Diagonalization of the Kondo Hamiltonian

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The Kondo Hamiltonian is exactly diagonalized with use of a modified Bethe *Ansatz*. The zero-temperature magnetic susceptibility is also calculated.

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The Kondo Hamiltonian,[1-4] describing the interaction of a localized magnetic impurity with electrons in a metal, is given by

$$H=-i\int \varphi_a^\dagger \partial_x \varphi_a dx + J\vec{S}\varphi_a^\dagger(0)\cdot\vec{\sigma}_{ab}\varphi_b(0). \tag{1}$$

Here $\varphi_a(x)$ is the electron field, $a=1,2$ are the spin indices, and $\vec{S}$ describes the spin-$\frac{1}{2}$ impurity. There is no kinetic energy associated with $\vec{S}$.

I slightly generalize the model, allowing the impurity to move, requiring, however, that it carry no kinetic energy. One may then form a localized wave packet for the impurity which will not disperse. In other words, since the energy is degenerate with respect to the motion of the impurity, one can sum over its momentum and localize it [see also Eq. (7)]. Our formalism allows us to consider an arbitrary but fixed number of impurities arbitrarily situated.

I introduce a new field ψ describing both the electrons and the impurities. Thus $\psi=\psi_{a\alpha}$ where a is the previous spin index and α is a "purity" index, with $\alpha=1$ ($\alpha=0$) corresponding to the electron (impurity). I impose on ψ canonical commutation relations and thus consider

$$H=-i\int \psi_{a\alpha}^\dagger \tfrac{1}{2}(1+\gamma^5)_{\alpha\beta}\partial_x\psi_{a\beta} - \tfrac{1}{4}J\int dx\,\bar{\psi}_{a\alpha}(\gamma_\mu)_{\alpha\beta}\vec{\sigma}_{ab}\psi_{b\beta}\bar{\psi}_{a'\alpha'}(\gamma^\mu)_{\alpha'\beta'}\vec{\sigma}_{a'b'}\psi_{b'\beta'}. \tag{2}$$

The matrices γ_μ ($\mu=0,1$) are the usual two-dimensional Dirac matrices and are introduced so that only electrons and impurities interact as is the case in (1). I choose the representation $\gamma^0=\sigma^x$, $\gamma^1=-i\sigma^y$, $\gamma^5=\sigma^z$, and $\bar{\psi}=\psi^\dagger\gamma^0$.

The Hamiltonian H is now similar to that of the chiral Gross-Neveu model[5] [or the SU(2) Thirring model[6]]. The only difference is that in the kinetic energy term the matrix $\frac{1}{2}(1+\gamma^5)$, with its eigenvalues $\alpha=0,1$, replaces the matrix γ^5 and its eigenvalues $\alpha=\pm 1$. H acts on states whose general form is

$$|\mathfrak{F}\rangle=\int\prod_{i=1}^N \mathfrak{F}(X_1,\ldots,X_N,\beta_1,\ldots,\beta_N,a_1,\ldots,a_N)\prod_{i=1}^N\psi^\dagger_{a_i\beta_i}(X_i)|0\rangle, \tag{3}$$

where $|0\rangle$ is the empty Fermi sphere defined by $\psi_{a\beta}(X)|0\rangle=0$. In order for $|\mathfrak{F}\rangle$ to be an eigenstate of H, $\mathfrak{F}(X,\beta,a)$ must be an eigenfunction of the N-particle Hamiltonian

$$h=-i\sum_{i=1}^N\beta_i\partial_i + J\sum_{i,j}^N\delta(X_i-X_j)\vec{\sigma}_i\cdot\vec{\sigma}_j(\beta_i-\beta_j)^2. \tag{4}$$

Note that the impurities, corresponding to $\beta_i=0$, do not carry kinetic energy and only electrons and impurities ($\beta_i\neq\beta_j$) interact. h may be rewritten as

$$h=-i\sum_{i=1}^N\beta_i\partial_i - 2J\sum_{i,j=1}^N\delta(X_i-X_j)P_\beta^{ij}(\beta_i-\beta_j)^2 - J\sum_{i,j=1}^N\delta(X_i-X_j)(\beta_i-\beta_j)^2, \tag{5}$$

where I have used the antisymmetry of the wave function to replace the spin exchange operator $\frac{1}{2}[1+\vec{\sigma}_i\cdot\vec{\sigma}_j]$ by a "purity exchange" operator P_β^{ij} given by $P_\beta^{ij}\mathfrak{F}(X,\beta_i,\ldots,\beta_j,a)=\mathfrak{F}(X,\beta_j,\ldots,\beta_i,a)$.

