Magnetization plateau and quantum phase transitions in a spin-orbital model

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Abstract. A spin-orbital chain with different Landé g factors and one-ion anisotropy is studied in the context of the thermodynamical Bethe ansatz. It is found that there exists a magnetization plateau resulting from the different Landé g factors. Detailed phase diagram in the presence of an external magnetic field is presented both numerically and analytically. For some values of the anisotropy, the four-component system undergoes five consecutive quantum phase transitions when the magnetic field varies. We also study the magnetization in various cases, especially its behaviors in the vicinity of the critical points. For the SU(4) spin-orbital model, explicit analytical expressions for the critical fields are derived, with excellent accuracy compared with numerics.

PACS. 75.30.Kz Magnetic phase boundaries (including magnetic transitions, metamagnetism, etc.) – 71.27.+a Strongly correlated electron systems; heavy fermions – 75.10.Jm Quantized spin models

1 Introduction

Orbital degeneracy in electron systems leads to rich and novel magnetic phenomena in many transitional metal oxides [1]. Among them are the orbital ordering and orbital density wave, which have been observed experimentally in a family of manganites [2]. A tractable model to describe 2-fold orbital degenerate system is the SU(4) model [3], which has attracted much attention [3–10]. In the one-dimensional case the model is exactly solvable by Bethe ansatz (BA) [5,11]. An interesting question is to study the critical behavior of such a system in an external magnetic field, especially when different Landé g factors for spin and orbital sectors are involved. One may expect that the difference of g factors will bring about new physics as a result of the competition of the spin and orbital degrees of freedom. In reference [9], the authors studied the magnetic properties of the SU(4) model via BA, without taking different g factors into account, whereas numerical calculation was performed in reference [10] for the model with different g factors for up to 200 lattice sites. However, a full picture about the critical fields is still lacking. Another motivation is to see whether or not any magnetization plateau (MP), an interesting magnetic phenomenon, occurs in such a spin-orbital model. As is well-known, antiferromagnetic chains with integer spin are gapful [12], whereas for half-integer spin there also exists a gapful phase with a MP in the presence of a large planar anisotropy [13]. Also fractional MP have been observed and can be explained by Shastry-Sutherland lattice [14]. But an MP arising from different Landé g factors has not been addressed yet.

Deviation from the SU(4) symmetry can be caused by variation in the interaction parameters of neighbor sites [4,6,8,15], while another possible deviation may result from the one-ion interaction. Since many compounds are magnetically anisotropic in which the orbital angular momentum (OAM) may be constrained in some direction due to crystalline field, the angle between spin and OAM determines the spin-orbital coupling (SOC) energy. This kind of one-ion SOC leads to magnetic anisotropy [16]. Under the influence of molecular field and an external field, the spin is parallel to the OAM. In such a case, $s^2\tau_i^2$ type of interaction describes well the SOC energy. Another possibility of such an interaction can be found when $\tau_i$ is pseudospin. In fact, some realizations of the SU(4) spin-orbital model were presented from tetrahis(dimethylamino) ethylene(TDAE)-C60 [15] and semiconducting quantum dot array [17] involving two orbitals $l^z = 1, -1$, while the $l^z = 0$ orbital is excluded due to a higher crystal field energy in TDAE-C60 or filled in the quantum dots due to lower energy in harmonic-oscillator potential. If the SOC is taken into account, we will have the anisotropy $s^2\tau_i^2$ by an effective relation $l \cdot s = 2\tau_i^2s^2$.

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since the $l^2 = 0$ orbital is excluded and the transition caused by $l^\pm$ in the SOC is prohibited. Here we shall introduce such an SU(2)$\otimes$SU(2) SOC interaction into the SU(4) model. A detailed investigation of the phase diagram is undertaken both numerically and analytically in the context of the thermodynamical Bethe ansatz (TBA). We find that the system exhibits an MP resulting from different $g$ factors when the SOC is sufficiently strong. The critical behavior of the magnetization in the vicinities of the critical points is revealed. For certain values of Landé $g$ factor, the model undergoes five consecutive quantum phase transitions when the external magnetic field varies. Further, the explicit analytic expressions for the critical fields for the SU(4) model are derived, with excellent accuracy compared to numerical results.

2 The model and TBA

We shall consider an L-site chain with the Hamiltonian

$$
H = H_0 + H_z + M, \quad H_0 = \sum_{i=1}^{L-1} P_{i,i+1},
$$

$$
H_z = \Delta_z \sum_i s^z_i \tau^z_i, \quad M = -g_s H \sum_i s^z_i - g_t H \sum_i \tau^z_i,
$$

(1)

