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Spinless impurities and Kondo-like behavior in strongly correlated electron systems

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We investigate magnetic properties induced by a spinless impurity in strongly correlated electron systems, i.e., the Hubbard model in spatial dimension $D=1, 2$, and 3 . For the one-dimensional (1D) system exploiting the Bethe ansatz exact solution we find that the spin susceptibility and the local density of states in the vicinity of a spinless impurity show divergent behaviors. The results imply that the induced local moment is not completely quenched at any finite temperatures. On the other hand, the spin lattice relaxation rate obtained by bosonization and boundary conformal field theory satisfies a relation analogous to the Korringa law, $1/T_1 T \sim \chi^2$. In the 2D and 3D systems, the analysis based upon the antiferromagnetically correlated Fermi liquid theory reveals that the antiferromagnetic spin fluctuation developed in the bulk is much suppressed in the vicinity of a spinless impurity, and thus magnetic properties are governed by the induced local moment, which leads to the Korringa law of $1/T_1$.

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I. INTRODUCTION

Recently, magnetic properties induced by spinless impurities in correlated electron systems have attracted much interest.¹⁻⁶ Especially, to probe antiferromagnetic correlations of high- T_c cuprates the substitution of Cu sites with nonmagnetic impurities such as Zn, Al, and Li has been studied experimentally.¹⁻⁴ According to NMR experiments, it was found that the substitution with spinless impurities induces local moments in the vicinity of impurities, which also show Kondo-like behaviors. For instance, the spin susceptibility in the vicinity of an impurity shows a temperature dependence like $\sim 1/(T+T_K)$, which implies the existence of the characteristic energy scale T_K analogous to the Kondo temperature.³ Moreover, the spin-lattice relaxation rate $1/T_1$ shows Korringa-like behaviors, $1/T_1 T \propto K^2$, for $T < T_K$.⁴ Here K is the Knight shift. It is noted that in the vicinity of a spinless impurity the antiferromagnetic spin correlation which is developed in the bulk is much suppressed, and the magnetic correlation is dominated by the induced local moment. From theoretical points of view, it is nontrivial how this induced local moment governs the magnetic properties around an impurity, suppressing the antiferromagnetic correlation. In this paper, we shall deal with this issue. Although the experiments are carried out for high- T_c cuprates which are essentially quasi-two-dimensional (quasi-2D) systems, it is expected that such effects may depend on the lattice structure and the dimensionality. Thus, we consider Hubbard models with a spinless impurity in spatial dimension $D=1, 2$, and 3 to investigate how the dimensionality affects the induced magnetic properties. For $D=1$, the effects of a spinless impurity are incorporated into an open boundary condition as will be explained in the next section. Thus we consider the 1D Hubbard model with boundaries which is exactly solvable in terms of the Bethe ansatz method. We analyze the magnetic properties of this model using the exact solution and boundary conformal field theory. For $D=2$ and 3 , we derive the Korringa relation satisfied in the vicinity of a spinless impurity which is observed in NMR experiments.

Our argument for $D=2, 3$ is based upon Fermi liquid theory in the presence of antiferromagnetic spin fluctuations.

The organization of this paper is as follows. In Sec. II, the 1D Hubbard model with a spinless impurity is considered. The spin susceptibility and the local density of states in the vicinity of an impurity are obtained based upon the Bethe ansatz exact solution. It is found that the induced moment is not screened completely at any finite temperatures. We also derive the spin-lattice relaxation rate $1/T_1$ which satisfies a relation analogous to the Korringa law. In Sec. III, we discuss the 2D and 3D systems, exploiting the antiferromagnetically correlated Fermi liquid theory. A summary is given in Sec. IV.

II. A SPINLESS IMPURITY IN THE ONE-DIMENSIONAL HUBBARD MODEL

A. Mapping to the Hubbard model with boundaries and the Bethe ansatz exact solution

The effects of a single impurity in one-dimensional correlated systems have been extensively studied so far.^{7,8} If the interaction between fermions is repulsive, a potential scattering in the 1D Hubbard model is renormalized to an infinite strength, eventually cutting the system into two half-infinite chains in the low-energy scaling limit. Thus at sufficiently low temperatures the system can be treated as a Hubbard chain with open boundaries, of which the Hamiltonian is given by

$$H = - \sum_{\sigma, i=1}^{L-1} c_{\sigma i}^{\dagger} c_{\sigma i+1} + \text{H.c.} + U \sum_{i=1}^L n_{\uparrow i} n_{\downarrow i} - \mu \sum_{\sigma, i=1}^L n_{\sigma i} - \frac{H}{2} \sum_{i=1}^L (n_{\uparrow i} - n_{\downarrow i}) + V \sum_{\sigma} n_{\sigma 1}, \quad (1)$$

where the last term is a boundary potential. As we will see below, the low-energy spin dynamics around the impurity with which we are concerned is mainly described by this model, and the interaction or hopping between the two half-

infinite chains is a subleading irrelevant interaction which can be incorporated by perturbative calculations.