If one drops the last term in Eq. (5), one obtains the N-particle Hamiltonian that was studied in Ref. (5). It was shown there that $\mathfrak{F}(X,\beta,a)$ could be constructed by means of a generalized Bethe-*Ansatz* technique,[7] which I briefly review.

As h no longer contains the spin, one may write $\mathfrak{F}(X,\beta,a)=F(X,\beta)\zeta(a)$, where $\zeta(a)$ is the spin wave function. It is described by a Young tableau $[N-M,M]$, and its conjugate describes $F(X,\beta)$. This part of the wave function is constructed as follows: In the region in configuration space defined by X_{Q1}

$\leqslant X_{Q2} \leqslant \cdots \leqslant X_{QN}$, F is given as a superposition of plane waves labeled by N momenta K_i and purities α_i,

$$F^{K,\alpha}(X,\beta) = \sum_P \xi_P(Q) \exp(i\sum_{i=1}^{N} K_{Pi}X_{Qi}) \prod_{l=1}^{N} \delta_{\alpha_{Pl},\beta_{Ql}}. \tag{6}$$

The energy eigenvalue is

$$E = \sum_i \alpha_i K_i. \tag{7}$$

Here $P=(P_1,\ldots,P_N)$ and $Q=(Q_1,\ldots,Q_N)$ are permutations of the numbers $(1,\ldots,N)$ and $\{\xi_P(Q)\}$ is a set of $N!\times N!$ real numbers to be determined. I denote by N^e (N^i) the number of electrons (impurities), namely the number of α's equal to 1 (0). N^e and N^i are conserved quantities and characterize the state.

The imposition of periodic boundary conditions on a line segment of length L and the requirement of proper discontinuities of the boundary of each region Q leads, via a lengthy algebraic analysis,[5] to the following condition on the momenta K_j of the electrons:

$$K_j = (2\pi/L)n_j + (N^i/L)\varphi + L^{-1}\sum_{\gamma=1}^{M}[\theta(2\Lambda_\gamma - 2) - \pi], \quad j=1,\ldots,N^e, \tag{8}$$

where the Λ's are a set of M numbers, all distinct, determined from

$$N^e\theta(2\Lambda_\gamma - 2) + N^i\theta(2\Lambda_\gamma) = -2\pi I_\gamma + \sum_{\delta=1}^{M}\theta(\Lambda_\gamma - \Lambda_\delta), \quad \gamma=1,\ldots,M, \tag{9}$$

where

$$\theta(X) = -2\tan^{-1}(X/C), \quad -\pi \leqslant \theta < \pi; \quad C = 2J/(1-J^2), \quad e^{i\varphi} = (1+iJ)/(1-iJ).$$

The I_γ's are half integers (integers) when $N-M$ is even (odd) and the n_j's are integers, cut off by the band width D, $|(2\pi/L)n_j| \leqslant D$. The inclusion of the last term in Eq. (5) does not change the *Ansatz* but merely modifies C and φ. One finds

$$C = 2J, \quad \varphi = 0. \tag{10}$$

Eigenstates thus are determined by the specification of the quantum numbers $\{n_j\}$ and $\{I_\gamma\}$, and the corresponding energy is

$$E = \sum_{i=1}^{N^e}(2\pi/L)n_j + (N^e/L)\sum_{\gamma=1}^{M}[\theta(2\Lambda_\gamma - 2) - \pi]. \tag{11}$$

One proceeds now to discuss the ground state and some of the excitations. I shall consider the antiferromagnetic case $J>0$ and assume N to be even.

The ground state is a singlet constructed by choosing the I_γ's to be consecutive and the n_j levels to be at their minimum.[5] For N large it is convenient to introduce the Λ density $\sigma(\Lambda)$ defined by: $1/\sigma(\Lambda_\gamma) = \Lambda_{\gamma+1} - \Lambda_\gamma$. For the ground state it must satisfy[5]

$$\sigma_0(\Lambda) = f(\Lambda) - \int_{-\infty}^{\infty} K(\Lambda - \Lambda')\sigma_0(\Lambda')d\Lambda', \tag{12}$$

where

$$K(X) = (C/\pi)/(C^2 + X^2), \quad f(X) = (2C/\pi)\{N^e/[C^2 + 4(X-1)^2] + N^i/(C^2 + 4X^2)\}.$$

