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Local Magnetic Moments in Nanoscale Systems

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ABSTRACT

The formation of local magnetic moments and its size effect in one- and three-dimension finite systems with magnetic impurity are investigated based on the Anderson hybridizing model in real space. By the exact diagonalization within the self-consistent mean field approximation, it is found that as contrast to that in infinite system, the formation of the local magnetic moment in finite system may strongly depend on the size of system up to a few nanometers. The spectral densities of the local electronic states and the spatial distribution of the magnetic moments for the conduction electrons polarized by the local moment are also obtained. The condition for the occurrence of local magnetic moments in such small systems is discussed. The strong size-dependence of the local magnetic

moments in finite system is attributed to the quantum size effect.

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I. INTRODUCTION

The magnetism of small particles has attracted great interests both in the theoretical and in the experimental study [1 - 7]. Nanosized magnetic particles are fundamentally important in cluster and nano-crystal physics and have extensive potential application. Experiments [1 - 3] have demonstrated that the magnetic properties of the 3d or 4d transition metal and the rare-earth metal clusters are different from those of the bulk materials. For example, the magnetic moments decrease with respect to the increase of cluster sizes, the ferromagnet-paramagnet transition temperature (Curie temperature) of the 3d transition metal clusters shows strong size-dependence [1 - 3]. Some 4d transition metal clusters may exhibit giant magnetic moments [4], though their bulk materials are nonmagnetic.

The theoretical study of the size effect on the magnetic properties of the transition metal and the rare-earth metal clusters has become an interesting subject [5 - 9]. Pastor et al. [5] studied the influence of the electron-electron correlation and the cluster geometry on the magnetism in the framework of the tight-binding Hubbard model. They found that the local magnetic moments of pure 3d transition-metal clusters, Fe_n, Cr_n and Ni_n (n < 10), have weak size-dependence, their prediction for the size-dependence of the magnetic moments of Fe_n clusters disagrees with the experimental results [1]. Recent electronic structure calculation performed by Reddy et al. [6] for pure 4d transition-metal clusters, Pd_{13}, Ru_{13} and Rh_{13}, shows the existence of the magnetic moment and magnetic order in Rh_{13} cluster, but the predicted magnetic moment per atom is larger than those found in the experiment [4]. This discrepancy might arise from the unreal geometries

for the clusters used in the calculation. Jena et al. [7] studied the Ising model for small magnetic clusters at finite temperature by using the Monte-Carlo technique. Linderoth et al. [8] discussed the finite size effect on the spin-wave spectrum in magnetic clusters in terms of the Heisenberg exchange model with structural relaxation, they showed that the spin-wave spectrum in these finite clusters is very different from that in the bulk cases, though the definition of the spin wave in such small systems is quite ambiguous. From these studies, it is clear that the magnetic properties in the finite systems are different from those in bulk phases.

The main subject of the studies mentioned above concentrates on the average magnetic moment, the magnetic order and the exchange interaction in magnetic clusters, the existence of local magnetic moment and its stability in nano-system are not deeply explored. Although some work on local moment of magnetic impurity in nonmagnetic clusters are investigated by several authors [10, 11], the general behavior of the formation of local magnetic moment in finite system is not clear. In the first-principle electronic structure calculation for FeR_n clusters (R=Al, Mg, Ca, Sr, etc.), Ellis and Guenzburger [10] found that Fe impurity is nonmagnetic for $FeAl_{42}$, while it is magnetic for $FeMg_{26}$, $FeCa_{42}$, and $FeSr_{18}$. Using the local spin density method, Callaway et al. [11] studied the electronic structure of Mn impurity in fcc Al matrix (a free $MnAl_{18}$ cluster), the Mn atom in the cluster is found to be magnetic, the magnetic moment is about 1.78 μ_B, which is much smaller than its atomic moment. But how and when the local magnetic moments can form in such small systems are not clear yet.

