PHYSICAL REVIEW B VOLUME 58, NUMBER 18 1 NOVEMBER 1998-II

Exactly solvable models of unconventional magnetic alloys: Bethe ansatz versus renormalization-group method

Valery I. Rupasov*
Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7
and Landau Institute for Theoretical Physics, Moscow, Russia
(Received 20 July 1998)

We propose toy models of unconventional magnetic alloys, in which the density of band states, $\rho(\epsilon)$, and hybridization, $t(\epsilon)$, are energy dependent; it is assumed, however, that $t^2(\epsilon)\propto\rho^{-1}(\epsilon)$, and hence an effective electron-impurity coupling $\Gamma(\epsilon)=\rho(\epsilon)t^2(\epsilon)$ is energy independent. In the renormalization-group approach, the physics of the system is assumed to be governed by $\Gamma(\epsilon)$ only rather than by separate forms of $\rho(\epsilon)$ and $t(\epsilon)$. However, an exact Bethe ansatz solution of the toy Anderson model demonstrates a crucial role of a form of inverse band dispersion $k(\epsilon)$. [S0163-1829(98)51642-6]

The Kondo problem in ''unconventional'' Fermi systems, where an effective density of states of band electrons vanishes either precisely at the Fermi level (''gapless'' systems) or on some interval around the Fermi level (''gapped'' systems), has been attracting a significant theoretical interest. Using poor-man's scaling, Withoff and Fradkin[1] have found that the Kondo effect in gapless systems takes place only if an effective electron-impurity coupling exceeds some critical value. Numerical renormalization-group (RG) calculations, large-N studies, and quantum Monte Carlo simulations of the gapless[2–7] and gapped[8–14] systems have confirmed this prediction and revealed a number of additional features of the physics of unconventional magnetic alloys.

In a conventional metallic system with (i) a linear dispersion of band electrons near the Fermi level and (ii) an energy independent electron-impurity hybridization, basic impurity models are exactly solved by the Bethe ansatz (BA).[15–18] It is well known that the Wilson's numerical RG[19,20] and BA methods lead to identical results. Moreover, renormalizability of the Kondo and Anderson models proved, respectively, by Abrikosov[21] and Haldane[22] has been reproven in the course of a BA solution. Therefore, it is reasonable to study the Kondo problem in unconventional Fermi systems, where the BA technique cannot be straightforwardly used, by making use of scaling arguments and the numerical RG approach.

However, it has recently been found[23] that integrability of the $U\rightarrow\infty$ nondegenerate and degenerate Anderson models is not destroyed because of a nonlinear dispersion of particles and an energy dependent hybridization, but it becomes only hidden.[24] The developed BA approach has allowed us to study[25] the thermodynamics of a $U\rightarrow\infty$ Anderson impurity in a BCS superconductor, and can be used to obtain an exact solution of the Kondo problem in other unconventional Fermi systems.

The results obtained[23,25] demonstrate a discrepancy between the RG and BA approaches to the Kondo problem in unconventional Fermi systems. In the RG approach, the separate forms of the density of states, $\rho(\epsilon)$, and an energy dependent hybridization, $t(\epsilon)$, are assumed to be *unimportant*. It is assumed that the impurity properties are governed only by an effective particle-impurity coupling $\Gamma(\epsilon)=\rho(\epsilon)t^2(\epsilon)$. However, BA equations contain both an effective coupling and an inverse band dispersion $k(\epsilon)$. The latter describes the spatial behavior of wave functions and enters BA equations via periodic boundary conditions imposed on system's eigenfunctions. A form of inverse dispersion plays an extremely important role in the physics of the system.

In this paper, we study a toy model describing an Anderson impurity embedded in a gapless Fermi system. In this model, the density of states and hybridization are energy dependent. It is assumed, however, that $t^2(\epsilon)=2\Gamma\rho^{-1}(\epsilon)$, where $\Gamma=\text{const}$, and an effective coupling is thus energy independent. Therefore, in the framework of RG approach, physical properties of the toy and Anderson models are obviously identical.