By integrating Eq. (12) with respect to Λ, one finds, $M = \int_{-\infty}^{\infty}\sigma_0(\Lambda)d\Lambda = \frac{1}{2}N$, which is the requirement for a singlet. The limits of integration in Eq. (12) being $\pm\infty$ the solution is easy to find and is given by

$$\sigma_0(\Lambda) = (2C)^{-1}\{N^e/\cosh[\pi(\Lambda-1)/C] + N^i/\cosh(\pi\Lambda/C)\}, \tag{13}$$

so that the ground-state energy is

$$E_0 = \sum_{j=1}^{Ne}(2\pi/L)n_j + (N^e/L)\int d\Lambda\, \sigma_0(\Lambda)[\theta(2\Lambda - 2 - \pi]. \tag{14}$$

Excited states are obtained by changing the quantum numbers $\{I_\gamma\}$ and $\{n_j\}$ from their ground-state values. Thus, for example, inserting two holes in the $\{I_\gamma\}$ sequence (i.e., $I_{\gamma+1} = I_\gamma + 1$, $\gamma \neq \gamma^1, \gamma^2$ and

$I_{\gamma_i+1}=I_{\gamma_i}+2,\ i=1,2)$ leads to a change $\Delta\sigma$ in the Λ density,[5]

$$\Delta\sigma(\Lambda)=-\int dp(2\pi)^{-1}e^{ip\Lambda}[\exp(-ip\Lambda^1)+\exp(-ip\Lambda^2)][1+\exp(-c|p|)]. \tag{15}$$

Here Λ^1 and Λ^2 are the Λ's corresponding to $I_{\gamma_1}+1$ and $I_{\gamma_2}+1$. The corresponding energy is

$$E^t=E_0+(N^e/L)\left\{\pi+2\tan^{-1}\{\tanh[2\pi(\Lambda^1-1)/C]\}+2\tan^{-1}\{\tanh[2\pi(\Lambda^2-1)/C]\}\right\}. \tag{16}$$

This state is a triplet as can be seen from calculating ΔM, $\Delta M=\int\Delta\sigma(\Lambda)d\Lambda=-1$.

A singlet excitation (i.e., $\Delta M=0$) is similarly constructed. One generates two holes at Λ^1 and Λ^2 but adds two complex Λ's at $\Lambda^{\pm}=\frac{1}{2}(\Lambda^1+\Lambda^2)\pm\frac{1}{2}iC$.[5,8] The singlet and triplet states are found to be degenerate in energy.

In a similar manner all further excitations can be discussed. One may now proceed, in the framework of the exact solution, to discuss the thermodynamics of the model, the magnetization curve, the scattering phase shifts and so on. Here I concentrate on the magnetic susceptibility at zero temperature, χ. One can follow methods developed earlier in the Heisenberg[9] and Hubbard[10] models.

The susceptibility is given by $\chi^{-1}=\mu^{-2}[\partial^2E(S)/\partial S^2]_{S=0}$, where $E(S)$ is the minimum energy of the system when magnetization μS is present. The magnetic moment μ is taken to be the same for electrons and impurities, and

$$S=N-2M, \tag{17}$$

where M is the number of down spins, given by

$$M=\int_{-B}^{\infty}\sigma_S(\Lambda)d\Lambda. \tag{18}$$

The density σ_S now satisfies

$$\sigma_S(\Lambda)=f(\Lambda)-\int_{-B}^{\infty}K(\Lambda-\Lambda')\sigma_S(\Lambda')d\Lambda'. \tag{19}$$

The energy $E(S)$ is then

$$E(S)=\sum(2\pi/L)n_j+(N^e/L)\int_{-\infty}^{-B}d\Lambda\,\sigma_S(\Lambda)[\theta(2\Lambda-2)-\pi]. \tag{20}$$

This is indeed the minimum energy for a given magnetization S as is obvious from Eq. (16). For Λ^1,Λ^2 large and negative, a very low-energy triplet is excited. The integration limit B, determined by the magnetization S, thus characterizes a macroscopic excitation of the ground state, in response to an external magnetic field in whose presence $S\neq 0$. As the absolute ground state ($S=0$) corresponds to $B_0=\infty$, we shall be interested in $B\gg\max(1,C)$.

