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Finite-size effect and Kondo screening effect in an A-B ring with a quantum dot*

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The properties of the ground state of a closed dot–ring system with a magnetic flux in the Kondo regime are studied theoretically by means of a one-impurity Anderson Hamiltonian. The Hamiltonian is solved by means of the slave-boson mean-field theory. It is shown that at T=0, a suppressed Kondo effect exists in this system even when the mean level spacing of electrons in the ring is larger than the bulk Kondo temperature. The physical quantities depend sensitively on both the parity of the system and the size of the ring; the rich physical behaviour can be attributed to the coexistence of both the finite-size effect and the Kondo screening effect. It is also possible to detect the Kondo screening cloud by measuring the persistent current or the zero field impurity susceptibility $\chi_{\rm imp}$ directly in future experiments.

Keywords: finite-size effect, Kondo screening effect, A-B ring, quantum dot
PACC: 7210, 7335, 7530H

1. Introduction

The Kondo effect is a well known and widely studied phenomenon in condensed-matter physics.[1] Recent advances in nanofabrication technology have made it possible to investigate various aspects of this effect using a quantum dot (QD) coupled to electrodes by tunnelling barriers under controlled experimentally conditions,[2,3] which has aroused new interest in this phenomenon. In contrast to the enhancement of the resistivity due to the Kondo effect in a bulk metal, the Kondo resonance near the Fermi level, localized at the QD, provides a new channel for the mesoscopic current and leads to an increase of the conductance in a QD.[4]

Very recently, great effort has also been dedicated to the study of the equilibrium properties of the ground state of an A-B ring with an in-line QD.[5−10] Main features of interest are: (i) the effect of the Kondo resonance on the persistent current (PC) induced by a magnetic flux and (ii) the possibility of detecting the Kondo correlation length $\xi_{\rm K}$ (= $\hbar V_{\rm F}/k_{\rm B}T_{\rm K}^0$, where $V_{\rm F}$ is the Fermi velocity and $T_{\rm K}^0$ the bulk Kondo temperature) by measuring the Kondo-assisted persistent current (PC). In spite of many approximate methods available for attacking those problems, little theoretical consensus has emerged on various aspects of the mesoscopic Kondo effect. On the one hand, it has been indicated that with the decrease of the ring circumference L such that the mean level spacing δ of electrons in the ring is larger than $k_{\rm B}T_{\rm K}^0$, namely $\delta > k_{\rm B}T_{\rm K}^0$, the finite-size effect will suppress the Kondo effect and eventually eliminates it in the limit $\delta \gg k_{\rm B}T_{\rm K}^0$.[11−13] However, some theoretical studies show that in the limit of $\delta \gg k_{\rm B}T_{\rm K}^0$, the Kondo effect does not vanish since the electrons have to go through the QD in order to encircle the magnetic flux due to the particular geometry of this system,[7,14] and the Kondo effect also exists in a nanosized system.[15] At the same time a strong enhancement of the PC due to the Kondo resonance has been found [7] in the limit $\delta \gg k_{\rm B}T_{\rm K}^0$, but no appreciable enhancement was obtained in Refs.[8] and [9]. It was also found that the Kondo-assisted PC is strongly suppressed for an odd number of electrons in the limit $\delta \gg k_{\rm B}T_{\rm K}^0$,[8] while an opposite

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result was also obtained.[9,10] On the other hand, it is believed that when increasing the ring circumference L such that $\xi_K/L \approx 0.5$, the system crosses over from an incompletely screened singlet ground state to a fully screened one, which will have a great effect on the physical properties of the system. Therefore, this closed dot–ring system has been proposed as an ideal system in search of the Kondo screening cloud,[9] but which was considered to be impossible since the charge degrees of freedom are decoupled from the spin degrees of freedom in the Kondo problem.[12] It is very clear that there exist two effects, namely the finite-size effect and the Kondo screening effect, in this system, and thus the physical properties of this system will undergo a dramatic change, respectively, at $\xi_K/L \approx 0.5$ and $\delta/k_B T_K^0 \approx 1$ with the variation of the ring circumference L. The coexistence of two effects gives rise to the rich physical behaviour, which makes it quite difficult to investigate. So far, theoretical studies of this system have focused on either the finite-size effect [7,8] or the effect of the Kondo screening cloud on the physical properties of this system only.[9]

We mainly concentrate on both the finite-size effect and the Kondo screening effect. The paper is organized as follows. In Section 2 we give a description about the theoretical models for this dot–ring system. Section 3 gives a detailed discussion of our calculated results. The last section summarizes our conclusions.

