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Effects of Berry phase and instantons in one dimensional Kondo-Heisenberg model

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Motivated by the global phase diagram of antiferromagnetic heavy fermion metals, we study the Kondo effect from the perspective of a nonlinear sigma model in the one dimensional Kondo-Heisenberg model away from half-filling. We focus on the effects of the instanton configurations of the sigma-model field and the associated Berry phase. Guided by the results derived using bosonization methods, we demonstrate that the Kondo singlet formation is accompanied by an emergent Berry phase. This Berry phase also captures the competition between the Kondo singlet formation and spin Peierls correlations. Related effects are likely to be realized in Kondo lattice systems in higher dimensions.

Introduction: Antiferromagnetic heavy fermion metals represent a prototype case study for quantum criticality [1]. Considerable theoretical work has emphasized the Kondo-breakdown local quantum criticality [2, 3]. Compared with the spin-density-wave picture [4–6], which is based on the Landau notion of order-parameter fluctuations, the Kondo breakdown introduces new low-energy degrees of freedom. The characteristic properties include, *e.g.*, a jump between large and small Fermi surfaces [7, 8].

Recently, experiments in YbRh_2Si_2 that is either doped [9, 10] or pressurized [11] have revealed a rich phase diagram. Under sufficient positive or negative (chemical) pressure, the Kondo-breakdown point can be separated from the antiferromagnetic (AF) transition. These results have been interpreted in terms of a global phase diagram, which was put forward several years ago and more extensively discussed recently [12–14].

The global phase diagram emphasizes the interplay between two effects. One is the Kondo screening and its breakdown, and the other the fluctuations in the quantum magnetism of local moments alone. The relevant zero-temperature phases can be either AF or paramagnetic, and can have “large” or “small” Fermi surfaces [12–14]. The large and small Fermi surfaces respectively correspond to the cases with Kondo screening and destruction. These results promise to take the study of heavy fermion phase diagram to an entirely new direction [1].

A promising approach to the global phase diagram starts from the AF state, using a quantum non-linear sigma model (QNL σ M) representation [13, 15]. In dimensions higher than one, the Kondo coupling turns out to be exactly marginal in the renormalization group (RG) sense, and this shows a stable AF phase with Kondo destruction. Such a phase serves as a basis to describe different types of phase transitions out of the AF state [12, 13]. The low-energy physics in the ordered state involves only the smooth space-time configurations of the sigma model field \mathbf{n} , for which the spin Berry phase vanishes. In order to access the Kondo-screened or otherwise paramagnetic phases, topologically non-trivial configurations of the \mathbf{n} field will also be important; for such configurations, the spin Berry phase is non-zero.

To gain insight into the effect of the Berry phase on the zero-temperature phases of Kondo lattice systems, here we

consider the case of AF spin-1/2 Kondo-Heisenberg model in one dimension. We use the QNL σ M basis to study the effect of topological spin excitations, with important guidance provided by the results derived from bosonization method. We show that, when the conduction electron moves in the topologically nontrivial instanton configurations of the \mathbf{n} fields, a Berry phase θ term with $\theta_c = \pi$ arises. The emergent Berry phase shifts the θ term of the spin chain from π to $0[\text{mod } 2\pi]$, which in turn gives rise to a spin gap that is characteristic [16–18] of the Kondo-screened state of the one-dimensional Kondo-Heisenberg lattice. Our results apply to both the insulating case at half-filling, where they are consistent with the result of Tsvelik [19], as well as the metallic case away from half-filling. As we discuss at the end of the paper, our results bring out considerable new insights into the Kondo-breakdown phenomena.