Equation (19) can be rewritten as

$$\sigma_S(\Lambda)=\sigma_0(\Lambda)+\int_{-\infty}^{-B}R(\Lambda-\Lambda')\sigma_S(\Lambda')d\Lambda', \tag{21}$$

where

$$R(\Lambda-\Lambda')=\int(dp/2\pi)e^{-ip(\Lambda-\Lambda')}/(1+e^{-C|p|})$$

is the resolvent of $K(\Lambda'-\Lambda'')$ satisfying

$$\int(1+K)(\Lambda-\Lambda')(1-R)(\Lambda'-\Lambda'')d\Lambda'=\delta(\Lambda-\Lambda'').$$

The energy and magnetization are given, respectively, by

$$E(S)=E_0+(N^e/L)\int_{-\infty}^{-B}d\Lambda\,\sigma_S(\Lambda)U(\Lambda),\quad S=\int_{-\infty}^{-B}\sigma_S(\Lambda)d\Lambda, \tag{22}$$

where

$$U(\Lambda)=\int d\Lambda'(1-R)(\Lambda-\Lambda')[\theta(2\Lambda-2)-\pi]=2\tan^{-1}\{\exp[-\pi(\Lambda-1)/C]\}-\pi.$$

For $\Lambda\leqslant -B$, $\sigma_S(\Lambda)$ satisfies

$$\sigma_S(\Lambda)=C^{-1}[N^e+N^ie^{\pi/C}]\exp[\pi(\Lambda-1)/C]+\int_{-\infty}^{-B}R(\Lambda-\Lambda')\sigma_S(\Lambda')d\Lambda'+O(e^{2\pi\Lambda/C}) \tag{23}$$

and we find (omitting steps detailed in the third paper of Ref. 9)

$$E(S)-E_0=\frac{N^e}{L}\frac{\pi}{2}\frac{S^2}{N^e+N^i\exp(\pi/C)}. \qquad (24)$$

The susceptibility thus is

$$\chi=\frac{1}{\pi}\mu^2\frac{N^e+N^i\exp(\pi/C)}{N^e/L}. \qquad (25)$$

The first contribution to χ (when $N^i=0$) is just the Pauli susceptibility $\chi_P=\pi^{-1}L\mu^2$. The second term $\delta\chi$, the change induced by the impurities, is

$$\delta\chi=\frac{N^i}{\pi}\frac{\mu^2}{(N^e/L)\exp(-\pi/C)},$$

exhibiting the quenching of the impurity moment.

The scale $T_0=(N^e/L)e^{-\pi/C}$ characterizes the physics in the scaling regime, $T\ll N^e/L$. To normalize it with the prescription of Ref. 3 one has to construct the high-temperature behavior ($T_0 \ll T \ll N^e/L$) of the model. This will be discussed in a forthcoming work.

The dependence of the physical scale T_0 on the coupling constant is determined by the cutoff procedure, specified after Eq. (9). The usual practice which restricts the *free* wave functions leads to an additional factor of the square root of the coupling constant.[11] But for a renormalizable model in the scaling regime cutoff effects can be neglected and various procedures are equivalent up to redefinition of the coupling constant.

The linear dependence of $\delta\chi$ on N^i is at first sight surprising. That the impurities do not interact is a special feature of the Kondo model and is related to its exact integrability and the infinite number of conserved charges resulting from it. This property is destroyed by various approximation schemes employed thus far.

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[1] J. Kondo, Prog. Theor. Phys. 32, 37 (1964).

[2] P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B 1, 4464 (1970).

[3] K. G. Wilson, Rev. Mod. Phys. 67, 773 (1975).

[4] A recent review is given by P. Nozières, in *Proceedings of the Fourteenth International Conference on Low Temperature Physics, Otaniemi, Finland, 1975*, edited by M. Krusius and M. Vuorio (North-Holland, Amsterdam, 1975).

[5] N. Andrei and J. H. Lowenstein, Phys. Rev. Lett. 43, 1698 (1979).

[6] A. A. Belavin, Phys. Lett. 87B, 117 (1979).

[7] M. Gaudin, Phys. Lett. 24A, 55 (1967); C. N. Yang, Phys. Rev. Lett. 19, 1312 (1967).

[8] N. Andrei and J. H. Lowenstein, New York University Report No. TR8/79 (to be published).

[9] R. B. Griffiths, Phys. Rev. 133, A768 (1964); C. N. Yang and C. P. Yang, Phys. Rev. 150, 321, 327 (1966).

[10] M. Takahashi, Prog. Theor. Phys. 42, 1098 (1969).

[11] The square root of the coupling constant is "universal" only as long as one uses cutoff procedures that lead to coupling constants that can be analytically related. This need not be the case.