The picture for the formation of local magnetic moment in bulk metal (infinite system)

had been established by Friedel, Anderson and many other authors [12 - 17] in the early of 1960s, they showed that an impurity dissolved in bulk metal may form Friedel's resonant states [12, 13] (or virtual bound-states) with the conduction electrons through the hybridizing interaction, the spin-split of the Friedel's resonant states leads to the formation of local magnetic moment. It is well known [16, 17] that the condition for the occurrence of local magnetic moment in bulk is $U\rho_{d\sigma}(E_F) > 1$, where $\rho_{d\sigma}(E_F)$ is the densities of states for the d-electrons at the Fermi surface and U is the on-site Coulomb interaction of the local d-electrons, the energy level of the d-electrons of the impurity with respect to the Fermi energy, ϵ_d, must be negative so as to form the local moment, and it is size-independent. However, when the size of bulk metal is reduced to just a few nanometers, does this condition still hold? Obviously, in this situation the quantum size effect will play an important role in the formation of local magnetic moment.

In this paper, we have studied the finite size effect on the formation of local magnetic moment by using the Anderson impurity model. It could provide the understanding on the magnetic behavior of small systems and the evolution of the magnetic properties from atom, through small cluster to bulk system. The rest of this paper is arranged as following: the formalism of the local magnetic moments in finite systems is described in Sec.II, the results and discussions for one-dimension (1D) and three-dimension (3D) cases are given in Sec. III, and the conclusion is drawn in Sec.IV.

II. FORMALISM

A magnetic impurity, such as a transition-metal atom dissolved in a nonmagnetic metal, can be described by the Anderson hybridization Hamiltonian [12]. The Anderson

model provides an essential description for the mechanism of the formation of a magnetic moment in solid, and plays an important role in our understanding on the existence of local magnetic moment in infinite system. This model is believed to be still valid in describing the physical process in the finite systems. In real space, the Hamiltonian of the Anderson hybridizing model with a magnetic impurity at site R_i can be expressed in matrix form:

$$H = \sum_{\sigma}[C_{\sigma}^{\dagger}\mathbf{T}C_{\sigma} + (\epsilon_d + \frac{U}{2}\sum_{\sigma'} d_{\sigma'}^{\dagger}d_{\sigma'})d_{\sigma}^{\dagger}d_{\sigma} + C_{\sigma}^{\dagger}\mathbf{P}d_{\sigma} + d_{\sigma}^{\dagger}\mathbf{P}^{\dagger}C_{\sigma}] \tag{1}$$

where $C_{\sigma}^{\dagger}$= ($c_{1\sigma}^{\dagger}$ $\ldots$ $c_{i-1\sigma}^{\dagger}$ 0 $c_{i+1\sigma}^{\dagger}$ $\ldots$ $c_{N\sigma}^{\dagger}$) denotes the creation operator matrix of the mobile (or conduction) electrons with spin σ, $d_{\sigma}^{\dagger}$ the creation operator of the *d*-electron of the impurity, and N is the electron number in the system. $\mathbf{T}$ represents the hopping matrix of the conduction electrons, which is a $N \times N$ matrix, it has simple tridiagonal form for 1D chain:

$$\mathbf{T} = \begin{pmatrix} \epsilon_c & t & 0 & \cdots & 0 \\ t & \epsilon_c & t & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \epsilon_c \end{pmatrix} \tag{2}$$

However it is more complicated in the case of higher dimensional systems, and it strongly depends on the structure of the small clusters. In Eq.(2), the matrix element t represents the hopping energy of the conduction electron from one site to its nearest-neighbor site; ϵ_d (or ϵ_c) denotes the difference between the impurity (or the conduction) electron energy level E_d (or E_c) and the chemical potential μ, and U is the on-site Coulomb interaction. $\mathbf{P}$ = ($\ldots$ v_{i-1} 0 v_{i+1} $\ldots$) refers the hybridizing matrix between the d-electron and the conduction electrons. In the present paper, only the nearest-neighbor interaction is

