Semiclassical Solution of One Dimensional Model of Kondo Insulator

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The model of a Kondo chain with an M-fold degenerate band of conduction electrons of spin 1/2 at half filling interacting with localized spins S is studied. It is shown that in the continuous limit the spectrum of spin excitations is described by the O(3) nonlinear sigma model with the topological term with $\theta = \pi(2S - M)$. Thus for $|M - 2S|$ =(even) the system is an insulator and single electron excitations at low energies are massive spin polarons. Otherwise the density of states has a pseudogap and vanishes only at the Fermi level.

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The problem of coexistence of delocalized and localized electrons in crystals remains one of the biggest unsolved problems in condensed matter physics. It is still unclear how conduction and localized electrons reconcile with each other when the local moments are arranged regularly (Kondo lattice problem). Empirically Kondo lattices resemble metals with very small Fermi energies of order of several degrees. It is widely believed that conduction and localized electrons in Kondo lattices hybridize at low temperatures to create a single narrow band. It is not clear, however, how this hybridization develops. In particular, it is not clear whether the localized electrons contribute to the volume of Fermi sea or not. If the answer is positive, a system with one conduction electron and one spin per unit cell must be an insulator. The available experimental data apparently support this point of view: all compounds with an odd number of conduction electrons per local moment are insulators [1] (Kondo insulators). At low temperatures they behave as semiconductors with very small gaps of the order of several degrees. The marked exception is FeSi where the value of the gap is estimated as $\sim$ 700 K [2]. The conservative approach to Kondo insulators would be to calculate their band structure treating the on-site Coulomb repulsion U as a perturbation. The advantage of this approach is that it gives an insulating state already in the zeroth order in U. The disadvantages are that it contradicts the principles of perturbation theory which prescribe that the strongest interactions are taken into account first and also does not lead to a satisfactory description of the experimental data: the band theory fails to explain many experimental observations (see Ref. [2] for a discussion).

In this Letter I study a one dimensional model of the Kondo lattice at half filling. It is shown that the insulating state forms not due to a hybridization of conduction electrons with local moments, but as a result of strong antiferromagnetic fluctuations. An interaction of electrons with kinks of the staggered magnetization converts them into massive spin polarons. This scenario does not require a global antiferromagnetic order, only an enhancement of the staggered magnetic susceptibility. The spin ground state remains disordered with a finite correlation length. The recent numerical calculations of Tsunetsugu *et al.* [3] and Yu and White [4] are in agreement with this point of view, demonstrating a sharp enhancement of the staggered susceptibility in one dimensional Kondo insulators and the formation of a spin gap. This scenario can be generalized for higher dimensions; Kondo insulators in this case are either antiferromagnets (then they have a true gap), or spin fluids with a strongly enhanced staggered susceptibility. In the latter case instead of a real gap one can expect a pseudogap—a drop in the density of states on the Fermi level.

Let us consider the following Hamiltonian describing a Kondo chain at half filling:

$$H = \sum_r \sum_{\alpha=1}^{M} [-\tfrac{1}{2}(c^\dagger_{r+1,\alpha,a} c_{r,\alpha,a} + c^\dagger_{r,\alpha,a} c_{r+1,\alpha,a}) + J(c^\dagger_{r,\alpha,a} \hat{\boldsymbol{\sigma}}_{ab} c_{r,\alpha,b}) \mathbf{S}_r]. \quad (1)$$

The conduction electrons have spin $S = 1/2$ and their band has an additional M-fold degeneracy. The value of local spins is S. In what follows I shall use the path integral approach. The path integral representation for spins has been discussed in detail by many authors, in particular in the book by Fradkin [5]. In the path integral approach spins are treated as classical variables $\mathbf{S} = S\mathbf{m}$ ($\mathbf{m}^2 = 1$); the corresponding Euclidean action for the model (1) is given by

$$A = \int d\tau \left(\sum_r \left[iS \int_0^1 du \{ \mathbf{m}_r(u,\tau) [\partial_u \mathbf{m}_r(u,\tau) \times \partial_\tau \mathbf{m}_r(u,\tau)] \} + c^*_{r,\alpha,a} \partial_\tau c_{r,\alpha,a} \right] - H(c^*, c; S\mathbf{m}) \right). \quad (2)$$

The first term is the spin Berry phase responsible for the correct quantization of local spins. The integrand in the Berry phase is a total derivative and the integral depends only on the value of $\mathbf{m}$ on the boundary, i.e., on $\mathbf{m}(u = 0, \tau) = \mathbf{m}(\tau), \mathbf{m}(u = 1, \tau) = (1, 0, 0)$. The introduction of the additional dummy variable u is the price one has to pay for the fact that the Berry phase cannot be written as a local functional of $\mathbf{m}_r(\tau)$.

