Identification of the physical parameters of the paramagnetic phase of the one-dimensional Kondo lattice model done by introducing a nonmagnetic quantum state with rotating order parameters

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(December 15, 2018)

The paramagnetic phase of the one-dimensional Kondo lattice model is investigated for electron densities below half-filling using a new mean-field approach. The physical parameters that govern this phase are identified to be the spin-flip processes of both the localized and itinerant spins. A new nonmagnetic-quantum state, where the local magnetization is a rotating vector with a nonzero average length, is proposed in order to describe this phase. This state does not break SU(2) symmetry in agreement with Mermin-Wagner theorem. The line boundary between this phase and the ferromagnetic phase is calculated in the coupling-density phase diagram. Also, expressions are calculated for the velocities of the conduction electrons excitations, and heat capacity and entropy versus temperature are analyzed. Good agreement with many of the available numerical data is achieved.

PACS numbers: 75.30.Mb

I. INTRODUCTION

Strong correlations between electronic degrees of freedom in several materials, like high-temperature superconductors, heavy-fermion materials, etc., are responsible, or are at least thought to be responsible, for the occurrence of various quantum phenomena such as quantum magnetism, superconductivity, non-conventional metallic phases, etc. Heavy-fermion materials may be modeled using the canonical Kondo-lattice model for which intensive studies have been reported in the last years about its one-dimensional version. In this case, the zero-temperature phase diagram in terms of the conduction-electrons density \( n \) below half-filling and the Kondo exchange coupling constant \( J_K \) between the localized and itinerant spins has been established mainly using numerical methods. For strong exchange couplings, the ground state is an unsaturated ferromagnet, whereas for weak couplings, it is a paramagnetic phase. At exactly half-filling, the phase is a spin-liquid insulator for any Kondo coupling, Fig. 1 (Ref. 1 contains detailed discussion of this phase diagram). The ferromagnetic and the spin-liquid phases are now well understood because these are characterized by order parameters which are the magnetization for the ferromagnetic phase, and the spin and charge energy gaps for the spin-liquid phase. For the paramagnetic phase however, no physical parameter has been proposed so far in order to describe it. One of the purposes of this work is to identify such a parameter (or parameters). Moreover, the question concerning the crossover from the high-temperature regime to the low-temperature region needs to be addressed. In the high-temperature regime, the conduction electrons and localized spins behave as being almost independent due to the fact that thermal fluctuations wash out any characteristic energy related to the Kondo exchange coupling. In the low-temperature regime, correlation effects become strong enough to dominate the physical properties of the Kondo lattice model. The paramagnetic phase was proposed to be a Luttinger liquid at zero temperature. If we were to assume that this true, then a crossover would take place between the high-temperature metallic and the low temperature Luttinger-liquid phases.

Our findings can be summarized as follows. The paramagnetic phase is found to be governed by the quantum dynamics (spin-flip processes) of both the localized and itinerant spins. We pave the way to a new quantum state in which the local magnetization is finite in the xy-plane if measured in a rotating reference frame, but vanishes once averaged over the angle of rotation, hence ensuring that Mermin-Wagner theorem is not violated; the magnetization along the z-axis being equal to zero. This is an example of a rotating order parameter with a finite length but a phase angle assuming any value between 0 and \( 2\pi \). We should mention that interpreting our findings in terms of the Luttinger liquid state is not a simple matter. We are still investigating this question. Note however that quantitative comparison between our results and the Luttinger-liquid description results is found to be fairly good (see below). What remains to do is understanding: why should the Fermi liquid picture give rise to the Luttinger liquid one at low temperature?

In section II, a full description of the present approach is provided. The physical foundations upon which our theoretical calculations are based, are explained. We identify the physical parameters as being the averages of spin-flip operators of the localized and itinerant electrons. Section III is devoted to showing some results and the Luttinger-liquid description results is found to be fairly good (see below). What remains to do is understanding: why should the Fermi liquid picture give rise to the Luttinger liquid one at low temperature?
II. DESCRIPTION OF THE APPROACH

A. Physical foundations

In this work, the numerical data available in the literature are considered as numerical experiments upon which the present approach is founded.