2. Formulation of the models

A dot–ring system can be described by an N_σ = 2-fold degenerate one-impurity Anderson Hamiltonian.[4,6,8] In the limit $U \to \infty$ (U is the Coulomb repulsion in the QD), the Hamiltonian can be written in terms of auxiliary slave-boson (SB) operators [1,16] with a constraint

$$\begin{aligned} H =& \sum_{m\sigma} \varepsilon_m c_{m\sigma}^+ c_{m\sigma} + \sum_\sigma \varepsilon_d f_\sigma^+ f_\sigma \\ &+ \sum_{m\sigma} (t_m c_{m\sigma}^+ b^+ f_\sigma + \text{H.c.}) \\ &+ \lambda \left(b^+ b + \sum_\sigma f_\sigma^+ f_\sigma - 1 \right). \end{aligned} \tag{1}$$

Here $c_{m\sigma}^+$ ($c_{m\sigma}$) are the creation (annihilation) operators for electrons in the ring and λ is the Lagrangian multiplier. ε_d represents the single particle energy in the QD, and $\varepsilon_m = -2t\cos\left(\frac{m}{N}\pi\right)$, $t_m = \sqrt{\frac{2}{N}} \mathrm{i} \sin\left(\frac{m}{N}\pi\right)(t_L + t_R e^{\mathrm{i}\phi}(-1)^{m+1})$ with $m = 1, 2, \ldots, N-1$. Here t and N are the nearest neighbour hopping amplitude and the number of lattice sites including a QD, respectively. t_L (t_R) is the hopping matrix element of the QD state with the left (right) neighbouring site, and the phase factor ϕ is defined by $\phi = 2\pi\Phi/\Phi_0$, where Φ and Φ_0 are the external flux and the flux quantum ($= hc/e$), respectively. In the SB representation, the dot level is represented as $d^+ = f_\sigma^+ b$, where the pseudo-fermion operator f_σ^+ and the SB operator b^+ describe the singly occupied and the empty dot states, respectively. Since the dot is either empty or singly occupied, the constraint $b^+ b + \sum_\sigma f_\sigma^+ f_\sigma = 1$ has to be fulfilled.

In the mean-field approximation (MFA), the SB operator b is replaced by one constant $b_0 = \langle b(t) \rangle$, neglecting the fluctuation around the average $\langle b(t) \rangle$ of the SB. At $T = 0$, this MFA is correct only for describing spin fluctuations (Kondo regime). In the chosen gauge in Eq.(1), the ring-electron contribution to the free energy is irrelevant to the flux ϕ and can be omitted in the calculation of the PC current. So we start from the impurity part of the free energy, which is given by [1,16]

$$\begin{aligned} F =& \frac{N_\sigma}{\pi} \int_{-\infty}^{\infty} f(\omega) \mathrm{Im}\ \mathrm{In} G_f(\omega^+) \mathrm{d}\omega \\ &+ (\tilde{\varepsilon}_d - \varepsilon_d)\left(\frac{\Delta}{\Delta_0} - 1\right), \end{aligned} \tag{2}$$

where $f(\omega)$ is the Fermi–Dirac distribution function. $\tilde{\varepsilon}_d = \varepsilon_d + \lambda$, $\Delta = b_0^2 \Delta_0$ and $\Delta_0 = \pi\rho(\varepsilon_F)\,|t(\varepsilon_F)|^2$. Δ_0 is the bare resonance level width, characterizing the coupling strength between the QD and the ring. $\rho(\varepsilon_F)$ and $t(\varepsilon_F)$ are the density of states and the hopping amplitude at the Fermi energy, respectively. For the half-filled case ($\varepsilon_F = 0$), $\rho(0) = 1/\delta = N/(2\pi t)$ and $|t(0)|^2 = \frac{2}{N}(t_L^2 + t_R^2 \mp 2t_L t_R \cos\phi)$, here the-holds for N even (even parity)and the+for N odd (odd parity). Thus, $\Delta_0 = (t_L^2 + t_R^2 \mp 2t_L t_R \cos\phi)/t$. $G_f(\omega^+)$ is the pseudo-fermion f_σ retarded propagator given by

$$G_f(\omega^+) = \left(\omega^+ - \tilde{\varepsilon}_d - \frac{\Delta}{\Delta_0} \sum_m \frac{|t_m|^2}{(\omega^+ - \varepsilon_m)}\right)^{-1}. \tag{3}$$

