x^++i\hat{p}_y^+),\quad \hat{p}_0^+=\hat{p}_z^+,$$
$$\hat{p}_{-1}^+=\frac{1}{\sqrt{2}}(\hat{p}_x^+-i\hat{p}_y^+). \qquad (9)$$

Multiplying both sides of Eq. (9) by -1, we obtain

$$(\hat{f}_\uparrow^+,\hat{f}_\downarrow^+)=(\hat{c}_\uparrow^+,\hat{c}_\downarrow^+)\begin{pmatrix}\hat{p}_z^+ & \hat{p}_x^+-i\hat{p}_y^+\\ \hat{p}_x^++i\hat{p}_y^+ & -\hat{p}_z^+\end{pmatrix}. \qquad (10)$$

Adding a spinless boson field $\hat{p}_0^+$, which transforms as a scalar and taking into account Eq. (10), we obtain Eq. (6). Expressions (6) were derived in Ref. 7 in a less transparent way. Thus, the spin of new fermions in the slave-boson approach turns out to be rigidly coupled to the vector boson moment.

The operator equivalence of the new Hamiltonian acting in the extended space is preserved by imposing the following constraints:

Completeness

$$\hat{Q}=\hat{e}^+\hat{e}+\hat{p}_0^+\hat{p}_0+\hat{\mathbf{p}}^+\cdot\hat{\mathbf{p}}+\hat{d}^+\hat{d}=1. \qquad (11)$$

Equivalence of the two ways of counting fermions

$$\hat{L}_0=\hat{p}_0^+\hat{p}_0+\hat{\mathbf{p}}^+\cdot\hat{\mathbf{p}}+2\cdot\hat{d}^+\hat{d}-\sum_\sigma \hat{c}_\sigma^+\hat{c}_\sigma=0. \qquad (12)$$

Total spin conservation

$$\hat{\mathbf{L}}=\hat{p}_0^+\hat{\mathbf{p}}+\hat{p}_0\hat{\mathbf{p}}^++i[\hat{\mathbf{p}}^+\times\hat{\mathbf{p}}]-\sum_{\sigma\sigma'}\hat{c}_\sigma^+\boldsymbol{\sigma}_{\sigma\sigma'}\hat{c}_{\sigma'}=0. \qquad (13)$$

Introduction of the Bose fields allows linearization of the Coulomb interaction term so that in the new representation the Hamiltonian becomes[6,7]

$$\hat{H}=\sum_{\substack{ij\\ \sigma\sigma'\sigma_1}} t_{ij}(\hat{c}_{i\sigma}^+\hat{z}_{i\sigma\sigma_1}^+)(\hat{z}_{j\sigma_1\sigma'}\hat{c}_{j\sigma'})+U\sum_i \hat{d}_i^+\hat{d}_i. \qquad (14)$$

The operators $\hat{z}$ in the hopping matrix elements are introduced to preserve the Hamiltonian equivalence and describe the following processes: (empty site→singly occupied site), (doubly occupied site→singly occupied site with time-reversed spin); explicitly they are given by the formulas

$$\hat{z}=[(1-\hat{d}^+\hat{d})\hat{I}-\hat{p}^+\hat{p}]^{-1/2}(\hat{e}^+\hat{p}+\hat{\tilde{p}}^+\hat{d})[(1-\hat{e}^+\hat{e})\hat{I}-\hat{\tilde{p}}^+\hat{\tilde{p}}]^{-1/2}. \qquad (15)$$

Constraints (11–13) are accounted for by introducing into the Hamiltonian the Lagrange factors

$$\hat{H}=\hat{H}'-\sum_i \lambda_i^{(1)}(\hat{Q}_i-1)+\sum_i(\lambda_{i0}^{(2)}\hat{L}_{i0}+\lambda_i^{(2)}\cdot\hat{\mathbf{L}}_i). \qquad (16)$$

The partition function is calculated by performing functional integration over the fermionic fields which appear in the Hamiltonian only bilinearly. Integration over the bosonic fields is carried out in the saddle-point approximation (assuming that the bosonic fields are time-independent and can be in fact replaced by their values at the saddle point).