The Kondo lattice Hamiltonian in one dimension is given by:

$$H = -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + J_K \sum_i S_i \cdot s_i,$$

where $S_i$ and $s_i$ are respectively the localized and itinerant spin operators. $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ are the creation and annihilation operators at site $i$ of an electron with the $z$-component of the spin being $\sigma = \pm 1/2$. $t$ is the hoping energy of conduction electrons. Because neither the Kondo singlets formation nor magnetic order occurs in the paramagnetic phase for densities below half-filling, a result that is strongly pointed out by numerical calculations, it is justified to choose the following Hamiltonian where only the averages $\langle S_i^- \rangle$ and $\langle S_i^+ \rangle$ and their complex conjugates are taken into account. These parameters represent spin-flip processes, and are therefore a good probe of the quantum dynamics of the system. We suppose that these processes dominate over all other processes which are the Kondo screening and magnetic ordering. We will see that our results turn out to be consistent with this hypothesis. It is worth noting here that in order to avoid breaking SU(2) symmetry, the phase angles of these parameters will not be calculated in mean-field theory. We, rather, perform a summation over all possible values of these angles. This procedure ensures that the physical phase we obtain is nonmagnetic because it does not break SU(2) symmetry.

B. Effective Hamiltonian

Using this new channel, we get the following approximate expression for the interacting term of (1):

$$S_i \cdot s_i \approx \frac{1}{2} \{ |S_i^- A_i^*| + s_i^- Q_i^* + \text{H.c.} - 2\text{Re}(Q_i A_i^*) \},$$

where $Q_i = \langle S_i^- \rangle \equiv |Q_i|e^{i\phi_i}$ and $A_i = \langle s_i^- \rangle \equiv |A_i|e^{i\psi_i}$. Then, the moduli $|Q_i|$ and $|A_i|$ are calculated in mean-field approximation, but summation over the phase angles $\psi_i$ and $\phi_i$ are performed to guarantee that the continuous SU(2) symmetry remains unbroken. The total Hamiltonian is averaged over $\phi_i$ and $\psi_i$, and the summation over the phases $\phi_i$ and $\psi_i$ of the lowering spin operators lead to $\langle S_i^- \rangle \phi_i = \int_0^{2\pi} d\phi |Q_i|^2 e^{i\phi} = 0$ and $\langle s_i^- \rangle \psi_i = \int_0^{2\pi} d\psi |A_i|^2 e^{i\psi} = 0$ where $|Q_i|$ and $|A_i|$ on one hand, and $|A_i|$ and $|Q_i|$ on the other hand are considered to be independent variables. The minimization of the average of the magnetic energy $J_K \langle S_i s_i \rangle = J_K |A_i||Q_i| \cos(\phi_i - \psi_i)$ imposes the constraint $\phi_i - \psi_i = \pi$ on the angles. For this reason, for example, the sum over these phases in the last term of (2), which involves $A_i^* Q_i$ is $\int d(\phi_i - \psi_i) |A_i Q_i|^2 e^{i(\phi_i - \psi_i)} [\cos(\phi_i - \psi_i - \pi) - |A_i Q_i|^2]$. The delta function implements the constraint $\phi_i - \psi_i = \pi$.

Using the second quantization form for the itinerant spins, the Hamiltonian (2) leads to the following effective Hamiltonian where averaging over the phase angles $\psi_i$ and $\phi_i$ is done:

$$\mathcal{H} = \frac{J_K}{2} \sum_i \int_0^{2\pi} \frac{d\psi_i}{2\pi} \langle S_i^+ |A_i|e^{i\psi_i} + \text{H.c.} \rangle + \frac{J_K}{2} \sum_i \int_0^{2\pi} \frac{d\psi_i}{2\pi} \{ Q_i c_{i,\uparrow}^\dagger c_{i,\downarrow} + Q_i^* c_{i,\downarrow}^\dagger c_{i,\uparrow} \} - t \sum_{i,\sigma=\uparrow,\downarrow} c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.} - \int d(\psi_i - \phi_i) \times \frac{J_K}{2} \{ |A_i| Q_i |e^{i(\phi_i - \psi_i)}| \delta(\phi_i - \psi_i - \pi) + \text{C.c.} \}.$$ (3)

