Field-induced SU(4) to SU(2) Kondo crossover in a half-filling nanotube dot: spectral and finite-temperature properties

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(Dated: March 31, 2020)

We study finite-temperature properties of the Kondo effect in a carbon nanotube (CNT) quantum dot using the Wilson numerical renormalization group (NRG). In the absence of magnetic fields, four degenerate energy levels of the CNT consisting of spin and orbital degrees of freedom give rise to the SU(4) Kondo effect. We revisit the universal scaling behaviour of the SU(4) conductance for quarter- and half-filling in a wide temperature range. We find that the filling dependence of the universality at low-temperatures $T$ can be explained clearly with an extended Fermi-liquid theory.

This theory clarifies that the $T^2$ coefficient of conductance becomes zero at quarter-filling whereas the coefficient at half-filling is finite. We also study a field-induced crossover from the SU(4) to SU(2) Kondo state observed at the half-filled CNT dot. It is caused by the matching of the spin and orbital Zeeman splittings, which lock two levels among the four at the Fermi level even in magnetic fields $B$. We find that the conductance shows the SU(4) scaling behaviour at $\mu_B B < k_B T_{K}^{SU(4)}$ and it exhibits the SU(2) universality at $\mu_B B \gtrsim k_B T_{K}^{SU(4)}$, where $T_{K}^{SU(4)}$ is the SU(4) Kondo temperature.

To clarify how the excited states evolve along the SU(4) to SU(2) crossover, we also calculate the spectral function. The results show that the Kondo resonance width of the two states locked at the Fermi level becomes sharper with increasing fields. The spectral peaks of the other two levels moving away from the Fermi level merge with atomic limit peaks for $\mu_B B \gtrsim k_B T_{K}^{SU(4)}$.

PACS numbers: 72.15.Qm, 73.63.Kv, 75.20.Hr

I. INTRODUCTION

Quantum dots provide an ideal testbed to investigate strong correlations between the electrons in localized levels and the conduction electrons in reservoirs. Kondo effect is a typical many-body phenomenon that occurs also in quantum dots having local spin degrees of freedom. The Kondo effect in quantum dots has been studied theoretically and experimentally. In addition to the spin degrees of freedom, carbon nanotube (CNT) quantum dots have also the orbital (valley) degrees of freedom, corresponding to clockwise and counter clockwise orbitals around the nanotube axis. Four energy levels consisting of the spin and orbital degrees of freedom give rise to the SU(4) Kondo effect in the case where the four localized states are degenerate. A number of experiments for non-equilibrium transport have observed the SU(4) Kondo effect. Perturbations such as spin-orbit coupling, valley mixing, and magnetic fields break the SU(4) symmetry. Effects of such perturbations on the Kondo state are theoretically studied for instance, using Wilson’s numerical renormalization group (NRG) approach which has been extended to explore transport coefficients and spectral functions with very high accuracy.

The main purpose of the present paper is to clarify the finite temperature properties of the Kondo effect in CNT dots. In the first half of this paper, we study the scaling behaviour of the SU(4) conductance at quarter- and half-filling. Although the scaling behaviour has been studied, we revisit it with an extended microscopic Fermi-liquid description, which describes transport phenomena at low-temperatures $T$. The Fermi-liquid description shows that the $T^2$ coefficient $C_T$ for the conductance is determined in terms of five Fermi-liquid parameters, i.e., electron filling, two linear-susceptibilities, and two non-linear susceptibilities which are defined with respect to the equilibrium ground state. We successfully explain the filling dependence of the scaling with the description. Specifically, we explore the filling dependence of $C_T$ by calculating the five parameters and find that $C_T$ becomes zero at quarter-filling whereas it is finite at half-filling.

In the second half of this paper, we examine a field induced crossover from SU(4) to SU(2) Kondo state at half-filling nanotube dot. At the valley where the
crossover occurs, the SU(4) Kondo resonance emerges in the absence of magnetic field, because \( \Delta_{K,K'} \) and \( \Delta_{SO} \) are smaller than the SU(4) Kondo energy scale, \( k_B T_K^{SU(4)} \). The field induced crossover is different from the other crossover occurring at quarter-filling.\(^{27, 28, 37–43} \) Specifically, this crossover at half-filling occurs in a situation where two localized levels among the four remain the Fermi level even in magnetic fields while the other two levels move away from the Fermi level. The situation realizes if the spin Zeeman splitting coincides the orbital splitting. Such a coincidence can be reasonably expected in real CNT dots.

In the previous work, we have studied the crossover occurring in this situation, by calculating quasi-particle parameters such as phase shift \( \delta \), wave function renormalization factor \( Z \) and Wilson ratio \( R \).\(^{29} \) We have found that the applied magnetic fields enhance the electron correlation.

In this paper, we calculate the temperature dependence of the conductance in magnetic fields to clarify the crossover in a wide range of temperature \( T \). We show that a temperature scale \( T^* \) around which the conductance shows log\( T \) dependence decreases with increasing magnetic fields. This decrease of \( T^* \) becomes clearer in a strong Coulomb interaction case and agree with the field dependence of \( Z \). We also examine the scaling behaviour of the conductance. Whereas the conductance follows the SU(4) scaling at \( \mu_B B < k_B T_K^{SU(4)} \), it shows the SU(2) scaling at \( \mu_B B \gg k_B T_K^{SU(4)} \).

In addition to the conductance, we calculate the level resolved spectral functions in magnetic fields. The component for the doubly degenerate levels shows that the Kondo resonance width becomes sharper with increasing magnetic fields. This field dependence of the width corresponds to that of \( T^* \). Spectral weights of the other two states transfer from the Fermi level, and the peaks merge with atomic limit peaks.

This paper is organized as follows. In the next section, we describe the microscopic Fermi-liquid theory and the NRG approach to CNT dots. In Sec. III, we examine the scaling behaviour of the SU(4) conductance at quarter- and half-filling. We discuss how the quasi-particle parameters evolve during the field induced crossover in Sec. IV. We present the NRG results of conductance and discuss the influence of magnetic fields on the temperature dependence of conductance in Sec. V. The spectral functions in increasing magnetic fields are shown in Sec. VI. Summary is given in Sec. VII.

II. FORMULATION

Transport properties of carbon nanotube quantum dots are determined by a linear combination of four one-particle levels, consisting of the spin (\( \uparrow, \downarrow \)) and valley (K, K') degrees of freedoms. The structure of these four states staying near the Fermi level depend on the inter-valley scattering, the spin-orbit coupling, and the Zeeman splittings of the spin and orbital degrees of freedoms. In this section we introduce the Anderson model for the CNT dot using a diagonal form for these local levels. We will provide a more microscopic description specific to a real CNT dot, for which high-resolution current and noise experiments have been carried out.\(^{30,33} \) The renormalized parameters that characterize the low-energy Fermi-liquid properties and details of the NRG calculations are also described in this section.

A. Anderson model for CNT quantum dots

We start with an Anderson impurity model for a CNT dot, which has \( N = 4 \) internal degrees of freedom and is connected to two noninteracting leads:

\[
\mathcal{H} = \mathcal{H}_0^d + \mathcal{H}_U + \mathcal{H}_e + \mathcal{H}_T, \tag{1}
\]

\[
\mathcal{H}_d^e = \sum_{m=1}^{N} \epsilon_m d_m^d d_m^\dagger, \quad \mathcal{H}_U = U \sum_{m < m'} n_{dm} n_{dm'}, \tag{2}
\]

\[
\mathcal{H}_e = \sum_{\nu=1}^{L,R} \sum_{m=1}^{N} \int_{-D}^{D} d\varepsilon \, \varepsilon^\dagger c_{\nu,\varepsilon,m} c_{\nu,\varepsilon,m} \tag{3}
\]

\[
\mathcal{H}_T = \sum_{\nu=1}^{L,R} \sum_{m=1}^{N} \nu \left( \psi_{\nu,m}^\dagger d_m + d_{m'}^\dagger \psi_{\nu,m} \right), \tag{4}
\]

\[
\psi_{\nu,m} \equiv \int_{-D}^{D} d\varepsilon \sqrt{\rho_{\nu,\varepsilon,m}}, \quad n_{dm} \equiv d_{m}^\dagger d_{m}. \tag{5}
\]

Here, \( d_{m}^\dagger \) and \( d_{m} \) are the creation and annihilation operators, respectively, for an electron with energy \( \varepsilon_m \) in the \( m \)-th discrete one-particle eigenstate of the dot (\( m = 1, 2, \ldots, N \)). We shall also call \( m \) the “flavour” in the following. The Coulomb interactions \( U \) between the electrons occupying the dot levels are assumed to be independent of \( m \), assuming that the intra- and inter-valley Coulomb repulsions to be identical. We also assume that Hund’s rule coupling can be neglected. This is consistent with the CNT dot in which the field-induced SU(4) to SU(2) Kondo crossover has been observed,\(^{19,35} \) and also with the other nanotube dots.\(^{12} \) Conduction bands in the leads on the left and right (\( \nu = L, R \)) are described by \( \mathcal{H}_L \). The conduction electrons are assumed to carry the flavour index \( m \), and the continuous energy states in the bands are normalized such that \( \{ c_{\nu,\varepsilon,m}, c_{\nu',\varepsilon',m'} \} = \delta(\varepsilon - \varepsilon') \delta_{\nu\nu'} \delta_{mm'} \). The Fermi level is chosen to be \( \varepsilon_F = 0 \), at the center of the flat conduction bands with the width \( 2D \). Charge transfer between the dot and leads are described by \( \mathcal{H}_T \). We assume that the tunneling matrix element \( \nu \) is independent of flavour \( m \), which can also be justified for a class of CNT dots.\(^{19,35} \) In this situation, the resonance width due to these hybridizations becomes \( \Delta = \Delta_L + \Delta_R \) with \( \Delta_{\nu} \equiv \pi \rho_{\nu} v_F^2 \).
and $\rho_c = 1/2D$ the density of states of the conduction band.

This Hamiltonian $\mathcal{H}$ conserves the total number of electrons for each flavour, $n_{dm} = \sum_{\nu} \int_{-D}^{D} e^{\nu}_{v,e,m} \tilde{e}_{v,e,m} \tilde{d}_{v,e,m}$. Correspondingly, it has a $U(1) \otimes U(1) \otimes U(1)$ symmetry. In the case that the dot levels are degenerate $\tilde{e}_m = \tilde{e}_d$ for $m = 1, 2, \ldots, N$, the system additionally has the $SU(N)$ symmetry. Furthermore, the system also has the electron-hole symmetry at $\tilde{e}_d = -(N-1)/2$. Unless other wise stated, we set the Boltzmann constant $k_B$ to unity i.e., $k_B = 1$.

