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Thermodynamics of the Kondo model with electronic interactions

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Abstract. On the basis of the Bethe ansatz solution of the one-dimensional Kondo model with electronic interaction, the thermodynamics equilibrium of the system at finite temperature is studied in terms of the strategy of Yang and Yang. The string hypothesis in the spin rapidity is discussed extensively. The thermodynamics quantities, such as the specific heat and the magnetic susceptibility, are obtained.

1. Introduction

It is known that the study of exact solutions is helpful in understanding non-perturbative effects in strongly correlated electronic systems. The exact solution of the one-dimensional Kondo [1] model with linearized dispersion in the absence of electronic interaction was found in [2, 3]. The model with quadratic dispersion in the presence of electronic interaction was shown to be exactly solvable at some value of electron-impurity coupling [4].

Here, we study the thermodynamics of the Kondo model in the presence of electronic interactions. The general thermal equilibrium is discussed exactly on the basis of the known Bethe ansatz solutions of the model [4]. The specific heat and magnetic susceptibility are obtained analytically, in general, and given explicitly in the strong-coupling limit. The specific heat and the magnetic susceptibility at low temperature are discussed. In the next section we briefly exhibit the model under consideration and its Bethe ansatz solution. In section 3, we demonstrate the string hypothesis and write out the Bethe ansatz equation in the presence of complex roots. In section 4, we consider the thermodynamics limit by introducing the density of roots and holes. In section 5 we derive the free energy of the system at thermal equilibrium according to the strategy of Yang and Yang [5]. In section 6, We calculate the thermodynamics quantities, such as the specific heat and the magnetic susceptibility. In the case of the strong-coupling limit, we find that the contributions of both electrons and impurities to the specific heat and the magnetic susceptibility is Fermi-liquid-like.

2. The model and its spectrum

The model Hamiltonian of a correlated electronic host with repulsive interaction ($u > 0$) reads

$$H_0 = \sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) C^*_{\boldsymbol{k}a} C_{\boldsymbol{k}a} + \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} u\delta(\boldsymbol{k}_1 + \boldsymbol{k}_2, \boldsymbol{k}_3 + \boldsymbol{k}_4) C^*_{\boldsymbol{k}_4 a} C^*_{\boldsymbol{k}_3 b} C_{\boldsymbol{k}_2 b} C_{\boldsymbol{k}_1 a}$$

where C_{ka} annihilates an electron with momentum $\boldsymbol{k}$ and spin component a, and $\varepsilon(k) = k^2/2$ (in units of $\hbar$ and of the electron mass). The electrons are coupled by both spin and charge interactions to a localized impurity,

$$H_I = J\Psi_a^*(0)\boldsymbol{S}_{ab}\Psi_b(0) \cdot \boldsymbol{S}^0 + V\Psi_a^*(0)\Psi_a(0)$$

where the field Ψ_a is the Fourier transform of C_{ka}, $\boldsymbol{S}^0$ is the spin of the impurity and $\boldsymbol{S}$ is the spin of the electrons in the band.

The present model was solved exactly on the basis of the Bethe ansatz with periodic boundary conditions by considering the system in the Hilbert space of N particles [4]. It was shown that the model is integrable [4, 6] when $u = -J$. The Bethe ansatz equations for the spectrum are

$$\begin{aligned} e^{-ik_jL} &= e^{-i\theta(k_j)} \prod_{\nu=1}^{M} \frac{\lambda_\nu - k_j + iu/2}{\lambda_\nu - k_j - iu/2} - \prod_{\nu=1}^{M} \frac{\lambda_\nu - \lambda_\mu + iu}{\lambda_\nu - \lambda_\mu - iu} \\ &= \frac{\lambda_\mu - iu/2}{\lambda_\mu + iu/2} \prod_{l=1}^{N} \frac{\lambda_\mu - k_l - iu/2}{\lambda_\mu - k_l + iu/2} \end{aligned} \tag{1}$$

where $\theta(k_j) = 2\tan^{-1}(k_j/u)$. It corresponds to the representation with the state of $N - M$ spin-up and M spin-down being the highest weight state. Except for the impurity contributions, the first factors on the right-hand sides of both equations of (1), they are the same as the Bethe ansatz equation of [7]. In the approximation $k_j \sim k_l$ for any j, l, the S-matrix of the electron–electron interaction will be independent of u. Then the Yang–Baxter equation will give no restrictions between u and J. This makes it easy to understand the usual Kondo problem where the linear dispersion relation is adopted, whence the model is solvable at any value of J.