Our task is to calculate the tunnel current between the two magnetically ordered systems (L and R). The tunneling Hamiltonian can be written as follows:

$$\hat{T}=\sum_{ij\sigma}(T_{LRij}\hat{f}_{Li\sigma}^+\hat{f}_{Rj\sigma}+\hat{f}_{Rj\sigma}^+\hat{f}_{Li\sigma}T_{RLji}), \qquad (17)$$

where T_{LRij} is the hopping integral which couples the sites that belong to the two systems. The tunnel current operator in the original representation has a standard form

$$\hat{I}(t)=\frac{ie}{\hbar}\sum_{ij\sigma}(T_{LRij}\hat{f}_{Li\sigma}^+(t)\hat{f}_{Rj\sigma}(t)-\hat{f}_{Rj\sigma}^+(t)\hat{f}_{Li\sigma}(t)T_{RLji}). \qquad (18)$$

In the new representation it transforms to

$$\hat{I}(t)=\frac{ie}{\hbar}\sum_{\substack{ij\\ \sigma\sigma'\sigma_1}}[T_{LRij}(\hat{c}_{Li\sigma}^+(t)\hat{z}_{Li\sigma\sigma_1}^+(t))\times(\hat{z}_{Rj\sigma_1\sigma'}(t)\hat{c}_{Rj\sigma'}(t))-\text{H.c.}]. \qquad (19)$$

The tunnel current itself can be calculated by evaluating the average of the operator (19), employing the following functional integral representation:

$$I=\int D\hat{e}^+D\hat{e}D\hat{p}^+\ldots D\hat{\lambda}^{(2)}D\hat{c}^+D\hat{c}\hat{I}(t)\times\exp\left\{-\int_p dt[\hat{L}_L(t)+\hat{L}_R(t)+\hat{T}(t)]\right\}, \qquad (20)$$

where $\hat{L}_{L,R}$ are the Lagrangians of the left (L) and right (R) systems, and $\hat{T}$ is the tunneling Hamiltonian in the slave-boson representation. Time integration in the exponential is performed over the closed-path contour.[10–14]

After the exponential is expanded to the first order in $\hat{T}$, the operators which are related to the left and right systems can be averaged independently, yielding

$$I=\frac{e}{\hbar}\int_p dt_1\left(\sum_{\substack{iji'j'\\ \sigma_1\sigma_2\sigma_3\sigma_4\\ \sigma\sigma'}} T_{LRij}\langle\hat{c}^+_{Li\sigma}(t)\hat{z}^+_{Li\sigma\sigma_1}(t)\hat{z}_{Li'\sigma_3\sigma_4}\right.$$

$$\times(t_1)\hat{c}_{Li'\sigma_4}(t_1)\rangle T_{RLj'i'}\langle\hat{z}_{Rj\sigma_1\sigma'}(t)\hat{c}_{Rj\sigma'}(t)\hat{c}^+_{Rj'\sigma_2}$$

$$\times(t_1)\hat{z}^+_{Rj'\sigma_2\sigma_3}(t_1)\rangle-\text{H.c.}). \quad (21)$$

Equation (21) can be transformed to

$$I=\frac{e}{\hbar}\int_{-\infty}^{\infty} dt_1[\hat{T}_{LR}\hat{z}_L\hat{g}^<_L(t-t_1)\hat{z}^+_L\hat{T}_{RL}\hat{z}_R\hat{g}^>_R(t_1-t)\hat{z}^+_R$$

$$-\text{H.c.}]. \quad (22)$$

In deriving the last formula we replaced the bosonic fields by their saddle-point values and introduced the matrix notation

$$\hat{g}^>_R(t-t_1)=\langle\hat{c}_{Rj\sigma'}(t)\hat{c}^+_{Rj'\sigma_2}\rangle,$$