B. Transport coefficients and Fermi-liquid parameters

Transport coefficients of quantum dots can be expressed in terms of the retarded Green’s function $G^r_m(\omega)$ defined with respect to the equilibrium state:

$$ G^r_m(\omega, T) = -i \int_0^\infty dt \, e^{i(\omega + i\delta) t} \langle \{ d_m(t), d^\dagger_m(0) \} \rangle $$

$$ = \frac{1}{\omega - \epsilon_m + i\Delta - \Sigma_m(\omega, T)/\omega}, $$

$$ A_m(\omega, T) = -\frac{1}{\pi} \text{Im} G^r_m(\omega, T). $$

(6) (7) (8)

Here, $\langle O \rangle \equiv \text{Tr} \left[ e^{-H/T} O e^{H/T} \right] / \Xi$ with $\Xi \equiv \text{Tr} e^{-H/T}$ is the thermal average of an observable $O$. The phase shift $\delta_m$, which is the primary parameter characterize the Fermi-liquid ground state, is determined by the self-energy $\Sigma_m(\omega, T)$ at the Fermi level $\omega = 0$ and zero temperature $T = 0$,

$$ \delta_m = \frac{\pi}{2} - \tan^{-1}\left[ \frac{\epsilon_m + \Sigma_m(0, 0)}{\Delta} \right]. $$

(9)

The Friedel sum rule relates the phase shift $\delta_m$ to the occupation number $\langle n_{dm} \rangle$ which is the first derivative of the free energy $\Omega = -T \ln e^{-H/T}$,

$$ \langle n_{dm} \rangle = \frac{\partial \Omega}{\partial \epsilon_m} \left. \right|_{T \to 0} \delta_m \left. \right|_{\pi}. $$

(10)

The linear-susceptibilities $\chi_{m_1, m_2}$ are important parameters to describe Fermi-liquid properties,

$$ \chi_{m_1, m_2} \equiv -\frac{\partial^2 \Omega}{\partial \epsilon_{m_1} \partial \epsilon_{m_2}} = -\frac{\partial \langle n_{dm_1} \rangle}{\partial \epsilon_{m_2}} T \to 0 A_{m_1}(0, 0) \left( \delta_{m_1, m_2} + \frac{\partial \Sigma_{m_1}(0, 0)}{\partial \epsilon_{m_2}} \right). $$

(11)

$$ \chi_{m_1, m_2} = \int_0^{1/T} d\tau \langle \delta n_{dm_1}(\tau) \delta n_{dm_2}(\tau) \rangle. $$

(13)

Here, $\delta n_{dm} \equiv n_{dm} - \langle n_{dm} \rangle$ is the fluctuation of the occupation number, and $\delta n_{dm}(\tau) = e^{i\mathcal{H} \tau} \delta n_{dm} e^{-i\mathcal{H} \tau}$. The Ward-Takahashi identities relate the linear-susceptibilities to the wave function renormalization factor $Z_m$ and the vertex function $\Gamma_{mm'; m'm}(0, 0, 0)$$^{45,46}$

$$ \chi_{m, m'} = \frac{A_m(0, 0)}{Z_m}, \quad 1 \equiv 1 - \frac{\partial \Sigma_m(\omega, 0)}{\partial \omega} \left. \right|_{\omega = 0}, $$

$$ \chi_{m, m'} = -A_m(0, 0) A_{m'}(0, 0) \Gamma_{mm'; m'm}(0, 0, 0). $$

(14) (15)

The linear-susceptibilities can be also expressed as two-body correlations,

$$ \chi_{m_1, m_2} = \int_0^{1/T} d\tau \langle \delta n_{dm_1}(\tau) \delta n_{dm_2}(\tau) \rangle. $$

(16)

The Ward-Takahashi identities determine another important Fermi-liquid parameter, the residual interaction between quasi-particles,$^{47}$

$$ \bar{U}_{m, m'} \equiv Z_m Z_{m'} \Gamma_{mm'; m'm}(0, 0, 0) \cdot $$

(17)

Wilson ratio $R_{m, m'}$ corresponds to a dimensionless residual interaction,$^{48}$ which generally depends on $m$ and $m'$:

$$ \bar{R}_{m, m'} \equiv 1 + \sqrt{\bar{A}_m \bar{A}_{m'} \bar{U}_{m, m'}}. $$

(18)

Static non-linear susceptibilities determine the next leading Fermi-liquid corrections,

$$ \chi^{[3]}_{m_1, m_2, m_3} = -\frac{\partial^3 \Omega}{\partial \epsilon_{m_1} \partial \epsilon_{m_2} \partial \epsilon_{m_3}} = \frac{\partial \chi_{m_2, m_3}}{\partial \epsilon_{m_1}}. $$

(19)

$$ \chi^{[3]}_{m_1, m_2, m_3} = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \left\langle T, \delta n_{dm_1}(\tau_3) \delta n_{dm_2}(\tau_2) \delta n_{dm_3}(\tau_1) \right\rangle. $$

(20)

When each of the impurity energy levels is different each other, i.e., $\epsilon_i \neq \epsilon_j, (i \neq j)$, the linear and non-linear susceptibilities have $N(N+1)/2$ and $N(N+1)(N+2)/6$
components, respectively. In the SU(N) symmetric case, i.e., $e_i \equiv e_d$ for all $i$. The numbers of independent parameters for $\chi_{m_1,m_2}$ and $\chi_{m_1,m_2,m_3}$ decrease to 2 and 3, respectively. Specifically, $\chi_{m,m}$ and $\chi_{m,m'}$ are the independent parameters of the linear-susceptibilities. Correspondingly, $\chi_{m,m,m}$, $\chi_{m,m',m'}$ and $\chi_{m_1,m',m'}$ are the independent parameters of the non-linear susceptibilities for $m \neq n' \neq m'' \neq m$.

The conductance $g_{\text{tot}}$ through a quantum dot can be expressed in the Landauer form\cite{22,23,24,62}.

$$g_{\text{tot}} = \sum_{m=1}^{N} g_m, \quad (22)$$

$$g_m = \frac{e^2}{h} \frac{4\Delta_L\Delta_R}{\Delta_L + \Delta_R} \int_{-\infty}^{\infty} d\omega \left( -\frac{\partial f(\omega)}{\partial \omega} \right) \pi A_m(\omega,T). \quad (23)$$

Here, $f(\omega) = 1/(e^{\omega/T} + 1)$ is the Fermi distribution function. Using the formulas given in Appendix A of Ref.\cite{33}, we obtain a low-temperature expansion for $g_m$ up to terms of order $T^2$ in the symmetric tunnel coupling case $\Delta_L = \Delta_R = \Delta/2$.

$$g_m = \frac{e^2}{h} \left[ \sin^2 \delta_m + c_{T,m} (\pi T)^2 + \cdots \right]. \quad (24)$$

$$c_{T,m} = \frac{\pi^2}{3} \left[ w_{T,m} + \theta_{T,m}. \right] \quad (25)$$

The $T^2$ coefficient $c_{T,m}$ consists of $w_{T,m}$ and $\theta_{T,m}$ which represent contributions from the two body correlations and those from the three body correlations, respectively. Specifically, the linear and non-linear susceptibilities determine $w_{T,m}$ and $\theta_{T,m}$,

$$w_{T,m} = -\cos 2\delta_m \left( \chi_{m,m}^2 + 2 \sum_{m' \neq m} \chi_{m,m'}^2 \right), \quad (26)$$

$$\theta_{T,m} = \frac{\sin 2\delta_m}{2\pi} \left( \chi_{m,m,m}^{[3]} + \sum_{m' \neq m} \chi_{m,m',m'}^{[3]} \right). \quad (27)$$

These coefficients take much simpler form in the SU(N) symmetric case,

$$g_{\text{tot}} = \frac{N e^2}{h} \left[ \sin^2 \delta - C_T \left( \frac{\pi T}{T^*} \right)^2 + \cdots \right], \quad (28)$$

$$C_T = \frac{\pi^2}{48} (W_T + \Theta_T), \quad (29)$$

$$W_T = -\left[ 1 + 2 (N - 1) (R - 1)^2 \right] \cos 2\delta, \quad (30)$$

$$\Theta_T = \frac{\sin 2\delta}{2\pi} \frac{1}{\lambda_{m,m}^2} \left[ \chi_{m,m,m}^{[3]} + (N - 1) \chi_{m,m',m'}^{[3]} \right]. \quad (31)$$

In the expression of $W_T$, Eq.\cite{30}. The subscripts of the phase shift $\delta$ and Wilson ratio $R$ are suppressed in this case. $T^*$ is a characteristic energy scale which corresponds to the Kondo temperature,$T^* = \frac{1}{4\chi_{m,m}}. \quad (32)$. 

C. NRG approach to the spectral function and transport coefficients

The NRG has successfully been applied to multi-orbital quantum dots including CNT dots since a seminal work of Izumida et al.\cite{10,11,37,40,52,55}. With the NRG, the renormalized parameters such as the phase shifts $\delta$, the wavefunction renormalization factor $Z$, and the Wilson ratio $R$ can be calculated\cite{22,23,24,62}. In the present work, we use this approach to calculate not only the renormalized parameters, but also the linear conductance $g$ and the spectral function $A_m(\omega,T)$\cite{24,62}.

The key approximation of the NRG is the logarithmic discretization of the conduction band, which is controlled by a parameter $\Lambda$ ($> 1$). The noninteracting part of the discretized Hamiltonian $H_d^0 + H_T + H_c$ is transformed into a one-dimensional tight-binding chain with exponentially decaying hopping matrix elements $t_n \sim DA^{-n/2}$. Then, the total Hamiltonian $H$ including the interactions can be diagonalized iteratively by adding the states on the tight-binding chain, starting from the impurity site. Owing to the exponential decay of $t_n$, high energy states can be discarded at each successive step without affecting low-lying energy states so much. Although this iteration itself is an artificial procedure, it can be interpreted as a process to probe lower energy scale, step by step, stating from high-energy scale\cite{22,62}. Furthermore, the quasi-particles parameters $Z_m$, $\tilde{c}_m$, and $U_{m,m'}$ can be deduced from the asymptotic behaviour of the low-lying eigenvalues near the fixed point of this iteration procedure\cite{22,23,62}.

In the present work, we explore the CNT dots in which the four-fold degeneracy is not completely lifted by the magnetic field but still a double degeneracy remains for the reason which will be discussed in more detail in Sec.\cite{11,23,48}.