considered. In finite system, the movement of the conduction electron can't be considered as a plane wave, therefore we can not describe the impurity effect by the usual scattering theory and the phase shift technique. In this paper, the real-space Green's function technique is employed to deal with the impurity effect in finite system. Within the self-consistent mean field approximation, by introducing the mean occupancy of the d-electrons, $\bar{n}_\sigma = < d^\dagger_\sigma d_\sigma >$, the propagator of the d-electron and the mixed propagator matrix between the conduction electrons and the d-electron are given as the follows:

$$<< d_\sigma; d^\dagger_\sigma >>= [\omega - (\epsilon_d + U\bar{n}_{\bar{\sigma}}) - \mathbf{P}(\omega\mathbf{I} - \mathbf{T})^{-1}\mathbf{P}^\dagger]^{-1} \tag{3}$$

$$<< C_\sigma; d^\dagger_\sigma >>= [\omega\mathbf{I} - \mathbf{T}]^{-1}\mathbf{P}^\dagger << d_\sigma; d^\dagger_\sigma >> \tag{4}$$

where $\mathbf{I}$ is the unit matrix. The propagator matrix of the conduction electrons is:

$$<< C_\sigma; C^\dagger_\sigma >>= [\omega\mathbf{I} - \mathbf{T} - \mathbf{P} \times \mathbf{P}^\dagger/(w - \epsilon_d - Un_{-\sigma})]^{-1} \tag{5}$$

The occupation number n_d and the magnetic moment m_d of the d-electrons can be obtained through the preceding propagators:

$$n_d = \frac{1}{\pi}\int d\omega f(\omega) Im[<< d_\uparrow; d^\dagger_\uparrow >>_{\omega - i\eta} + << d_\downarrow; d^\dagger_\downarrow >>_{\omega - i\eta}] \tag{6}$$

and

$$m_d = \frac{1}{\pi}\int d\omega f(\omega) Im[<< d_\uparrow; d^\dagger_\uparrow >>_{\omega - i\eta} - << d_\downarrow; d^\dagger_\downarrow >>_{\omega - i\eta}] \tag{7}$$

Where f(ω)=1/(exp(β (ω-μ))+1) is the Fermi-Dirac distribution function. The total spectral density of the excited states for the local electrons is:

$$\rho_d(\omega) = \frac{1}{\pi} Im[<< d_\uparrow; d^\dagger_\uparrow >>_{\omega - i\eta} + << d_\downarrow; d^\dagger_\downarrow >>_{\omega - i\eta}] \tag{8}$$

Once upon a local magnetic moment forms, its surrounding conduction electrons will be polarized, the magnetic moment of the polarized conduction electrons at site R_i can be expressed as:

$$m_s(i) = \frac{1}{\pi}\int d\omega f(\omega) Im[<< c_{i\uparrow}; c^{\dagger}_{i\uparrow} >>_{\omega - i\eta} - << c_{i\downarrow}; c^{\dagger}_{i\downarrow} >>_{\omega - i\eta}] \tag{9}$$

The occupation number and the magnetic moments are obtained by the self-consistent mean field approximation. Although the mean field approach is somewhat simple and approximate, it might produce some misleading results at finite temperature, however at T=0 K, it indeed provides many physical results [12,17]. For example, the mean-field results for the formation of local magnetic moments give a good qualitative description of an impurity in a nonmagnetic metal, so it remains sense near the temperature of absolute zero degree. As the first step, the mean-field approximation is a good approach to outline tthe basic picture of the local magnetic moment in finite systems.

In infinite system, the matrix product $\mathbf{P}(\omega\mathbf{I} - \mathbf{T})^{-1}\mathbf{P}^{\dagger}$ in Eq.(3) can be expressed in terms of a summation over the wavevectors of the conduction electrons. However, in finite case, the translation symmetry is broken, the evolution of the local magnetic moment with respect to the size of systems has to been studied numerically. In this paper, the closed set of the self-consistent equations (3) to (6) are solved by exact diagonalization to calculate the Green's function and the local spectral density. In the following, all the energies are measured in units of the hopping integral t and the magnetic moment in units of the Bohr magneton, μ_B.