3. String hypothesis

For the ground state (i.e. at zero temperature), the ks and λs are real roots of the Bethe ansatz equation (1). For the excited state (i.e. at non-zero temperature), however, they can be complex roots [8, 9]. We will not take account of the complex roots in the charge sector k for repulsive interaction since it does not happen at low temperature. The complex roots λ in the spin sector are always for a 'bound state' with several other λs, which arises from the consistency of both sides of the Bethe ansatz equation [8]. The complex roots with the same real part λ_β^n form an n-string,

$$\begin{aligned} &\Lambda_\beta^{nm} = \lambda_\beta^n + i\frac{u}{2}m + O(\exp(-\delta N)) \qquad (\delta > 0) \\ &m = -n+1, -n+3, \ldots, n-3, n-1. \end{aligned} \tag{2}$$

The set of roots $\{\lambda_\nu | \nu = 1, 2, \ldots, M\}$ is then partitioned into a set of n-strings $\{\Lambda_\beta^n | m = -n+1, -n+3, \ldots, n-3, n-1; \beta = 1, 2, \ldots, M_n\}$. Obviously,

$$M = \sum_{n=1}^{\infty} nM_n$$

where M_n denotes the number of n-strings.

Substituting these n-strings into equation (1), we can find that the product of the fractions for the roots within the same n-string reduces to $(\lambda_\beta^n - k_j + inu/2)/(\lambda_\beta^n - k_j - inu/2)$ because of the alternative elimination between the denominator and numerator. Hence the Bethe ansatz equation (1) becomes

$$e^{-ik_jL} = e^{-i\theta(k_j)} \prod_{\beta n} \frac{\lambda_\beta^n - k_j + inu/2}{\lambda_\beta^n - k_j - inu/2} \tag{3}$$

and

$$-\prod_{\beta m} \prod_{q=-m+1}^{m-1} \frac{\Lambda_\beta^{mq} - \Lambda_\alpha^{np} + iu}{\Lambda_\beta^{mq} - \Lambda_\alpha^{np} - iu} = \frac{\Lambda_\alpha^{np} - iu/2}{\Lambda_\alpha^{np} + iu/2} \prod_{l=1}^{N} \frac{\Lambda_\alpha^{np} - k_l - iu/2}{\Lambda_\alpha^{np} - k_l + iu/2}. \tag{4}$$

The product of equation (4) for $p = -n+1, -n+3, \ldots, n-3, n-1$ gives rise to

$$\begin{aligned}(-1)^n \prod_{\beta m} & \frac{\lambda_\beta^m - \lambda_\alpha^n + i(m+n)u/2}{\lambda_\beta^m - \lambda_\alpha^n - i(m+n)u/2} \\ & \times \left[\frac{\lambda_\beta^m - \lambda_\alpha^n + i(m+n-2)u/2}{\lambda_\beta^m - \lambda_\alpha^n - i(m+n-2)u/2} \cdots \frac{\lambda_\beta^m - \lambda_\alpha^n + i(|m-n|+2)u/2}{\lambda_\beta^m - \lambda_\alpha^n - i(|m-n|+2)u/2} \right]^2 \\ & \times \frac{\lambda_\beta^m - \lambda_\alpha^n + i|m-n|u/2}{\lambda_\beta^m - \lambda_\alpha^n - i|m-n|u/2} = \frac{\lambda_\alpha^n - inu/2}{\lambda_\alpha^n + inu/2} \prod_{l}^{N} \frac{\lambda_\alpha^n - k_l - inu/2}{\lambda_\alpha^n - k_l + inu/2}. \end{aligned} \tag{5}$$

Taking the logarithm of equations (3) and (5) we have

$$\begin{aligned} k_j &= \frac{2\pi}{L} I_j + \frac{1}{L}\theta(k_j) + \frac{1}{L} \sum_{\beta n} \Theta_{n/2}(\lambda_\beta^n - k_j) \\ \Theta_{n/2}(\lambda_\alpha^n) &+ \sum_{l=1}^{N} \Theta_{n/2}(\lambda_\alpha^n - k_l) = 2\pi J_\alpha^n - \sum_{\beta m p} A_{nmp} \Theta_{p/2}(\lambda_\beta^m - \lambda_\alpha^n) \end{aligned} \tag{6}$$

where $\Theta_\rho(x) = 2\tan^{-1}(\frac{x}{\rho u})$ and

$$A_{nmp} = \begin{cases} 1 & \text{for } p = m+n, |m-n| \ (\neq 0) \\ 2 & \text{for } p = n+m-2, n+m-4, \ldots, |n-n|+2 \\ 0 & \text{otherwise.} \end{cases}$$

I_j and J_α^n are quantum numbers, I_j are integers or half-integers depending on whether M is even or odd, the J_α^n are integers or half-integers depending on whether $N - M_n - n + 1$ is even or odd.