III. FIELD-INDUCED SU(4) TO SU(2) CROSSOVER OF KONDO SINGLET STATE

A. Microscopic description for the CNT-dot levels

The Hamiltonian $H$ defined in Eqs.\cite{11,23,48} are described using the representation in which the dot part $H_d^0$ has already been diagonalized. However, to see a mi-
The matrix \( H^0_d \) can be expressed in the following form, using the dot-electron operator \( \psi^\dagger_{d,\ell,s} \) for orbital \( \ell (=K, K') \) and spin \( s (=\uparrow, \downarrow) \),

\[
H^0_d = \sum_{\ell, \ell', s, s'} \psi^\dagger_{d,\ell,s} H^0_{\ell,d,\ell',s'} \psi_{d,\ell',s'} = \psi^\dagger_d H^0_d \psi_d .
\]

The matrix \( H^0_d \equiv \{ H^0_{\ell,d,\ell',s'} \} \) is given by \(7,28,37\)

\[
H^0_d = \varepsilon_d 1_s \otimes 1_{orb} + \frac{\Delta_{KK'}}{2} 1_s \otimes \tau^x + \frac{\Delta_{SO}}{2} \sigma^z \otimes \tau^z - \vec{M} \cdot \vec{b},
\]

\[
\vec{M} \equiv - \frac{1}{2} g_b \vec{\sigma} \otimes 1_{orb} - g_orb 1_s \otimes \tau^z \vec{e}_z.
\]

Here, \( \sigma^j = \{ \sigma^j_{ss'} \} \) and \( \tau^j = \{ \tau^j_{\ell\ell'} \} \) for \( j = x, y, z \) are the Pauli matrices for the spin and the valley pseudo-spin spaces, respectively. Correspondingly, \( 1_s = \{ \delta_{ss'} \} \) and \( 1_{orb} = \{ \delta_{\ell\ell'} \} \) are the corresponding unit matrices. In a finite magnetic field \( \vec{b} \equiv \mu_B \vec{B} \), where \( \mu_B \) is the Bohr magneton, both the spin and orbital moments contribute to the magnetization \( \vec{M} \). The g-factor for the spin is \( g_s = 2.0 \). The orbital moment couples to the magnetic field along the nanotube axis, and the orbital Zeeman splitting is given by \( \pm g_{orb} |\vec{b}| \cos \Theta \). Here, \( g_{orb} \) is the orbital Landé factor and \( \Theta \) is the angle of the magnetic field relative to the nanotube axis, which is chosen as the \( z \)-axis with \( \vec{e}_z \) the unit vector. The one-particle Hamiltonian of the dot levels \( H^0_d \) can be diagonalized via the unitary transform with the matrix \( U_d = (u_1, u_2, u_3, u_4) \), constructed with the eigenvectors,

\[
H^0_d u_m = \epsilon_m u_m , \quad u^\dagger_m \cdot u_{m'} = \delta_{mm'} .
\]

The operator \( d^\dagger_m \) that annihilates an electron in the eigenstate with energy \( \epsilon_m \) can be expressed in a linear combination of \( \psi^\dagger_{d,\ell,s} \)'s via this transform with \( U_d \).

In the case that \( \Delta_{SO} = \Delta_{KK'} = 0 \), the spin component of the magnetization becomes parallel to the field \( \vec{e}_z \) so \( \epsilon_\uparrow = \cos \Theta \vec{e}_z + \sin \Theta \vec{e}_\parallel \) while the orbital component is in the direction along the nanotube axes \( (\Theta \leq \pi/2) \). Then, the eigenvalues of \( H^0_d \) can be written as \( \epsilon_1 = \varepsilon_d - (g_{orb} \cos \Theta + g_{orb}/2) b, \epsilon_2 = \varepsilon_d - (g_{orb} \cos \Theta - g_{orb}/2) b, \epsilon_3 = \varepsilon_d + (g_{orb} \cos \Theta - g_{orb}/2) b, \) and \( \epsilon_4 = \varepsilon_d + (g_{orb} \cos \Theta + g_{orb}/2) b \). The eigenstates, for \( m = 1, 2, 3 \) and 4, correspond to \( |K\uparrow\downarrow\rangle, |K\uparrow\uparrow\rangle, |K\downarrow\downarrow\rangle \) and \( |K\uparrow\downarrow\rangle \), respectively, with \( \uparrow \) and \( \downarrow \) the spin defined with respect to the direction along the field \( \vec{b} \). Therefore, the thermal average of \( \vec{M} \) can be written in the form

\[
\langle \psi^\dagger_d \vec{M} \psi_d \rangle = M_{orb} \epsilon_z + M_s \epsilon_\parallel .
\]

\[
M_{orb} = g_{orb} \left[ \langle n_{d1} \rangle - \langle n_{d4} \rangle + \langle n_{d2} \rangle - \langle n_{d3} \rangle \right],
\]

\[
M_s = \frac{g_s}{2} \left[ \langle n_{d1} \rangle - \langle n_{d4} \rangle - \langle n_{d2} \rangle + \langle n_{d3} \rangle \right].
\]

**B. CNT level structure & field-induced crossover**

In recent experiments reported in Refs.\(^\text{19,35}\), non-linear current and current noise were measured for a CNT dot with the orbital Landé factor \( g_{orb} \approx 4 \) at finite magnetic fields with an angle \( \Theta \approx 75^\circ \). These values of \( g_{orb} \) and \( \Theta \) imply that the magnitude of the orbital Zeeman splitting becomes almost the same as the spin Zeeman splitting in this particular situation,

\[
g_{orb} \cos \Theta \approx \frac{1}{2} g_{orb} = 1 .
\]

This situation can take place for CNT dots as the orbital Landé factor \( g_{orb} \) depends significantly on the diameter of nanotube and takes a value around \( g_{orb} \approx 10 \). In the case where this matching of the orbital and spin Zeeman splittings is satisfied, the energy level of the dot has a double degeneracy which remains unlifted in magnetic fields:

\[
\epsilon_1 = \varepsilon_d - 2b, \quad \epsilon_2 = \varepsilon_d, \quad \epsilon_3 = \varepsilon_d + 2b, \quad \epsilon_4 = \varepsilon_d .
\]

In this case the occupation numbers of the degeneracy become the same \( \langle n_{d2} \rangle = \langle n_{d4} \rangle \). Thus, both the orbital and spin magnetizations are determined by the occupation numbers of the other two levels \( m = 1 \) and \( m = 4 \): \( M_{orb} = g_{orb} M_{14} \) and \( M_s = \frac{g_s}{2} M_{14} \), with

\[
M_{14} = \langle n_{d1} \rangle - \langle n_{d4} \rangle .
\]

We note that \( \Delta_{SO} \) and \( \Delta_{KK'} \) are less important for the examined CNT dot.\(^\text{22,23}\) In this situation, the system has an SU(2) rotational symmetry defined with respect to the degenerate states in the middle, and the U(1) symmetry that conserves the sum of the occupation numbers \( n_2 + n_4 \), in addition to the other two U(1) symmetries corresponding to \( n_1 \) and \( n_4 \) for the levels \( m = 1 \) and \( m = 4 \), respectively. Therefore, the SU(4) symmetry that the total Hamiltonian has at zero field breaks down to the U(1)\((m=1) \otimes SU(2) \otimes U(1)\)|\(m=2,3 \otimes U(1)\)|\(m=4 \) symmetry at finite magnetic fields. This SU(2) symmetric part plays a central role in the field-induced SU(4) to SU(2) Kondo crossover, occurring at half-filling point \( N_2 = 2 \). At this point, due to the matching condition given in Eq.\(^\text{41}\), the Hamiltonian \( H \) is invariant under an extended electron-hole transformation:

\[
d^\dagger_1 \Rightarrow h_4 , \quad d^\dagger_2 \Rightarrow h_3 , \quad d^\dagger_3 \Rightarrow h_2 , \quad d^\dagger_4 \Rightarrow h_1 ,
\]

and correspondingly, \( f_{\nu\epsilon_m,m'} \Rightarrow -f_{\nu,-\epsilon_m,m'} \) for \( (m, m') = (1, 4), (2, 3), (3, 2), (4, 1) \). Here, \( h_m \) and \( f_{\nu\epsilon_m,m'} \) annihilate hole in the dot and the conduction bands, respectively.
NRG calculations are carried out for an asymmetric half-filling $V$ at $V = 16\text{mK}$, $2\text{K}$, and $4.5\text{K}$. These two energies dominate the other energy scales; the valley mixing and spin-orbit interaction are much smaller than $U$ and $\Delta$: $\Delta_{\text{KK}} \approx \Delta_{\text{SO}} \approx 0.2\text{meV}$.

In Fig. 1, we compare the NRG results of the conductance at $T = 0$ with the experimental results obtained at $T = 16\text{mK}$ which is much lower than the Kondo temperature at half-filling $T_K^{\text{SU(4)}} = 4.3\text{K}$. The asymmetry in the lead-dot tunneling couplings is estimated as $4\Delta_L\Delta_R/\Delta_{\text{L}} + \Delta_L + \Delta_R = 0.92$. The comparisons which have been done also in Ref. 33 show that the NRG results nicely agree with the experimental results. We can clearly see in this figure that the Kondo ridge emerges near half-filling $V_g \approx 26\text{V}$ in the absence and presence of magnetic fields. Its height reduces from the SU(4) value $4e^2/h$ to the SU(2) value $2e^2/h$ as magnetic field increases. This reduction of the height implies that the observed SU(2) behavior is caused by the doubly degenerate states, which are labeled as $m = 2$ and $m = 3$ in Eq. (41) and are shifted towards the Fermi level in the half-filled case where $e_d = -3U/2$. Furthermore, the additional sub-peaks that emerge outside the Kondo ridge for large magnetic fields $B \gtrsim 4\text{T}$ can also be regarded as the resonances corresponding to the other two non-degenerate levels, labelled as $m = 1$ and $m = 4$. Note that the Kondo ridges corresponding to the 1/4 and 3/4 fillings are not so pronounced at $B = 0$ because the Coulomb interaction for this CNT dot $U/(\pi\Delta) = 2.0$ is not very large.

We have also examined in the previous work how $\Delta_{\text{KK}}$, $\Delta_{\text{SO}}$ and also the other perturbations that cause violations of the matching condition $g_{\text{orb}}\cos \Theta = \frac{1}{4}g_{\text{orb}}$ afield-induced SU(4) to SU(2) crossover. Our NRG results obtained for realistic situations show that this crossover is robust in a rather wide magnetic field range $0 \lesssim B \lesssim 5.0\text{T}$, where the energy scale of these perturbations is smaller than the Kondo temperature $T_K^{\text{SU(4)}}$.

Our NRG results for the CNT dots, reported so far, were restricted to ground-state properties. The present work sheds light also on the finite-temperature and dynamic properties of the Kondo crossover. First of all, we consider the zero field case $B = 0$. Figure 2 compares the experimental results of the zero-field conductance measured at $T = 16\text{mK}$, $2\text{K}$, and $4.5\text{K}$ with the corresponding NRG results, calculated for slightly lower temperatures $T = 0\text{K}$, $1.7\text{K}$, and $3.8\text{K}$ to demonstrate how these comparisons work at the best. We see a reasonable agreement between the theoretical results and experimental results. The height of the Kondo ridge emerging near half-filling $V_g \approx 26\text{V}$ decreases as temperature increases. At temperatures of order $T \sim T_K^{\text{SU(4)}} = 4.3\text{K}$, Four peaks corresponding to the Coulomb oscillation emerge. This agreement also indicates that the experimental results of the conductance can be explained by the theory of the SU(4) Kondo effect.

C. Comparison of NRG and experiments results: gate-voltage dependence at finite $B$ or $T$

In the previous work, we showed that the level scheme, defined in Eq. (41), nicely explain the field-induced SU(4) to SU(2) Kondo crossover observed at half-filling $N_d = 2$ where two electrons occupy the local levels of the CNT dot. The Coulomb interaction for this CNT dot is estimated to be $U \approx 6\text{meV}$, and the hybridization energy is $\Delta \equiv \Delta_L + \Delta_R \approx 0.9\text{meV}$ and it is nearly symmetric $\Delta_L \approx \Delta_R$. We can clearly see in this figure that the Kondo ridge emerges near half-filling $V_g \approx 26\text{V}$ in the absence and presence of magnetic fields. Its height reduces from the SU(4) value $4e^2/h$ to the SU(2) value $2e^2/h$ as magnetic field increases. This reduction of the height implies that the observed SU(2) behavior is caused by the doubly degenerate states, which are labeled as $m = 2$ and $m = 3$ in Eq. (41) and are shifted towards the Fermi level in the half-filled case where $e_d = -3U/2$. Furthermore, the additional sub-peaks that emerge outside the Kondo ridge for large magnetic fields $B \gtrsim 4\text{T}$ can also be regarded as the resonances corresponding to the other two non-degenerate levels, labelled as $m = 1$ and $m = 4$. Note that the Kondo ridges corresponding to the 1/4 and 3/4 fillings are not so pronounced at $B = 0$ because the Coulomb interaction for this CNT dot $U/(\pi\Delta) = 2.0$ is not very large.