The PC is defined by the relation

$$I(\phi, T) = -\frac{e}{\hbar} \frac{\partial}{\partial\phi} F(\phi, T). \tag{4}$$

At zero temperature, by using the free energy in Eq.(2) and the retarded propagator in Eq.(3), we ob-

tain the following expression for the current:

$$I(\phi) = \frac{4et_{\rm L}t_{\rm R}\Delta}{\hbar N\Delta_0} \times \sum_{m\sigma} \frac{(-1)^{m+1}\sin^2\left(\frac{m}{N}\pi\right)(\varepsilon_m - \tilde{\varepsilon}_d)}{(\varepsilon_m - \tilde{\varepsilon}_d)^2 + \Delta^2}\sin\phi. \quad (5)$$

The renormalized parameters $\tilde{\varepsilon}_d$ and Δ represent, respectively, the position and width of the resonance peak in the QD, and the Kondo correlation energy is $T_{\rm K} = \sqrt{\tilde{\varepsilon}_d^2 + \Delta^2}$. At $T = 0$, by minimizing F with respect to $\tilde{\varepsilon}_d$ and Δ, we obtain a set of two self-consistent equations for the two unknown quantities $\tilde{\varepsilon}_d$ and Δ as follows:

$$\frac{\partial F}{\partial \tilde{\varepsilon}_d} = \frac{\Delta}{\Delta_0}\left(1 + \sum_{m\sigma}\frac{|t_m|^2}{(\varepsilon_m - \tilde{\varepsilon}_d)^2 + \Delta^2}\right) - 1 = 0,$$

$$\frac{\partial F}{\partial \Delta} = (\tilde{\varepsilon}_d - \varepsilon_d) + \sum_{m\sigma}\frac{|t_m|^2(\varepsilon_m - \tilde{\varepsilon}_d)}{(\varepsilon_m - \tilde{\varepsilon}_d)^2 + \Delta^2} = 0. \quad (6)$$

The zero field impurity susceptibility $\chi_{\rm imp}$ can be calculated by including a magnetic field h in the free energy $F(h)$, then taking the derivative with respect to h and setting h equal to zero. At $T = 0$, this gives

$$\chi_{\rm imp} = \left(-\frac{\partial^2 F}{\partial h^2}\right)_{h=0} = -(g\mu_\beta)^2\frac{\Delta}{\Delta_0}\sum_m \frac{|t_m|^2(\varepsilon_m - \tilde{\varepsilon}_d)}{[(\varepsilon_m - \tilde{\varepsilon}_d)^2 + \Delta^2]^2}. \quad (7)$$

It has been shown that physical properties of this system are universal scaling functions of $\xi_{\rm K}/L$ or $\delta/k_{\rm B}T_{\rm K}^0$ in the Kondo regime,[8,9] and so we solve numerically the set of Eqs.(6) as functions of the phase factor ϕ for various values of $\xi_{\rm K}/L$. The parameters are taken as $\varepsilon_d = -0.6$, $t_{\rm L} = t_{\rm R} = 0.25$ (Kondo regime), by which the bulk Kondo temperature $T_{\rm K}$, namely $T_{\rm K}^0$, in the bulk ($\delta \to 0$) Kondo limit is given as 7.8×10^{-4}, the bulk impurity susceptibility $\chi_{\rm imp}^0$ is $202(g\mu_\beta)^2$ and the bulk occupation number n_f^0 of the QD is 0.9938 (all energies in units of t) at $\phi = 0.5\pi$. It should be pointed out that the parameters do not affect the physics in the Kondo limit but only shift the value of the characteristic quantities $k_{\rm B}T_{\rm K}^0$, $\chi_{\rm imp}^0$ and n_f^0, thus it is sufficient to choose only one set of parameters for the calculation.[8]

