Phase diagram and quantum critical behavior of an integrable Kondo lattice model

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An integrable Kondo lattice model describing a strongly correlated electron host interacting with a spin-$\frac{1}{2}$ lattice is proposed. It is found that with the variations of the Kondo coupling J, the hole concentration n_h, and the magnetic field H, the system may fall into a variety of phases. The phase boundaries of the ground state are determined exactly. The marginal excitations and the quantum critical behavior at the phase boundaries are discussed.

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Metallic compounds containing partially filled f bands belong to the general category of heavy fermions.[1] Recently, with the discovery of the Kondo insulators[2] and the non-Fermi-liquid behavior,[3] the interest in this field has been greatly renewed. Especially, the non-Fermi-liquid behavior found in some heavy fermion compounds, which stimulates a strong challenge to Landau's Fermi-liquid theory, reveals the quantum critical behavior of these systems at low temperatures.[4] The heavy fermion systems are usually modeled by the periodic Anderson model or the Kondo lattice model in some limiting cases. The single-impurity Kondo problem has been studied extensively and exact solutions[5,6] were obtained. In addition, important progress has been achieved recently for the Kondo problem in strongly correlated hosts.[7–10] Nevertheless, the understanding to the Kondo lattice systems is rather unsatisfactory. Though many efforts have been made, an exactly solvable Kondo lattice model, which may provide us some crucial information of a heavy fermion system, is still absent. In fact, a generic two-impurity problem is very hard to be solved even in one dimension. We note a few integrable models consisting of many impurities have been proposed.[11,12] The impurities in these models are very artificial and are almost independent of each other since only forward scattering between the conduction electrons and the impurities survive. The physical effect of these impurities is additive and therefore the problem is still at the single-impurity level.

In this paper, we propose an exactly solvable Kondo lattice model consisting of a correlated electron host interacting with a spin-$\frac{1}{2}$ lattice. In one dimension, we show the model is exactly solvable via algebraic Bethe ansatz. The model Hamiltonian reads

$$H=t\sum_{i,\delta} h_{i,i+\delta}(1+\vec{\tau}_i\cdot\vec{\tau}_{i+\delta})+J\sum_i \vec{S}_i\cdot\vec{\tau}_i,$$

$$h_{i,j}=\sum_{\sigma=\uparrow,\downarrow}\mathcal{P}\left[c^\dagger_{i,\sigma}c_{j,\sigma}+c^\dagger_{j,\sigma}c_{i,\sigma}+2\left(\vec{S}_i\cdot\vec{S}_j+\frac{3}{4}n_in_j\right)\right]\mathcal{P}-(n_i+n_j)+1, \quad (1)$$

where $c^\dagger_{i,\sigma}$ ($c_{i,\sigma}$) are the creation (annihilation) operators of the conduction electrons with spin σ on site i, $\vec{S}_i=\frac{1}{2}\Sigma_{\sigma,\sigma'}c^\dagger_{i,\sigma}\vec{\tau}_{\sigma,\sigma'}c_{i,\sigma'}$ are the spin operators of the conduction electrons ($\vec{\tau}$ the Pauli matrices), n_i denotes the electron number on site i, $\mathcal{P}$ means the constriction $n_i\leqslant 1$, $\vec{\tau}_i$ are the Pauli matrices indicating the local spin on site i, t, and J are two real constants indicating the hoping amplitude and the Kondo coupling constant, respectively, $i=(i_1,\ldots,i_d)$ in d dimension, and δ are the basic vectors of the lattice, $\delta=1$ in one dimension and (1,0), (0,1) in two dimensions etc. Obviously, Eq. (1) describes an SU(3)-invariant t-J system[13] coupled with a spin lattice. The first term of Eq. (1) represents the hoping and interactions of the conduction electrons, which depend not only on the local electron states, but also on the local spin environment. As discussed in some previous works,[14] the electron-spin interactions contained in the first term can be mediated either by phonons or ordinary Coulomb repulsions. The second term describes the usual Kondo interactions.