We have also examined in the previous work how $\Delta_{\text{KK}}$, $\Delta_{\text{SO}}$ and also the other perturbations that cause violations of the matching condition $g_{\text{orb}}\cos \Theta = \frac{1}{4}g_{\text{orb}}$ affect the field-induced SU(4) to SU(2) crossover. Our NRG results obtained for realistic situations show that this crossover is robust in a rather wide magnetic field range $0 \lesssim B \lesssim 5.0\text{T}$, where the energy scale of these perturbations is smaller than the Kondo temperature $T_K^{\text{SU(4)}}$.

Our NRG results for the CNT dots, reported so far, were restricted to ground-state properties. The present work sheds light also on the finite-temperature and dynamic properties of the Kondo crossover. First of all, we consider the zero field case $B = 0$. Figure 2 compares the experimental results of the zero-field conductance measured at $T = 16\text{mK}$, $2\text{K}$, and $4.5\text{K}$ with the corresponding NRG results, calculated for slightly lower temperatures $T = 0\text{K}$, $1.7\text{K}$, and $3.8\text{K}$ to demonstrate how these comparisons work at the best. We see a reasonable agreement between the theoretical results and experimental results. The height of the Kondo ridge emerging near half-filling $V_g \approx 26\text{V}$ decreases as temperature increases. At temperatures of order $T \sim T_K^{\text{SU(4)}} = 4.3\text{K}$, Four peaks corresponding to the Coulomb oscillation emerge. This agreement also indicates that the experimental results of the conductance can be explained by the theory of the SU(4) Kondo effect.
D. Scaling behaviour of SU(4) conductance at quarter and half-filling

In this section, we examine the scaling behaviours of conductance as functions of temperature especially at quarter-filling $N_d = 1$ and half-filling $N_d = 2$. In Fig. 3, the valley is quarter and half-filled at gate voltages, $V_g \simeq 25V$ and $V_g \simeq 26V$, respectively. The first value of $V_g$ corresponds to the theoretical value $\epsilon_d/U = -1/2$, and the second one corresponds to $\epsilon_d/U = -3/2$. If the interaction $U$ is not so large, $N_d$ at $\epsilon_d/U = -1/2$ is larger than 1. However, the valley becomes almost quarter filled as $U$ becomes large. For instance, an NRG result of the filling number is $N_d \simeq 1.06$ for $U/\pi\Delta = 3.0$. Although the temperature dependence has been studied\textsuperscript{12}, we revisit it using the extended microscopic Fermi-liquid theory\textsuperscript{22}.

Figures 3(a) and (b) shows the temperature dependence of $g_{tot}$ at half-filling and quarter-filling, respectively. We choose four values of the interaction, $U/\pi\Delta = 2.0, 3.0, 4.0$, and 5.0, assuming the symmetric tunnel couplings $\Delta_L = \Delta_R = \Delta/2$. The first value is the experimental value for the valley where the SU(4) Kondo effect occurs. In other valleys, the experimental values of $U/\pi\Delta$ can be larger than 2.0, and we also consider the larger interaction cases. The temperatures are scaled by the Kondo energy scales $T^*$ defined in Eq. 32 for each $N_d$ and $U$. In each of the two figures, we find that the scaled conductance curves collapse into a single curve over a wide range of temperatures $T \lesssim T^*$ for $U/\pi\Delta \gtrsim 3.0$, and thus the conductance shows the universality for each filling.

To clarify the filling dependence of the universality, we replot the curves of quarter and half filling in Fig. 3(c). For the two curves, we choose the largest $U$ among the four, $U/\pi\Delta = 5.0$. We find that whereas these two curves almost overlap each other around $T \simeq T^*$, the conductance of quarter-filling is slightly larger than that of half-filling at low-temperatures $T < T^*$, especially around $T \simeq 0.1T^*$. The inset of Fig. 3(c) clearly shows such different behaviours depending on the filling.

This filling dependence of the scaling can be explained by the Fermi-liquid theory\textsuperscript{23,24}. The three-body fluctuation $\Theta_T$ for the $T^2$ coefficient $C_T$ defined in Eq. 29 vanishes in a wide range of filling $1 \lesssim N_d \lesssim 3$ because a charge susceptibility $\chi_C$ and its derivative $\partial \chi_C/\partial \epsilon_d$ are suppressed\textsuperscript{32}. Thus, $C_T$ is dominated by the two body fluctuation, $C_T = - (\pi^2/48) [1 + 3(R - 1)^2] \cos (\pi N_d/2)$ as can be seen in this expression, $C_T$ becomes 0 at quarter-filling $N_d = 1$, whereas it takes a finite value, $C_T = (\pi^2/48) [1 + 3(R - 1)^2]$ at half-filling $N_d = 2$. Thus, the conductance at $N_d = 1$ persists the zero temperature value up to $T/T^* \simeq 0.1$ as shown in the inset of Fig. 3. The finite value at $N_d = 2$ approaches $5\pi^2/144$ as the interaction becomes strong. This is because the Wilson ratio saturates to the strong coupling limit value $R \rightarrow 3/4$. At a finite value of the interaction $U/\pi\Delta = 3.0$, an NRG result of the coefficient is $C_T \simeq 0.34$ which is already close to the strong coupling limit value $5\pi^2/144$.

![FIG. 3. SU(4) conductance curves are plotted as functions of temperature $T$. (a) and (b) shows the results at half-filling and quarter-filling, respectively. In these figures, the conductance curves are plotted for four values of the interaction, $U/\pi\Delta = 2.0, 3.0, 4.0$, and 5.0. (c) shows the curves of half-filling and quarter-filling for the largest value $U/\pi\Delta = 5.0$. The inset of (c) is an enlarged view for $0.01 \leq T/T^* \leq 1$.

This inset clearly shows that the $T^2$ coefficient $C_T$ given in Eq. 29 vanishes at quarter-filling whereas that at half-filling does not. In (a)-(c), the x-axes are scaled by the Kondo temperature $T^* \equiv 1/(4\chi_{m,m})$. The values of $T^*/\Delta$ at half-filling are 0.41, 0.29, 0.20, and 0.13 for $U/\pi\Delta = 2.0, 3.0, 4.0$, and 5.0, respectively. Similarly, the values at quarter-filling are 0.82, 0.57, 0.37, and 0.23. The y-axes are normalized by the zero temperature values of conductance, $g_0 = (4e^2/h)\sin^2 \delta$. At half-filling, $\sin^2 \delta \equiv 1$ for any value of $U$, and at quarter-filling, $\sin^2 \delta = 0.56, 0.55, 0.54,$ and 0.54.
IV. EVOLUTION OF QUASI-PARTICLES ALONG THE FIELD-INDUCED CROSSOVER

Low energy properties of quantum dots are determined by the Fermi-liquid parameters for renormalized quasi-particles, i.e., $\tilde{\epsilon}_m$, $Z_m$, and $\tilde{U}_{m,m'}$. In this section, we describe how these related parameters evolve as magnetic field $b$ increases, during the SU(4) to SU(2) crossover of the Kondo single state, occurring for the dot levels defined in Eq. (11). Specifically, we consider the half-filled case corresponding to the point $V_g \approx 26$ V in the middle of the Kondo ridge seen in Fig. 1. The center of the dot levels is chosen to be $\epsilon_d = -(3/2)U$, and thus the average number of electrons in the dot levels conserves in a way such that $(n_{d1}) = \langle n_{d3} \rangle = 1/2$ and $\langle n_{d1} \rangle \rightarrow 1$ at finite magnetic fields.

We examine two different values for the Coulomb interaction in the following: (i) $U/(\pi \Delta) = 2.0$ and (ii) $U/(\pi \Delta) = 4.0$. The first one, (i), simulates the situation of the CNT dot, in which the field-induced crossover has been observed and the parameters have been estimated as $U \approx 6$ meV and $\Delta \approx 0.9$ meV. We can see more clearly the renormalization effects due to strong correlations in the second case (ii).

A. Fermi-liquid parameters for the real CNT dot

First of all, we consider the case $U/(\pi \Delta) = 2.0$ that is estimated by the recent experiments. The NRG results for this case are shown in Fig. 3. Figure 3a shows the transmission probability $T_m(0) = \sin^2 \delta_m$ and magnetization $M_{14} = \langle n_{d1} \rangle - \langle n_{d4} \rangle$, as a function of magnetic field at half-filling. The degenerate levels, $m = 2$ and $m = 3$, keep their positions just on the Fermi level for finite magnetic fields, and show the unitary limit transport $\sin^2 \delta_m \approx 1$, $d_2 = d_3 = \pi/2$. The magnetic field partly lifts the degeneracy and the other two states, $m = 1$ and
\( m = 4 \). For these orbitals, \( \sin^2 \delta_m \) decreases as magnetic field increases. The magnetization \( M_{14} \), which in the present case is determined by the occupation number or these two levels, increases as the magnetic field increases. It saturates to \( M_{14} \to 1 \) in the the limit of \( b \to \infty \), and the charge fluctuations are suppressed as \( \langle n_{d,1} \rangle \to 1 \) and \( \langle n_{d,4} \rangle \to 0 \).

Figure 4(b) shows the renormalized resonance level position \( \tilde{\varepsilon}_m \) as a function of magnetic field \( b \). The two-fold degenerate states at the center, \( \tilde{\varepsilon}_2 = \tilde{\varepsilon}_3 = 0 \), remain just on the Fermi level at arbitrary magnetic fields. The other two levels, \( \tilde{\varepsilon}_1 \) and \( \tilde{\varepsilon}_4 \) move away from the Fermi level as \( b \) increases. Slopes of them are steeper than those for the noninteracting electrons \( 2b \) (dashed line).

In the large field limit \( b \to \infty \), the renormalized level positions approach the one described in the mean-field theory, i.e., \( \tilde{\varepsilon}_1^{HF} = -(2b + U/2) \) and \( \tilde{\varepsilon}_4^{HF} = (2b + U/2) \). These asymptotic form can be obtained as follows, substituting the mean values \( \langle n_{d,1} \rangle = 1 \), \( \langle n_{d,4} \rangle = 0 \) and \( \langle n_{d,2} \rangle = \langle n_{d,3} \rangle = 1/2 \) into the dot-part of the Hamiltonian with \( \tilde{\varepsilon}_m = -(3/2)U \):

\[
\mathcal{H}_d^0 + \mathcal{H}_U = 2b(n_{d_1} - n_{d_4}) - \frac{3U}{2}(n_{d_2} + n_{d_3} + n_{d_1} + n_{d_4}) + U\left[n_{d_2}n_{d_3} + n_{d_1}n_{d_4} + (n_{d_2} + n_{d_3})(n_{d_1} + n_{d_4})\right] \\
\quad \xrightarrow{b \to \infty} U\left[n_{d_2}n_{d_3} - \frac{1}{2}(n_{d_2} + n_{d_3})\right] + \left(2b + \frac{U}{2}\right)(n_{d_4} - n_{d_1}) + \text{const.} \tag{44}
\]

Here, the Coulomb interaction between the orbitals \( m = 2 \) and \( 3 \) is kept undecoupled. This asymptotic Hamiltonian also shows that the symmetric SU(2) Anderson model describes the Fermi-liquid properties of these two orbitals.