The Bethe ansatz exact solutions of 1D correlated systems with boundaries have been studied by many authors.⁹⁻²¹ In connection with the spin dynamics in the vicinity of the boundary, an intriguing result was obtained for the supersymmetric t - J model by Essler.¹⁶ He obtained the divergent behavior of the boundary spin susceptibility as a function of a magnetic field H , i.e., $\chi_{\text{boundary}} \sim 1/H(\ln H)^2$. It was first predicted by de Sa and Tselik that such a Curie-like behavior is universal for integral models with boundaries.¹⁴ Later, similar behavior was also found for the Hubbard model at half-filling by Asakawa and Suzuki.¹⁷ In the next subsection, we shall show that this divergent behavior holds also for the case away from half-filling with finite U .

Here we summarize the basic equations which are relevant to the following arguments. The Bethe ansatz equations of the 1D Hubbard model with boundaries obtained by Schulz many years ago are¹⁰

$$e^{i2k_j L} e^{i\phi_0(k_j)} = \prod_{\beta=1}^M e_1(\sin k_j - \lambda_\beta) e_1(\sin k_j + \lambda_\beta), \quad (2)$$

$$\prod_{j=1}^N e_1(\lambda_\alpha - \sin k_j) e_1(\lambda_\alpha + \sin k_j)$$

$$= \prod_{\substack{\beta=1 \\ \beta \neq \alpha}} e_2(\lambda_\alpha - \lambda_\beta) e_2(\lambda_\alpha + \lambda_\beta), \quad (3)$$

where $e_n(x) = (x + inu)/(x - inu)$, $u = U/4$, and $\phi_{0,L}$ is a potential at boundaries. N is the total number of electrons. M is the total number of down spins. k_j and λ_α are rapidities for charge and spin degrees of freedom, respectively. In the following, we consider only the case of repulsive boundary potentials. Thus the above equations have real roots. Putting $k_{-j} = -k_j$, $\lambda_{-\alpha} = -\lambda_\alpha$, and taking a continuum limit, we have the integral equations for the distribution functions of rapidities,

$$\rho(k) = \frac{1}{\pi} + \frac{1}{\pi L} \phi_0'(k) - \frac{1}{2\pi L} \frac{2u \cos k}{(\sin k)^2 + u^2}$$

$$+ \cos k \int_{-B}^B \frac{d\lambda}{\pi} \frac{u}{(\sin k - \lambda)^2 + u^2} \sigma(\lambda), \quad (4)$$

$$\sigma(\lambda) = \frac{1}{\pi L} \frac{2u}{\lambda^2 + 4u^2} + \int_{-Q}^Q \frac{dk}{\pi} \frac{u}{(\lambda - \sin k)^2 + u^2} \rho(k)$$

$$- \int_{-B}^B \frac{d\lambda'}{\pi} \frac{2u}{(\lambda - \lambda')^2 + 4u^2} \sigma(\lambda'). \quad (5)$$

N and M are given by

$$\int_{-Q}^Q \rho(k) dk = \frac{2N+1}{L}, \quad (6)$$

$$\int_{-B}^B \sigma(\lambda) d\lambda = \frac{2M+1}{L}. \quad (7)$$

Then the magnetization is expressed as

$$\frac{S_z}{L} = \frac{1}{4} \int_{-Q}^Q \rho(k) dk - \frac{1}{2} \int_{-B}^B \sigma(\lambda) d\lambda + \frac{1}{4L}. \quad (8)$$

The total energy is expressed in terms of the dressed energies,

$$\frac{E}{L} = \int_{-Q}^Q dk \left(\frac{1}{\pi} + \frac{1}{\pi L} \phi_0'(k) - \frac{1}{2\pi L} \frac{2u \cos k}{(\sin k)^2 + u^2} \right) \varepsilon_c(k)$$

$$+ \int_{-B}^B \frac{d\lambda}{\pi L} \frac{2u}{\lambda^2 + 4u^2} \varepsilon_s(\lambda), \quad (9)$$

where the dressed energies $\varepsilon_c(k)$ and $\varepsilon_s(\lambda)$ are determined by the integral equations

$$\varepsilon_c(k) = -2 \cos k - \frac{H}{2} - \mu + \int_{-B}^B \frac{d\lambda}{\pi} \frac{u}{(\sin k - \lambda)^2 + u^2} \varepsilon_s(\lambda), \quad (10)$$

$$\varepsilon_s(\lambda) = H + \int_{-Q}^Q \frac{dk}{\pi} \frac{u}{(\sin k - \lambda)^2 + u^2} \varepsilon_c(k)$$

$$- \int_{-B}^B \frac{d\lambda'}{\pi} \frac{2u}{(\lambda - \lambda')^2 + 4u^2} \varepsilon_s(\lambda'). \quad (11)$$