$$\hat{g}^<_R(t-t_1)=-\langle\hat{c}^+_{Rj'\sigma_2}(t_1)\hat{c}_{Rj\sigma'}\rangle, \quad (23)$$

and similarly for $\hat{g}^{<,>}_L$. The retarded Green's function (GF) is the inverse matrix of the Hamiltonian (14), where the bosonic operators are replaced by their saddle-point values, so that

$$\hat{g}^r(\varepsilon)=(\varepsilon-\hat{H}+i0)^{-1}. \quad (24)$$

After the Fourier transform, the Keldysh GF are defined as

$$\hat{g}^{<,>}(\varepsilon)=-\frac{1}{\pi}\,\text{Im}\{\hat{g}^r(\varepsilon)\}\begin{cases} f(\varepsilon)\\ f(\varepsilon)-1\end{cases}. \quad (25)$$

The retarded GF $\hat{g}^r$ is a linear combination of the Pauli matrices, since $\hat{H}$ contains the terms of the $\hat{z}^+_i\hat{z}_j$ type in the hopping integrals

$$\hat{z}^+_i\hat{z}_j=\hat{I}(P^+_{0i}P_{0j}+\mathbf{P}^+_i\cdot\mathbf{P}_j)+\boldsymbol{\sigma}\cdot\mathbf{M}_{ij},$$

$$P_{i0}=\text{Tr}\{\hat{I}\hat{z}^+_i\},$$

$$\mathbf{P}_i=\text{Tr}\{\boldsymbol{\sigma}\hat{z}^+_i\},$$

$$\mathbf{M}_{ij}=\mathbf{P}^+_iP_{0j}+\mathbf{P}_jP^+_{0i}+i[\mathbf{P}^+_i\times\mathbf{P}_j]. \quad (26)$$

If the subscripts i and j refer to the same site, the vector $\mathbf{M}_{ij}$ has the meaning of magnetization. According to Eqs. (24)–(26), the Keldysh GF can be represented in the form

$$\hat{g}^{<,>}_{L,R}(\varepsilon)=(\hat{\rho}_{0L,R}(\varepsilon)+\hat{\rho}_{sL,R}(\varepsilon)\boldsymbol{\sigma}\cdot\hat{\mathbf{M}}_{L,R})\begin{cases} f_{L,R}(\varepsilon)\\ f_{L,R}(\varepsilon)-1,\end{cases}$$

$$\hat{\mathbf{M}}_{L,R}=\{\mathbf{M}_{L,Rij}\}. \quad (27)$$

Finally, taking into account Eqs. (26) and (27), we obtain for the tunnel current a formula similar to that for noninteracting electrons, but with spin-dependent tunneling matrix elements:

$$I=\frac{2\pi e}{\hbar}\int d\varepsilon\,\text{Tr}\{\tilde{\hat{T}}_{RL}\hat{\rho}_L(\varepsilon)\tilde{\hat{T}}_{LR}\hat{\rho}_R(\varepsilon)\}[f_L(\varepsilon)-f_R(\varepsilon)], \quad (28)$$

where

$$\tilde{\hat{T}}_{LR,RL}=\hat{z}^+_{R,L}\hat{T}_{LR,RL}\hat{z}_{L,R}.$$

Physically, the tunneling matrix element renormalization can be explained in the following way. In the slave-boson approach (in the saddle-point approximation) the new fermions are the free quasiparticles (eigenstates of the interacting system). Bosonic fields play the role of a spin-dependent potential, where the spin of a new fermion is rigidly coupled to the vector boson spin. However, tunneling involves transfer of a real particle (electron with its spin and charge), which is a superposition of a new fermion and vector boson, rather than an eigenstate of the interacting system. The original fermion spin can also be obtained by adding the moments of a new fermion and the vector boson, so that tunneling results in the transfer of the vector boson spin together with the spin of a new fermion, which is manifested in the tunneling matrix element renormalization.