3. Results

Figure 1 displays the variation of the impurity susceptibility $\chi_{\rm imp}$ with $\xi_{\rm K}/L$. At $\xi_{\rm K}/L \approx 16$, it can be found that although the finite-size effects increase the charge fluctuation of the QD, there still exists a finite zero-field impurity susceptibility at T=0. However, the impurity susceptibility $\chi_{\rm imp}$ is quite small compared with the bulk limit value $\chi_{\rm imp}^0$, which is the result of both the incompletely screened singlet ground state and the finite-size effects. The existence of a finite zero-field impurity susceptibility at T=0 indicates that the Kondo correlation is present in this system even at $\xi_{\rm K}/L > 1$ (i.e. $\delta/k_{\rm B}T_{\rm K}^0 > 1$). When reducing the scaling variable $\xi_{\rm K}/L$, the impurity susceptibility $\chi_{\rm imp}$ increases, and reaches the bulk limit value $\chi_{\rm imp}^0$ at $\xi_{\rm K}/L \approx 0.5$ for even parity due to the formation of a fully screened singlet ground state. In the $0.15 < \xi_{\rm K}/L < 0.5$ region, the impurity susceptibility $\chi_{\rm imp}$ is slightly greater than $\chi_{\rm imp}^0$ and approaches to $\chi_{\rm imp}^0$ at $\xi_{\rm K}/L \approx 0.15$ ($\delta/k_{\rm B}T_{\rm K}^0 \approx 1$). However, the situation is quite different for odd parity systems, where the impurity susceptibility $\chi_{\rm imp}$ also goes up with the decrease of $\xi_{\rm K}/L$, but it reaches $\chi_{\rm imp}^0$ at $\xi_{\rm K}/L \approx 2$, and comes to the maximum value of $1.5\chi_{\rm imp}^0$ at $\xi_{\rm K}/L \approx 0.5$ as the result of a fully screened singlet ground state, and then begins to go down and reaches the minimum value of $0.8\chi_{\rm imp}^0$ at $\xi_{\rm K}/L \approx 0.15$ due to the disappearance of the finite-size effects. In addition, the impurity susceptibility $\chi_{\rm imp}$ is smaller for even N than for odd N when $\xi_{\rm K}/L > 0.25$. The behaviour of the impurity susceptibility can be partly explained by the charge fluctuations in the QD. It is well known that $\chi_{\rm imp} \propto n_f^2/(1 - n_f)$,[1] and thus the smaller charge fluctuations means the greater susceptibility. In comparison with an even parity system, the charge fluctuations are small for odd N, which is clearly shown in Fig.1(b). The small charge fluctuations for odd N are due to the fact that high positions of peaks will suppress the charge fluctuations, and thus it is more favourable for the d electrons to develop a moment in the odd relative to the even system. This is different from that of Ref.[11], where an opposite result is obtained. This reflects the difference of physical properties between the two systems just as discussed in Ref.[12]. However, there is no evident change of n_f corresponding to the fluctuation of the impurity susceptibility $\chi_{\rm imp}$ around $\chi_{\rm imp}^0$ at $\xi_{\rm K}/L \approx 0.5$, especially the appearance of the peak and valley, respectively, at $\xi_{\rm K}/L \approx 0.5$ and $\xi_{\rm K}/L \approx 0.15$, for odd N, which only shows that the magnetic properties of impurities undergo a great change as a result of the formation of a fully screened singlet ground state and the vanishing of the finite-size effects, respectively, at $\xi_{\rm K}/L \approx 0.5$ and $\xi_{\rm K}/L \approx 0.15$.

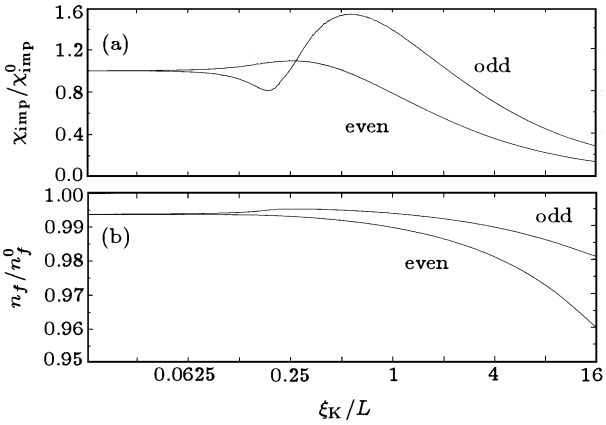


Fig.1. (a) The impurity susceptibility $\chi_{\rm imp}$ vs $\xi_{\rm K}/L$ and (b)the occupation number n_f of the QD vs $\xi_{\rm K}/L$ at $\phi = \pi/2$.