If one fixes the magnetic field H , B is determined by the equilibrium condition $\partial E / \partial B = 0$, which is equivalent to the condition $\varepsilon_s(B) = 0$. In the subsequent sections, we calculate the spin susceptibility and the local density of states using the above equations.

B. Spin susceptibility

In order to derive the spin susceptibility, we solve Eqs. (4) and (5) for $\sigma(\lambda)$ using the Wiener-Hopf method, and obtain the magnetization, Eq. (8).

Applying the Fourier transformation and shifting the argument, $\lambda \rightarrow \lambda + B$, we rewrite Eq. (5) as,

$$\sigma(\lambda + B) = f_0(\lambda + B) + \int_0^\infty \frac{d\lambda'}{\pi} R(\lambda - \lambda') \sigma(\lambda' + B)$$

$$+ \int_0^\infty \frac{d\lambda'}{\pi} R(\lambda + \lambda' + 2B) \sigma(\lambda' + B), \quad (12)$$

where

$$f_0(\lambda + B) = \frac{1}{L} \int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{e^{-u|\omega|} e^{-i\omega(\lambda+B)}}{2 \cosh u\omega}$$

$$+ \int_{-Q}^Q dk \frac{\rho(k)}{2 \cosh \frac{\pi}{u} (\lambda + B - \sin k)}, \quad (13)$$

$$R(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-u|\omega|} e^{-i\omega x}}{2 \cosh u\omega}. \quad (14)$$

The last term of the right-hand side of Eq. (12) is $O(1/B^2)$ for small magnetic fields. Thus we neglect it. Then Eq. (12) can be solved by using the standard Wiener-Hopf method.²² The solution is expressed in terms of the following functions:

$$G^+(\omega) = \sqrt{2\pi} \frac{\left(-i \frac{u\omega}{\pi}\right)^{-iu\omega/\pi}}{\Gamma\left(\frac{1}{2} - i \frac{u\omega}{\pi}\right)} e^{iu\omega/\pi}, \quad (15)$$

$$G^-(\omega) = [G^+(-\omega)]^{-1}, \quad (16)$$

$$Q^+(\omega) + Q^-(\omega) = G^-(\omega) \tilde{f}_0(\omega), \quad (17)$$

$$\tilde{f}_0(\omega) = \int_{-\infty}^{\infty} d\lambda f_0(\lambda + B) e^{i\omega\lambda}, \quad (18)$$

where $Q^+(\omega)[Q^-(\omega)]$ is the analytic part of $G^-(\omega)\tilde{f}_0(\omega)$ defined in the upper [lower] half-plane. Fourier transforming Eq. (12) and introducing the function $\sigma^+(\omega) = \int_0^\infty d\lambda e^{i\omega\lambda} \sigma(\lambda + B)$, we obtain the solution as $\sigma^+(\omega) = G^+(\omega)Q^+(\omega)$.

Now we derive $Q^+(\omega)$ as follows. For small magnetic fields, i.e., large B , and $\lambda > 0$ the second term of $f_0(\lambda + B)$ is approximated as

$$\int_{-Q}^Q dk \frac{\rho(k)}{2 \cosh \frac{\pi}{u}(\lambda + B - \sin k)} \approx \frac{2N+1}{L} \frac{1}{2 \cosh \frac{\pi}{u}(\lambda + B)}. \quad (19)$$

This driving term is essentially the same as the bulk contribution, with which we are not concerned. The first term of $f_0(\lambda + B)$ gives rise an interesting boundary effect. Using $e^{-u|\omega|/2 \cosh u\omega} = \sum_{n=1}^{\infty} (-1)^{n-1} e^{-2nu|\omega|}$ and the Laplace transformation

$$\frac{2nu}{(\lambda + B)^2 + (2nu)^2} = \int_0^\infty dt e^{-(\lambda+B)t} \sin(2nut), \quad (20)$$

we rewrite the first term of $f_0(\lambda + B)$ as

$$\begin{aligned} & \frac{1}{L} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-u|\omega|} e^{-i\omega(\lambda+B)}}{2 \cosh u\omega} \\ &= \frac{1}{\pi L} \sum_{n=1}^{\infty} (-1)^{n-1} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_0^\infty dt \sin(2nut) \\ & \times \left[\frac{1}{\omega + it} - \frac{1}{\omega - it} \right] i e^{-i\omega(\lambda+B)}. \end{aligned} \quad (21)$$