III. RESULTS AND DISCUSSIONS

The formation of a local magnetic moment and its dependence on the size of the

finite system are studied in this section. To explore the explicit interrelation of the local magnetic moment, the cluster size and the dimensionality of the system, we first consider a linear quantum chain with an impurity situated at the center at T=0 K, the formation of a local magnetic moment in 3D system with an impurity will be discussed later. The maximum numbers of the atoms in the systems we have studied are 30 for 1D case, and 15 for 3D case, respectively, which correspond to several nanometers.

From the numerical calculations for various systems with different parameters, we find two points: (a) When the impurity energy level ϵ_d is far below the chemical potential and the Coulomb interaction U is strong enough, the local moment can form and is almost not affected by the variation of cluster size. (b) If the energy level ϵ_d approaches or lies above the chemical potential μ, and the Coulomb interaction is not strong enough, there will be no local moment. In this situation, the impurity level is too shallow to form localized Friedel's resonant states, or the Coulomb interaction is too weak to lead to the spin-split of the Friedel's resonant states. These two points are similar to the results of infinite systems [12]. These results are reasonable, since the former corresponds to the isolated atom limit when the impurity level is deep and the on-site Coulomb interaction is strong enough, the magnetic moment of the impurity is almost not affected by the environment; and the latter corresponds to the free electron limit. These results are valid both for 1D quantum chains and for 3D nano-clusters. However, there are also other distinct and interesting behavior when the finite systems lie between these two extreme cases, we will address it in detail in the following.

III.1 One-Dimensional Finite Systems

To avoid the effect of the asymmetry on the formation of the local magnetic moment in the cases of even-number-particle systems, we consider only the systems with odd-number atoms. Fig.1 and Fig.2 show the local magnetic moment as a function of the size for 1D linear quantum chains with different parameters. A strong dependence of the magnetic moment on the number of the atoms can be seen clearly. It is found that the value of the magnetic moment mainly depends on three factors: the system size, the impurity energy level and the on-site Coulomb interaction. The local moment will approach a constant (the bulk value) when the cluster size increases. A non-monotonous descent of the local magnetic moment with respect to the increase of the size can be seen in Fig.2 for the 1D systems with small Coulomb interaction and shallow energy level. The shallower the impurity energy level is, the stronger the variation of the local magnetic moment is. The d-electron will be delocalized and lose its magnetic moment when the energy level becomes shallow and the size of the system becomes large enough (See the curves (b) and (c) in Fig.1). The reason is that the impurity electron would be influenced by the surrounding electronic field, when more nonmagnetic metal atoms, correspondingly more conduction electrons, are added to the finite system, the local environment of the system is changed, the modification to the electrons in shallow energy level is stronger than that in deep energy level. In the mean time, because of the quantum size effect, the difference between the energy levels and the density of states for the conduction electrons are also changed, therefore for the small system, the Friedel's resonant states, hence the formation of the local magnetic moments is very sensitive to the local environment.

So far there is no any direct experimental data on the magnetic properties of the "dilute

clusters" available for comparison with the present results. We have noted that similar behavior of the local electronic structure is observed experimentally for Co impurity in nonmagnetic matrix, such as in $CoAl_n$ (n = 1-35) [18] clusters. It reflects that the local environment of the magnetic impurity changes with the variation of the nonmagnetic atoms in cluster. As seen from Fig.2., the delocalization of the d-electron happens abruptly rather than in a gradual way [1, 2]. This can be attributed to the absence of the Coulomb correlation between d-electrons at different sites and the less coordinate number in 1D case.