In the present form, the solvability of Eq. (1) is rather hidden. We note that the first term can be rewritten as $\Sigma_{i,\delta}P_{i,i+\delta}$, where $P_{i,j}$ is the permutation operator between the ith site and the jth site. For any given orthogonal and complete set of Dirac states $\{|\alpha_i\rangle\}$ spanning the Hilbert space of the ith site, $P_{i,j}$ can be expressed as $\Sigma_{\alpha,\beta}X_i^{\alpha\beta}X_j^{\beta\alpha}$, where $X_i^{\alpha\beta}\equiv|\alpha_i\rangle\langle\beta_i|$ represent the Hubbard operators. Now we check the possible states of a single site. A natural choice of $\{|\alpha_i\rangle\}$ is $|\gamma_i,\tau_i^z\rangle$, where $\gamma_i=\uparrow,0,\downarrow$ denote one electron with spin up, no electron, and one electron with spin down, respectively, and $\tau_i^z=\uparrow,\downarrow$ denote the two components of the local spin. Obviously, the local Hilbert space is six dimensional and therefore the first term of Eq. (1) is SU(6) invariant. To diagonalize the whole Hamiltonian, we introduce the following notations:

$$|0\rangle=\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle),$$

$$|1\rangle=|0,\uparrow\rangle,\quad |2\rangle=|0,\downarrow\rangle,\quad |3\rangle=|\uparrow,\uparrow\rangle,$$

$$|4\rangle=\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle),\quad |5\rangle=|\downarrow,\downarrow\rangle. \quad (2)$$

$|0\rangle$ represents a Kondo singlet; $|1\rangle,|2\rangle$ denote two hole states and $|3\rangle,|4\rangle$ and $|5\rangle$ indicate the Kondo triplets. Obviously, $\langle\alpha|\beta\rangle=\delta_{\alpha,\beta}$. Therefore, we can rewrite Eq. (1) as (up to an irrelevant constant)

$$H=2t\sum_{i,\delta}\sum_{\alpha,\beta=0}^{5}X_i^{\alpha\beta}X_{i+\delta}^{\beta\alpha}-2J\sum_i X_i^{00}-J\sum_i(X_i^{11}+X_i^{22}). \tag{3}$$

Now it is clear that the Kondo interaction term represents one of the conserved quantities of the system. In fact, we have six types of conserved charges $N_\alpha=\Sigma_i X_i^{\alpha\alpha}$, which correspond to the number of local state $|\alpha\rangle$ in the whole system. After this transformation, the Hamiltonian (3) takes the exact form of an SU(6)-invariant spin chain model introduced by Sutherland[13] but with the Kondo coupling J as an effective field. In any dimensions, we have five branches of elementary excitations relative to a reference state $|\alpha\rangle_g=|\alpha_1\rangle\otimes\cdots\otimes|\alpha_N\rangle$. For example, if we choose $|0\rangle_g$ as the pseudovacuum, we have two degenerate hole bands (corresponding to $|0,\uparrow\rangle$ and $|0,\downarrow\rangle$) and three degenerate triplet bands. For the half-filled case, no hole state is allowed and the one-dimensional model is reduced to the SU(4)-invariant spin ladder considered by one of the present authors.[15] There is a critical value of the Kondo coupling J. When $J>J_c$, $|0\rangle_g$ becomes the ground state and the degenerate triplet bands are empty. Consider a single excitation upon the ground state with momentum $\vec{k}=(k_1,\ldots,k_d)$. The corresponding wave function reads $|\vec{k}\rangle=\Sigma_{\vec{r}}\exp(i\vec{k}\cdot\vec{r})X_{\vec{r}}^{\alpha 0}|0\rangle_g$, where $\vec{r}$ runs all sites and $\alpha=3,4,5$ in the half-filled case. This excitation is a generalized spin wave and its energy is $\epsilon(\vec{k})=4t\Sigma_{j=1}^d[\cos(k_j)-1]+2J$. Therefore, $J_c=4|t|d$. For $J\rangle J_c$, the triplet excitations are massive, while for $J=J_c$, these excitations are marginal and the system may show quantum critical behavior. For the latter case, the dispersion relation of the low-lying excitations behaves as $\epsilon(\vec{k})\sim4|t|\vec{k}^2$ and the asymptotic density of states is $\rho(\epsilon)\sim\epsilon^{d/2-1}$ as for the spin waves in an ordinary ferromagnet. This allows us to derive the leading temperature dependence of some thermodynamic quantities easily. For example, the low-temperature specific heat and susceptibility at the critical point behave as $C\sim T^{d/2}$, $\chi\sim T^{d/2-1}$. In fact, the massive spin excitations in the half-filled case correspond to a Kondo insulator phase if we allow double occupation of electrons on a single site. This can be realized by replacing the SU(3) t-J term $h_{i,j}$ in Eq. (1) by the SU(4) or SU(2|2) Hubbard term.[16] In the latter case, the system exhibits also a charge gap which takes the same value of the spin gap $\Delta=2(J-J_c)$ at half filling. For any non-half-filling case, we have two degenerate "hole seas" in the ground-state configuration and the charge and spin excitations are always gapless. However, there is still a critical point J_c. When $J>J_c$, the triplet states are forbidden in the ground state. This critical value is generally filling dependent and is hard to be derived in higher dimensions. The Kondo singlets behave as spin polarons. Because there is a finite gap to excite a triplet when $J>J_c$, we expect some type of condensation of the Kondo singlets at low temperatures.