The analytic property of Eq. (21) solves Eq. (17),

$$Q^+(\omega) = \frac{1}{L} \sum_{n=1}^{\infty} \int_0^\infty dt \sin(2nut) \frac{e^{-tB}}{\omega + it} i G^+(-it) + \text{bulk terms}. \quad (22)$$

Finally, using Eq. (8), we obtain the magnetization,

$$S_z = \frac{1}{2} \int_0^\infty d\lambda \sigma(\lambda + B) = \frac{1}{2} \sigma^+(0) \sim \frac{1}{LB} + \text{bulk terms}, \quad (23)$$

for large B , i.e., small magnetic fields. B is related to H from the condition $\varepsilon_s(B) = 0$. From Eqs. (10) and (11), we have $H = C e^{-\pi B/2u}$ for $H \ll u$. Here C is a constant. Then the spin susceptibility $\chi = \partial S_z / \partial H$ behaves like

$$\chi \sim \frac{1}{L} \frac{1}{H(\ln H)^2} + \text{bulk terms}. \quad (24)$$

This H dependence is the same as that found for the half-filling case.¹⁷ The above result implies that in 1D systems the magnetic moment induced by a nonmagnetic impurity is not screened completely even at zero temperature. This behavior is analogous to the underscreening multichannel Kondo effect, as pointed out by de Sa and Tsvelik.¹⁴ The leading H dependence of Eq. (24) is not altered, even if one includes irrelevant interactions such as the hopping between the two half-infinite chains.

In this section, we restrict our discussion to the zero-temperature case. It is expected that at finite temperatures the boundary spin susceptibility behaves like $\chi_{\text{boundary}} \sim 1/T(\ln T)^2$. In order to confirm this prediction, we need to explore the thermodynamic Bethe ansatz method in the presence of boundaries. However, in the presence of boundaries, the entropy cannot be expressed in terms of rapidity distribution functions in the continuum limit, because of the presence of spurious states for vanishing rapidities, and thus the usual technique of the thermodynamic Bethe ansatz method is not applicable. If we limit the argument to sufficiently low-temperature regions, undesirable contributions from the spurious state around the bottom of the energy spectrum may be small, and not give rise to serious errors. Even if we admit this approximation, it is still a cumbersome task to solve the thermodynamic Bethe ansatz equations numerically for low temperatures. Thus here we just give a field-theoretical argument to justify the above speculation. According to the boundary conformal field theory, the above divergent behavior of the spin susceptibility is due to the presence of a boundary entropy $S_{\text{bound}} = T \ln(\sqrt{4\pi}R)$.^{23,17} Here R is the radius of the boson field of the Gaussian model which is the low-energy effective theory. If the leading irrelevant interaction is the marginal operator in the spin degrees of freedom, $\mathbf{J}_L \cdot \mathbf{J}_R$, we have $R \sim R_0 - g/\ln T$ for small T .²⁴ Then, the boundary spin susceptibility should behave like $\chi_{\text{boundary}} \sim 1/T(\ln T)^2$. Thus we expect that this temperature dependence which signifies the presence of an unquenched local moment may realize in this system.

C. Local density of states

In models solvable in terms of the Bethe ansatz method, the local density of states is defined as the derivative of the quantum number, which parametrizes rapidities, with respect to the pseudoenergy, i.e., $\partial I_j / \partial \varepsilon(k_j)$.²⁵ For the 1D Hubbard model, we can consider the density of states of holons and spinons, respectively. An interesting singular behavior due to the boundary appears in the spin degrees of freedom.