4. The thermodynamics limit

The transcendental equations (6) for the real parts of the complex roots are obviously difficult to solve. It will be convenient to consider the thermodynamics limit (see, for example, [11]), i.e. $N \to \infty$, $L \to \infty$ but $D = N/L$ is fixed. Introducing the density distribution of roots and holes

$$\begin{aligned} \frac{1}{L}\frac{dI(k)}{dk} &= \rho(k) + \rho^h(k) \\ \frac{1}{L}\frac{dJ^n(\lambda)}{d\lambda} &= \sigma_n(\lambda) + \sigma_n^h(\lambda) \end{aligned} \tag{7}$$

we obtain from (6) the following set of integral equations:

$$\begin{aligned}\rho(k)+\rho^h(k) &= \frac{1}{2\pi}-\frac{1}{L}K_1(k)+\sum_{n=1}^{\infty}K_{n/2}(k|\lambda')\sigma_n(\lambda')\\ \sigma_n(\lambda)+\sigma_n^h(\lambda) &= \frac{1}{L}K_{n/2}(\lambda)+K_{n/2}(\lambda|k')\rho(k')-\sum_{mp}A_{nmp}K_{p/2}(\lambda|\lambda')\sigma_m(\lambda')\end{aligned} \tag{8}$$

where $K_n(x)=\pi^{-1}nu/(n^2u^2+x^2)$. We have adopted a notation convention $K_n(x|y)\rho(y) = \int K_n(x-y)\rho(y)\,\mathrm{d}y$, etc in the above.

In term of the density distributions, the energy and the concentration of electrons as well as the number of down spins are given by

$$E = L\int_{-\infty}^{\infty}\mathrm{d}k\,\rho(k)k^2$$

$$D=\frac{N}{L}=\int_{-\infty}^{\infty}\mathrm{d}k\,\rho(k)$$

$$\frac{M}{L}=\sum_{n=1}^{\infty}n\int_{-\infty}^{\infty}\mathrm{d}\lambda\,\sigma_n(\lambda).$$

Thus the magnetic moment of the system is

$$\mathcal{M}=\frac{1}{2}(N-2M)+S^z_{imp} \tag{9}$$

$$=\frac{L}{2}\int_{-\infty}^{\infty}\rho(k)\,\mathrm{d}k - L\sum_{n=1}^{\infty}n\int_{-\infty}^{\infty}\sigma_n(\lambda)\,\mathrm{d}\lambda+S^z_{imp} \tag{10}$$

where S^z_{imp} denotes the spin of the impurity, and the g factor is set to unity.

The ground state of the present model is a Fermi sea described by $\rho(k)$ with real rapidity λ, i.e. $\rho(k)=0$ for $|k|>k_F$ and $\rho^h(k)=0$ for $|k|<k_F$; $\sigma_1(\lambda)\neq 0$ but $\sigma_n(\lambda)=0$ $(n>1)$, which is the case at zero temperature. Away from zero temperature, the density distributions of roots and holes with respect to the momentum k and the spin rapidity λ should be determined by the principles of statistical physics. In the next section we will discuss this issue extensively on the basis of the strategy of Yang and Yang [5].

5. Thermal equilibrium

For a given $\rho(k)$ and $\rho^h(k)$, the number of roots and that of holes in the neighbourhood $\mathrm{d}k$ are $L\rho\,\mathrm{d}k$ and $L\rho^h\,\mathrm{d}k$, respectively. Obviously, the total number of roots and holes in the neighbourhood is $L(\rho+\rho^h)\,\mathrm{d}k$. For a given $\sigma_n(\lambda)$ and $\sigma_n^h(\lambda)$, $L\sigma_n\,\mathrm{d}\lambda$ and $L\sigma_n^h\,\mathrm{d}\lambda$ give rise to the number of n-strings and the number of the vacancies of n-strings (holes) in the neighbourhood $\mathrm{d}\lambda$, while $L(\sigma_n+\sigma_n^h)\,\mathrm{d}\lambda$ gives rise to the total number of n-strings and vacancies of n-strings. Thus the total number of possible choices of the state in $\mathrm{d}k\,\mathrm{d}\lambda$ being consistent with the given distribution functions in both charge and spin sectors is

$$\Xi(k,\lambda)=\frac{[L(\rho+\rho^h)\,\mathrm{d}k]!}{[L\rho\,\mathrm{d}k]![L\rho^h\,\mathrm{d}k]!}\prod_n\frac{[L(\sigma_n+\sigma_n^h)\,\mathrm{d}\lambda]!}{[L\sigma_n\,\mathrm{d}\lambda]![L\sigma_n^h\,\mathrm{d}\lambda]!}.$$