In one dimension, the Hamiltonian (3) can be solved with the standard method,[13] which is in fact related to a class of integrable spin-ladder models.[15,17] Not losing generality, we set $2t=1$ in the following text and choose the Kondo insulator state $|0\rangle_g$ as the pseudovacuum state. We note that here the Kondo hole states $|1\rangle$ and $|2\rangle$ are fermion states while the Kondo singlet and Kondo triplets are boson states, i.e., $[X_i^{\alpha0},X_j^{\beta0}]=0$ for $\alpha,\beta=0,3,4,5$, $i\neq j$ and $\{X_i^{\alpha0},X_j^{\beta0}\}=0$ for $\alpha,\beta=1,2$, $i\neq j$. However, the fermion states can be transformed to boson states with the Jordan-Wigner transformation. For $\alpha=1,2$, we define

$$X_i^{\alpha0}=\tilde{X}_i^{\alpha0}\prod_{j=1}^{i-1}e^{i\pi(\tilde{X}_j^{11}+\tilde{X}_j^{22})},$$

$$X_i^{0\alpha}=\prod_{j=1}^{i-1}e^{-i\pi(\tilde{X}_j^{11}+\tilde{X}_j^{22})}\tilde{X}_i^{0\alpha},\quad \tilde{X}_i^{\alpha\alpha}=X_i^{\alpha\alpha}.$$

We have $[\tilde{X}_i^{\alpha0},\tilde{X}_j^{\beta0}]=0$ for $i\neq j$. With the identity $X_i^{\alpha\beta}=X_i^{\alpha0}X_i^{0\beta}$ we can check that the Hamiltonian (1) is invariant under the Jordan-Wigner transformation but with a slightly different boundary condition, which is not important in the thermodynamic limit. In such a sense, the local states $|\alpha_i\rangle$ ($\alpha\geqslant1$) can be treated as colored hardcore bosons with the single occupation condition $\Sigma_{\alpha=0}^5X_i^{\alpha\alpha}\equiv1$. Therefore, our model is just the B^6 case of Ref. 13 and the Bethe ansatz equations read

$$\left(\frac{\lambda_j^{(1)}-\frac{i}{2}}{\lambda_j^{(1)}+\frac{i}{2}}\right)^N=-\prod_{l=1}^{M_1}\frac{\lambda_j^{(1)}-\lambda_l^{(1)}-i}{\lambda_j^{(1)}-\lambda_l^{(1)}+i}\prod_{k=1}^{M_2}\frac{\lambda_j^{(1)}-\lambda_k^{(2)}+\frac{i}{2}}{\lambda_j^{(1)}-\lambda_k^{(2)}-\frac{i}{2}},$$

$$\prod_{l=1}^{M_n}\frac{\lambda_j^{(n)}-\lambda_k^{(n)}-i}{\lambda_j^{(n)}-\lambda_k^{(n)}+i}=-\prod_{t=n\pm1}\prod_{k=1}^{M_t}\frac{\lambda_j^{(n)}-\lambda_k^{(t)}-\frac{i}{2}}{\lambda_j^{(n)}-\lambda_k^{(t)}+\frac{i}{2}},$$