C. Uniform rotating configuration

In the rest of this work, we focus our attention on the uniform configuration, which is obtained for $Q_i = |Q|e^{i\phi}$ and $A_i = |A|e^{i\psi}$. $Q$, $A$, $\phi$, $\psi$ are considered to be site independent but angles vary between 0 and $2\pi$ while satisfying the constraint $\phi - \psi = \pi$. This state realized in this way is called the uniform rotating configuration (URC). In this state, the vector parameters $Q_i = \langle S_i^- \rangle$ and $A_i = \langle s_i^- \rangle$ point in opposite directions while rotating at the same rate. The local and total magnetizations are equal to zero.

In addition, we treat the up and down fermions as being different, and use the following canonical transformation:

$$c_{k\uparrow} = e^{i\phi/2}(\rho_k + \sigma_k)/\sqrt{2}$$
$$c_{k\downarrow} = e^{-i\phi/2}(\rho_k - \sigma_k)/\sqrt{2}$$

(4)
in order to diagonalize the effective Hamiltonian \( H \) in the case of the URC. Here, \( c_i^{(t)} = \sum_k c_i^{(t)} e^{-i \epsilon_k / \sqrt{N}} \) with \( N \) being the number of lattice sites. Next, we perform the following transformation to absorb the phase terms in the transformations (3):

\[
ck,\uparrow \rightarrow e^{i \phi / 2} ck,\uparrow, \quad ck,\downarrow \rightarrow e^{-i \phi / 2} ck,\downarrow
\]

which is equivalent to making a rotation by angle \( \phi \) about the z-axis for the x- and y-components of the itinerant spin operator, with the matrix of rotation given by

\[
\begin{pmatrix}
\cos \phi & \sin \phi \\
-\sin \phi & \cos \phi
\end{pmatrix}
\]

Due to the constraint \( \phi - \psi = \pi \), rotating the itinerant-spins x and y components causes the rotation of the x and y components of the localized spins by angle \( \psi = \phi - \pi \) about the z axis. The matrix of rotation in this case is given by:

\[
\begin{pmatrix}
\cos \psi & \sin \psi \\
-\sin \psi & \cos \psi
\end{pmatrix}
\]

Because we sum over the angles \( \phi \) and \( \psi \) between 0 and \( 2\pi \), the spin components are continuously rotating, and the Hamiltonian may be written in the rotating reference frame for which the x axis and y axis coincide with the rotating x and y components of the itinerant spins.

D. Mean field Hamiltonian in the rotating reference frame

The fact that the effective Hamiltonian is invariant under the above rotations by angles \( \phi \) and \( \psi \) is consistent with the absence of SU(2) symmetry breaking. Here we perform such rotations before diagonalizing the simplified Hamiltonian obtained in the URC approximation. This is equivalent to using the transformations

\[
ci,\uparrow \rightarrow e^{i \phi / 2} ci,\uparrow, \\
ci,\downarrow \rightarrow e^{-i \phi / 2} ci,\downarrow, \\
S_i^+ \rightarrow e^{-i \psi} S_i^+
\]

on both the itinerant and localized spins. The result is a much simpler expression for the Hamiltonian:

\[
H - \mu N = \sum_k \{ E_{\rho}(k) p_k^+ p_k + E_{\sigma}(k) \sigma_k^+ \sigma_k \} \\
+ AJ_K \sum_i S_i^+ + J_K \sum_i AQ
\]

where \( A \) and \( Q \) stand now for the magnitudes \( |A| \) and \( |Q| \) respectively. Here, \( E_{\rho,\sigma} = \epsilon(k) - \mu \pm |Q| J_K / 2; \epsilon(k) = -2t \cos k \) is the tight-binding spectrum, and \( \mu \) is the chemical potential. Note that we should keep in mind that (3) is obtained in a rotating frame as \( \phi \) and \( \psi \) take values in the interval \([0, 2\pi]\) subject to the constraint \( \phi - \psi = \pi \). Therefore, it is inappropriate to interpret this Hamiltonian as that of conduction electrons and localized spins coupled to magnetic fields along the x-direction in a reference frame at rest. Now, we understand that the up and down spins could be treated differently as a consequence of the effective rotating magnetic fields \( AJ_K \) for the localized spins, and \( QJ_K \) for the itinerant spins. Note also that the energy spectrum of the itinerant electrons splits into two bands under the effect of the Kondo exchange interaction.