The magnetic field dependence of the wavefunction renormalization factors \( Z_m \), plotted in Fig. 4(c) more clearly shows the crossover. At finite magnetic fields, only two of the four \( Z_m \)'s become independent: \( Z_2 = Z_3 \) and \( Z_1 = Z_4 \) because of the particle-hole symmetry given in Eq. (43). The first one is for the degenerate levels remaining on the Fermi level, and the second one is for the levels moving away from the Fermi level. At zero field, where the system has the SU(4) symmetry, these two factors for the different orbitals become identical each other: \( Z_2 = Z_1 = Z_{SU(4)} = 0.52 \) for \( U/(\pi \Delta) = 2.0 \). Substituting this SU(4) value into Eq. (52) gives the SU(4) Kondo energy scale \( T_{K_{SU(4)}}^{SU(4)}/\Delta = 0.41 \). Many-body effects significantly renormalize \( Z_2 \) from the SU(4) value as magnetic field increases. In the limit of \( b \to \infty \), it approaches the SU(2) symmetric value \( Z_{SU(2)} = 0.23 \), which determines the SU(2) Kondo energy scale \( T_{K_{SU(2)}}^{SU(2)}/\Delta = 0.19 \). The many-body effects become less important for \( Z_1 \) with increasing field, and \( Z_1 \) approaches the non-interacting value \( Z_1 \to 1 \) for the large magnetic field.

In order to clarify the many-body effects between electrons occupying the different orbitals, we also examine the orbital dependent Wilson ratio \( R_{m,m'} \) and corresponding residual interaction \( \tilde{U}_{m,m'} \). Figures 4(d) and 4(e) respectively show \( R_{m,m'} \to 1 \) and \( \tilde{U}_{m,m'} \) as functions of \( b/2K_{SU(4)} \). Magnetic field dependence of \( \tilde{U}_{m,m'} \) are plotted also in Fig. 4(f), where the magnetic field is scaled by \( U \) to examine behaviours of \( \tilde{U}_{m,m'} \) at larger fields \( b \gg T_{K_{SU(4)}}^{SU(4)} \). Owing to the particle-hole symmetry, only three of the six \( \tilde{U}_{m,m'} \) are independent: \( \tilde{U}_{2,3}, \tilde{U}_{1,4}, \) and \( \tilde{U}_{1,2} = \tilde{U}_{1,3} = \tilde{U}_{2,4} = \tilde{U}_{3,4} \). Correspondingly, three independent parameters of the Wilson ratios, \( R_{2,3}, R_{1,4}, \) and \( R_{1,2} \), can be deduced from Eq. (45):

\[
R_{2,3} - 1 = \frac{1}{Z_2} \frac{\tilde{U}_{2,3}}{\pi \Delta}, \tag{45}
\]
\[
R_{1,4} - 1 = \frac{\sin^2 \delta_1}{Z_1} \frac{\tilde{U}_{1,4}}{\pi \Delta}, \tag{46}
\]
\[
R_{1,2} - 1 = \sqrt{\frac{\sin^2 \delta_1}{Z_1}} \frac{1}{Z_2} \frac{\tilde{U}_{1,2}}{\pi \Delta}. \tag{47}
\]

Among the three independent parameters of \( R_{m,m'} \) and \( \tilde{U}_{m,m'} \), \( R_{2,3} - 1 \) and \( \tilde{U}_{2,3} \) are for the doubly degenerate orbitals on the Fermi level. At zero field, \( R_{2,3} \) and \( \tilde{U}_{2,3} \) take the SU(4) values \( R_{2,3} - 1 = 0.31 \) and \( \tilde{U}_{2,3}/(\pi \Delta) = 0.16 \) for \( U/(\pi \Delta) = 2.0 \), and \( R_{2,3} - 1 \) already approaches very closely to the value for the infinite Coulomb interaction: \( R_{SU(4)}^{max} \to 1 \approx 1/3 \). These parameters continuously evolve from the SU(4) values to the SU(2) symmetric values: \( R_{SU(2)} - 1 = 0.96 \) and \( \tilde{U}_{2,3}/(\pi \Delta) = 0.23 \).

We also discuss the field dependence of the other parameters, \( R_{1,2}, R_{1,4}, \tilde{U}_{1,2}, \) and \( \tilde{U}_{1,4} \). \( \tilde{U}_{1,2} \) decreases from the SU(4) value with increasing magnetic field, and the corresponding Wilson ratio \( R_{1,2} - 1 \) decreases to the non-interacting value 0. In contrast to \( \tilde{U}_{1,2}, \tilde{U}_{1,4} \) increases from the zero field value and becomes larger than \( \tilde{U}_{2,3} \) and \( \tilde{U}_{1,2} \) for \( b > T_{K_{SU(4)}}^{SU(4)} \). It further increases at the larger magnetic field regions \( b \gg T_{K_{SU(4)}}^{SU(4)} \) as shown in Fig. 4(f).

This field dependence of \( \tilde{U}_{1,4} \) is similar to that of \( U \) for a single orbital Anderson model\cite{66, 67}, although \( \tilde{U}_{1,4} \) does not approach to the bare value \( U \). We briefly discuss the field dependence of \( \tilde{U} \) and of the other Fermi liquid parameters also for the single orbital Anderson model in Appendix A. This enhancement of \( \tilde{U}_{1,4} \) does not result in the enhancement of \( R_{1,4} \). In fact, \( R_{1,4} - 1 \) as well as \( R_{1,2} - 1 \) decreases to 0 since the factor \( \sin^2 \delta_1 \) goes to 0. We note that \( R_{1,2} \) is slightly larger than \( R_{1,4} \) at arbitrary \( b \) in this case of \( U/(\pi \Delta) = 2.0 \).
FIG. 5. (a) $\sin^2 \delta_m$ and magnetization $M_{14} = \langle n_{d1} \rangle - \langle n_{d4} \rangle$, (b) renormalized level position $\bar{\varepsilon}_m$, (c) renormalization factor $Z_m$, (d) Wilson ratio $R_{m,m'} - 1$, and (e) residual interaction $\tilde{U}_{m,m'}$ are plotted as functions of magnetic field $b$ at half-filling $\varepsilon_d/U = -3/2$ for $U/(\pi \Delta) = 4.0$. The x axes in (a)-(e) are scaled by the SU(4) Kondo temperature $T^{SU(4)}_K = 0.2 \Delta = (0.016U)$ determined at $b = 0$. The axis in (f) is scaled by $U$ for examining the behaviour of $\tilde{U}_{m,m'}$ at larger magnetic fields. The dot levels $\varepsilon_m$ are chosen in a such way that is described in Eq. (41). In (a), $\sin^2 \delta_m$ and $M_d$ for $U/(\pi \Delta) = 2.0$ are also plotted by dashed lines to compare them with those for the present case $U/(\pi \Delta) = 4.0$. Similarly, $\bar{\varepsilon}_m$ for $U/(\pi \Delta) = 2.0$ are plotted in (b). The dash-dotted lines indicate the mean-field splitting $\varepsilon^{MF} = -(2b + U/2)$ and $\varepsilon^{MF} = (2b + U/2)$. In the limit of $b \to \infty$, $Z_2$, $R_{2,3} - 1$, and $\tilde{U}_{2,3}$ approach the SU(2) values for $U/(\pi \Delta) = 4.0$: $Z_2 \to 0.026$, $R_{2,3} \to 1.99$, and $\tilde{U}_{2,3}/\pi \Delta \to 0.026$.

B. Fermi-liquid parameters for larger $U$

We next consider a strong coupling case, taking the Coulomb repulsion to be $U/(\pi \Delta) = 4.0$, which is twice as large as the one studied in the above. For this case, effects on the interactions on the field-induced SU(4) to SU(2) emerges pronounced way. Such a situation is also realistic because the experimental values of $U$ and $\Delta$ depend on individual quantum dots and on the valleys to be measured.

In Fig. 5(a), ground-state values of $T_m(0) = \sin^2 \delta_m$ and $M_{14}$ are plotted vs magnetic field $b/T^{SU(4)}_K$ for both $U/(\pi \Delta) = 4.0$ and $U/(\pi \Delta) = 2.0$. The results for $U/(\pi \Delta) = 4.0$ and $U/(\pi \Delta) = 2.0$ are plotted with solid lines and dashed lines, respectively. The energy scale depends on the coupling constant as $T^{SU(4)}_K/\Delta = 0.2$ for $U/(\pi \Delta) = 4.0$ and $T^{SU(4)}_K/\Delta = 0.41$ for $U/(\pi \Delta) = 2.0$. We see that $\sin^2 \delta_m$ and $M_d$ of $U/(\pi \Delta) = 4.0$ show almost same $b$ dependences as those of $U/(\pi \Delta) = 2.0$, and thus they show the universality. The universal behaviour is determined by the $b$ dependence of a single parameter $\delta_1 (= \pi - \delta_4)$. Renormalized levels $\bar{\varepsilon}_m$ for $U/(\pi \Delta) = 4.0$ plotted in Fig. 5(b) show the different $b$ dependence from those for $U/(\pi \Delta) = 2.0$. Specifically, $\bar{\varepsilon}_m$ and $\bar{\varepsilon}_d$ stay closer to the Fermi level than those for $U/(\pi \Delta) = 2.0$. However, this different $b$ dependence does not affect the universal behavior of $\delta_1$ because the phase shift is determined by the ratio of $\bar{\varepsilon}_m$ and $\bar{\Delta}_m$, i.e., $\delta_m = \cot^{-1}(\bar{\varepsilon}_m/\bar{\Delta}_m)$.

Figures 5(b) and 5(c) show the renormalization factors $Z_m = \bar{\Delta}_m/\Delta$ and the Wilson ratios $R_{m,m'}$, respectively. As in the $U/(\pi \Delta) = 2.0$ case, the quasi-particle parameters $Z_2$ and $R_{2,3}$ for the doubly degenerate states at the Fermi level continuously evolve from the SU(4) value to the SU(2) value as $b$ varies from 0 to $\infty$. At zero field, these parameters take the SU(4) values: $Z_{SU(4)} = 0.25$ and $R_{SU(4)} = 0.33$ for $U/(\pi \Delta) = 4.0$. Note that the Wilson ratio is almost saturated to the maximum possible value $R^{max}_{SU(4)} - 1 = 1/3$ at zero field. In the opposite limit $b \to \infty$, these parameters for the two-fold degenerate states $(m = 2, 3)$ approach those for the...
symmetric SU(2) Anderson model: \( Z_{\text{SU}(2)} \rightarrow 0.026 \) and \( R_{23}^{\text{SU}(2)} - 1 \rightarrow 0.99 \) for the same \( U \). These results show that the renormalization factor \( Z_2 \) or \( \tilde{\Delta}_2 \), is most significantly affected by the strength of the Coulomb interaction. It determines the energy scale for large field as \( T_{K}^{\text{SU}(2)} = 0.02\Delta \) with Eq. (22). The quasi-particle parameters \( Z_1, R_{12} \) and \( R_{14} \), for the states moving away from the Fermi level approach the noninteracting value in the limit of \( b \rightarrow \infty \); i.e, \( Z_1 \rightarrow 1, R_{12} \rightarrow 1, \) and \( R_{14} \rightarrow 1 \). Notably, \( R_{14} \) becomes larger than \( R_{12} \) for \( U/(\pi\Delta) = 4.0 \) at finite \( b \). This is quite different what we have found for the smaller interaction case \( U/(\pi\Delta) = 2.0 \).