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I shall follow the semiclassical approach assuming that all fields can be separated into fast and slow components. Then the fast components will be integrated out and as a result we shall obtain an effective action for the slow ones. This approach is self-consistent if the obtained correlation length for spins is much larger then the lattice spacing. In ordinary antiferromagnets this requirement is fulfilled only for large spins $S \gg 1$. As we shall see later, the Kondo chain is semiclassical even for $S = 1/2$ provided $JM \ll 1$. I suggest the following decomposition of variables:

$$\mathbf{m}_r = a\mathbf{k}(x) + (-1)^r \mathbf{n}(x)\sqrt{1 - a^2\mathbf{k}(x)^2}, \quad (\mathbf{k}\cdot\mathbf{n}) = 0,$$
$$c_r = i^r \psi_R(x) + (-i)^r \psi_L(x), \tag{3}$$

where $|\mathbf{k}|a \ll 1$ is the quickly varying ferromagnetic component of the local magnetization. Substituting Eqs. (3) into Eq. (2) and keeping only nonoscillatory terms, we get

$$L = iS(\mathbf{k}\cdot[\mathbf{n}\times\partial_\tau\mathbf{n}]) + \bar\psi_j\{i\gamma_\mu\partial_\mu\hat I + JS[\hat{\boldsymbol\sigma}\cdot\mathbf{n}(x)]\sqrt{1-a^2\mathbf{k}(x)^2}\}\psi_j + 2\pi S\times(\text{top term}), \tag{4}$$

where

$$(\text{top term}) = \frac{i}{8\pi}\int d\tau dx \epsilon_{\mu\nu}(\mathbf{n}\cdot[\partial_\mu\mathbf{n}\times\partial_\nu\mathbf{n}]) \tag{5}$$

is the topological term first derived by Haldane [6]. As far as the nonelectronic part of the action is concerned, the present derivation repeats the one of Ref. [5]. The interaction of ferromagnetic fluctuations with electronic currents has been omitted; it can be shown that at small $JM \ll 1$ it gives insignificant corrections.

The fermionic determinant is calculated later [see Eqs. (24) and (25)]. Besides the trivial static part it contains the topological term, but with $-M$ instead of $2S$. This is what one should expect: this change reflects the fact that local spins couple with conduction electrons to give the total spin $S - M/2$. Substituting expression (25) into Eq. (4), we get

$$L = iS(\mathbf{k}\cdot[\mathbf{n}\times\partial_\tau\mathbf{n}]) + \frac{M}{2\pi}[(\partial_x\mathbf{n})^2 + (\partial_\tau\mathbf{n})^2] + \frac{2M}{\pi}(JS)^2\ln\frac{1}{JS}(\mathbf{k})^2 + \pi(2S-M)\times(\text{top term}). \tag{6}$$

Integrating over $\mathbf{k}$, we get

$$A = \frac{M}{2\pi}\int d\tau dx\,[v^{-2}(\partial_\tau\mathbf{n})^2 + (\partial_x\mathbf{n})^2] + \pi(2S-M)\times(\text{top term}), \tag{7}$$

$$v^{-2} = 1 + \frac{2\pi^2}{J^2M^2\ln(1/JS)}. \tag{8}$$

After the rescaling of the coordinates $v\tau = x_0, x = x_1$ we get the action of the O(3) nonlinear sigma model with the dimensionless coupling constant

$$g = \frac{\pi v}{M} = \frac{\pi}{\sqrt{M^2 + \frac{2\pi^2}{J^2\ln(1/JS)}}}. \tag{9}$$

This constant is small at $JM \ll 1$ which justifies the entire semiclassical approach. At $|M - 2S| =$ (even) one can omit the topological term. Then the model Eq. (7) is the ordinary O(3) nonlinear sigma model whose ground state is disordered and the spectral gap is given by [7,8]

$$\Delta = Jg^{-1}\exp[-2\pi/g]. \tag{10}$$

The correlation length $\xi \sim Ja/\Delta \gg a$. If $|M - 2S| =$ (odd) the topological term is essential [6]. The model becomes critical and the correlation functions of staggered magnetization have a power law decay. The specific heat is linear at small temperatures without requiring, however, the single electron density of states to be constant at the Fermi level.