As the total number of all possible states for a given distribution function is

$$\Xi=\prod_{k\lambda}\Xi(k,\lambda)$$

the total entropy S will be obtained by taking the logarithm of Ξ,

$$S/L = \int \left\{[\rho(k) + \rho^h(k)] \ln[\rho(k) + \rho^h(k)] - \rho(k) \ln \rho(k) - \rho^h(k) \ln \rho^h(k)\right\} \mathrm{d}k$$
$$+ \sum_n \int \left\{[\sigma_n(\lambda) + \sigma_n^h(\lambda)] \ln[\sigma_n(\lambda) + \sigma_n^h(\lambda)]\right.$$
$$\left. - \sigma_n(\lambda) \ln \sigma_n(\lambda) - \sigma_n^h(\lambda) \ln \sigma_n^h(\lambda)\right\} \mathrm{d}\lambda \tag{11}$$

where the Boltzmann constant is set to unity.

In the presence of the external magnetic field H, we must add a Zeeman term to the original Hamiltonian. As the Zeeman term commutes with the original Hamiltonian, the Bethe ansatz solution is still valid for the present case. Therefore, the energy of the system in the presence of an external magnetic field will be

$$E/L = \int (k^2 - H)\rho(k) \,\mathrm{d}k + \sum_{n=1}^{\infty} 2nH \int \sigma_n(k) \,\mathrm{d}k. \tag{12}$$

In order to obtain the thermal equilibrium at temperature T, we should maximize the contribution to the partition function from the state described by the density distributions of roots and holes. As maximizing the partition function is equivalent to minimizing the free energy $F = E - TS - \mu N$. Here S and E are given by equations (11) and (12), μ is the chemical potential for canonical ensembles. μ plays the role of the Lagrangian multiplier for the condition $L \int \rho(k) \,\mathrm{d}k = N =$ constant if one minimizes the Helmholtz free energy $\Omega = E - TS$. This constraint implies that the assembly has a fixed number of particles. The constraint that the number of down spins is fixed was imposed in [10] when discussing a delta Fermi gas, whereas we will not impose any physical constraints in the following discussion.

Making use of the relations derived from equation (8)

$$\begin{aligned} \delta\rho^h(k) &= -\delta\rho(k) + \sum_n K_{n/2}(k|\lambda)\delta\sigma_n(\lambda) \\ \delta\sigma_n^h(\lambda) &= -\delta\sigma_n(\lambda) + K_{n/2}(\lambda|k)\delta\rho(k) - \sum_{mp} A_{mnp} K_{p/2}(\lambda|\lambda')\delta\sigma_m(\lambda') \end{aligned} \tag{13}$$

we obtain the following conditions from the minimum condition $\delta F = 0$, namely

$$\epsilon(k) = -\mu + k^2 - H - T \sum_n K_{n/2}(k|\lambda) \ln(1 + \mathrm{e}^{-\xi_n(\lambda)/T}) \tag{14}$$

$$\xi_n(\lambda) = 2nH - T K_{n/2}(\lambda|k) \ln(1 + \mathrm{e}^{-\epsilon(k)/T}) + T \sum_{mp} A_{nmp} K_{p/2}(\lambda|\lambda') \ln(1 + \mathrm{e}^{-\xi_m(\lambda')/T}) \tag{15}$$

where we have written

$$\frac{\rho^h(k)}{\rho(k)} = \exp[\epsilon(k)/T]$$
$$\frac{\sigma_n^h(\lambda)}{\sigma_n(\lambda)} = \exp[\xi_n(\lambda)/T].$$

Principally, once $\epsilon(k)$ and $\xi(\lambda)$ are solved from equations (14) and (15), the equilibrium distributions $\rho(k)$ and $\sigma_n(\lambda)$ at temperature T will be known from the following relations:

$$\begin{aligned} \rho(k)[1 + \mathrm{e}^{\epsilon(k)/T}] &= \frac{1}{2\pi} - \frac{1}{L} K_1(k) + \sum_n K_{n/2}(k|\lambda')\sigma_n(\lambda') \\ \sigma_n(\lambda)[1 + \mathrm{e}^{\xi_n(\lambda)/T}] &= \frac{1}{L} K_{n/2}(\lambda) + K_{n/2}(\lambda|k')\rho(k') - \sum_{mq} A_{nmq} K_{q/2}(\lambda|\lambda')\sigma_m(\lambda'). \end{aligned} \tag{16}$$