In order to clarify this difference, we plot the residual interactions \( U_{m,n} \) as functions of magnetic fields in Figs. 5(c) and 5(f). The magnetic fields of Figs. 5(c) and 5(f) are respectively scaled by \( T_{K}^{\text{SU}(4)} \) and \( U \). In these figures, especially in Fig. 5(f), we can see that \( U_{14} \) becomes much larger than the other two residual interactions \( U_{12} \) and \( U_{2,3} \) as \( b \) increases. This field dependence of \( U_{14} \) clearly explain why the corresponding Wilson ratio \( R_{14} \) becomes larger than \( R_{12} \). We also note that \( U_{2,3} \) for the doubly degenerate levels approach the SU(2) symmetric value \( U_{2,3}/(\pi\Delta) \rightarrow 0.026 \).

All these results discussed in this section indicate that the quantum fluctuations and many-body effects are enhanced for large magnetic fields as the number of active channel decreases from 4 to 2. We have also shown the enhancement of the fluctuations are more clearly seen for strong interactions by comparing the results for \( U/(\pi\Delta) = 4.0 \) to those for \( U/(\pi\Delta) = 2.0 \).

V. TEMPERATURE DEPENDENCE OF MAGNETOCO nductance

The above discussions about the Fermi-liquid parameters have mainly focused on the zero temperature properties of the crossover. The results show that the quasiparticles are strongly renormalized as the ground state undergoes the crossover from the SU(4) Kondo state to the SU(2) Kondo state.

In this section, we study the crossover at finite temperatures by calculating each component of the conductance \( g_m \) for \( m = 1,2,3,4 \) and the total conductance \( g_{\text{tot}} \) in a wide range of magnetic field. At half-filling, \( \varepsilon_d = -\frac{\pi}{2}U \) only two components are independent, i.e., \( g_2 = g_3 \) and \( g_1 = g_4 \) due to the level structure described in Eq. (11). The finite-temperature conductance, defined in Eq. (29), depends also on the excited states whose contributions enter through the spectral function \( A_m(\omega,T) \) which also depends on \( T \). We calculate the T-dependent \( A_m(\omega,T) \), using the NRG with some extended methods for dynamic correlation functions described in Sec. II C and Appendix B, to obtain \( g_m \). We examine two different interactions, \( U/(\pi\Delta) = 2.0 \) and 4.0, also for these components of the conductance assuming symmetric couplings \( \Delta_L = \Delta_R = \Delta/2 \).

A. Conductance for \( U/(\pi\Delta) = 2.0 \) at half-filling

In Figs. 6(a)-(d), we present results for the total conductance \( g_{\text{tot}} \) and the components \( g_2 = g_3 \) and \( g_1 = g_4 \) as functions of the temperature for six values of magnetic fields, \( b/T_{K}^{\text{SU}(4)} = 0.0, 0.25, 0.5, 1.0, 2.0, \) and 4.0. The SU(4) Kondo energy scale, determined at \( b = 0 \) for \( U/(\pi\Delta) = 2.0 \), is estimated to be \( T_{K}^{\text{SU}(4)} = 0.41\Delta \) as mentioned in Sec. IV A.

The total conductance in Fig. 6(a) at \( b = 0 \) logarithmically increases around \( T \sim T_{K}^{\text{SU}(4)} \). This logarithmic temperature dependence is a hallmark of the SU(4) Kondo effect. \( g_{\text{tot}} \) increases to the unitary-limit value \( 4e^2/h \) as temperature goes down to \( T \rightarrow 0 \). As the magnetic field increases, the low-temperature conductance at \( T = T_{K}^{\text{SU}(2)} \) decreases from the SU(4) unitary limit value \( 4e^2/h \) to the SU(2) one \( 2e^2/h \). We can also see that in a temperature range of \( 0.1T_{K}^{\text{SU}(2)} \lesssim T \lesssim T_{K}^{\text{SU}(4)} \), the conductance curve deforms continuously into the curve for the SU(2) symmetric case completed for \( b \rightarrow \infty \) where the characteristic energy scale becomes \( T_{K}^{\text{SU}(2)} = 0.19\Delta \). Therefore, the crossover can also be observed through the finite temperature measurements of the magnetocconductance. To examine how the magnetocconductance \( g_{\text{tot}} \) evolves with increasing \( b \) in more detail, we discuss the two components, \( g_2 \) and \( g_1 \).

Figure 6(b) shows the first component \( g_2 \) for the two states remaining at the Fermi level. As can be seen in this figure, \( g_2 \) decreases as \( b \) increases in the temperature range of \( 0.1T_{K}^{\text{SU}(2)} \lesssim T \lesssim T_{K}^{\text{SU}(4)} \). To clarify this decrease of \( g_2 \) in the range, we define an energy scale \( T^* \) by the renormalization factor \( Z_2 \) shown in Fig. 4(c),

\[
T^*_2 = \frac{\pi}{4}Z_2\Delta. \tag{48}
\]

This energy scale \( T^*_2 \) coincides \( T_{K}^{\text{SU}(4)} = 0.41\Delta \) at \( b = 0 \), and \( T_{K}^{\text{SU}(2)} = 0.19\Delta \) in the opposite limit \( b \rightarrow \infty \). The inset of Fig. 6(b) shows the energy scale \( T^* \) as functions of \( b \). We can see that \( T^*_2 \) decreases from \( T_{K}^{\text{SU}(4)} \) to \( T_{K}^{\text{SU}(2)} \) with increasing \( b \). Correspondingly, a region where \( g_2 \) shows the log T dependence moves towards low temperature side as \( b \) increases. Although \( g_2 \) decreases with increasing \( b \) at the finite temperatures, it approaches the unitary limit \( e^2/h \) for \( T \rightarrow 0 \) at arbitrary magnetic fields. This is because the phase shifts for these two levels, \( m = 2 \) and 3, are locked at \( \delta_2 = \delta_3 = \pi/2 \) even for
strong magnetic fields due to the compensation of the spin and orbital Zeeman effects described in Eq. \[\text{Eq. (11)}.\]

Another important aspect of the crossover is the scaling behaviour of the conductance. In Ref. [28], Mantell and his coworkers examine effects of the spin-orbit interaction on the scaling behavior at quarter filling, \(\varepsilon_d = -\frac{U}{2} \). We examine how the magnetic field affects the scaling at half-filling, \(\varepsilon_d = -\frac{U}{4} \). To explore the scaling behaviour, we rescale temperatures by the field dependent energy scale \(T_2^*\) and plot \(g_2^*\) for different \(b\) as functions of the rescaled temperatures \(T/T_2^*\) in Fig. \[\text{Fig. 6}\](c). At low-fields \(b \ll T_K^\text{SU(4)}\), the conductance curves almost collapse into a single SU(4) universal curve over a wide temperature range. The universality is lost when \(b\) becomes comparable with \(T_K^\text{SU(4)}\). At the high-fields \(b \gg T_K^\text{SU(4)}\), the curves deform into the other universal curve for the SU(2) symmetric case. At half-filling points \(\varepsilon_d = -\frac{U}{4}\), since the three body fluctuations \(\Theta_T\) vanish, the \(T^2\) coefficient \(C_T\) for the SU(N) conductance is determined only by the Wilson ratio, \(C_T = (\pi^2/48) [1 + 2(N-1)(R-1)^2]\). Substituting the Wilson ratios for the SU(4) case \(C_T^\text{SU(4)} = 0.32\) and for the SU(2) case \(C_T^\text{SU(2)} = 0.96\) into the formula of \(C_T\), we obtain the \(T^2\) coefficients \(C_T\) of each case for \(U/(\pi\Delta) = 2.0\): \(C_T^\text{SU(4)} \approx 0.33\) and \(C_T^\text{SU(2)} \approx 0.59\). Since \(C_T^\text{SU(4)} < C_T^\text{SU(2)}\), the conductance for \(N = 4\) is larger than that for \(N = 2\) in the low-temperature regions \(T/T_2^* \ll 0.1\). Figure \[\text{Fig. 6}\](c) shows this magnitude relation of the conductance, and thus demonstrate that the scaling behaviour depends on the number of orbitals \(N\) and the Wilson ratio \(R\).

Figure \[\text{Fig. 6}\](d) shows the other component \(g_1(= g_4)\) which...
correspond to the contributions of the other two state moving away from the Fermi level. At low temperatures $T \lesssim T_K^{SU(4)}$, these components decrease as $b$ increases and eventually vanish at the high magnetic fields $b \gg T_K^{SU(4)}$. We can also see that $g_1$ has a peak at large magnetic fields $b \lesssim 0.52T_K^{SU(4)}$. The emergent peak is caused by thermal excitations from (to) the renormalized level $\tilde{\varepsilon}_1$ ($\tilde{\varepsilon}_4$) which situates deep inside (far above) the Fermi level for large fields as shown in Fig. 5(b). Furthermore, for the large fields, the level structure of the CNT dot approaches the mean-field levels described in Eq. (44), and the atomic-limit peak also emerges at $U/2 + 2b$ [see also Appendix B].

These results obtained for $U/(\pi\Delta) = 2.0$ show a rather moderate evolution of the crossover and the Kondo energy scale $T^*$ as $T_K^{SU(2)}$ is only half of $T_K^{SU(4)}$. We will discuss a large $U$ case in the following.

---

**Fig. 7.** Temperature dependence of the linear conductance for $U/(\pi\Delta) = 4.0$ are plotted for six values of magnetic fields $b/T_K^{SU(4)} = 0.0, 0.25, 0.5, 1.0, 2.0, 4.0$ at half-filling $\varepsilon_d = -3U/2$. (a) shows the total conductance $g_{\text{tot}} = \sum_{m=1} g_m$. The conductance consists of two components, i.e., $g_2 = g_3$ and $g_1 = g_4$. (b) and (c) show the first one $g_2$, and (d) shows the second one $g_1$. Figures (a)-(c) also show the results for the SU(2) symmetric case by the symbols (+). The $x$-axes in (a), (b), and (d) are normalized by characteristic energy scales $T_2^{SU(2)}$. The inset of (b) shows $T_2^{SU(2)}$ as functions of $b/T_K^{SU(4)}$. At $b = 0$, $T_2^{SU(2)}$ takes the SU(4) symmetric value, $T_2^{SU(4)} = 0.20$. In the opposite limit $b = \infty$, it takes SU(2) value, $T_K^{SU(2)}/\Delta = 0.02$ which is indicated by the dashed line. The vertical arrows at the bottom of the panels indicate $T_K^{SU(2)}$, $T_K^{SU(4)}$, $U/2$, $\tilde{\varepsilon}_4$ and $U/2 + 2b$; specifically the last two, $\varepsilon_4$ and $U/2 + 2b$, are defined with respect to $b/T_K^{SU(4)} = 4.0$. 