For ferro- and antiferromagnetic ordering the vector $\mathbf{P}$ is real. If the magnetization direction does not depend on the site, then $\mathbf{M}\|\mathbf{P}$. Expanding the double vector products in Eq. (28), we find that under these conditions the tunnel current structure is similar to that for free electrons; i.e., the spin-dependent contribution to the tunnel current is proportional to the scalar product of magnetizations $I_s\propto\mathbf{M}_L\cdot\mathbf{M}_R$.

For a nonuniform magnetization distribution, the spin-dependent contribution in the case of noninteracting electrons due to tunneling from the site Li to site Rj is $I_{sj}\propto\Sigma_i a(i,j)\mathbf{M}_{Li}\cdot\mathbf{M}_{Rj}$. Here the amplitude $a(i,j)$ is independent of the magnetization direction. For the interacting electrons the amplitude contains an angular dependence which does not reduce to the scalar product of magnetizations.

The physics beyond the tunneling matrix element renormalization can qualitatively be understood in the following way. Let us first consider the origin of the scalar product of magnetizations which appears in the tunneling current between the two spin-polarized free-fermion systems. Different orientations of magnetization in the left and right systems actually correspond to different choices of the spin quantization axes in these systems. Let the quantization axes z and z' (in the L and R systems, respectively) be directed along the magnetization directions, where the angle between them is θ. The fermion states in the L system are described by the spinor

$$\hat{\Psi}_L=\begin{pmatrix}\Psi_{L\uparrow}\\ \Psi_{L\downarrow}\end{pmatrix},$$

which is quantized with respect to the z axis. Similarly, in the right system the states are described by the spinor

$$\hat{\Psi}'_R=\begin{pmatrix}\Psi'_{R\uparrow}\\ \Psi'_{R\downarrow}\end{pmatrix},$$

where z' is the quantization axis.

The tunneling current is proportional to the absolute value of the square of the scalar product of these spinors

$$I\propto\text{Sp}|\hat{\Psi}^+_L\hat{\Psi}_R|^2, \quad (29)$$

where the trace is over the spin indices (the hopping integrals themselves do not depend on the spin). The spinors that appear in Eq. (29) should be brought to the common quantization axis, e.g., the axis in the left system. In the latter case the states in the right system, which are quantized along the z' axis, should be expressed in terms of the states quantized along the z axis. This transformation is performed with the spin-1/2 rotation matrix,

$$\hat{\Psi}_R=\hat{D}_{1/2}(\theta)\hat{\Psi}'_R. \qquad (30)$$

For simplicity we assume that both z' and z lie in the same plane, which is normal to the interface between the systems (one-dimensional tunneling). In the latter case the rotation matrix is known to have the form

$$\hat{D}_{1/2}(\theta)=\begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}. \qquad (31)$$

According to Eq. (29), the spin-dependent contribution to the tunneling current has the components $\cos(\theta)(|\Psi_{L\uparrow}\Psi_{R\uparrow}|^2+|\Psi_{L\downarrow}\Psi_{R\downarrow}|^2)$ [we used the known relation $\cos(\theta/2)^2=(1+\cos(\theta))/2$]. The latter term is exactly the scalar product of the magnetizations.

Physically, when tunneling occurs between the two systems with different magnetization directions the scalar product appears because one should express the states which are quantized along the original quantization axis in terms of the states with the definite angular moment projection onto the z axis of a new coordinate system which serves as the common quantization axis.

For the interacting fermions the original fermion states (which are no longer the system's eigenstates) are in fact the superpositions of the spin-1 vector boson field and the new spin-1/2 fermions. Calculating the tunneling current, we should bring to the common quantization axis not only the fermionic, but also the bosonic degrees of freedom. However, the bosonic degrees of freedom posses different transformation properties with respect to spatial rotation (described by the spin-1 rotation matrix). This consideration results in an additional angular dependence of the expression for the tunneling current, which in the saddle-point approximation reduces to the tunneling matrix element renormalization.

The case of the complex vector **P** corresponds to the spin-flux states and requires special treatment.

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