The local density of states of spinon as a function of energy is given by

$$\rho_{\text{spin}}(\varepsilon) = \frac{\partial \lambda}{\partial \varepsilon_s} \sigma(\lambda). \quad (25)$$

In the absence of magnetic fields, $B \rightarrow \infty$, the solution of Eq. (5) is expressed as

$$\begin{aligned} \sigma(\lambda) = & \frac{1}{L} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{u|\omega|} e^{-i\omega\lambda}}{2 \cosh u\omega} \\ & + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega\lambda}}{2 \cosh u\omega} \int_{-Q}^Q dk \rho(k) e^{i\omega \sin k}. \end{aligned} \quad (26)$$

For $\lambda \gg 1$, the first term of Eq. (26) behaves like $\sim 1/\lambda^2$, while the second term is just the order of $O(e^{-\pi\lambda/u})$. Thus the main singular contribution comes from the former which is nothing but the boundary term. In a similar manner, from Eq. (11) we obtain the asymptotic form of $\varepsilon_s(\lambda)$ for large λ , i.e., $\varepsilon_s(\lambda) \sim A e^{-\pi\lambda/u}$, where A is a constant. Then from Eqs. (25) and (26), we have

$$\rho_{\text{spin}}(\varepsilon) \sim \frac{1}{\varepsilon (\ln \varepsilon)^2}, \quad (27)$$

for small ε . Thus the local density of states also shows singular divergent behavior because of the presence of the boundary. It is noted that this result is similar to that of the underscreened multichannel Kondo effect.²⁵

$$\chi(x, y, t) \sim \left(\frac{\pi T}{v_s} \right)^2 \left[\sinh \frac{\pi T}{v_s} (x - y - vt) \right]^{-2} + e^{2ik_F(x-y)}$$

$$\times \prod_{\nu=s,c} \left[\left(\frac{\pi T}{v_\nu} \right)^2 \frac{\sinh \frac{2\pi T x}{v_\nu} \sinh \frac{2\pi T y}{v_\nu}}{\sinh \frac{\pi T}{v_\nu} (x+y+v_\nu t) \sinh \frac{\pi T}{v_\nu} (x+y-v_\nu t) \sinh \frac{\pi T}{v_\nu} (x-y+v_\nu t) \sinh \frac{\pi T}{v_\nu} (x-y-v_\nu t)} \right]^{K_\nu/2}. \quad (28)$$

Here v_s and v_c are the velocities of spinons and holons, respectively. K_c is the Luttinger liquid parameter in the charge sector, and $1/2 \leq K_c \leq 1$. $K_s = 1$ because of the SU(2) symmetry of the spin sector. In the vicinity of the boundary, i.e., $x, y, |x-y| \ll v_s t$, the staggered part (the second term) of Eq. (28) is less relevant in comparison

The important message of this and the previous subsections is that in 1D correlated electron systems the localized moment induced by a nonmagnetic impurity is not quenched at any temperatures. The inclusion of irrelevant interactions such as hopping between semi-infinite chains does not change the result qualitatively. It should be stressed that this unquenched local moment is a particular property of the 1D systems where an impurity divides the system into two semi-infinite chains. Such a separation of the system is not possible in higher-dimensional systems.

D. Spin-lattice relaxation rate

Here we calculate the spin-lattice relaxation rate $1/T_1$ in the vicinity of a spinless impurity, i.e., a boundary, using the bosonization method and boundary conformal field theory. The same kinds of calculations have been done for Heisenberg spin chains before.^{26,27} Some parts of the following results are similar to those obtained in Refs. 26 and 27. However, combining them with the results from the Bethe ansatz exact solution, we shall see some new aspects. In the previous subsections, it was shown that the induced moment is not screened completely at any temperatures. Then one might expect that $1/T_1$ behaves like that of an isolated spin, $1/T_1 \sim T\chi$. However, as will be seen below, this naive expectation is incorrect.

According to the boundary conformal field theory, correlation functions for any operators in the vicinity of boundaries are obtained by the analytic continuation of the antiholomorphic part to the holomorphic part, $O(z, \bar{z}) = O_L(vt + ix) O_R(vt - ix) \sim O_L(vt + ix) O_L(vt - ix)$.^{28,29} Following the standard technique, we have the asymptotic behaviors of the spin-spin correlation function in the presence of the boundary,^{28,23,30}

with the uniform part (the first term). Thus in contrast to the bulk behavior, the antiferromagnetic spin fluctuation is much suppressed, and the uniform part gives the dominant contribution to $1/T_1$ near the boundary. Fourier transforming Eq. (28),^{31,32} we obtain, up to logarithmic corrections,

$$\frac{1}{T_1 T} = \lim_{\omega \rightarrow 0} \frac{1}{\omega} \sum_{q, q'} \text{Im} \chi(q, q', \omega) \sim \frac{C}{v_s^2} + O(T^{2K_c}). \quad (29)$$