B. Conductance for $U/(\pi \Delta) = 4.0$ at half-filling

We next examine the conductance for a strong interaction $U/(\pi \Delta) = 4.0$ in order to see more clearly the field-induced crossover at finite temperatures. In this case, the characteristic energy scale for the SU(2) case is significantly suppressed $T_K^{SU(2)} = 0.02\Delta$, which becomes much smaller than the SU(4) energy scale $T_K^{SU(4)} = 0.2\Delta$, i.e., the difference is about one order of magnitude.

We see in Fig. 7(a) that the total conductance $g_{tot}$ for a temperature region $0.1T_K^{SU(2)} \lesssim T \lesssim T_K^{SU(4)}$ decreases as magnetic field increases. Since the characteristic energy scale $T_2$ defined in Eq. (13) in this case becomes much smaller than that for $U/(\pi \Delta) = 2.0$, the region where the crossover occurs moves towards a low-temperature region, $T \lesssim T_K^{SU(4)} = 0.2\Delta$. Furthermore, the shoulder structures emerging in the high temperature region are more pronounced because of the strong interaction.

Figure 7(b) clearly shows that the curves of $g_2$ evolve from the SU(4) curve to the SU(2) curve during the crossover. Specifically, the energy scale $T_2^2$ around which $g_2$ shows log$^2$ dependence decreases with increasing magnetic field. The inset of Fig. 8(b) shows the suppression of $T_2^2$: it decreases from $T_K^{SU(4)} = 0.2\Delta$ to $T_K^{SU(2)} = 0.02\Delta$.

The scaling behaviour of $g_2$ in Fig. 8(c) also becomes clear because of this suppression. In wide range of temperatures, we can see that the scaled results collapse into two different universal curves, i.e., the SU(4) curves for small fields $b/T_K^{SU(4)} \lesssim 0.25$, and SU(2) curves for large fields $b/T_K^{SU(4)} \gtrsim 1$. Since the Wilson ratios for $N = 4$ and $N = 2$ are respectively saturated to the maximum possible values $R^{SU(4)} - 1 = 1/3$ and $R^{SU(2)} - 1 = 1$, the $T_2$ coefficients $C_T$ for each $N$ are also saturated: $C_T^{SU(4)} \simeq 0.34$ and $C_T^{SU(2)} \simeq 0.62$. Figure 8(c) clearly shows that $g_2$ for $b = 0$ is larger than that for $b \to \infty$ at $T < T_K^{SU(4)}$ because of $C_T^{SU(4)} > C_T^{SU(2)}$.

Furthermore, we can recognize that a broad peak emerges for $b \gg T_K^{SU(4)}$ at $T \approx U/2$. It corresponds to an thermal energy needed to add an electron or a hole to the degenerate states. Thus, this atom-like peak and the quasi-particle excitation peak in Fig. 8(d) at $T \approx 2b + U/2$ yield the shoulder structure of $g_{tot}$ at the high temperatures, as shown in Fig. 7(a).

VI. SPECTRAL PROPERTIES ALONG THE FIELD-INDUCED CROSSOVER

Spectral functions at finite magnetic fields also reflect the crossover from the SU(4) to SU(2) Kondo states. In addition to the Kondo resonance near the Fermi level, the Zeemann splitting causes a shift of the atomic-limit peak to $\pm (2b + U/2)$. The spectral functions for the doubly degenerate states remain the same $A_2(\omega, T) = A_3(\omega, T)$ for finite magnetic fields owing to the dot level structure given in Eq. (11). Following relations additionally hold in the particle-hole symmetric case $\varepsilon_d = -(3/2)U$,

$$
A_2(\omega, T) = A_2(-\omega, T), \quad A_1(\omega, T) = A_1(-\omega, T).
$$

The second relation shows that $A_1$ is a mirror image of $A_2$, and we discuss $A_1$ and $A_2$ in the following. We examine the spectral functions at $T = 0$, and hence we drop the second argument of the functions, namely, $A_m(\omega) = A_m(\omega, T = 0), (m = 1, 2, 3, 4)$. As in the previous sections, we consider the two cases for the interaction: (i) $U/(\pi \Delta) = 2.0$ and (ii) $U/(\pi \Delta) = 4.0$.

A. Spectral function for $U/(\pi \Delta) = 2.0$

Figure 8(a) shows the total spectral function $A_{tot}(\omega) = \sum_{m=1}^{4} A_m(\omega)$ for several magnetic fields and $U/(\pi \Delta) = 2.0$. At zero magnetic field, we can see that a single SU(4) Kondo resonance peak emerges on the Fermi level $\omega = 0$. As the magnetic field increases in the range of $0 < b < \infty$, the height of the Kondo peak decreases from 4 to 2 in units of $\pi \Delta$ since the resonance peak positions for $m = 1$ and $m = 4$ move away from the Fermi level, leaving the other positions for $m = 2$ and $m = 3$ just on the Fermi level, as shown in Fig. 8(a). This field dependence of the peak positions results in deforming the peak shape of the SU(4) Kondo resonance into that of the SU(2) Kondo resonance on the Fermi level, and the emergence of two sub peaks at higher energies, $\pm (2b + U/2)$.

Figure 8(b) shows $A_2 (= A_3)$ for the several values of $b$ shows such deformation of the peak shape. In the case of $U/(\pi \Delta) = 2.0$, the evolution of $A_2$ is not so clear since $T_K^{SU(2)}$ is only half as large as $T_K^{SU(4)}$. Nevertheless, the inset of Fig. 8(b) which is an enlarged view around the Fermi level shows that the resonance width on the Fermi level becomes sharper. As the magnetic field increases, $A_2$ also develops two sub peaks at $\omega = \pm U/2$, which correspond to the excitation energies on adding an electron or hole to the dot. In the Appendix B we provide analytic expression of the spectral functions in the atomic limit $\nu_r \to 0$, where the CNT dot is disconnected from the metallic leads. In the limit of $b \to \infty$, the remaining degenerate states turn into the SU(2) Kondo state, indicating that the ground state undergoes the crossover from the SU(4) to SU(2) Kondo state.

Figure 8(c) shows the other component $A_1(\omega)$, which corresponds to the component of the level going down from the Fermi level. Note that $A_1(\omega) = A_1(-\omega)$, as mentioned. We can see that the spectral weight transfers to the negative frequency region $\omega < 0$, and an evolution of its resonance peak position shows good agreement with the field dependence of $\varepsilon_1$ presented in Fig. 4(a). This transfer leads to the development of the sub peaks and decrease of the Kondo peak of $A_{tot}$. With increasing magnetic fields, the resonance peak at $\omega = \varepsilon_1$ merges with the atomic-limit peak at $\omega = -U/2 - 2b$ which shifts from the zero field position $-U/2$ in the presence of $b$. 


FIG. 8. Zero temperature spectral functions for $U/(\pi \Delta) = 2.0$ are plotted for five values of magnetic fields, $b/T^{SU(4)}_K = 0.0, 0.5, 1.0, 2.0, 4.0$ at half-filling $\varepsilon_d = -3U/2$: (a) $A_{tot}(\omega) = \sum_{m=1}^{15} A_m(\omega)$; (b) $A_2(\omega)$, and (c) $A_1(\omega)$. Vertical arrows at the bottom of the panels indicate the points $\omega = \pm U/2$ and $\pm (2b + U/2)$ where peaks emerge in the atomic limit. The peaks of $\omega = \pm (2b + U/2)$ are for the largest value of $b$ among the five, $b/T^{SU(4)}_K = 4.0$. The position of the renormalized resonance level $\tilde{\varepsilon}_1$ for the same value of $b$ are also shown in the bottom.

This shift of the atomic-limit peak, which we discuss in the appendix [3], results from the descent of the energy level $\varepsilon_1$ described in Eq. (11). For much larger fields $b \gg T^{SU(4)}_K$, the curve of $A_1$ approaches the Lorentzian form. Therefore, the quasiparticle state of $m = 1$ are unrenormalized from the correlated Kondo state to the bare state.

B. Spectral function for $U/(\pi \Delta) = 4.0$

In order to investigate the effects of the strong interaction on the spectral functions, we next discuss the spectral functions for $U/(\pi \Delta) = 4.0$. We present the results of $A_{tot}$, $A_2$ and $A_1$ in Fig. 9 and compare them with the corresponding results for the weak interaction case in Fig. 8. $A_{tot}$ for the strong interaction in Fig. 9(a) shows a similar trend as that for $U/(\pi \Delta) = 2.0$ in Fig. 8(a). However, the width of resonance for $U/(\pi \Delta) = 4.0$ in Fig. 9(a) is smaller than that for $U/(\pi \Delta) = 2.0$ in Fig. 8(a) in arbitrary magnetic fields, because $U$ is larger.

The component $A_2$ in Fig. 9(b) more clearly shows the narrowing of the resonance width than that for $U/(\pi \Delta) = 2.0$, because $T^{SU(2)}_K$ is smaller than $T^{SU(4)}_K$ by one order of magnitude in this case i.e., $T^{SU(2)}_K = 0.02\Delta$ and $T^{SU(4)}_K = 0.2\Delta$. The narrowing of the width leads to a loss of the spectral weight around the Fermi level, which is compensated by an enhancement of the atomic-limit peak at $\pm U/2$.

The atomic limit peak around $-U/2 - 2b$ of $A_1$ is broader in the strong interaction case shown in Fig. 9(c) than in the weak interaction case, because the quasiparticle resonance position $\tilde{\varepsilon}_1$ presented in Fig. 9(b) still remains around the Fermi level at the higher fields, $b \gg T^{SU(4)}_K$. Owing to this remaining, the quasiparticle state is still renormalized even at the higher fields, and thus the shape of $A_1$ differs from the Lorentzian form.

VII. SUMMARY

We have studied the Kondo effect in a carbon nanotube quantum dot in a wide range of temperature and magnetic field using the numerical renormalization group.

In the first half of the present paper, we have studied finite temperature properties of the $SU(4)$ Kondo state by calculating the finite temperature conductance in a wide range of electron filling $N_d$. The NRG results nicely agree with the experimental results in the wide range, supporting an emergence of the $SU(4)$ Kondo resonance at low-temperatures, $T \lesssim T^{SU(4)}_K$. Furthermore, we have precisely examined the temperature dependence of conductance especially at two fixed values of $N_d$: quarter-filling $N_d = 1$ and half-filling $N_d = 2$. The obtained results show that the scaled conductance of $N_d = 1$ is larger than that of $N_d = 2$ at the low-temperatures. A
panels indicate the points $\omega = \pm \Delta$. The peaks of $b/T$ are for the largest value of $b$.}

In a strong interaction case because a characteristic energy scale $T_K^2$ clearly decreases from the $SU(4)$ Kondo energy scale $T_K^SU(4)$ to the $SU(2)$ Kondo energy scale $T_K^SU(2)$.