The free energy per unit length reads

$$F/L = \int \mathrm{d}k\,\rho(k)\left[k^2 - \epsilon(k) - H - T(1 + \mathrm{e}^{\epsilon(k)/T})\ln(1 + \mathrm{e}^{-\epsilon(k)/T})\right]$$
$$+\sum_n \int \mathrm{d}\lambda\,\sigma_n(\lambda)\left[2nH - \xi_n(\lambda) - T(1 + \mathrm{e}^{\xi_n(\lambda)/T})\ln(1 + \mathrm{e}^{-\xi_n(\lambda)/T})\right]. \tag{17}$$

Integrating equation (14) over k after multiplying it with $D^{-1}\rho$, we obtain the chemical potential

$$\mu = \frac{1}{D}\int (k^2 - \epsilon(k) - H)\rho(k)\,\mathrm{d}k - \frac{T}{D}\sum_n \iint K_{n/2}(k-\lambda)\ln(1 + \mathrm{e}^{-\xi_n(\lambda)/T})\rho(k)\,\mathrm{d}\lambda\,\mathrm{d}k. \tag{18}$$

Integrating equation (15) over λ and summing over n after multiplying it with $D^{-1}\sigma_n$, we obtain the following relation:

$$\sum_n \int \xi_n(\lambda)\sigma_n(\lambda)\,\mathrm{d}\lambda = \sum_n 2nH \int \sigma_n(\lambda)\,\mathrm{d}\lambda$$
$$-T\sum_n \iint K_{n/2}(\lambda - k)\ln(1 + \mathrm{e}^{-\epsilon(k)/T})\sigma_n(\lambda)\,\mathrm{d}k\,\mathrm{d}\lambda$$
$$+T\sum_{mnq} A_{mnq} \iint K_{q/2}(\lambda - \lambda')\ln(1 + \mathrm{e}^{-\xi_m(\lambda')/T})\sigma_n(\lambda)\,\mathrm{d}\lambda'\,\mathrm{d}\lambda. \tag{19}$$

Using the relations (18) and (19), we can write out the free energy in terms of ϵ and ξ only,

$$F = \mu N + T\int \left(K_1(k) - \frac{L}{2\pi}\right)\ln(1 + \mathrm{e}^{-\epsilon(k)/T})\,\mathrm{d}k - T\sum_n \int K_{n/2}(\lambda)\ln(1 + \mathrm{e}^{-\xi_n(\lambda)/T})\,\mathrm{d}\lambda. \tag{20}$$

Consequently, the partition function is given by

$$Z = \mathrm{e}^{-F/T} \tag{21}$$

where the Boltzmann constant is set to unity.

The thermodynamics functions, partition function Z, free energy F and thermal potential Ω, etc, are of importance, as knowing either of them, one is able to calculate all thermodynamics properties of the system in principle. However, it is difficult to obtain an analytic expression of $\epsilon(k)$ and $\xi_n(\lambda)$ from the coupled nonlinear integral equations (14) and (15). So we are not able to derive explicit results for thermodynamics quantities. Moreover, we will obtain some plausible results for some special cases in the next section.

6. Thermodynamic quantities

In general, the free energy of our model should be calculated using formula (20), where $\epsilon(k)$ and $\xi(\lambda)$ are determined from equations (14) and (15). Then the other thermodynamic quantities are obtainable from thermodynamic relations.

In the appendix, we show that if μ, ϵ and ξ_n are implicit functions of some thermodynamic quantities x (such as T, L), the derivative of equation (20) with respect to x is the same as the partial derivative of equation (20) with respect to the explicit variable x. It is easy to obtain the pressure of the system

$$P = -\frac{\partial F}{\partial L} = \frac{T}{2\pi}\int \ln(1 + \mathrm{e}^{-\epsilon(k)/T})\,\mathrm{d}k \tag{22}$$

which is formally the same as Yang and Yang's expression. However, the integral equation that $\epsilon(k)$ obeys is different. In our present case the contributions from both the impurity and the spin rapidity are involved.