Here we have assumed that the hyperfine coupling constant is independent of q , and omitted it. C is a temperature-independent constant. In the case that v_s is a constant, the above result is equivalent to that obtained by Brunel *et al.* for Luttinger liquids with boundaries.²⁶ The spinon velocity v_s is related to the spin susceptibility obtained before, $1/v_s = \chi_{\text{bulk}} + \chi_{\text{boundary}}/L$. As claimed in the previous subsections, χ_{boundary} should show enhanced local correlations like $\chi_{\text{boundary}} \sim 1/T(\ln T)^2$. Thus, near the boundary,

$$\frac{1}{T_1 T} \sim (\chi_{\text{boundary}})^2. \quad (30)$$

Surprisingly, this relation is analogous to the Korringa relation. However, it is noted that in contrast to the conventional Korringa law, the right-hand side of Eq. (30) shows a strong temperature dependence. As mentioned in the previous subsections, the induced local moment is not quenched completely. In spite of such an unscreened character of the moment, the Korringa-like relation holds in the vicinity of a spinless impurity.

III. SPINLESS IMPURITY IN 2D AND 3D HUBBARD MODELS

In this section, we discuss the local magnetic properties caused by a spinless impurity in 2D and 3D Hubbard models in the presence of bulk antiferromagnetic fluctuations, i.e., very close to the half-filling. The main purpose of this section is to derive the Korringa relation satisfied at the nearest neighbor of the impurity site, which is observed in the NMR experiment for cuprates.⁴ The model Hamiltonian is given by

$$H = \sum_{k\sigma} E_k c_{\sigma k}^\dagger c_{\sigma k} + U \sum_i n_{\uparrow i} n_{\downarrow i} + E_0 \sum_{\sigma} n_{\sigma 0}. \quad (31)$$

Here $E_k = -2t \sum_{a=1}^D \cos k_a$ ($D=2$ or 3), and the last term represents a spinless impurity localized at site 0. We restrict our discussion to the case of the square lattice in 2D and the cubic lattice in 3D. Because of the presence of an impurity, correlation functions are nonlocal. In the case of $U=0$, the single-particle Green's function is given by

$$G_{kk'}^0(\varepsilon_n) = \frac{\delta_{kk'}}{i\varepsilon_n + \mu - E_k} + \frac{1}{i\varepsilon_n + \mu - E_k} \times \frac{E_0}{1 - E_0 \sum_{k''} \frac{1}{i\varepsilon_n + \mu - E_{k''}}} \frac{1}{i\varepsilon_n + \mu - E_{k'}}, \quad (32)$$

where μ is a chemical potential. For $U \neq 0$, the single-particle Green's function is obtained by solving the equation

$$\sum_{k''} [(i\varepsilon_n + \mu - E_k) \delta_{kk''} - \Sigma_{kk''}(\varepsilon_n) - E_0] G_{k''k'}(\varepsilon_n) = \delta_{kk'}. \quad (33)$$

The self-energy $\Sigma_{kk'}(\varepsilon)$ may be obtained by perturbative calculation in terms of U . However, in the following qualitative argument we do not need an explicit expression of $G_{kk'}(\varepsilon_n)$.

Before discussing the magnetic properties, it is useful to sketch the spatial dependence of the density of states in the vicinity of an impurity. The density of states at the Fermi level is given by

$$\rho(x, x') = -(1/\pi) \sum_{kk'} \text{Im} G_{kk'}^R(0) e^{ikx} e^{-ik'x'}. \quad (34)$$

To simplify the calculation, we consider the strong limit of an impurity potential, i.e., $E_0 \gg U, t$. The following arguments do not change qualitatively even in the case of a finite E_0 . Using Eq. (32), we obtain the density of states at the Fermi level for the noninteracting system, $U=0$,

$$\rho_0(x, x') = N_{x-x'}(\mu) - \frac{N_x(\mu) N_{x'}(\mu)}{N_0(\mu)}, \quad (35)$$

$$N_x(\varepsilon) \equiv \sum_k \delta(\varepsilon - E_k) e^{ikx} = \int_{-\infty}^{\infty} \frac{ds}{2\pi} e^{is\varepsilon} \prod_{i=1}^D J_{n_i}(ts), \quad (36)$$