The finite temperature conductance in the magnetic fields also shows such decrease of the energy scale. In addition, the scaling behaviour at half-filling shows that the excited states undergoes the crossover. Specifically, as soon as the magnetic fields $b$ become comparable to $T_K^SU(4)$, the $SU(4)$ universality is lost, and for the much larger fields, $b \gg T_K^SU(4)$, the $SU(2)$ universality emerges. Furthermore, the NRG results for both $SU(2)$ and $SU(4)$ symmetric cases indicate that the Wilson ratio and the Kondo energy scale determine the low-temperature behaviour of half-filled quantum dots.

We have also calculated total spectral functions and their components in magnetic fields. The obtained spectral functions shows that the resonance states remaining on the Fermi level becomes sharper as the magnetic field increases, showing a good agreement with the field dependence of the corresponding renormalized resonance width. Furthermore, a spectral weight of the other two states transfer toward the higher frequency region, because the Zeeman splitting shifts the two peak positions upward and downward from the Fermi level. Such transfer results in the emergence of two sub-peaks whose positions approach atomic-limit peak positions.

**ACKNOWLEDGMENTS**

This work was supported by Grant-in-Aid for JSPS Research Fellow Grant Number JP18J10205 and JSPS KAKENHI Grand Numbers JP18K03495, JP19H00656, JP19H05826, JP16K17723, 19K14630, and JST CREST Grant No. JPMJCR1876, the French program Agence nationale de la Recherche DYMESYS (ANR2011- I00-001-01), and Agence nationale de la Recherche MASH (ANR-12-BS04-0016).
Appendix A: Fermi-liquid parameters for single orbital Anderson impurity

![Diagram of Fermi liquid parameters](image)

**Fig. 10.** (a) Magnetic field dependence of Fermi liquid parameters for single orbital Anderson impurity at the electron-hole symmetric point $\varepsilon_d/U = -1/2$ for $U/(\pi \Delta) = 2.0$. At this point, a total occupation number is locked at one, i.e., $\langle n_{d\uparrow} + n_{d\downarrow} \rangle = 1$ at arbitrary magnetic fields, and thus $\langle n_{d\uparrow} \rangle$ can be expressed in terms of the magnetization $M_\uparrow \equiv \langle n_{d\uparrow} \rangle - \langle n_{d\downarrow} \rangle$ as follows: $\langle n_{d\uparrow} \rangle = (1 + \text{sgn}(\sigma) M_\downarrow)/2$. Furthermore, $\sin^2 \delta_{\uparrow} = \sin^2 \delta_{\downarrow}$ and $Z_{\uparrow} = Z_{\downarrow}$. (b) Residual interaction $U$ as a function of $b$. The x-axes are scaled by the Coulomb interaction $U$. Each inset shows an enlarged view of the region around $b = 0$. In the insets, the axes are scaled by the Kondo temperature $T_K^{SU(2)} = 0.19\Delta = (0.03U)$.

We briefly discuss how the Fermi liquid state of the single Anderson impurity evolves with increasing magnetic field. The field dependence of the Fermi liquid parameters have been discussed also in Refs. In Fig. 10(b) also show NRG results of the Fermi liquid parameters and the residual interaction, respectively. In the NRG calculations, the spin-dependent impurity level is locked at $1.5$ level, and correspondingly, the induced magnetization is rapidly saturated to $1$, i.e., $M_\uparrow \rightarrow 1$. In contrast, $Z$ and $R - 1$ vary more slowly than $T(0)$ and $M_\downarrow$ with the scales of $U$. As shown in the inset of Fig. 10(a), $\Delta$ and $R - 1$ are still renormalized for small magnetic fields $b \lesssim T_K^{SU(2)}$. For large magnetic fields $b \gg T_K^{SU(2)}$, these parameters approaches the non-interacting values, $Z \rightarrow 1$ and $R - 1 \rightarrow 1$.

The residual interaction plotted in Fig. 10(b) also vary from a zero field value $4T_K^{SU(2)} = 0.23\Delta$ with increasing $b$. For small magnetic fields $b \leq 0.2U$, $U$ is enhanced and its value becomes larger than a bare Coulomb interaction $U$. As magnetic field further increases, it decreases from the enhanced value to the bare value $U$.

Appendix B: Spectral function in the atomic limit

We consider the atomic limit in order to show how the spectral weight of the impurity states evolves as magnetic increases at high-energies in the case that the Zeemenn splittings of the impurity levels are given by Eq. (41).

At zero temperature, the flavour $m$-resolved single-particle spectral function can be written in the Lehmann representation as,

$$A_m(\omega) = \frac{1}{M} \sum_{i=1}^{M} \sum_{n} \left[ |\langle n| d_m^\dagger |\Psi_{GS,i} \rangle|^2 \delta(\omega - (E_n - E_{GS})) + |\langle n| d_m |\Psi_{GS,i} \rangle|^2 \delta(\omega + (E_n - E_{GS})) \right].$$

Here, $|n\rangle$ and $E_n$ are the eigenstate and eigenenergy of Hamiltonian $H$, respectively. The ground state $|\Psi_{GS,i} \rangle$ with the energy $E_{GS}$ can generally be degenerate, and the summation over $i$ represents an average over $M$-fold degenerate states.

In the atomic limit, the CNT dot whose eigen energies are defined is Eq. (11) is disconnected from the leads $(\epsilon_i = 0$ for $\nu = L, R)$, and there remains two-fold degeneracy for the ground state at half-filling $\epsilon_d = -3U/2$,

$$|\Psi_{GS,2} \rangle = d_1^\dagger d_2^\dagger |0 \rangle,$$

$$|\Psi_{GS,3} \rangle = d_1^\dagger d_3^\dagger |0 \rangle.$$  

Either of the two one-particle states, $m = 2$ or $3$ situated on the Fermi level, is occupied, and the lowest one-particle level with the energy $\epsilon_1$ is occupied while the highest one with $\epsilon_4$ is empty. Therefore, the ground energy for these two-electron states becomes

$$E_{GS} = \epsilon_1 + \epsilon_2 + U = 2\epsilon_d - 2b + U.$$  

We next consider a single-particle excitation to add an electron into the level of $m = 4$, and a single-hole excitation to remove the electron occupying the $m = 1$ level,

$$|\Psi_{p4} \rangle = d_4^\dagger |\Psi_{GS,i} \rangle,$$

$$E_{p4} = 3\epsilon_d + 3U,$$

$$|\Psi_{h1} \rangle = d_1^\dagger |\Psi_{GS,i} \rangle,$$

$$E_{h1} = \epsilon_d.$$
The excitation energies from the ground state \( i = 2, 3 \) to these two states are given by

\[
E_{p4} - E_{GS} = \varepsilon_d + 2b + 2U = 2b + \frac{U}{2}, \tag{B7}
\]

\[
E_{GS} - E_{h1} = \varepsilon_d - 2b + U = -2b - \frac{U}{2}. \tag{B8}
\]

Therefore, the spectral weights of these processes are given by

\[
A_4(\omega) = \delta \left( \omega - \left( 2b + \frac{U}{2} \right) \right),
\]

\[
A_1(\omega) = \delta \left( \omega + \left( 2b + \frac{U}{2} \right) \right). \tag{B9}
\]

These weights shift towards high-energy region from the usual atomic limit position \( \pm U/2 \). We have observed the corresponding shifts of the spectral weight in the NRG results shown in Fig. 8(c) and Fig. 9(c) although these atomic peaks merge with the resonance peak which also moves away from the Fermi level as \( b \) increases.

The other single electron (hole) excitation from the ground state \( |\Psi_{GS,2}\rangle \) corresponds to an addition of an electron to the level \( m = 3 \) (annihilation of an electron from \( m = 2 \)). The similar excitations also occur from \( |\Psi_{GS,3}\rangle \). The peaks corresponding to these excitations appear at \( \omega = \pm U/2 \) in the spectral functions for \( m = 2 \) and 3,

\[
A_2(\omega) = A_3(\omega) = \frac{1}{2} \delta \left( \omega - \frac{U}{2} \right) + \frac{1}{2} \delta \left( \omega + \frac{U}{2} \right). \tag{B10}
\]

These two peaks are equivalent to the Hubbard peaks for the SU(2) symmetric case.

### Appendix C: NRG for dynamical correlations

#### 1. Spectral function and finite \( T \) conductance

In this work, the spectral function \( A_m(\omega) \) has been calculated using the “complete Fock-space basis set”, developed by Andes et al.\(^\text{24,25}\) and by Weichselbaum and von Delft.\(^\text{26}\) In this approach, contributions of the high energy states which are discarded at the NRG steps can be recovered to form a complete basis for the Wilson’s NRG chain, by carrying out the backward iteration. The merit of this approach is that the sum rule for the spectral weights can be fulfilled.

In addition, we have employed the method due to Bulla, Hewson, and Pruschke,\(^\text{22}\) we have calculated not only \( G_m(\omega) \) but also the higher-order Green’s function \( F_m(\omega) \)

\[
F_m(\omega) = -i \int_0^\infty dt e^{i(\omega + i\delta)t} \times \sum_{m' \neq m} \langle \{n_{dm'}(t) d_m(t), d_m^\dagger(0) \} \rangle. \tag{C1}\]

Then, the self-energy can be determined directly through the relation \( \Sigma_m(\omega) = UF_m(\omega)/G_m(\omega) \). The final form of the Green’s function has been obtained from \( \Sigma_m(\omega) \) and the noninteracting Green’s function \( G^0_m(\omega) \) using the Dyson equation given in Eq. (7). The merit to treat the self-energy as an input is that the fully analytic expression which is not affected by the logarithmic discretization can be used for \( G^0_m(\omega) \).

#### 2. The \( z \) averaging

The size of the Hilbert space to be diagonalized at each NRG step increases as the number of conduction electron channels increases. To ensure the accuracy of the NRG calculation, a large \( \Lambda \) is used for quantum impurities with a number of internal degrees of freedom.

Oliveira and Oliveira found that thermodynamic averages which are calculated for large \( \Lambda \) show an artificial oscillation at low temperatures,\(^\text{62,63}\) and they proposed the \( z \) averaging for removing such an artificial oscillation. The parameter \( z \) which slides a set of discretization points from that of the standard Wilson chain,\(^\text{22}\)

\[
\pm \Lambda^{-n} \rightarrow \pm \Lambda^{-(n+1-z)}, \quad n = 0, 1, 2, \cdots, \tag{C2}\]

with \( 0 \leq z \leq 1 \). For \( z = 1 \), it coincides with the standard Wilson chain. The discretized conduction band can be transformed into a \( z \) dependent Wilson chain

\[
\mathcal{H}_c \Rightarrow \sum_{n=0}^\infty \sum_{m=1}^4 t_n(z) \left( f_{n,m}^\dagger f_{n+1,m} + f_{n+1,m}^\dagger f_{n,m} \right). \tag{C3}\]

The hopping matrix element \( t_n(z) \) that can be determined using the Householder algorithm summarized in Refs. 59 and 61. We have carried out NRG calculations for some fixed values of \( z \), and calculate expectation values using the obtained eigenstates. Then, an average is taken over “\( z \)” for two different values \( z = 0.5 \) and 1, which is enough to eliminate the artificial oscillations in our case.

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