The spectral density of the excited states for the d-electrons can be obtained from the propagators in Eq.(8). The total spectral densities of the excited states in the systems with N=15 and N=25 are shown in Fig.3 and Fig.4, respectively. There exist two local modes near the lower energy level ϵ_d and upper energy level $\epsilon_d + U$, these two local modes correspond to the single-electron levels. Similar to the infinite systems, there are a series of closely spaced states lying between them, which may form a narrow hybridizing band when N approaches infinity, these two bands might correspond to the Friedel's resonant states, the fact that the levels are discrete and the width of the resonant states is very narrow implies that the finite system exhibits strongly localized character. The quantum size effect of the energy level cann't seen clearly from the Fig.3 and Fig.4 since the energy-level shift is relatively small, it is about 0.001 to 0.01, which is difficult to reflect in the figures. It is found that the electrons most probably occupy the spin-up lower energy level, and the present distribution of one-electron energy levels has some similarity to that obtained by the local density functional technique [9].

When a local magnetic moment is situated at a nonmagnetic metal, it will polarize the spins of its surrounding conduction electrons, therefore the local moment will be partially or completely "screened" by the conduction electrons. An exactly screened local moment by the conduction electrons will form a singlet and may lead to the abnormality of the conductivity and the specific heat. This phenomenon is the so-called "Kondo effect" [19, 20]. Recently, the size-dependence of the Kondo energy scale, i.e. the Kondo temperature, is studied both in point contacts [21] and in thin film, an explicit size-dependence of the Kondo temperature and the Kondo peak in the differential resistance is observed in [21]. The magnetic moment distribution of the polarized conduction electrons around the local magnetic moment is an important physical properties in such a dilute magnetic cluster. We have calculated the spatial distribution of the spins of the conduction electrons for two systems with N=15 and N=25. The distribution of the polarized magnetic moments is shown in Fig.5. The nearest-neighbor polarized spins are antiparallel to the local moment, it may be parallel in the next-nearest-neighbor site. the nearest-neighbor polarized moment in the 1D system is -0.09 μ_B for N=15 and -0.12 μ_B for N=25. It is found that the period and amplitude of the Friedel's oscillation change with respect to the size, although these two systems (with different sizes N=25 and N=15) has the same parameters. It is found that the larger the system is, the shorter the period of the Friedel's oscillation is. Because of the hybridization interaction between the conduction electrons and the d-electron, the conduction electrons have some possibilities to enter the impurity atom, so the number and the magnetic moment of the conduction electrons don't vanish at the impurity site.

III.2 Three-Dimensional Finite Systems

In the following, we have studied the formation of the local magnetic moment and the size effect on the magnetic properties in 3D dilute clusters, however, for the 3D cases, one may meet the difficulty of the giant possible configurations when the number of atoms in clusters exceeds 8-10 [5, 9]. The real geometry must be determined by other methods, such as the first-principle electronic structure calculation by minimizing the total energy or the molecular-dynamic simulation by ensuring the structure in the lowest equilibrium state. To determine the optimal cluster structure is beyond our scope. In the present paper, we investigate some small 3D systems with the high-symmetry structure, these systems consist of 5, 7, 9 and 15 atoms. The corresponding structures of these systems are chosen as tetrahedron for 5-atom clusters, octahedron for 7-atom clusters, cube for 9-atom clusters and 6-capped-cube for 15-atom clusters. The impurity is situated at the center of the clusters, and the nonmagnetic metal atoms surround it.

A typical size-dependence of the local magnetic moments in 3D finite systems is shown in Fig.6. The local magnetic moments decrease monotonously with the increasing atoms when ϵ_d is shallow and U is small. Comparing with the 1D case, the local magnetic moment in 3D systems varying smoothly with the size may result from the increase of the coordination number. Though the absence of the valley feature in 3D cases, the dependence of the local magnetic moment on the cluster size are obvious. The strong size-dependence of the formation of the local magnetic moments originates from the quantum size effect. Because in these situations, the mean coordination number and the overlap of the wavefunction of atoms are reduced, which lead to the narrowing of the d-electron and

the conduction electron bands, the localized character become important for these finite systems. From Fig.6, one also finds that the impurity atom becomes nonmagnetic if the cluster size is large enough.