$$n=2,3,4,5, \tag{4}$$

with the eigenvalue of the Hamiltonian (3) as

$$E=-\sum_{j=1}^{M_1}\left(\frac{\frac{1}{2}}{\lambda_j^{(1)2}+\frac{1}{4}}-2J\right)-J(N_1+N_2), \tag{5}$$

where $M_n=N_n+\cdots+N_5$ and $M_6\equiv0$, $\lambda_j^{(n)}$ are the rapidities of the flavor waves (holons and spinons). Note that the boundary condition $X_1^{\alpha\beta}=X_{N+1}^{\alpha\beta}$ has been used in deriving Eq. (4) and an irrelevant constant has been omitted in Eq. (5). Relative to the Kondo insulator state $|0\rangle_g$, the unoccupied states $|0,\uparrow\rangle$ and $|0,\downarrow\rangle$ can be treated as Kondo holes which are responsible to the dynamical properties of a doped Kondo insulator. For large enough $J>J_c$, there is no triplet states in the ground-state configuration, i.e., $M_3=0$. The effective low-energy hamiltonian of the system is therefore equivalent to an SU(3)-invariant t-J model.

For a given Kondo-hole concentration $n_h=(N_1+N_2)/N$, there is a phase boundary $J_c(n_h)$ above which the spin triplet states will be eliminated from the ground state. Set $\rho_n(\lambda)$ as the distribution of $\lambda^{(n)}$ modes in the ground state. When $J>J_c$, from Eq. (4) we have

$$\rho_1(\lambda)=a_1(\lambda)+\int_{-\Lambda_2}^{\Lambda_2}a_1(\lambda-\nu)\rho_2(\nu)d\nu-\int_{-\Lambda_1}^{\Lambda_1}a_2(\lambda-\nu)\rho_1(\nu)d\nu,$$

$$\rho_2(\lambda)=\int_{-\Lambda_1}^{\Lambda_1}a_1(\lambda-\nu)\rho_1(\nu)d\nu-\int_{-\Lambda_2}^{\Lambda_2}a_2(\lambda-\nu)\rho_2(\nu)d\nu,\rho_n(\lambda)=0,\ \ n\geqslant 3, \tag{6}$$

where $a_n(\lambda)=n/[2\pi(\lambda^2+n^2/4)]$ and the cutoffs $\Lambda_{1,2}$ are determined by

$$\int_{-\Lambda_1}^{\Lambda_1}\rho_1(\lambda)d\lambda=n_h,\quad \int_{-\Lambda_2}^{\Lambda_2}\rho_1(\lambda)d\lambda=\frac{1}{2}n_h. \tag{7}$$

By integrating the second equation of Eq. (6), we obtain $\Lambda_2=\infty$. The excitation energy of a triplet mode can be exactly derived by considering the process $M_1\to M_1+1$, $M_2\to M_2+1$, and $M_3=1$. Such an excitation can be realized by adding a $\lambda^{(1)}$ mode $\lambda_p^{(1)}$ above the $\lambda^{(1)}$ sea, a $\lambda^{(3)}$ mode $\lambda_p^{(3)}$, and a $\lambda^{(2)}$ hole $\lambda_h^{(2)}$ in the $\lambda^{(2)}$ sea. After some manipulation we obtain the excitation energy $\Delta E(\lambda_p^{(1)},\lambda_h^{(2)},\lambda_p^{(3)})$ as

$$\Delta E=\epsilon_1(\lambda_p^{(1)})-\epsilon_2(\lambda_h^{(2)})+\epsilon_3(\lambda_p^{(3)}), \tag{8}$$

where the dressed energy $\epsilon_n(\lambda)$ satisfy (see, for example, Ref. 16)

$$\epsilon_1(\lambda)=-\pi a_1(\lambda)-\mu+\int_{-\infty}^{\infty}a_1(\lambda-\nu)\epsilon_2(\nu)d\nu-\int_{-\Lambda_1}^{\Lambda_1}a_2(\lambda-\nu)\epsilon_1(\nu)d\nu,$$

$$\epsilon_2(\lambda)=\int_{-\Lambda_1}^{\Lambda_1}a_1(\lambda-\nu)\epsilon_1(\nu)d\nu-\int_{-\infty}^{\infty}a_2(\lambda-\nu)\epsilon_2(\nu)d\nu,$$