Now let us evaluate the fermionic determinant

$$D[g] = M\,\mathrm{Tr}\ln[\, i\,\gamma_\mu\partial_\mu + (1+i\gamma_5)mg/2 + (1-i\gamma_5)mg^\dagger/2], \tag{11}$$

where g is a matrix from SU(N) group and m is some constant energy scale. In the context of the model (1) $m = JS$ and $g = (\boldsymbol\sigma\mathbf{n})$. Therefore in the original problem $N = 2$, but it is worth doing the calculation for general N. I shall study the expansion of the determinant (11) in terms of $m^{-1}\nabla g$. The first terms of this expansion are independent of m and survive even at $m \to \infty$. I claim that the gradient expansion contains a Berry phase. To prove this point I take a route which may seem exotic, but I do not know any better way to get the right answer. The basic idea is that the determinant (11) coincides with an effective action for *gapless* excitations of the chiral Gross-Neveu model with the U(M) × SU(N) symmetry. For this particular model there is an alternative way to calculate this effective action; this way leads to Eq. (24). The above mentioned Gross-Neveu model is described by the following action:

$$A = \int d^2x\left(i\bar\eta_{a,\alpha}\gamma_\mu\partial_\mu\eta_{a,\alpha} - \frac{c}{2}[(\bar\eta_{a,\alpha}\eta_{b,\alpha})(\bar\eta_{b,\beta}\eta_{a,\beta}) - (\bar\eta_{a,\alpha}\gamma_5\eta_{b,\alpha})(\bar\eta_{b,\beta}\gamma_5\eta_{a,\beta})]\right). \tag{12}$$

The Greek indices belong to the group SU(M) and the Latin ones to SU(N). Let us show that low-lying excitations of this model are described by the actions (11) and (24) which are thus equivalent to each other.

First, let us show that the low-lying excitations of the model (12) are indeed described by the effective action (11). For this purpose let us separate massive excitations and show that the remaining action is given by (11). I do it with an auxiliary field Q_{ab} which decouples the interaction term in (12) via the Hubbard-Stratonovich transformation. Integrating over the fermions we obtain the partition function for the tensor Q_{ab}:

$$Z = \int DQ^\dagger DQ \exp\Big(-\int d^2x L\Big),$$

$$L = \frac{1}{2c}\mathrm{Tr}Q^\dagger Q - M\,\mathrm{Tr}\ln[i\gamma_\mu\partial_\mu + (1+i\gamma_5)Q/2 + (1-i\gamma_5)Q^\dagger/2]. \tag{13}$$

The action (13) has a saddle point with respect to $Q^\dagger Q$ and thus fluctuations of $\det Q$ are massive. This can be done in the standard fashion, the resulting mass being

$$m = \Lambda \exp[-\pi/Mc]. \tag{14}$$

Therefore for slowly varying fields Q one can substitute Q_{ab} in the Tr ln in Eq. (13) by mg_{ab} where g is an SU(N) matrix. As a result we get (11) as the effective action for those excitations of the model (12) whose energies are $\ll m$, where m is given by Eq. (14). Thus the first goal is accomplished.

The second goal is to find an alternative way to calculate the effective action for the massless modes of the model (12). This way exists and it will give us an explicit expression for this action in the form of Eq. (11). Using the identity $2\tau_1^a\tau_2^a = 1/2 - P_{12}$, where P_{12} is the permutation operator, we can rewrite the interaction term in (12) in terms of fermionic currents:

$$A = \int d^2x\{i\bar\eta_{a,\alpha}\gamma_\mu\partial_\mu\eta_{a,\alpha} + 4cJ_\mu^\lambda J^{\mu\lambda}\},$$

$$J_\mu^\lambda = (\bar\eta_{a,\alpha}\gamma_\mu\tau^\lambda_{\alpha\beta}\eta_{a,\beta}), \tag{15}$$