with $J_n(x)$ the Bessel function and $x = (n_1, n_2)$ for $D=2$ and $x = (n_1, n_2, n_3)$ for $D=3$. Note that if x or x' is the impurity site, the density of states vanishes, $\rho_0(x, 0) = \rho_0(0, x') = 0$. We can easily show that if the electron density is close to half-filling, i.e., $|\mu|/t \ll 1$, then $N_x(\mu) \sim O((\mu/t)^2)$ for the site x on the sublattice which includes the nearest-neighbor site of the impurity, x_{NN} (denoted by the A sublattice), and $N_x(\mu) \sim N_0(\mu)$ for the site x on the sublattice which includes the impurity site (B sublattice). Thus from Eq. (35) we immediately see that the local density of states around the impurity site shows strong spatial modulation similar to the Friedel oscillation. The period of the oscillation is $\sim 1/k_F$ which is close to the half-filling value in this case. If x and x' belong to the A sublattice, the local density of states is nearly equal to that of bulk systems, $\rho_0(x, x') \sim \rho_0(|x| \rightarrow \infty, |x'| \rightarrow \infty)$. On the other hand, if $x \neq 0$ and $x' \neq 0$ belong to the B sublattice, $\rho_0(x, x') \sim O((\mu/t)^2)$. Since the density of states at the Fermi level is not renormalized by electron-electron interactions, this Friedel oscillation occurs for $U \neq 0$. This observation leads to an important implication for local magnetic properties on the nearest-neighbor site of the impurity, x_{NN} . Because of the Friedel oscillation and the bipartite lattice structure, the local density of states on all the sites surrounding the site x_{NN} is much suppressed provided that the impurity potential is sufficiently strong. Thus the spin on the site x_{NN} is less screened than spins of electrons in the bulk. As a result, the local spin susceptibility on the site x_{NN} is strongly enhanced.

Now we consider the spin-lattice relaxation rate $1/T_1$ in the vicinity of a spinless impurity. For simplicity, we assume

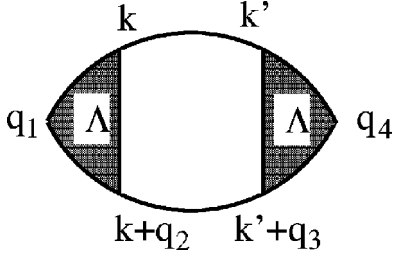


FIG. 1. diagram of the ω -linear term of $\text{Im}\chi(q_1, q_4, \omega)$. The shaded part is the three-point vertex.

that the hyperfine coupling constant does not depend on q . We apply the general argument from the Fermi liquid theory to the case with a single spinless impurity.^{33,34} Then $1/T_1$ at site x_i is given by, up to constant factors,

$$\begin{aligned} \frac{1}{T_1 T} &= \lim_{\omega \rightarrow 0} \sum_{q, q'} \frac{\text{Im}\chi(q, q', \omega)}{\omega} e^{iqx_i} e^{-iq'x_i} \\ &= \sum_{q_1, q_2, q_3, q_4, k, k'} \text{Re}\Lambda(q_1, k+q_2, k) \\ &\quad \times \text{Im}G_{kk'}^R(0) \text{Im}G_{k+q_2, k'+q_3}^R(0) \\ &\quad \times \text{Re}\Lambda(q_4, k'+q_3, k') e^{iq_1 x_i} e^{-iq_4 x_i}, \end{aligned} \quad (37)$$

where $\Lambda(q, k+q', k)$ is a three-point vertex function. The diagrammatic expression of Eq. (37) which is the ω -linear term of $\text{Im}\chi(q, q', \omega)$ is shown in Fig. 1. The detail derivation of this formula is given in Refs. 33 and 34. In the presence of strong antiferromagnetic fluctuations, it is plausible to assume that $\Lambda(q, k+q', k)$ depends mainly on q and q' . Thus in the following we discard the k dependence of $\Lambda(q, k+q', k)$. It is useful to rewrite Eq. (37) in terms of quantities in coordinate space,

$$\begin{aligned} \frac{1}{T_1 T} &= \pi^2 \sum_{s, t} \rho(-x_i - s, -x_i + t) \rho(x_i + s, x_i - t) \\ &\quad \times \Lambda(x_i, x_i + s) \Lambda(x_i - t, x_i). \end{aligned} \quad (38)$$

Here,

$$\Lambda(x, x') = \sum_{q, q'} \text{Re}\Lambda(q, q') e^{iqx} e^{-iq'x'}. \quad (39)$$

In the case that site x_i is far from the impurity, i.e., $|x_i| \gg a$, where a is a lattice constant, $\rho(x_i + s, x_i - t) \rightarrow \rho(s + t)$, $\Lambda(x_i, x_i + s) \rightarrow \Lambda(-s)$, and thus the above expression is reduced to the usual formula of $1/T_1$ in bulk systems. It is also noted that if $x_i = 0$, $1/T_1 T$ vanishes, since $\Lambda(0, s)$ includes $G(0, x_j)$ which vanishes as mentioned above. Here we are concerned with the case that the site x_i is the nearest neighbor of the impurity site, $x_i = x_{\text{NN}}$.