Kondo-Heisenberg model and QNL σ M mapping: We study the following one dimensional Hamiltonian

$$H = -t \sum_{i,\alpha} c_{i,\alpha}^\dagger c_{i+1,\alpha} + h.c. + J_K \sum_i \mathbf{s}_i \cdot \boldsymbol{\tau}_i + J_H \sum_i \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_{i+1}, \quad (1)$$

where the fermion spins and spin-half local moments are respectively described by $\mathbf{s}_i = \frac{1}{2} c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta}$, and $\boldsymbol{\tau}_i$. The Kondo (J_K) and nearest neighbor (J_H) exchange couplings are both antiferromagnetic, and t is the fermion hopping strength. We will work in the regime $J_K \ll J_H, t$, where we can use a continuum approximation for the spin chain. For the latter, we first consider the semiclassical QNL σ M mapping[20], followed by the bosonization method[21, 22].

In the semiclassical approximation we take $\boldsymbol{\tau}_i = (-1)^i S \mathbf{n}_i (1 - \frac{a^2 \mathbf{L}_i^2}{S^2})^{1/2} + a \mathbf{L}_i$, where the unit vector field \mathbf{n}_i is the staggered magnetization, and \mathbf{L}_i is a canting field that satisfies the constraint $\mathbf{n}_i \cdot \mathbf{L}_i = 0$. After integrating out \mathbf{L}_i we obtain the effective action $S_{eff} = S[\mathbf{n}] + S_f + S_K$. The three terms respectively describe the QNL σ M for the lo-

cal moments, the free electrons, and the Kondo interactions:

$$S[\mathbf{n}] = \frac{\rho_s}{2} \int d^2x [(\partial_1 \mathbf{n})^2 + \frac{1}{c^2} (\partial_0 \mathbf{n})^2] + i\theta W[\mathbf{n}] \quad (2)$$

$$S_f = \int d^2x \bar{\psi}_s [\gamma_0 \partial_0 + v\gamma_1 \partial_1] \psi_s \quad (3)$$

$$S_K = \int d^2x \left[\lambda_b e^{-i\pi r_j} \bar{\psi} e^{-i2k_F r_j \gamma_5} \sigma \psi \cdot \mathbf{n} + i\lambda_f \bar{\psi} \gamma_0 \sigma \psi \cdot (\mathbf{n} \times \partial_0 \mathbf{n}) \right] + \dots \quad (4)$$

In Eq. 2, $\rho_s = J_H S^2 a$, $c = 2J_H S a$ respectively denote the spin stiffness and spin-wave velocity. The topological term $i\theta W[\mathbf{n}]$ corresponds to the Berry's phase due to the instanton configurations of \mathbf{n} , with $\theta = 2\pi S$, and the Pontryagin index $W[\mathbf{n}] = \frac{1}{4\pi} \int d^2x \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_0 \mathbf{n})$ counts the winding number of the instantons. In the semiclassical approximation only the Berry's phase term retains the information about the quantized value of the spin. Based on this mapping, Haldane conjectured that half-integer spin chains characterized by $\theta = \pi$ are gapless, and in contrast the integer spin chains with $\theta = 2\pi$ are gapped[20]. In Eqs. 3,4, v is the Fermi velocity, k_F is the Fermi momentum, and the anticommuting gamma matrices are $\gamma_0 = \eta_1$, $\gamma_1 = \eta_2$ and $\gamma_5 = i\gamma_0 \gamma_1 = -\eta_3$, with η_i 's being Pauli matrices. These Pauli matrices operate on the fermionic spinor $\psi^\dagger = (R^\dagger, L^\dagger)$, where R and L are the right and left moving fields, and $\bar{\psi} = \psi^\dagger \gamma_0$.

The two terms in Eq. 4 with coupling constants λ_b and λ_f respectively correspond to the back scattering and forward scattering interactions between the fermions and local moments; both are $\propto J_K$. The ellipsis indicates a four-fermion interaction term, obtained after integrating out \mathbf{L}_i , that is not important for our purpose. The back scattering term describes the coupling of the staggered magnetization densities of the electrons and spin chain, and the forward scattering term describes the coupling of the uniform magnetization densities. At half-filling, the product of the exponential phase factors is unity due to the commensurability of the conduction electrons and spin chain, and the back scattering term contributes as a relevant operator. Away from half-filling, the product is oscillatory in space, which makes the back scattering term irrelevant and the low energy physics is governed by the forward scattering term.