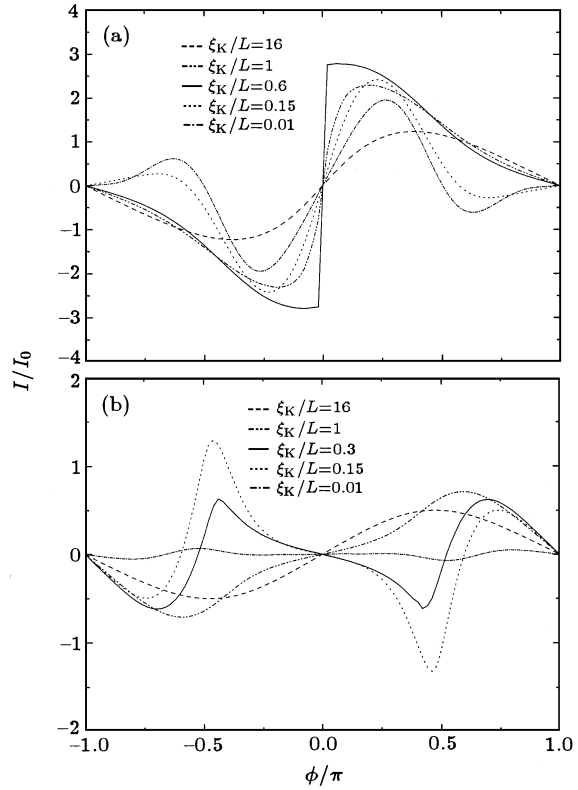


Fig.2. PC vs phase ϕ for rings of various size (a) for even parity and (b) for odd parity.

The I–ϕ characteristic curves are plotted for several values of $\xi_{\rm K}/L$ in Fig.2(a) for even N and 2(b) for odd N, respectively. It is found that the PC also goes through a great change, respectively, at $\xi_{\rm K}/L \approx 0.5$ and $\xi_{\rm K}/L \approx 0.15$, just as the impurity susceptibility $\chi_{\rm imp}$ does. Especially, we obtain three kinds of the functional forms of PC for the rings of various sizes but not two as found in Ref.[9]. At $\xi_{\rm K}/L \approx 16$, the resonance peaks are wide and are far from the Fermi energy, and the impurity susceptibility $\chi_{\rm imp}$ is small compared with $\chi^0_{\rm imp}$. In that case all levels of electrons in the ring can be neglected except for the Fermi level,[6] and thus sinusoidal oscillations of the PC with the magnetic flux are the obvious results. The functional form of PC begins to cross over from a sine function to a sawtooth-like at $\xi_{\rm K}/L \approx 1$, and a sawtooth-like with period 2π occurs at $\xi_{\rm K}/L \approx 0.5$ for even N, while a sawtooth-like with period π occurs at $\xi_{\rm K}/L \approx 0.3$ for odd N. At the same time the current peaks increase from I_0 ($= eV_{\rm F}/L$, which is the intensity of PC of a perfect ring with the same size) at $\xi_{\rm K}/L \approx 16$ to $2.7I_0$ at $\xi_{\rm K}/L \approx 0.5$ for even N, and from $0.5I_0$ at $\xi_{\rm K}/L \approx 16$ to $0.7I_0$ at $\xi_{\rm K}/L \approx 0.3$ for odd N. When the ring circumference increases further, the PC goes through the second change from a sawtooth-like to a Fano-like line shape at $\xi_{\rm K}/L \approx 0.15$, and here we describe the third kind of line shape of PC as a Fano-like line shape, since it looks similar to the Fano line shape.[17] In the limit of $\xi_{\rm K}/L \ll 1$, the PC retains a Fano-like line shape with a peak value of $2I_0$ for even N, but is strongly suppressed compared to I_0 for odd N. As far as the other case of the parity (i.e. an odd number of electron pairs for even parity and an even number of electron pairs plus one extra electron for odd parity) is concerned, it influences only the direction of the current and not the current–phase relation $I_N(\phi) = -I_{N+2}(\phi)$.