To proceed further, we use a phenomenological expression for $\Lambda(q, q')$. We assume that the three-point vertex function $\Lambda(q, q')$ consists of a part which is strongly enhanced by antiferromagnetic spin fluctuations and a local part which depends on q and q' weakly,

$$\Lambda(q, q') \sim \Lambda_{\text{AF}}(q) \delta_{q, q'} + \Lambda_{\text{loc}}(q, q'). \quad (40)$$

The antiferromagnetically correlated part $\Lambda_{\text{AF}}(q)$ has a strong peak at $q = Q$, the staggered vector, and then is approximated as $\text{Re}\Lambda_{\text{AF}}(q) \sim \text{Re}\chi(q \sim Q) = \chi(Q) / \{1 + [\xi_{\text{AF}}(q - Q)]^2\}$. Here we used the phenomenological expression for $\chi(q \sim Q)$.³⁵ As mentioned above, $\Lambda_{\text{loc}}(q, q')$ is enhanced by local magnetic correlations at site x_{NN} , i.e., $\Lambda_{\text{loc}}(q, q') \sim \Lambda_{\text{loc}} e^{-iqx_{\text{NN}}} e^{iq'x_{\text{NN}}}$. Then, Eq. (37) is rewritten as

$$\begin{aligned} \left(\frac{1}{T_1 T} \right)_{\text{NN}} &\sim \left[\frac{\chi(Q)}{(\xi_{\text{AF}})^m} \right]^2 \sum_{k, k'} \text{Im}G_{k, k'}^R(0) \text{Im}G_{k+Q, k'+Q}^R(0) \\ &\quad + [\text{Re}\Lambda_{\text{loc}}]^2 \sum_{k, k', q_2, q_3} \text{Im}G_{k, k', q_2, q_3}^R(0) \\ &\quad \times \text{Im}G_{k+q_2, k'+q_3}^R(0), \end{aligned} \quad (41)$$

where $m = 2$ for 2D systems and $m = 3$ for 3D systems. Since $\chi(Q) \sim (\xi_{\text{AF}})^2$,³⁵ the first term of Eq. (41), which is the antiferromagnetically correlated part, is much suppressed compared to the second term, i.e., the local correlation part. Thus we obtain

$$\left(\frac{1}{T_1 T} \right)_{\text{NN}} \sim (\text{Re}\Lambda_{\text{loc}})^2. \quad (42)$$

Here we neglect all factors which are not enhanced by electron correlation. On the other hand, the local spin susceptibility at x_{NN} is approximately given by $\chi_{\text{loc}} \sim \text{Re}\Lambda_{\text{loc}}$. Thus Eq. (42) establishes the Korringa relation satisfied at the nearest-neighbor site of the impurity. As mentioned before, this relation is actually observed in NMR experiments.⁴

IV. SUMMARY AND DISCUSSION

We have discussed some magnetic properties analogous to the Kondo effect induced by a spinless impurity in strongly correlated electrons systems. In the 1D system, we have shown that the spin susceptibility and the local density of states near the impurity indicate divergent behaviors, implying the presence of an unquenched local moment at any temperatures. We have also obtained a Korringa-like relation between the spin-lattice relaxation rate and the local spin susceptibility, $1/T_1 T \sim (\chi_{\text{boundary}})^2$. In 2D and 3D systems, the antiferromagnetically correlated Fermi liquid theory has been applied. It has been shown that magnetic properties in the vicinity of a spinless impurity are dominated by the induced moment rather than the antiferromagnetic spin fluctuation developed in the bulk, and that the Korringa relation holds at the near-neighbor site of the impurity.

The results obtained for the 1D system have an interesting implication to higher-dimensional systems. Suppose a semi-infinite 2D Hubbard model with a boundary line, which is regarded as the coupled semi-infinite Hubbard chains. According to the results obtained in Sec. II, it is expected that at some finite temperatures 1D-like strong spin correlations occur in the vicinity of the boundary line, leading to a strongly enhanced density of states near the boundary. Such an en-

hanced electron correlation and one dimensionality of the boundary line may give rise to strong fluctuations toward some surface phase transition. For instance, if there exists a pairing interaction in the bulk system, the pairing correlation may be enhanced near the boundary, leading to a higher transition temperature than the bulk superconductivity. Actually, it is reported that Sr_2RuO_4 with lamellar microdomains of Ru metal shows a superconducting transition at a temperature higher than T_c of the pure system, and that superconductivity with higher T_c occurs in the vicinity of the bound-

ary between Sr_2RuO_4 and Ru metal.³⁶ We would like to pursue this possible mechanism of the enhanced transition temperature in the near future.

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