In terms of ϵ and ξ, the entropy $S = -(\partial F/\partial T)$ becomes

$$\begin{aligned} S = &-\int \ln(1+\mathrm{e}^{-\epsilon(k)/T})\left[-\frac{L}{2\pi}+\frac{1}{\pi}\frac{u}{u^2+k^2}\right]\mathrm{d}k \\ &-\int \frac{\mathrm{e}^{-\epsilon(k)/T}}{1+\mathrm{e}^{-\epsilon(k)/T}}\frac{\epsilon(k)}{T}\left[-\frac{L}{2\pi}+\frac{1}{\pi}\frac{u}{u^2+k^2}\right]\mathrm{d}k \\ &+\sum_n\int\frac{1}{\pi}\frac{nu/2}{(nu/2)^2+\lambda^2}\ln(1+\mathrm{e}^{-\xi_n(\lambda)/T})\,\mathrm{d}\lambda \\ &+\sum_n\int\frac{1}{\pi}\frac{nu/2}{(nu/2)^2+\lambda^2}\frac{\xi_n(\lambda)/T}{1+\mathrm{e}^{\xi_n(\lambda)/T}}\,\mathrm{d}\lambda. \end{aligned} \tag{23}$$

The other thermodynamics quantities are formally obtainable, for example,

$$C_V = T\left(\frac{\partial S}{\partial T}\right) \qquad M = -\left(\frac{\partial F}{\partial H}\right) \qquad \chi = \left(\frac{\partial M}{\partial H}\right). \tag{24}$$

For the sake of saving space, we do not write them out.

The free energy (20) is conveniently partitioned as two parts. $F = F_e + F_i$, here F_i denotes the contribution from the impurity,

$$F_i = \frac{T}{\pi}\int\frac{u}{u^2+k^2}\ln(1+\mathrm{e}^{-\epsilon(k)/T})\,\mathrm{d}k - \frac{T}{\pi}\sum_n\int\frac{nu/2}{(nu/2)^2\eta^2+\lambda^2}\ln(1+\mathrm{e}^{-\xi_n(\lambda)/T})\,\mathrm{d}\lambda$$

and F_e for that from the electrons.

6.1. Strong-coupling limit

For strong coupling $u \to \infty$ and non-vanishing external magnetic field, we keep the leading term in equations (14) and (15),

$$\begin{aligned} \epsilon(k) &= k^2 - H - \mu \\ \xi_n(\lambda) &= 2nH. \end{aligned} \tag{25}$$

The free energy related to the impurity and electrons becomes

$$\begin{aligned} F_i &= T\int\frac{\mathrm{d}k}{\pi}\frac{u}{u^2+k^2}\ln[1+\mathrm{e}^{(\eta-k^2)/T}] - T\sum_n\int\frac{\mathrm{d}\lambda}{\pi}\frac{nu/2}{(nu/2)^2+\lambda^2}\ln[1+\mathrm{e}^{-2nH/T}] \\ F_e &= \mu N - T\frac{L}{2\pi}\int\ln[1+\mathrm{e}^{(\eta-k^2)/T}]\,\mathrm{d}k \end{aligned} \tag{26}$$

where $\eta = \mu + H$. Since $\tan^{-1}(k/u) \simeq k/u$ for $u \to \infty$, integrating equation (26) we have

$$\begin{aligned} F_i &= \frac{4}{\pi u}\int_0^\infty\frac{k^2}{1+\mathrm{e}^{(k^2-\eta)/T}}\,\mathrm{d}k - T\sum_n\ln(1+\mathrm{e}^{-2nH/T}) \\ F_e &= \mu N - \frac{2L}{\pi}\int_0^\infty\frac{k^2}{1+\mathrm{e}^{(k^2-\eta)/T}}\,\mathrm{d}k. \end{aligned} \tag{27}$$

Now we compute the common integration in equation (27),

$$I = \int_0^\infty \frac{k^2}{1 + e^{(k^2 - \eta/T)}}\, dk. \tag{28}$$

Changing variables of $z = (k^2 - \eta)/T$ brings it to

$$I = \frac{T}{2} \int_{-\eta/T}^\infty \frac{(zT + \eta)^{1/2}}{1 + e^z}\, dz \tag{29}$$

which is conveniently split up into three terms,

$$I = \frac{T}{2} \int_0^{\eta/T} (\eta - zT)^{1/2}\, dz - \frac{T}{2} \int_0^{\eta/T} \frac{(\eta - zT)^{1/2}}{1 + e^z}\, dz + \frac{T}{2} \int_0^\infty \frac{(\eta + zT)^{1/2}}{1 + e^z}\, dz. \tag{30}$$