This size dependence of PC can be understood as follows. First of all, the Kondo ground state is a singlet state in which the impurity spin is screened by a cloud of ring-electron spins with length $\xi_{\rm K}$, so the Kondo effect is weaker due to the incomplete screening of the impurity spin for $\xi_{\rm K}/L > 1$ than it is for $\xi_{\rm K}/L < 1$. Secondly, the density of states at the Fermi energy will increase with reducing $\xi_{\rm K}/L$, which means that more and more levels of the ring are effectively coupled with the QD by quantum-mechanical tunnelling, and thus will contribute to the PC with the decrease of $\xi_{\rm K}/L$. Therefore, the appearance of a sawtooth-like at $\xi_{\rm K}/L \approx 0.5$ is a result of the complete screening of the impurity spin, while at $\delta/k_{\rm B}T^0_{\rm K} > 1$, it is believed that the finite-size effects suppress the Kondo effect,[11] and so one can say that the appearance of a Fano-like line shape at $\delta/k_{\rm B}T^0_{\rm K} \approx 1$ is a signature of the full Kondo resonance. The main factors for the parity dependence of the PC are: (i) the suppression of both charge fluctuations and the PC due to the high positions of peaks in odd relative to even system; (ii) the cancellation between the current resulting from up spins and the current resulting from

down spins:[8] namely, on the basis of Leggett's theorem, the direction of the PC in an A-B ring depends only on the parity of the electron numbers with the given spin σ, N_e^σ. For an odd number of electrons, the sign of the current resulting from up spins is opposite to the one resulting from down spins due to $N_e^\uparrow = N_e^\downarrow \pm 1$, but with almost the same magnitude when $\xi_K/L \ll 1$, so they almost cancel out.

Our results are partly in agreement with the results of Ref.[9], but the difference is also obvious. The main distinction between those results is that the functional form of the PC changes twice in our approximation, i.e. from a sine function to sawtooth-like at $\xi_K/L \approx 0.5$, then to a Fano-like line shape at $\delta/k_B T_K^0 \approx 1$, whereas it changes only once as shown in Ref.[9], where the functional form of the PC crosses over from a sine function for $\xi_K/L \gg 1$ to a sawtooth at $\xi_K/L \ll 1$. The Fano-like line shape is reminiscent of the Fano resonance in condensed-matter physics.[17] Fano resonances are ubiquitous in resonant scattering,[18] and are observed whenever resonant and non-resonant scattering paths interfere. In this one-dimensional dot–ring system, there is only one resonant scattering channel, thus there are no Fano resonances. In the SB MFA, the Hamiltonian is particle–hole asymmetric, and the electrons in the ring will suffer a pure potential scattering besides interacting antiferromagnetically with the impurity spin,[1] whereas a scattering state yields non-harmonic oscillations of the PC, and the sum of many non-harmonics will lead to the formation of the Fano-like line shape in the limit $\xi_K/L \ll 1$. The situation is different in the approaches of Ref.[5,9], where the particle–hole symmetry is present, and thus in the ground state the oscillations of the PC are sawtooth-like arising from the sum of many harmonics.[5] In addition, the PC is predicted to be small for N odd for small ξ_K/L but not for large ξ_K/L in our calculation, opposite to the results of Ref.[5,9]. The subject has also been attacked by the variational approximation in Ref.[9], where an opposite behaviour of the PC was found, i.e, the functional form of the PC crosses over from a sawtooth for $\xi_K/L \gg 1$ to a sine function at $\xi_K/L \ll 1$; whereas the scaling behaviour of the correlation energy and the results of a small PC for an odd number of electrons at $\xi_K/L \ll 1$ are in agreement with ours.

4. Conclusions

In conclusion, we have conducted a theoretical study of various aspects of the Kondo resonance occurring in a dot–ring system by employing the slave-boson technique in mean-field approximation. Our results demonstrate that at T=0, a suppressed Kondo effect exists in this system when $\delta/k_B T_K^0 > 1$, and the physical quantities depend sensitively on both the parity of this system and the size of rings, as well as that the rich physical behaviour can be attributed to the coexistence of both the finite-size effect and the Kondo screening effect. On the one hand, when increasing the ring circumference such that $\xi_K/L \approx 0.5$, the system crosses over from a incompletely screened singlet ground state to a fully screened one. On the other hand, when $\delta/k_B T_K^0 < 1$, the finite-size effect will disappear. Therefor, the physical properties of this system will undergo a dramatic change, respectively, at $\xi_K/L \approx 0.5$ and $\delta/k_B T_K^0 \approx 1$, with the change of the ring circumference. Our results also show that it is possible to detect the Kondo screening cloud by measuring the PC or the zero field impurity susceptibility χ_{imp} directly in future experiments.

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