

Spatial Correlations around a Kondo Impurity

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We present a method for calculating zero-frequency, spatially varying response and correlation functions around a magnetic impurity in metals. We illustrate the procedure, which involves a combination of perturbative scaling and nonperturbative renormalization-group methods for the spin- $\frac{1}{2}$ Kondo impurity. We explain the factorization of the temperature and spatial dependence of the Knight shift observed in NMR experiments.

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In this Letter we use perturbative, thermodynamic scaling theory¹ to develop a method for calculating zero-frequency, spatially varying response functions and correlation functions involving spin and charge densities around magnetic impurities in nonmagnetic metals.² Such functions are experimentally accessible. For example, spin-density response functions at zero frequency have been measured³ from the new satellite NMR lines that arise as a result of the extra Knight shifts induced in the host metal (e.g., Cu) by magnetic impurities (Cr, Mn, or Fe). A notable feature of the experimental data is the factorization of the spatial and temperature dependence of such response functions (see below), notwithstanding the Kondo effect. We employ our method to explain⁴ this factorization in the context of the spin- $\frac{1}{2}$ Kondo Hamiltonian. We also show that this factorization can only be approximate and discuss the accuracy with which it is obeyed.

Consider the spin- $\frac{1}{2}$ Kondo Hamiltonian⁵ $H_K(D_0)$ given by

$$H_K(D_0) = H_{e1}(D_0) - J_0 \mathbf{S} \cdot \mathbf{s}(\mathbf{0}), \quad (1)$$

where the first term describes a band of conduction electrons with bandwidth $2D_0$, \mathbf{S} is a spin- $\frac{1}{2}$ operator representing the impurity at the origin, and $\mathbf{s}(\mathbf{0})$ is the conduction-electron spin density at the impurity.

We will focus on the zero-frequency response function $C(\mathbf{r}, T)$ given by⁶

$$C(\mathbf{r}, T) \equiv \langle \langle s_z(\mathbf{r}); g_d S_z + g_e s_z \rangle \rangle_{H_K(D_0)}, \quad (2)$$

where g_d and g_e are the impurity and electron g factors, $s_z(\mathbf{r})$ denotes the conduction-electron spin density at \mathbf{r} , and s_z denotes the total spin density of the conduction electrons. $C(\mathbf{r}, T)$ is directly related to the extra Knight shift for a host nucleus at \mathbf{r} . Let K denote the Knight shift of the pure host,⁷ i.e., it determines the position of

the main resonance line due to the Cu nuclei far away from the impurity. Cu nuclei near a magnetic impurity produce weak resonances, called satellites, in the tail of the main resonance, with a Knight shift given by $K + \Delta K$. One has^{3,4,7}

$$\Delta K = C(\mathbf{r}, T) - K. \quad (3)$$

For short distances ($k_F |\mathbf{r}| < 10$) the behavior of $C(\mathbf{r}, T)$ depends on the details of the band structure of the host metal. For simplicity, we will assume an isotropic band with a constant density of states ρ_0 cut off at $\pm D_0$ about the Fermi level, and a linear dispersion relation $k_\varepsilon = k_F + \varepsilon/v_F$, where v_F is the Fermi velocity.⁸

Our method for calculating response functions such as $C(\mathbf{r}, T)$, in outline, is as follows: We employ the thermodynamic scaling procedure to eliminate iteratively the high-energy (near the band edge) electron and hole degrees of freedom and reduce the cutoff from D_0 to D , but in such a way as to preserve the free energy. This generates an effective Hamiltonian $H(D)$, and correlation functions evaluated with $H_K(D_0)$ are linear combinations of correlation functions evaluated with $H_K(D)$. When the bandwidth is D the most localized state that can be formed at the origin has a spatial width $O(v_F/D)$ which is much larger than r if $rD/v_F \ll 1$. Then the correlation functions evaluated with $H_K(D)$ reduce to local correlation functions. Hence, we get a result of the form

$$C(\mathbf{r}, T) = \sum_i f_i(r) C_i(T), \quad (4)$$

i.e., the correlation or response function of interest is a sum of terms which are products of functions of r (which are essentially independent of T) multiplied by local correlation or response functions C_i , involving operators with the same symmetries as C , evaluated with $H_K(D)$. These local correlation functions contain essentially all

the temperature dependence. Depending on the quantity at hand, one or more of these terms can dominate. We show that in the case of the Knight shift, ΔK is dominated by a single product, and hence it factorizes; if no single term dominates, factorization fails to occur. Furthermore, we show that the temperature-dependent part of the dominant term in ΔK is proportional to the susceptibility. We emphasize that even though perturbative methods have been employed, the factorization when it occurs is valid at all low T . This is because the condition $rD/v_F \ll 1$ can be satisfied for D in a regime in which perturbative scaling and the form in Eq. (4) are valid, and given factorization at that stage it persists for all

lower T . However, the T -dependent factors may have to be computed by nonperturbative methods such as the Wilson numerical renormalization-group method.⁹