The right end of the interval for integration in the second term can be regarded as ∞ as the contribution from large values of z is negligible. Integrating equation (30) after expanding the numerator as Taylor series, we obtain

$$I = \frac{1}{3}\eta^{3/2} + \frac{T}{2} \sum_{n=0}^\infty (-1)^n \frac{\Gamma(n + 1/2)}{2\sqrt{\pi}} T^{2(n+1/2)} \left[1 - \left(\frac{1}{4}\right)^{n+1/2}\right] \zeta(2n + 2) \left(\frac{1}{\eta}\right)^{n+1/2} \tag{31}$$

where $\zeta(2n + 2)$ is the Riemann zeta function. Consequently, the free energy is obtained as

$$\begin{aligned} F_i &= \frac{4}{\pi u} I - T \sum_{n=1}^\infty \ln[1 + e^{-2nH/T}] \\ F_e &= \mu N - \frac{2L}{\pi} I. \end{aligned} \tag{32}$$

6.2. *Thermodynamic quantities at low temperature*

In the low-temperature approximation, equation (32) becomes

$$F_i = \frac{4}{\pi u} I - T \sum_{n=1}^\infty e^{-2nH/T}. \tag{33}$$

The magnetization. The contributions of electrons and the impurity to the magnetization are obtained

$$\begin{aligned} M_e &= \frac{2L}{\pi} I_h \\ M_i &= -\frac{4}{\pi u} I_h - 2 \sum_{n=1}^\infty n e^{-2nH/T} \end{aligned} \tag{34}$$

where

$$I_h = \frac{\partial I}{\partial H} \qquad I_{hh} = \frac{\partial^2 I}{\partial H^2} \qquad I_{tt} = \frac{\partial^2 I}{\partial T^2}. \tag{35}$$

Clearly, the system has spontaneous magnetization,

$$\begin{aligned} M_e(H \to 0) &= \frac{L}{\pi} \mu^{1/2} - \frac{\pi L}{24} T^2 \mu^{-3/2} \\ M_i &= -\frac{2}{\pi u} \mu^{1/2} + \frac{\pi}{12u} \mu^{-3/2}. \end{aligned}$$

Specific heat and magnetic susceptibility. The specific heat and the magnetic susceptibility are

$$\begin{aligned} C_e &= \frac{2LT}{\pi} I_{tt} \\ \chi_e &= -\frac{2L}{\pi} I_{hh} \\ C_i &= -\frac{4T}{\pi u} I_{tt} + \frac{4H^2}{T^2} \mathrm{e}^{-2H/T} \\ \chi_i &= -\frac{4}{\pi u} I_{hh} + \frac{4}{T} \mathrm{e}^{-2H/T} \end{aligned} \tag{36}$$

where C_e (C_i) is the specific heat of electrons (impurity), and χ_e (χ_i) is the magnetic susceptibility of electrons (impurity).

Wilson's treatment of the Kondo model by a renormalization-group calculation has made it possible to determine the proportionality factor ('Wilson ratio') relating low- and high-temperature dimensional scales. When $T \to 0$, because $\mathrm{e}^{-2H/T}$ decreases more rapidly than T, the second term of equation (36) can be neglected. Then we are able to evaluate the Wilson ratio

$$R = \frac{\chi_i / \chi_e}{C_i / C_e} = 1.$$

As is known $R = 2$ in the usual Kondo model [2] where the linear dispersion was adopted. In the present model the charge sector and spin sector is not completely decoupled due to the electron–electron interaction. In the usual Kondo model, however, the impurity modifies only the spin sector.

Furthermore, if we ignore the small term in I_{tt} and I_{hh}, that is we only keep the first term of each, we find that the impurity's contribution to the specific heat at low temperature is Fermi-liquid-like

$$C_i = -\frac{\pi}{3u} (\mu + H)^{-1/2} T \tag{37}$$

and so is the magnetic susceptibility

$$\chi_i = -\frac{1}{\pi u} (\mu + H)^{-1/2} - \frac{\pi T^2}{8u} (\mu + H)^{-5/2}. \tag{38}$$

Obviously, the zero-temperature susceptibility is finite

$$\chi_i (T = 0) = -\frac{1}{\pi u} (\mu + H)^{-1/2} \tag{39}$$

indicating that the impurity spin manifest in the high-temperature regime by Curie's law, $\chi_i \propto 1/T$, is now completely screened. We interpret the effect as being due to effective coupling of impurity–electron and the electron–electrons leading to the formation of singlet, and the infrared physics is dominated by a strong-coupling fixed point. The impurity's contribution is to suppress the magnetization and give a negative Zeeman energy so that we obtain the minus sign in (37)–(39).