E. Phase fluctuations

Allowing for the summation over the phase angles means that we do not minimize free energy with respect to these angles. However, to satisfy the requirement that the magnetic energy is minimized we constrained their difference to be \( \pi \). This leads us to questioning whether this minimum is stable against fluctuations about the value \( \phi - \psi = \pi \). To study the effect of these fluctuations, the following treatment is done. We replace the delta function in the last term of \( H \) in Eq. (3) by the broader Gaussian distribution

\[
\frac{1}{\epsilon \sqrt{\pi}} e^{-\epsilon^2} (\phi - \psi - \pi)^2 / \epsilon^2
\]

to allow for other angles difference to contribute. If \( \epsilon \to 0 \) the Gaussian distribution reduces to the Dirac distribution. The last term in (3) takes the form:

\[
\frac{J_K}{2} \sum_i (|AQ| e^{\pm i \phi - \psi} \frac{1}{\epsilon \sqrt{\pi}} e^{-\epsilon^2} (\phi - \psi - \pi)^2 / \epsilon^2 + C.c.).
\]

Integration over \( \epsilon \) from \(-\infty\) to \(+\infty\) is undertaken, once the integration over \( \phi - \psi \) is done, to guarantee that all possible fluctuations of the phase angles are embodied in the present approach. The result in the URC is

\[
-\alpha J_K \sum_i |AQ|
\]

which differs from the result \(-J_K \sum_i |AQ|\), obtained without fluctuations, by the factor \( \alpha \). \( \alpha \) is a number larger than 1 but smaller than \( 2\sqrt{\pi} \) which is the value obtained when the integrations are carried out to infinity in the integral of \( \phi - \psi \). This reduces the values of the mean-field parameters (as one would expect) by a factor \( \alpha \sim 1 \) without destroying the mean-field picture. Thus this means that the mean-field solution \( \phi - \psi = \pi \) is stable against phase fluctuations.

III. RESULTS
A. Parameters of the KLM model

In the rest of this paper, we set $\alpha = 1$, and seek some quantitative understanding of the present approach. To calculate the parameters $Q$ and $A$, we use the self-consistent equations obtained by minimizing the free energy:

$$F = -\frac{1}{N\beta} \sum_{k,\nu=\rho,\sigma} \ln\{1 + e^{-\beta E_\nu(k)}\}$$
$$- \frac{1}{\beta} \ln\{2 \cosh[\beta A J_K / 2]\} + J_K Q A.$$  \hfill (8)

with respect to $A$ and $Q$. This yields:

$$Q = \frac{1}{2} \tanh(\beta J_K A / 2)$$
$$A = \frac{1}{2N} \sum_k \{f[E_\sigma(k)] - f[E_\rho(k)]\},$$  \hfill (9)

where the summation $\sum_k$ runs over the Brillouin zone of the conduction electrons, and $f(x) = 1/(1 + e^{\beta(x-\mu)})$ is the Fermi distribution factor. $\beta = 1/k_B T$ with $k_B$ is the Boltzmann constant. $\mu \approx \epsilon_F$ with $\epsilon_F$ being the Fermi energy of the conduction electrons.

As the paramagnetic phase occurs for $J_K < 4t$, we expand $f(E_\rho) - f(E_\sigma)$ to first order in $Q J_K / 2$. We obtain:

$$A = -\frac{1}{2} Q J_K \sum_k \frac{\partial f(\epsilon(k))}{\partial \epsilon(k)} = \frac{1}{2} Q \chi J_K,$$  \hfill (10)

which leads to

$$A = \frac{1}{4} \chi J_K \tanh(\beta A J_K / 2)$$  \hfill (11)

when $\sum_k$ is used. Here $\chi = -\sum_k \frac{\partial f(\epsilon(k))}{\partial \epsilon(k)}$ is the uniform susceptibility of the free conduction electrons in one dimension.