Bosonization results: Before proceeding with the calculations within the QNL σ M approach, we will use bosonization method to gain insight into the Kondo singlet formation [17, 18] and the emergent Berry phase. We show that the abelian-bosonization description of the Kondo-singlet state, when transformed in terms of a non-abelian bosonization method, already suggests an emergent Berry phase.

In the bosonization approach the spin chain is first described in terms of fermions Ψ with frozen charge fluctuations, and the Kondo interaction term is expressed as

$$S_K = \int d^2x [\lambda_b \bar{\psi} e^{-i2k_F r_j \gamma_5} \sigma \psi \cdot \bar{\Psi} e^{-i\pi r_j \gamma_5} \sigma \Psi + \lambda_f \bar{\psi} \gamma_0 \sigma \psi \cdot \bar{\Psi} \gamma_0 \sigma \Psi]. \quad (5)$$

Within the Abelian bosonization, the collective charge and spin fluctuations of the electrons are respectively described by the bosonic fields φ_c , φ_s and their corresponding dual fields θ_c , θ_s . The spin fluctuations of the local moments are described by the bosonic field φ_τ and its dual θ_τ . The kinetic energy of the fermions are described in terms of Gaussian actions involving φ_c , φ_s , and φ_τ , and S_K becomes

$$S_K \propto \int d^2x \left[\lambda_b \cos((2k_F + \pi)r_j + \sqrt{2\pi}\varphi_c)(\cos \sqrt{2\pi}\varphi_- - \cos \sqrt{2\pi}\varphi_+ + 2 \cos \sqrt{2\pi}\theta_-) + \lambda_f \partial_x \varphi_s \partial_x \varphi_\tau + \lambda_f \cos \sqrt{2\pi}\theta_- (\cos \sqrt{2\pi}\varphi_- + \cos \sqrt{2\pi}\varphi_+) \right], \quad (6)$$

where $\varphi_\pm = \varphi_s \pm \varphi_\tau$ and $\theta_- = \theta_s - \theta_\tau$.

Away from the half filling, the low energy physics is controlled by the forward scattering term that is marginally relevant [18]. (The $\cos \sqrt{2\pi}\theta_- \cos \sqrt{2\pi}\varphi_-$ coupling is irrelevant and can be ignored.) Since the forward scattering operators do not couple the charge and spin sectors, the charge field remains a free field and leads to the metallic behavior in the charge sector. However the spin fields still satisfy one of the following locking conditions:

$$\sqrt{2\pi}\varphi_+ = 2n_1\pi, \quad \sqrt{2\pi}\theta_- = (2n_2 + 1)\pi \quad (7)$$

$$\sqrt{2\pi}\varphi_+ = (2n_1 + 1)\pi, \quad \sqrt{2\pi}\theta_- = 2n_2\pi, \quad (8)$$

which signals the Kondo singlet formation and an emergent spin gap [17, 18, 23]. As a result of the Kondo singlet formation there is a gapless charge density wave mode at wavevector $2k_F^* = 2k_F + \pi$, described by $\langle \mathbf{N}^\tau \cdot \mathbf{N}^s \rangle \propto \cos((2k_F + \pi)r_j + \sqrt{2\pi}\varphi_c)$.

The above can be compared with the insulating system at half filling, where the back scattering and forward scattering operators are respectively relevant and marginally relevant operators. Consequently[16–18], the low energy physics is governed by the back scattering term, a potential energy of the form $\mathbf{N}^\tau \cdot \mathbf{N}^s$, where $\mathbf{N}_{s,\tau}$ are the staggered magnetization densities. This form implies that the spin fields will lock into a configuration such that $\mathbf{N}^\tau \cdot \mathbf{N}^s = -1$. Combining the energy minimum criterion with the fact that $\cos \sqrt{2\pi}\varphi_-$ and $\cos \sqrt{2\pi}\theta_-$ can not have simultaneous vacuum expectation values, we find two possibilities for the charge and spin fields, either with Eq. (7) and $\sqrt{2\pi}\varphi_c = 2n_3\pi$, or with Eq. (8) and $\sqrt{2\pi}\varphi_c = (2n_3 + 1)\pi$. The nonzero $\langle \cos \sqrt{2\pi}\varphi_c \rangle$ causes a charge gap, leading to a charge insulator behavior. In the spin sector, the above reveals an important insight, which appears not to have been appreciated before: the locking conditions for the spin bosons in the half-filled insulating case and away-from-half-filled metallic cases are identical. This insight will be important in guiding our subsequent analysis of the Berry phase effect in the QNL σ M representation.