where τ^r are matrices—generators of the SU(M) group. The two models (12) and (15) differ by a term containing a diagonal scattering. This term does not renormalize and therefore is not important. Now I apply to the model (15) the non-Abelian bosonization procedure suggested by Witten [9] (see also [10]). Namely, let us rewrite its Hamiltonian in the Sugawara form:

$$H = H_{\mathrm{U}(1)} + H_{\mathrm{SU}(N)} + H_{\mathrm{SU}(M)}, \tag{16}$$

$$H_{\mathrm{U}(1)} = \pi\int dx[:J_R(x)J_R(x):+:J_L(x)J_L(x):], \tag{17}$$

$$H_{\mathrm{SU}(N)} = \frac{2\pi}{N+M}\sum_{i=1}^{G_N}\int dx[:J_R^i(x)J_R^i(x):+:J_L^i(x)J_L^i(x):], \tag{18}$$

$$H_{\mathrm{SU}(M)} = \sum_{\lambda=1}^{G_M}\int dx\Big\{\frac{2\pi}{N+M}[:J_R^\lambda(x)J_R^\lambda(x):+:J_L^\lambda(x)J_L^\lambda(x):] + 4c:J_R^\lambda(x)J_L^\lambda(x):\Big\}, \tag{19}$$

where the chiral currents for the group SU(N) are

$$J_R^i = \eta^\dagger_{R,a\alpha}t^i_{ab}\eta_{R,b\alpha}, J_L^i = \eta^\dagger_{L,a\alpha}t^i_{ab}\eta_{L,b\alpha}, \tag{20}$$

where t^i are the generators of the SU(N) (spin) group and η_R, η_L are right and left components of the Dirac spinor η. J and J^λ are the U(1) and the SU(M) (flavor) currents, the latter defined as in Eq. (15). $G_N = N^2-1$ and $G_M = M^2-1$ are the total number of generators of the su(N) and the su(M) algebras. Currents from different algebras commute. Therefore the Hamiltonian (16) is a sum of three mutually commuting operators. Now notice that the interaction term transits from Eq. (12) into Eq. (19) and thus does not affect the spectra of SU(M) singlets. It is well known that the spectrum of $H_{\mathrm{SU}(M)}$ is gapful for the given sign of the coupling constant (see, for example, Ref. [11]). From the previous discussion we can conclude that the gapful excitations correspond to fluctuations of $\det Q$. Therefore the spectrum below the gap m described by the action (11) is also described by the rest of the Hamiltonian (16), in other words by $H_{\mathrm{U}(1)}$ and $H_{\mathrm{SU}(N)}$ given by Eqs. (17) and (18). The Hamiltonian (18) is the Hamiltonian of the Wess-Zumino-Witten model on the group SU(N). Its spectrum is the subsector of the free fermionic spectrum generated by the SU(N) current operators. The model is conformally invariant and exactly solvable [12,13]. In order to extract from these results an expression for the determinant (11), I rewrite the model in the Lagrange representation [9–13]:

$$A_{\mathrm{U}(1)} = \frac{NM}{8\pi}\int d^2x(\partial_\mu\phi)^2. \tag{21}$$

$$A_{\mathrm{SU}(N)} = \int d^2x\Big(\frac{M}{16\pi}\mathrm{Tr}(\partial_\mu g^\dagger\partial_\mu g) + \frac{M}{24\pi}\int_0^1 d\xi\epsilon_{abc}\mathrm{Tr}(g^\dagger\partial_a g g^\dagger\partial_b g g^\dagger\partial_c g)\Big), \tag{22}$$

where g is a matrix from the SU(N) group ($g^\dagger g = I, \det g = 1$). The second term on the right-hand side of Eq. (22) is called the Wess-Zumino term. This term is topological; its actual value (modulus $2\pi iN$) depends on the boundary values of $g(x,\xi=0) = g(x)$ [$g(x,\xi=1)=0$].