The electron's contributions to the specific heat and the magnetic susceptibility are

$$\begin{aligned} C_e &= \frac{\pi L}{6} (\mu + H)^{-1/2} T \\ \chi_e &= \frac{L}{2\pi} (\mu + H)^{-1/2} + \frac{\pi L T^2}{16} (\mu + H)^{-5/2}. \end{aligned} \tag{40}$$

We have analysed the thermodynamics of the Kondo model with electronic interactions and, in particular, discussed the case of the strong-coupling limit extensively. In that case we have shown the impurity's contribution to the specific heat and the magnetic susceptibility of the system is Fermi-liquid-like and shown that at very low temperature the system has the property of spontaneous magnetization.

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Appendix

Since ϵ and ξ which solve equations (14) and (15) evidently depend on μ, we should consider them as functionals of μ which is usually a function of some thermodynamic variable x (such as T or L). The derivative of the free energy (20) is given by

$$\frac{\partial F}{\partial x} = \left(\frac{\partial F}{\partial x}\right)_{\mu,\epsilon,\xi} + N\frac{\partial \mu}{\partial x} + \int \mathrm{d}k \frac{L/2\pi - K_1(k)}{1 + \mathrm{e}^{\epsilon(k)/T}} \frac{\partial \epsilon}{\partial \mu}\frac{\partial \mu}{\partial x} + \sum_n \int \mathrm{d}\lambda \frac{K_{n/2}(\lambda)}{1 + \mathrm{e}^{\xi_n(\lambda)/T}} \frac{\partial \xi_n}{\partial \mu}\frac{\partial \mu}{\partial x} \tag{A1}$$

where $(\partial F/\partial x)_{\mu,\epsilon,\xi}$ denotes the partial derivative of F with respect to the explicit variable x, while μ, ϵ, and ξ are regarded as irrelevant to x.

The derivative of (14) with respect to μ is

$$\frac{\partial \epsilon}{\partial \mu} = -1 + \sum_n \int \mathrm{d}\lambda \frac{K_{n/2}(k-\lambda)}{1 + \mathrm{e}^{\xi_n(\lambda)/T}} \frac{\partial \xi_n}{\partial \mu}. \tag{A2}$$

Integrating (A2) after multiplying both sides with ρ, we obtain

$$\int \mathrm{d}k \frac{\partial \epsilon}{\partial \mu}\rho(k) = -\frac{N}{L} + \sum_n \int \mathrm{d}\lambda\, \frac{\partial \xi_n}{\partial \mu}\sigma_n(\lambda) - \frac{1}{L}\sum_n \int \mathrm{d}\lambda\, \frac{K_{n/2}(\lambda)}{1 + \mathrm{e}^{\xi_n(\lambda)/T}} \frac{\partial \xi_n}{\partial \mu}$$
$$+ \sum_{nmq} \iint \mathrm{d}\lambda\, \mathrm{d}\lambda' \frac{\partial \xi_n}{\partial \mu} \frac{A_{nmq}}{1 + \mathrm{e}^{\xi_n(\lambda)/T}} K_{q/2}(\lambda - \lambda')\sigma_m(\lambda'). \tag{A3}$$

In deriving the above equation, the second equation of equation (16) has been used. We take a derivative of equation (15), then multiply both sides with σ_n and integrate over λ. Summing over the subscript n in what we obtained, we have

$$\sum_n \int \mathrm{d}\lambda\, \frac{\partial \xi_n}{\partial \mu}\sigma_n(\lambda) = \sum_n \iint \mathrm{d}k\, \mathrm{d}\lambda\, \frac{K_{n/2}(\lambda - k)\sigma_n(\lambda)}{1 + \mathrm{e}^{\epsilon(k)/T}}$$
$$- \sum_{nmq} \iint \mathrm{d}\lambda\, \mathrm{d}\lambda'\, \frac{\partial \xi_m}{\partial \mu} \frac{A_{nmq}}{1 + \mathrm{e}^{\xi_m(\lambda')/T}} K_{q/2}(\lambda - \lambda')\sigma_n(\lambda). \tag{A4}$$

With the help of the first equation of equation (16), equations (A4) and (A3) give rise to

$$N + \int \mathrm{d}k\, \frac{L/2\pi - K_1(k)}{1 + \mathrm{e}^{\epsilon(k)/T}} \frac{\partial \epsilon}{\partial \mu} + \sum_n \int \mathrm{d}\lambda\, \frac{K_{n/2}(\lambda)}{1 + \mathrm{e}^{\xi_n(\lambda)/T}} \frac{\partial \xi_n}{\partial \mu} = 0. \tag{A5}$$

Thus the complete cancellation of the last three terms in equation (A1) concludes that

$$\frac{\partial F}{\partial x} = \left(\frac{\partial F}{\partial x}\right)_{\mu,\epsilon,\xi}.$$

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