$$\epsilon_3(\lambda)=\mu+2J+\int_{-\infty}^{\infty}a_1(\lambda-\nu)\epsilon_2(\nu)d\nu, \tag{9}$$

where $\mu=-\pi a_1(\Lambda_1)$ denotes the chemical potential. The energy gap associated with this excitation is given by $\Delta(n_h)=\epsilon_3(0)$. [Note that $\epsilon_1(\pm\Lambda_1)=0$ and $\epsilon_2(\pm\infty)=0$.] Δ is a monotonically increasing function of n_h and ranges from $2(J-2)$ for $n_h=0$ to $2J$ for $n_h=1$, while J_c is a monotonically decreasing function of n_h and ranges from $J_c=2$ for $n_h=0$ to $J_c=0$ for $n_h=1$. For $n_h=2/3$, the dressed energy $\epsilon_3(\lambda)$ reads

$$\epsilon_3(\lambda,n_h=2/3)=-\frac{1}{2}\int\frac{e^{-1/2|\omega|}e^{-i\omega\lambda}}{4\cosh^2\frac{\omega}{2}-1}d\omega+2J. \tag{10}$$

The energy gap $\Delta(2/3)$ and the critical value $J_c(2/3)$ can be easily derived as

$$\Delta(2/3)=2J-\frac{\pi}{2\sqrt{3}}+\frac{1}{2}\ln 3,\quad J_c(2/3)=\frac{\pi}{4\sqrt{3}}-\frac{1}{4}\ln 3. \tag{11}$$

When $J<J_c(n_h)$, the triplet excitations become massless and the system behaves as a Luttinger liquid with a holon band and four-spinon bands. Exactly at the critical point $J=J_c(n_h)$, the triplet excitations are marginal, indicating a quantum phase transition at this point. To see it clearly, let us consider the dispersion relation of the triplet excitations for $J=J_c(n_h)$. From the third equation of the Bethe ansatz equations (4) we know that a single $\lambda^{(3)}$ mode with rapidity λ is quantized as

$$\frac{2\pi I}{N}=\frac{1}{N}\sum_{j=1}^{M_2}2\arctan[2(\lambda-\lambda_j^{(2)})], \tag{12}$$

where I is an arbitrary integer or half integer depending on the parity of M_2. Therefore, the left-hand side of Eq. (12) can be treated as the quasimomenta $k(\lambda)$ of the $\lambda^{(3)}$ mode.[18] In the thermodynamic limit $N\to\infty$,

$$k(\lambda)=2\int_{-\infty}^{\infty}\arctan[2(\lambda-\nu)]\rho_2(\nu)d\nu. \tag{13}$$

From Eqs. (6) and (9) one finds that the velocity of the $\lambda^{(3)}$ mode $v_3=\lim_{k\to 0}\partial\epsilon_3(\lambda)/\partial k(\lambda)=0$, implying a finite mass of this excitation. Therefore, the dispersion relation takes the following form:

$$\epsilon_3[k(\lambda)]=k^2/(2m)$$

for $k\to 0$. The effective mass of the excitation reads

$$m=\lim_{\lambda\to 0}\left[\frac{\partial^2\epsilon_3(\lambda)}{\partial k^2(\lambda)}\right]^{-1}. \tag{14}$$

It can be easily demonstrated that m takes positive values for any given n_h. At very low temperatures, only few excitations exist and behave as a quasi-ideal quantum gas obeying the Pauli exclusion principle but with a zero effective chemical potential. The quantum critical behavior at $J=J_c(n_h)$ is mainly governed by the marginal excitations. For example, the low-temperature specific heat and susceptibility of the system behave as

$$C\sim T^{1/2},\quad \chi\sim T^{-1/2}. \tag{15}$$

The divergence of the susceptibility at $T=0$ is due to the singularity of the density of states of the marginal excitations.