At zero temperature, the non-zero solution is given by $A = \chi J_K / 4$ and $Q = 1/2$; $\chi \approx \mathcal{D}(\epsilon_F) = 1/(2\pi v_F)$ is the density of states of the conduction electrons; $v_F = 2t \sin k_F$ being their Fermi velocity. Slightly above zero temperature, we get for $k_B T \ll \mathcal{D}(\epsilon_F) J_K^2 / 4$:

$$A \approx \frac{1}{4} \chi J_K (1 - 2e^{-\beta \chi J_K^2 / 4})$$
$$Q \approx \frac{1}{2} - e^{-\beta \chi J_K^2 / 4},$$

where again $\chi \approx \mathcal{D}(\epsilon_F)$ is evaluated at $T = 0$ because $\chi(T)$ does not deviate much from its zero-temperature value for temperature well below the Fermi temperature of the free conduction electrons. In the rest of this paper we will consider this value for $\chi$.

B. Crossover temperature

The parameters $A$ and $Q$ decrease as temperature increases, and vanish at a temperature $T_{cf}$. Indeed, expanding the tangent hyperbolic to third order in the vicinity of this critical temperature in Eq. (11) and using Eq. (13), we find:

$$A \approx A_0 (1 - T/T_{cf})^{1/2}, \quad Q \approx Q_0 (1 - T/T_{cf})^{1/2},$$

with $A_0 = 2\sqrt{3} k_B T_{cf} / J_K$, and $Q_0 = \sqrt{3}/2$, and the temperature:

$$T_{cf} = \chi J_K^2 / 8 k_B.$$  \hfill (12)

Below $T_{cf}$, the Kondo lattice system deviates from the system of independent localized spins and conduction electrons. As might be expected $T_{cf}$ is proportional to $J_K^2$, a result that is reminiscent of the RKKY interaction which dominates over Kondo screening, although not leading to magnetic order. Above $T_{cf}$, the magnitude of the magnetization is zero. Below, $T_{cf}$, the magnitude becomes finite, but averaging about its phase angles gives zero magnetization. It is for this reason that this change in behavior is not a true phase transition. The present approach leads to a sharp change of regime at $T_{cf}$. We do not exclude that if the change in the regime is rather a smooth crossover, the crossover temperature will be given by $T_x \sim T_{cf}$. $T_{cf}$ is called the crossover temperature. Shiba and Tsunetsugu \cite{JPSJ} reported the existence of a crossover temperature, but said that it is determined by the velocity of the excitations of the itinerant spins at zero temperature.

C. Ground-state energy and the phase diagram

The idea behind calculating the ground-state energy is to find how the correction (due to $J_K$) to the ground-state energy of the conduction electrons behaves. This will indicate the type of correlations that dominant. This correction is found to be given by the equation:

$$\Delta E_{GS} \approx -\frac{J_K^2}{8} \mathcal{D}(\epsilon_F), \quad (|\Delta E_{GS}| / k_B T_{cf} \approx 1).$$  \hfill (13)

for $J_K \ll 4t$. Interestingly, this correction is of order $J_K^2 / t$, and is again reminiscent of the RKKY interaction between localized spins. As $J_K / t$ increases (but keeping $J_K / t < 4$), we found that the correction to the ground-state energy deviates from a $J_K^2 / t$ law. Estimating the points where the change takes place for different values of $J_K$, we determined the line boundary, $J_{K,c}(n)/t$ versus the conduction electrons density $n$, separating the paramagnetic phase from the ferromagnetic phase at strong coupling $J_K / t$. This line is found to be very well fitted by:

$$J_{K,c}(n)/t \approx 2\pi n \sin(\pi n).$$  \hfill (14)
This is consistent with the fact that the weak coupling regime is equivalent to $J_K/t < \epsilon_F/t$. Linearizing the energy spectrum of the conduction electrons around $k_F$, one finds the linear spectrum $\epsilon(k) - \epsilon_F = v_F(k - k_F)$, where $v_F$ is the Fermi velocity. For a particle with momentum $k$ ($h = 1$) and velocity $v_F$, the energy is given by $v_F k_F$. Thus, within the linear approximation, it is natural to consider an effective Fermi energy given by $\epsilon_F = v_F k_F = 2k_F \sin k_F$. This yields $J_K < v_F k_F = 2\pi n \sin(n \pi)$, which leads to (6).