To anticipate the QNL σ M analysis, we now demonstrate the relation between the Kondo singlet formation and topological Berry phase using the non-Abelian bosonization method[21, 22]. The spin sector for the electrons and local

moments are described by the $SU(2)$ matrix fields $\mathcal{U}_{s,\tau}$ and the corresponding $SU(2)$ -WZW actions

$$S_{s,\tau} = \frac{1}{16\pi} \int d^2x Tr[\partial_\mu \mathcal{U}_{s,\tau}^\dagger \partial_\mu \mathcal{U}_{s,\tau}] + \Gamma_{WZ}[\mathcal{U}_{s,\tau}]$$

$$\Gamma_{WZ}[\mathcal{U}_{s,\tau}] = \frac{-i}{24\pi} \int_0^\infty d\xi \int d^2x \epsilon_{\alpha\beta\gamma} Tr[\mathcal{U}_{s,\tau}^\dagger \partial_\alpha \mathcal{U}_{s,\tau} \mathcal{U}_{s,\tau}^\dagger \partial_\beta \mathcal{U}_{s,\tau} \mathcal{U}_{s,\tau}^\dagger \partial_\gamma \mathcal{U}_{s,\tau}] \quad (9)$$

where Γ_{WZ} is the topological Wess-Zumino term. For the electrons and local moments the space-time coordinates are respectively described by $(v_{s,\tau}x_0, x_1)$. The topological WZ term is crucial to maintaining the gapless behavior of the $\mathcal{U}_{s,\tau}$ fields. The matrix fields can be decomposed as $\mathcal{U}_{s,\tau} = u_{0,s,\tau} + i\mathbf{u}_{s,\tau} \cdot \boldsymbol{\sigma}$, with $u_{0,s,\tau}^2 + \mathbf{u}_{s,\tau}^2 = 1$, where $u_{0,s,\tau}$ and $\mathbf{u}_{s,\tau}$ respectively describe singlet spin-Peierls and staggered magnetization correlations. The relationship among the non-Abelian and Abelian bosonization fields are described by

$$u_{0,s} \pm iu_{3,s} = e^{\pm i\sqrt{2\pi}\phi_s}, \quad u_{1,s} \pm iu_{2,s} = \pm ie^{\mp i\sqrt{2\pi}\theta_s} \quad (10)$$

The locking conditions of the Abelian fields, Eqs. (7,8), translate into $\mathcal{U}_s = \pm \mathcal{U}_\tau^\dagger$. Using the property $\Gamma_{WZ}[\mathcal{U}^\dagger] = -\Gamma_{WZ}[\mathcal{U}]$, we find that the Kondo-singlet formation is accompanied by the cancellation between the WZ terms of the spin chain and the electrons. This leaves an effective matrix sigma model without the topological term, which is known to be gapped. If the Peierls type singlet correlation u_0 is suppressed, the WZW action reduces to a QNL σ M, and the WZ term transforms into a topological $\theta = \pi$ Berry phase for the QNL σ M. Therefore we anticipate that the Kondo singlet formation within a sigma model approach will be associated with an emergent $\theta = \pi$ Berry phase from the electronic part of the action.