We now present some more details of our scheme for computing $C(\mathbf{r}, T)$. The response function $C(\mathbf{r}, T)$ can be expressed as a zero-field second derivative of the free energy F with respect to h and h_1 of the following Hamiltonian:

$$H(D_0) = H_K(D_0) - h(g_d S_z + g_e s_z) - h_1 s_z(\mathbf{r}). \quad (5)$$

We label the conduction-electron operators by their energy ε and $\hat{\mathbf{k}}$ instead of \mathbf{k} and thus write the Hamiltonian as

$$H(D_0) = \int_{\varepsilon \hat{\mathbf{k}} \mu}^{D_0} \varepsilon c_{\varepsilon \hat{\mathbf{k}} \mu}^\dagger c_{\varepsilon \hat{\mathbf{k}} \mu} - \frac{1}{2} J_0 \mathbf{S} \cdot [\psi_\mu^\dagger(\mathbf{0}) \boldsymbol{\sigma}_{\mu\mu'} \psi_{\mu'}(\mathbf{0})] - h g_d S_z - h g_e s_z - \frac{1}{2} h_1 \psi_\mu^\dagger(\mathbf{r}) \boldsymbol{\sigma}_{\mu\mu'} \psi_{\mu'}(\mathbf{r}), \quad (6)$$

where

$$\psi_\mu^\dagger(\mathbf{r}) = \int_{\varepsilon}^{D_0} \int_{\hat{\mathbf{k}}} c_{\varepsilon \hat{\mathbf{k}} \mu}^\dagger e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (7a)$$

$$\int_{\varepsilon}^{D_0} \int_{\hat{\mathbf{k}}} = \int_{-D_0}^{D_0} \rho_0 d\varepsilon \int d\Omega_{\hat{\mathbf{k}}} / 4\pi. \quad (7b)$$

Our procedure involves two steps. First, we derive the effective Hamiltonian $H(D)$ with bandwidth D . Next we relate $C(\mathbf{r}, T)$ evaluated with $H(D_0)$ to response functions evaluated with $H(D)$.

In the process of perturbative scaling the Hamiltonian evolves from $H(D_0)$ to a D -dependent effective Hamiltonian $H(D)$ with new couplings but so as to preserve the free energy to terms $O(\exp(-D/T))$. To order h , h_1 , and hh_1 , at the level of *second-order* scaling, the effective Hamiltonian assumes the following form¹⁰:

$$\begin{aligned} H(D) = & \int_{\varepsilon} \int_{\hat{\mathbf{k}} \mu} [\varepsilon c_{\varepsilon \hat{\mathbf{k}} \mu}^\dagger c_{\varepsilon \hat{\mathbf{k}} \mu}] - \frac{1}{2} J(D) \mathbf{S} \cdot \psi(\mathbf{0}) \boldsymbol{\sigma} \psi(\mathbf{0}) + E_0 + [-\rho_0 g_e / 2 + E_1] h h_1 + S_z [U_0 h + U_1(r, D) h_1 + U_2(r, D) h h_1] \\ & + h_1 \{ K_1(r, D) S_z \psi^\dagger(\mathbf{0}) \psi(\mathbf{0}) - \frac{1}{2} J_1(r, D) \psi^\dagger(\mathbf{0}) \sigma_z \psi(\mathbf{0}) - \frac{1}{2} K_t(r, D) S_z [\psi^\dagger(\mathbf{r}) \psi(\mathbf{0}) + \psi^\dagger(\mathbf{0}) \psi(\mathbf{r})] \\ & - \frac{1}{2} J_x(r, D) i \varepsilon^{mn3} S_m [\psi^\dagger(\mathbf{r}) \sigma_n \psi(\mathbf{0}) - \psi^\dagger(\mathbf{0}) \sigma_n \psi(\mathbf{r})] - \frac{1}{2} \psi^\dagger(\mathbf{r}) \sigma_z \psi(\mathbf{r}) \}. \quad (8) \end{aligned}$$