These results show that the formation of the local magnetic moment in finite system is different from that in bulk case. Since the size is finite, the electronic structure and the density of states are modified by the quantum size effect, the condition of the occurrence for local magnetic moments in infinite systems, $\mathrm{U}\rho_{d\sigma}(\mu) > 1$, might need to be modified for the formation of local magnetic moment in small system. The condition should show explicit size dependence, can it be $\mathrm{U(N)}\rho_{d\sigma}(\mu, N) > 1$? But the finite boundary and the broken translation-symmetry make it too difficult to obtain an explicit expression in the momentum space as in the case of infinite system. According to the experimental results [1, 2], it seems that the deviation of the local moment in small systems to that in bulks, $\delta\mu$, may be the order of $\frac{1}{N}$ in magnitude, i.e., $\delta\mu \sim O(\frac{1}{N})$, when N exceeds a certain critical value. In our group, some work are being done to try to elucidate the problem by the first-principle electronic structure calculation for the clusters with the 3d or 4d transition metal impurity.

The peak and valley of the local magnetic moments in certain sizes of 1D systems might be related to the magic number of the total electrons. It should be pointed out that in 1D systems, the scattering of the conduction electrons by the impurity are dominant, however, near the absolute zero temperature, the quantum interference effect will play an important role in 3D case, the movement of the conduction electrons may be ballistic, and this might contribute another correction to the formation of the local magnetic moment.

As a result of the mean-field approach, there are two disadvantages. First the dynamic fluactuation effect, such as the local spin fluctuation and the spatial fluctuaction, are neglected; Second, the quantum interference effect and the weak localization, which may play a role in nanoscale systems, are not considered. Our next aim is to study the influence of these dynamic and quantum effects on the formation of local magnetic moments in nanoscale systems.

IV. CONCLUSIONS

In summary, the magnetic properties of small finite systems up to a few nanometers have been studied in framework of the Anderson impurity model, we find that the formation of the local magnetic moment depends not only on the energy level and the Coulomb interaction of the d-electron but also on the dimensionality and the size of finite system, the spectral densities of the local electronic states and the spatial distribution of the magnetic moment for the polarized conduction electrons exhibit strong size dependence both for 1D and 3D systems. These indicate that the difference of the magnetic behaviors between the small systems and the infinite systems is not only due to the size effect of exchange interaction between atoms but also due to the size-dependence of the formation of the local magnetic moments.

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FIGURE CAPTIONS

Fig.1. The size-dependence of the local magnetic moments for several linear quantum chains. Theoretical parameters: (a) U =8.5, V =0.8, ϵ_d =-2.5, (b) U =4.0, V =0.4, ϵ_d =-0.5, (c) U =4.0, V =0.8, ϵ_d =-0.5.

Fig.2. The dependence of the local magnetic moment on the size of 1D systems. Parameters: (a) U=4.0, V = 0.4, ϵ_d= -1.0, (b) U=8.0, V = 0.8, ϵ_d= -3.0 .

Fig.3. The total spectral densities of the local electrons for the 1D system with N=15. The parameters are U=8.5, V=0.8 and ϵ_d=-2.5.

Fig.4. The total spectral densities of the local electrons for the 1D system with N=25. The parameters are U=8.5, V=0.8 and ϵ_d=-2.5.

Fig.5. The spatial distribution of the spins for the conduction electrons polarized by local moments in the 1D systems with N=15 (dash line) and with N=25 (solid line). Theoretical parameters in both two systems: U=8.5, V=0.8 and ϵ_d=-2.5. The local magnetic moments of the impurity are $m_d = 0.945\mu_B$ and m_d=0.976, respectively.

Fig.6. The dependence of the local magnetic moment on the size for the 3D systems. Parameters: (a) U=20.0, V = 0.4, ϵ_d= -10.0, (b) U= 3.0, V = 0.8, ϵ_d= - 1.5.