QNL σ M at half-filling : After gaining insight into the Kondo-singlet formation via bosonization analysis, we turn to the QNL σ M approach. At half-filling the problem can be solved in an elegant manner due to Tsvelik[19]. Introducing the non-Abelian bosonization field \mathcal{U}_s for the conduction electrons, the relevant back scattering term can be expressed as $4\lambda_b \mathbf{u}_s \cdot \mathbf{n} \cos \sqrt{2\pi}\varphi_c$. The energy minimization is achieved for $\mathbf{u}_s = \mathbf{n}$, $\sqrt{2\pi}\varphi_c = (2n+1)\pi$ or $\mathbf{u}_s = -\mathbf{n}$, $\sqrt{2\pi}\varphi_c = 2n\pi$. The conditions $\mathbf{u}_s = \pm \mathbf{n}$ imply $u_{0,s} = 0$, and the WZ term becomes $\pm i\pi W[\mathbf{n}]$ which cancels the $\theta = \pi$ Berry phase term of the spin chain. Consequently we obtain charge and spin gaps. However this approach does not account for the forward scattering terms and can not be applied to the metallic case away from half filling, where a new treatment is required.

Berry's phase from non-Abelian chiral anomaly: We now analyze the Kondo effect and emergent Berry phase in the QNL σ M representation at arbitrary filling. Based on the bosonization results, we see that Kondo singlet formation is accompanied by the $2k_F^*$ charge density wave oscillation described by $\langle \mathbf{N}_s \cdot \mathbf{N}_\tau \rangle$. Therefore in the sigma model approach we need to find an appropriate fermionic basis such that the

component of \mathbf{N}_s parallel to \mathbf{n} has $2k_F^*$ charge oscillation (at half-filling due to commensurability $2k_F^*$ charge mode remains gapped).

Recognizing that \mathbf{N}_s contains the combination of left and right moving fields, we anticipate that a spin dependent chiral transformation will be needed to describe the appropriate fermionic basis. In the following section we demonstrate that both at and away from half-filling the emergent Berry's phase can be calculated by using a non-Abelian chiral rotation and the associated chiral anomaly [24–26]. In Ref. 26 the non-Abelian chiral rotation technique has been applied to calculate the Berry phase at half-filling in the absence of the forward scattering term. However the relation between the emergent Berry phase and Kondo singlet formation has not been addressed. We consider this relationship and, in addition, study the forward scattering term to address the metallic case away from half-filling.

We perform a spin-dependent chiral rotation $\psi \rightarrow \exp(i\phi \mathbf{n} \cdot \boldsymbol{\sigma} \gamma_5) \chi$. The staggered magnetization transforms into

$$\bar{\psi} e^{-i2k_F r_j \gamma_5} \frac{\boldsymbol{\sigma}}{2} \psi = \frac{1}{2} \bar{\chi} [\boldsymbol{\sigma} - \mathbf{n}(1 - \cos 2\phi) \mathbf{n} \cdot \boldsymbol{\sigma} + i\gamma_5 \sin 2\phi \mathbf{n}] e^{-i2k_F r_j \gamma_5} \chi \quad (11)$$

After taking a dot product with \mathbf{n} , we find that only for $\phi = \pm\pi/4$, $\mathbf{N}_s \cdot \mathbf{n}$ demonstrates pure charge density oscillations with $2k_F^*$ wavevector. Therefore $\phi = \pi/4$ is the required chiral rotation angle, which removes the spin dependence of the back scattering term and converts it into $i\lambda_b \exp(-i\pi r_j - 2ik_F r_j \gamma_5) \bar{\chi} \gamma_5 \chi$. Therefore at half-filling, the back scattering term becomes $i\lambda_b \bar{\chi} \gamma_5 \chi$, and causes a charge gap. One can also perform a successive $U(1)$ chiral rotation $\exp(-i\frac{\pi}{4}\gamma_5)\chi$, to transform $i\bar{\chi} \gamma_5 \chi$ into an ordinary mass term $\lambda_b \bar{\chi} \chi$. However this is not necessary for the physics in the spin-sector.