Here $J(D)$ is the scaled, effective J determined by

$$D dJ/dD = \rho_0 J^2(D). \quad (9a)$$

The recursion relations for the most important of these couplings are

$$-D dK_t/dD = -\rho_0 J J_x + \frac{1}{2} \rho_0 J (\phi_D - \phi_{-D}), \quad (9b)$$

$$-D dJ_x/dD = -\frac{1}{2} \rho_0 (J J_x + J K_t) + \frac{1}{2} \rho_0 J (\phi_D - \phi_{-D}), \quad (9c)$$

$$-D dJ_1/dD = -\frac{1}{2} \rho_0 (\phi_D - \phi_{-D}) (J J_x - \frac{1}{2} J K_t), \quad (9d)$$

$$dU_1/dD = \rho_0^2 \int_0^D d\varepsilon / D + \varepsilon [2J_1 J + J J_x (\phi_D + \phi_\varepsilon - \phi_{-D} - \phi_{-\varepsilon}) + J (\phi_D \phi_{-\varepsilon} + \phi_{-D} \phi_\varepsilon)], \quad (9e)$$

where

$$\phi_D = \sin k_D r / k_D r, \quad k_{\pm D} = k_F \pm D / v_F.$$

The initial conditions for solving (9a)–(9e) are $J(D_0) = J_0$, $U_0 = -[g_d + g_e (\rho_0 J_0)^2 (\ln 2) / 4]$, all other coupling constants zero. It is through ϕ_D that the coupling con-

stants develop their r dependence. The recursion relation for E_1 is complicated and will not be needed in detail.

Since the scaling procedure preserves the free energy F , we can calculate $C = -\partial^2 F / \partial h \partial h_1$ using $H(D)$ given by Eq. (8) instead of $H(D_0)$. Since the original Hamil-

tonian is spherically symmetric we perform an angular average over \hat{r} and obtain $C(r, T)$. We assume that the bandwidth D has been reduced so that $rD/v_F \ll 1$ for the r 's we are interested in. [$rD/v_F = k_{FR}(D/2D_0) \ll 1$ is easily satisfied¹¹ for $k_{FR} \lesssim 10$ if $D = 10^{-2}D_0$. If, for example, $T, T_K \sim 10^{-3}D_0$ the scaling relations are still valid.] Hence, we can replace $k_e r$ by k_{FR} and consequently $\psi(r)$ by $(\text{sink}_{FR}/k_{FR})\psi(0) = \phi_F\psi(0)$. We conclude that

$$C(r, T) - \frac{1}{2} g_e \rho_0 = -E_1 + U_0 [U_1 \langle \langle S_z; S_z \rangle \rangle_{H_K(D)} + (K_1 \phi_F - K_1) \langle \langle S_z; S_z \psi^\dagger(0) \psi(0) \rangle \rangle_{H_K(D)} + \frac{1}{2} (J_1 + \phi_F^2) \langle \langle S_z; \psi^\dagger(0) \sigma_z \psi(0) \rangle \rangle_{H_K(D)}]. \quad (10)$$

Equation (10) exemplifies the result stated earlier [Eq. (4)]. We now argue that the second term in the sum dominates the other term, and, hence, $\Delta K/K$ factorizes. First with the use of the recursion relations for E_1 and U_1 it is straightforward (though tedious) to show that the constant term E is down by a factor of $\max[(T/D_0)\ln(D_0/D), (T_K/D_0)\ln(D_0/D)]$ compared to the second term. This factor is at most a few percent for reasonable values of T . Next particle-hole symmetry can be invoked to show that the third term vanishes. Third, the last term can be neglected on the basis of the general grounds that terms with larger numbers of electron operators will be down by factors of D/D_0 , one for each pair of electron operators. To see this note that $\psi(0)$ as defined by (7a) contains only energies less than D and is not normalized. Let $\tilde{\psi}_D(0) = (2\rho_0 D)^{-1/2} \psi_D(0)$ be the normalized annihilation operator at the origin, where we have added a subscript to emphasize that the operators refer to a reduced bandwidth D . Thus the last term is proportional to $(D/D_0) \langle \langle O_3 \rangle \rangle$, where

$$\langle \langle O_3 \rangle \rangle \equiv \langle \langle S_z; \tilde{\psi}_D^\dagger(0) \sigma_z \tilde{\psi}_D(0) \rangle \rangle_{H_K}.$$

We expect that the last term is down by D/D_0 and can

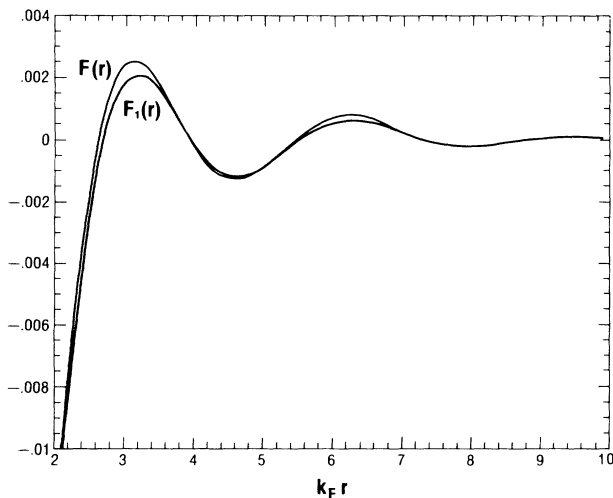


FIG. 1. Spatial dependence of the extra Knight shift $F(r)$ given in Eq. (11). F_1 is the first-order (in J_0) approximation. $F(r)$ includes higher-order contributions. The calculations were performed for $\rho_0 J_0 = -0.1$. The ordinate is in units of $|U_0|$ defined in the text.