Eq. (14) is in very good agreement with the available exact numerical data, Fig. 1. For $n = 0.35$, Eq. (4) yields $J_{K,c} \approx 1.96$, which is very close to the density-matrix-renormalization-group exact result, 24.

The agreement is however less accurate for $n = 1/6$ where we obtained $J_{K,c} \approx 0.5$ compared to the result of Ref. 24, namely $J_{K,c} \approx 1$, obtained using quantum Monte Carlo simulation. The reason for this discordance may however be attributed to the fact that Monte Carlo simulations are difficult to implement at very low temperatures, and to the fact that the present theory is mean-field like. Using the bosonization technique [5], Honner and Gulacsi, reported $J_{K,c}(n) \approx 2.5 \sin(n \pi)$. But as we notice on figure 1, this does not capture the general trend, while Eq. (4) does it fairly well. Honner and Gulacsi noted that a dependence as that I report here is also possible.

Finally, we would like to briefly analyze the entropy $S = -\partial F/\partial T$ and heat capacity $C = T \partial S/\partial T$. In Fig. 3, we display $C$, for $n = 0.35$ and $J_K/t = 1.6$ where $T_{c,f} = 0.057/t$/$k_B$ agrees very well with the crossover temperature predicted by Shibata and Tsunetsugu in their numerical work [20]. The entropy $S$ is also reported on the same figure. It behaves as predicted in Ref. 20. For $T/T_{c,f} \rightarrow 0$, the entropy $S \approx 1.24 T$ yields a slope in very good agreement with the Tomonaga-Luttinger result $S = \pi T(v^{-1}_\sigma + v^{-1}_\rho)/3 \approx 1.20T$. A sharp maximum is found in $C$ at $T_{c,f}$ as a consequence of the change in the regime from high temperature to temperatures below $T_{c,f}$. The linear behavior of entropy in terms of temperature is consistent with the gapless quasi-particle excitations, and is an indication of the metallic character of the paramagnetic state.

**IV. CONCLUSIONS**

In summary, the paramagnetic phase of the one-dimensional Kondo lattice model is investigated using a new mean-field approach. This approach is valid
away from half-filling where Kondo screening is negligible. We predict that this phase is described by a new nonmagnetic-quantum state characterized by two rotating order parameters with nonzero magnitudes below a crossover temperature. We calculated the ground-state line boundary in the density-coupling phase diagram, the elementary-excitation velocities of the conduction electrons, heat capacity, and entropy. The crossover temperature separating the low-temperature paramagnetic quantum phase from the normal high-temperature phase is evaluated as a function of the Kondo coupling constant and the density of states of the conduction electrons. Overall, our results agree very well with many of the available numerical data well below half-filling, and are compatible with the Luttinger-liquid picture as put forward by several authors, (see Ref.[1] and references therein). Note that it is not yet clear how we could interpret the results of our approach in terms of the Luttinger-liquid description. For densities close to half-filling, residual effects due to Kondo screening have to be taken into account. It is then natural that, quantitatively, our approach is less accurate in this limit. This is what we come face when we compare Shibata and Tsunetsugu’s results with ours for the entropy $S$ for example. The results start to agree well only for conduction-electrons densities below 0.35. Finally, the RKKY oscillations constitute an issue that needs to be addressed within the present approach. One possible avenue is to allow for the parameters $A Q$ to be $k$-dependent. However, even with these two limitations, the present approach is very promising because it is very simple to use, and the calculations can, to a very large extent, be done analytically. And most importantly, it leads to many very satisfactory physical results.

The author would like to thank Prof. P. Fulde for his comments on the manuscript.

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