Now let us compare Eq. (22) with Eq. (11). The part of Eq. (22) which does not contain the Wess-Zumino term represents the first term in the gradient expansion of Tr ln term in Eq. (13). Indeed, at small momenta $|p| \ll m$ this term is equal to

$$\frac{M}{16\pi m^2}\int d^2x\,\mathrm{Tr}(\partial_\mu Q^\dagger\partial_\mu Q). \tag{23}$$

Now let us write down the Q field as follows:

$$Q(x) = mg(x)e^{i\sqrt{M}\phi(x)},$$

where g belongs to the SU(N) group. Substituting this expression into Eq. (23) we reproduce Eq. (21) and the first term of Eq. (22). It is not entirely unexpected that the naive gradient expansion, being an adiabatic approximation, misses the important Wess-Zumino term. This term is a Berry phase and thus requires special care. Thus we conclude that the determinant (11) is equal to

$$D[g] = A_{\mathrm{SU}(N)}[g] + \frac{Mm^2}{2\pi}\ln(\Lambda/m) + O(m^{-2}), \qquad (24)$$

where $A_{\mathrm{SU}(N)}[g]$ is given by Eq. (22) and the second term represents the static part of the determinant. For the particular case $g = (\hat{\boldsymbol{\sigma}}\mathbf{n})$ the Wess-Zumino term becomes the topological term (5) and we get

$$A_{\mathrm{SU}(2)}[(\hat{\boldsymbol{\sigma}}\mathbf{n})] = \frac{M}{2\pi}(\partial_\mu \mathbf{n})^2 - \pi M(\text{top term}). \qquad (25)$$

I shall discuss the excitation spectrum only for $M = 1$. In this case the original model has a combined symmetry SU(2)$\times$SU(2) [the additional SU(2) symmetry arises as a particle-hole symmetry at half filling]; excitations carry two quantum numbers—spin S and an isotopic spin I. We have established that spin excitations, i.e., excitations with $I = 0$, are described by the nonlinear sigma model with the topological term (7). The leading contributions to the low energy dynamics come from antiferromagnetic fluctuations. It agrees with the results of numerical calculations [3,4]. The corresponding energy scale (10) formally resembles the expression for the Kondo temperature. $m(J)$ is larger, however, due to the presence of the large logarithm. Therefore at small JM the RKKY interaction always plays a stronger role than the Kondo screening—it also agrees with the conclusions of Refs. [3,4]. The topological term can be omitted if $|M - 2S|$ = (even); in particular, it cancels for the most physical case $S = 1/2, M = 1$. The low-lying magnetic excitations are in this case massive triplets, as it is for the O(3) nonlinear sigma model [7,8]. This picture is in qualitative agreement with the strong coupling limit of the model (1). Indeed, for $J \gg 1$ the ground state of the Kondo chain consists of local singlets. Excited states are triplets separated by the gap $\sim J$ from the ground state. That is what one can expect from a one dimensional model: usually in 1D there is no discontinuity between strong and weak coupling, which in the present case is supported by the numerical calculations of Ref. [3] showing a smooth crossover between $J \gg 1$ and $J \ll 1$.

Fermionic excitations carry quantum numbers $S = 1/2$, $I = 1/2$. It follows from (4) that the fermionic fields live in a slowly fluctuating field $JS\{\hat{\boldsymbol{\sigma}}\mathbf{n}(x,\tau)\}$. For constant $\mathbf{n}$ the electrons would have a spectral gap JS, but since $\mathbf{n}$ fluctuates, there are states in the gap. These are bound states of electrons with solitons of the unit vector field $\mathbf{n}$. Formation of bound states is a typical feature of relativistic field theories (see, for example, Ref. [14]). Following Ref. [14] let us consider a slowly varying static configuration $\mathbf{n}(x)$ such that $\mathbf{n}(-\infty)$ is antiparallel to the z axis and $\mathbf{n}(\infty)$ is parallel to it. Then a straightforward calculation shows that there is an electronic bound state on this domain wall whose energy is zero and wave function is equal to

$$\Psi(x) = \hat{T}\exp\left(-\int_0^\infty dy(\boldsymbol{\sigma}\cdot\mathbf{n}(y))\right)\Psi(0). \qquad (26)$$

Therefore the total energy of this bound state is equal to the energy necessary to create the domain wall, which is the gap for the spin excitations. Thus in the energy interval between JS and m single electron excitations are massive spin polarons. It is no longer the case if $|M-2S|$ = (odd), when the nonlinear sigma model becomes critical and belongs to the universality class of the isotropic $S = 1/2$ Heisenberg chain. In the critical phase the spin solitons do not have a fixed scale and the corresponding bound states can have an arbitrary small energy. It is reasonable to suggest that the single particle density of states in this case has a pseudogap on the Fermi surface decaying as a power law: $\rho(\omega) \sim |\omega|^\alpha$.

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