be neglected. We have confirmed this by explicitly calculating $\langle \langle O_3 \rangle \rangle$ with the use of the Wilson renormalization-group method, thus providing the first nonperturbative calculation of this response function. Finally we have¹²

$$C(r, T) - \frac{1}{2} g_e \rho_0 = U_0 U_1 \langle \langle S_z; S_z \rangle \rangle = F(r) \chi(T). \quad (11)$$

We have computed $F(r)$ from the recursion relations for U_0 and U_1 ; it is displayed in Fig. 1. We denote $F(r)$ evaluated to first order in J_0 by F_1 ; this is essentially of the Ruderman-Kittel-Kasuya-Yosida form except for a change of sign. The other terms which account for part of the $O(J^2)$ contributions, as seen from Fig. 1, are important only at the quantitative level ($\sim 10\%$). Thus we have shown that the experimental observation of factorization can be understood from first principles for temperatures $T \lesssim 10T_K$. As discussed earlier this is valid only if $v_F/r \gg (T, T_K)$. Also, factorization obtains only approximately, only to the extent that one of the terms in Eq. (10) dominates. Nonperturbative methods⁹ can be used to compute the deviations from factorization as well, when they are important.

We have also worked out the charge density and $\langle \mathbf{s}(r) \cdot \mathbf{S} \rangle$ for the Kondo problem and extended our method to the Anderson model¹³ which includes spin and charge fluctuations. These will be reported elsewhere. The extension of the perturbative part of the calculation to a realistic model⁴ with higher spin can be performed and is under investigation.

In summary, we have developed a procedure for calculating zero-frequency response functions and correlation functions for magnetic impurities in metals. The method uses a combination of perturbative scaling that extracts the spatial dependence and nonperturbative methods such as the Wilson renormalization-group technique to calculate local correlation functions and extract the T dependence. We have used it to demonstrate factorization of the Knight shift observed experimentally.

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⁶We have employed standard notation (apart from a sign) for $\langle\langle A;B \rangle\rangle$. See D. N. Zubarev, Usp. Fiz. Nauk. **71**, 71 (1960) [Sov. Phys. Usp. **3**, 320 (1960)].

⁷Note that $K = \langle\langle s_z(\mathbf{r}); g_e s_z \rangle\rangle_{H_0}$, which is the Pauli susceptibility of the conduction electrons, and is simply $\rho_0 g_e / 2$.

⁸These two features are not fully consistent since $\rho(\epsilon)$

$= k^2 (dk/d\epsilon) / 2\pi^2$. However, this is unimportant. See, e.g., C. Jayaprakash, H. R. Krishna-Murthy, and J. W. Wilkins, Phys. Rev. Lett. **47**, 737 (1981).

⁹See Wilson, Ref. 5.

¹⁰The term $-hg_e s_z$ in Eq. (6) leads to different densities of states for up (+) and down (-) spins: $\rho_{\pm}(\epsilon) = \rho_0$ for ϵ in $[-D_0 \mp hg_e/2, D_0 \mp hg_e/2]$. We have integrated out the asymmetric part of the high energies to obtain a band with $\rho_{\pm} = \rho_0$ for ϵ in $[-\tilde{D}_0, \tilde{D}_0]$ with $\tilde{D}_0 = D_0 - hg_e/2$ and an initial Hamiltonian

$$\tilde{H}(\tilde{D}_0) = H_K(\tilde{D}_0) + U_0 h S_z - (\rho_0 g_e / 2) h h_1 - h_1 s_z(\mathbf{r})$$

Further scaling leads to $H(D)$ in Eq. (8).

¹¹In the experiments, only satellites corresponding to the first four or five neighbors are observable.

¹²We have tacitly ignored irrelevant operators. It is easy to establish that their contributions are $O(J\delta)$ and they give small contributions to $F(r)$. Also they can contribute temperature dependence, but this is very weak, $O(T/D)$.

¹³In the Anderson model, H. Ishii [Prog. Theor. Phys. **55**, 1373 (1976)] has argued that at $T=0$, the conduction-electron spin polarization $\langle s_z(r) \rangle$ is proportional to $\chi f(r)$ for large r . For small r , he believes that $f(r)$ has the Ruderman-Kittel-Kasuya-Yosida form.