When $J<J_c(n_h)$, the system behaves as a five-component Luttinger liquid, while for $J>J_c(n_h)$, an external magnetic field may drive some quantum phase transitions at zero temperature. For a given hole concentration n_h, there are three critical fields H_c^1, H_c^2, and H_c^3. In a very weak field, the susceptibility is Pauli type due to the response of the Kondo holes. When H reaches H_c^1, the Kondo holes are completely polarized, while when $H=H_c^2$, the Kondo singlets begin to be broken and the zero-temperature susceptibility has a singularity at this point, $\chi(H)\sim(H-H_c^2)^{-1/2}$ $(H\geqslant H_c^2)$. For a strong enough $H\geqslant H_c^3$, the Kondo holes are completely polarized and the spin singlets are completely broken. H_c^1 ranges from 0 $(n_h=0)$ to 4 $(n_h=1)$, $2(J-2)\leqslant H_c^2\leqslant 2J$ and H_c^3 ranges from $2(J+2)$ $(n_h=0)$ to 4 $(n_h=1)$. For $H_c^1 < H < H_c^2$, a magnetization plateau occurs since in this case, the Kondo holes are completely polarized while H is still not strong enough to excite the triplet modes. For $H_c^2 < H_c^1$, singlet broken occurs before the saturation of the holes' magnetization. There is no magnetization plateau for $H<H_c^3$ but there are a singularity at $H=H_c^2$ and a kink at $H=H_c^1$ in the χ-H curve. To see the situation clearly, let us consider the ground-state properties of $n_h=1/2$ and $J>J_c(1/2)$ case. With a magnetic field, the eigenenergy reads (up to an irrelevant constant)

$$E=-\sum_{j=1}^{M_1}\frac{\frac{1}{2}}{\lambda_j^{(1)}+\frac{1}{4}}-2JN_0-H(N_3-N_5)-\frac{1}{2}H(N_1-N_2). \tag{16}$$

In this case, $H_c^1<H_c^2<H_c^3$. When $H=H_c^1$, the ground-state configuration is described by $N_0=N/2=N_1=M_1$ and $N_n=0$ for $n>2$. The density of $\lambda^{(1)}$ is still given by Eq. (6) but with $\rho_2(\lambda)=0$ and $\Lambda_1=\infty$. The critical field H_c^1 can be derived by considering the excitation process $N_1\to N/2-1$, $N_2\to 1$. This is realized by putting a hole in the $\lambda^{(1)}$ sea and adding a particle to the $\lambda^{(2)}$ band. Denoting the rapidities of the hole and the particle as λ_h and λ_p, respectively, and setting $\delta\rho_1(\lambda)/N$ as the change of $\rho_1(\lambda)$ due to λ_h and λ_p, from Eq. (6) we have

$$\delta\rho_1(\lambda)=-\int_{-\infty}^{\infty}a_2(\lambda-\nu)\,\delta\rho_1(\nu)d\nu+a_1(\lambda-\lambda_p)-\delta(\lambda-\lambda_h). \tag{17}$$

The excitation energy associated with this excitation is

$$\epsilon(\lambda_h,\lambda_p)=-\pi\int_{-\infty}^{\infty}a_1(\lambda)\,\delta\rho_1(\lambda)d\lambda+H. \tag{18}$$

Solving Eq. (17) by Fourier transformation and substituting it into Eq. (18), we readily obtain the energy gap $\Delta_1=\epsilon(\infty,0)=H-\ln 2$. Obviously, $H_c^1=\ln 2$. H_c^2 can be derived in a similar way. For convenience, we choose $|1\rangle_g$ as the vacuum state. The excitation breaking a Kondo singlet corresponds to $M_1=N_0\to N/2-1$, $M_2\to 1$. The energy gap associated with this excitation is $\Delta_2=2J-H-\ln 2$. Therefore, $H_c^2=2J-\ln 2$. To derive H_c^3, we choose still $|1\rangle_g$ as the vacuum state. When $H>H_c^3$, the ground state is described by $N_1=N_3=N/2$. With the same procedure we readily obtain the energy gap associated with this excitation reads $\Delta_3=H-2J-\ln 2$. Therefore $H_c^3=2J+\ln 2$.

In conclusion, we introduce an integrable Kondo lattice model describing a strongly correlated electron gas interacting with a Heisenberg spin chain. The ground-state phase boundaries and the critical behaviors around the phase boundaries are derived exactly. We remark that though the model is somehow artificial, it is indeed related to some experimental observations, such as the Kondo insulators, the quantum critical behavior in some heavy fermion compounds and the magnetization plateau in some low-dimensional systems.

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