where $s$ and $\tau$ are spin-1/2 operators for spin and orbital sectors. The $g_s$ denotes the Landé $g$ factor in $z$-direction for spin sector and the orbital $g$ factor $g_t$ depends on the orbitals the system involves. For example, $g_t = 0$ in $z$-direction if only $e_g$ orbitals involve and $t_2g$ orbitals are already occupied [1], since the field energy is zero for the orbital $d_{x^2-y^2}$ while it is prohibited for the orbital $d_{3z^2-r^2}$ from the field by the orbital $d_{3z^2-r^2}$ to the occupied $d_{xy}$; for $l^z = \pm 1$ orbitals [15,17] $g_t$ is the real orbital $g$ factor in $z$-direction multiplied by 2. We shall discuss generally and assume $g_s > g_t$ throughout the paper, the results for $g_s < g_t$ are similar when the spin and orbital sectors are exchanged. $H_0$ is the SU(4) model with $P_{i,j} = (2s_i \cdot s_j + 1/2)(\tau_i \cdot \tau_j + 1/2)$ exchanging the four site states $|s^z_i \tau^z_i>: (||), \phi_2 = [||], \phi_3 = [\|\], \phi_4 = [\|\|].$ It should be noted that electrons have positive $\Delta_z$ whereas holes have negative $\Delta_z$ according to their SOC [18]. The symmetry is broken into SU(2)$\otimes$SU(2) by $\mathcal{H}$ and further into four U(1)’s by the external magnetic field $H$. The model can be solved exactly via BA approach. The BA equations are the same as the SU(4) model [5,11] under the periodic boundary conditions, with the energy eigenvalues given by

$$
E = -2\pi \sum_{i=1}^{M^{(i)}} a_i(\lambda_i) + \sum_{k} E_k N_k,
$$

(2)

where $a_n(\lambda) = 1/(2\pi n/\lambda^2 + n^2/4)$, and $E_1 = -\Delta_z/4 - g_s H/2$, $E_2 = -\Delta_z/4 + g_s H/2$, $E_3 = -\Delta_s/4 + g_s H/2$, $E_4 = -\Delta_s/4 + g_s H/2$, with $g_s = g_s + g_t$ $N_k$ is the total site number in state $\phi_k$ and $M^{(i)} (i = 1, 2, 3)$ is the rapidity number. For a certain choice of the basis order, which depends on whether or not the component is energetically favorable, the energy can be rewritten as $E = \sum_{i=1}^{M^{(i)}} g^{(1)}(\lambda_i) + g^{(2)} M^{(2)} + g^{(3)} M^{(3)}$. Following references [19,20], one may obtain the ground state (GS) equations for the dressed energies $\epsilon^{(i)} (i = 1, 2, 3)$,

$$
\epsilon^{(i)} = g^{(1)}(\lambda_i) - a_2 \epsilon^{(i+1)} \epsilon^{(i-1)} + a_1 \epsilon^{(i-1)},
$$

(3)

where $\epsilon^{(0)} = \epsilon^{(4)} = 0$ and the symbol $*$ denotes the convolution. The GS is composed of Fermi seas filled by negative dressed energies $\epsilon^{(i-1)}$. According to an energetics argument, we may divide the external field $H$ into three regions: (I) $0 \leq H < H_{R1}$, (II) $H_{R1} < H < H_{R2}$, (III) $H_{R2} < H < \infty$ with $H_{R1} = |\Delta_z|/(2g_s)$, $H_{R2} = |\Delta_z|/(2g_t)$. For $\Delta_z > 0$, the corresponding basis order are: (I+) $(\phi_1, \phi_2, \phi_3, \phi_4)^T$, (II+) $(\phi_1, \phi_3, \phi_2, \phi_4)^T$, (III) $(\phi_3, \phi_1, \phi_2, \phi_4)^T$; for $\Delta_z < 0$: (II-) $(\phi_3, \phi_1, \phi_2, \phi_4)^T$, (II-) $(\phi_3, \phi_1, \phi_4, \phi_2)^T$, (III) the same as $\Delta_z > 0$. These five basis orders provide a full description of the phase diagram of the system.

3 Magnetization plateau

The competition between the anisotropy parameter $\Delta_z$ and the magnetic field $H$ results in a novel quantum phase diagram. In the absence of the magnetic field, it is easy to find that the states $\phi_3$ and $\phi_4$ are gapful for $\Delta_z > \Delta_z^c = 4 \ln 2$. Whereas for $\Delta_z < -\Delta_z^c$, the components $\phi_1$ and $\phi_2$ are gapful. Therefore, the GS is in an $su(2)$ spin-orbital liquid state in strong anisotropy regime in the absence of the field. However, the presence of the magnetic field completely splits all four components energetically. The magnetization $M^z = g_s s^z + g_t \tau^z$ increases from zero. For large positive $\Delta_z$, the field bring the component $\phi_3$ closer to the GS, while the component $\phi_2$ gradually gets out of the GS. Certainly, if the field reaches the first critical field where the component $\phi_3$ has not yet involved in the GS, a quantum phase transition from the spin-orbital liquid phase to a ferromagnetic phase occurs. Thus a magnetization plateau opens with a constant magnetization $M^z = g_s /2$. Nevertheless, this plateau will end when the field is strong enough $H > H_{c2}$. The component $\phi_3$ becomes involved in the GS. The critical field $H_{c2}$ indicates a quantum phase transition from the ferromagnetic GS into a spin-orbital liquid phase. If the field continues to increase, the spin and orbital sectors become fully-polarized at the third critical point $H_{c3}$. From the TBA equations (3), we get the exact expressions for the critical fields

$$
H_{c1}^p = \frac{4}{g_s}, \quad H_{c2}^p = \frac{\Delta_z^c/2 - 4}{g_t}, \quad H_{c3}^p = \frac{\Delta_z^c/2 + 4}{g_t},
$$

(4)

Notice that the plateau opens only if $\Delta_z > \Delta_z^c = 8 g_s /g_t$ and $0 < g_t < g_s$. If the $g$ factors are the same, the plateau disappears because the components $\phi_1$ and $\phi_2$ remain degenerate in the field. The critical behavior of the magnetization in the vicinities of the critical points may be