Since the functional measure is not invariant under chiral rotation, we need to find the Jacobian of the transformation which leads to the chiral anomaly terms. After an explicit calculation detailed in the supplementary materials [27], we find the Jacobian

$$J\left(\phi = \frac{\pi}{4}\right) = \exp \left[-i\pi W[\mathbf{n}] + \int d^2x \left\{ \frac{v}{4\pi} (\partial_1 \mathbf{n})^2 + \frac{(1-2\lambda_f)^2}{4\pi v} (\partial_0 \mathbf{n})^2 \right\} \right] \quad (12)$$

The Jacobian consists an emergent $\theta = \pi$ Berry phase term, and two additional terms which renormalize the spin stiffness and spin wave velocity of the QNL σ M. The emergent Berry phase cancels the existing π Berry phase of the spin chain, and renders the sigma model field gapped. As a result of the $\pi/4$ chiral rotation, the spin sector of the χ fermions also becomes gapped. This can be demonstrated by considering the bosonization of the χ fermions. In the non-abelian bosonization formulation, the spin sector of the χ fermion does not contain the topological WZW term, and the matrix sigma

model becomes gapped. The fermionic action transforms into

$$S_f = \int d^2x \bar{\chi} [\gamma_\mu \partial_\mu + \frac{i}{2} \gamma_\mu \gamma_5 \boldsymbol{\sigma} \cdot \partial_\mu \mathbf{n} + \frac{i}{2} \gamma_\mu \boldsymbol{\sigma} \cdot (\mathbf{n} \times \partial_\mu \mathbf{n}) - i \lambda_f \gamma_0 \gamma_5 \boldsymbol{\sigma} \cdot \partial_0 \mathbf{n} + i \lambda_b e^{-i(\pi+2k_F)r_j \gamma_5} \gamma_5] \chi + \dots \quad (13)$$

Since the \mathbf{n} field, and the spin sector of χ field are gapped, the interaction between these fields describe the innocuous fluctuations about Kondo singlet phase.

To summarize, the spin dependent chiral rotation by angle $\pi/4$ incorporates the Kondo singlet formation. In the metallic case away from half-filling, a $\theta = \pi$ Berry phase emerges as a consequence of chiral anomaly. The effects of the Berry phase and instantons in the spin sector turn out to be the same as those at half-filling. The difference between the two cases exists only in the charge sector, and the term causing the gap at half-filling no longer operates away from half-filling.

Competition with spin-Peierls correlations: The emergent theta term highlights the role of instanton configurations of the \mathbf{n} field. We now discuss its connection with the spin-Peierls order parameter. In the semiclassical language spin Peierls order parameter $(-1)^i \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ corresponds to the instanton density $a^2 \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_0 \mathbf{n})$. Therefore it can be argued that the instantons of the sigma model are manifestations of the competition between the spin Peierls and Néel order. For the spin one-half case we consider, $\theta = \pi$ and the gaplessness of the spin chain implies the same power law correlation of the Peierls and the Néel order parameters. The Kondo singlet formation is detrimental to both singlet Peierls and triplet Néel correlations, as the system moves away from the gapless point; this competition between two types of singlet correlations is encoded in the emergent π Berry phase term.

This conclusion demonstrates the effect of the emergent Berry phase beyond the description of how Kondo-singlet paramagnetic phase transitions out of a Kondo-breakdown spin-liquid reference point. The Berry phase also characterizes the competition between the Kondo paramagnet and Kondo-breakdown spin-Peierls phase. While the Fermi momenta of the Kondo-singlet paramagnet are large, those of the spin-Peierls state are small. These paramagnetic phases and their transitions resemble the paramagnetic portion of the global phase diagram that has been proposed for heavy-fermion metals.

In higher dimensions there is a stable Néel ordered AF state, and the instantons are suppressed by finite spin stiffness in the magnetically ordered phase. However in the quantum disor-

dered region the consideration of the instantons becomes relevant, and the associated Berry phase is critical in determining the nature of the emergent valence bond solid phase[28, 29]. Therefore it is conceivable that Berry phase effects related to what we have considered here will be important in dimensions higher than one.

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