As in many publications on the Kondo problem in gapless Fermi systems, we assume a simple form of the density of band states,

$$\rho(\epsilon)=\frac{|\epsilon|^r}{|\epsilon|^r+\beta^r}, \tag{1}$$

where the energy ϵ is taken relative to the Fermi level. The parameter β determines the size of a region with an unconventional behavior of the density of states. At $\beta=0$, we come back to the Anderson model. In the region near the Fermi level, $|\epsilon|\ll\beta$, the density of the states exhibits a power-law variation, $\rho(\epsilon)\sim|\epsilon|^r$.

The toy model is obviously integrable. It is clear also that a corresponding integrable toy version can be constructed in the above-described manner for any conventional integrable impurity model. The physical properties of the toy versions of the exchange models, such as the *s-d* (Kondo) and Coqblin-Schrieffer models, are not affected by a form of dispersion, because in these models charge and spin excitations of a system are decoupled from each other.[15–18] The physics of the toy versions of the Anderson model, where charge and spin excitations strongly interact, is shown to be governed by a form of inverse dispersion $k(\epsilon)$.

We start with a general Anderson model with the arbitrary band electron dispersion, $\epsilon(k)$, and hybridization, $t(k)$.

In terms of the energy dependent Fermi operators $c^{\dagger}_{\sigma}(\epsilon)$ $[c_{\sigma}(\epsilon)]$ which create (annihilate) an electron with a spin $\sigma=\uparrow,\downarrow$ in an s-wave state of energy ϵ, the model Hamiltonian is written as

$$H=H_c+H_d+H_h. \tag{2a}$$

Here

$$H_c=\int_{-D}^{D}\frac{d\epsilon}{2\pi}\epsilon c^{\dagger}_{\sigma}(\epsilon)c_{\sigma}(\epsilon), \tag{2b}$$

$$H_d=\epsilon_d d^{\dagger}_{\sigma}d_{\sigma}+Ud^{\dagger}_{\uparrow}d_{\uparrow}d^{\dagger}_{\downarrow}d_{\downarrow}, \tag{2c}$$

$$H_h=\int_{-D}^{D}d\epsilon\sqrt{\Gamma(\epsilon)}[c^{\dagger}_{\sigma}(\epsilon)d_{\sigma}+d^{\dagger}_{\sigma}c_{\sigma}(\epsilon)] \tag{2d}$$

are the conduction band, impurity and hybridization terms, respectively. All notation in Eqs. (2) are standard. The electron energies and momenta are taken relative to the Fermi values, which are set to be equal to zero. The integration over the energy variable ϵ is restricted by the band half width D. In what follows, we assume that D is the largest parameter on an energy scale, $D\to\infty$. In the energy representation, the effective particle-impurity coupling $\Gamma(\epsilon)=\rho(\epsilon)t^2(\epsilon)$ combines the density of band states, $\rho(\epsilon)=[d\epsilon(k)/dk]^{-1}$, and the energy dependent hybridization $t(\epsilon)$.

The metallic version of the general Anderson model, where $\rho(\epsilon)=\text{const}$, $t(\epsilon)=\text{const}$, is solved by BA. Hereafter we call this model the Anderson model. In this paper we study a toy version of the general Anderson model assuming that

$$t^2(\epsilon)=2\Gamma\rho^{-1}(\epsilon), \tag{2e}$$

where $\Gamma=\text{const}$, and hence the effective coupling is energy independent as in the Anderson model. Therefore, the toy model is also integrable at an arbitrary U. Indeed, let us introduce the Fourier images of the electron operators,

$$c_{\sigma}(\tau)=\int\frac{d\epsilon}{2\pi}c_{\sigma}(\epsilon)\exp(i\epsilon\tau),$$

and transform thus Eqs. (2) to the auxiliary τ space. In this space related to the particle energy, the model Hamiltonian coincides with the Hamiltonian of the Anderson model written in terms of the operators in the auxiliary x space,

$$c_{\sigma}(x)=\int\frac{dk}{2\pi}c_{\sigma}(k)\exp(ikx),$$

related to the particle momentum. Therefore, in the τ space the N-particle wave functions of the system, $\Phi_{\sigma_1\ldots\sigma_N}(\tau_1,\ldots,\tau_N)$, are given by the standard Bethe ansatz formulas derived by Wiegmann.[26] However, periodic boundary conditions must be imposed on a wave function $\Psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N)$ on an interval of size L in the x space rather than in the τ space. These different representations of wave functions are related by

$$\Psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N)=\int_{-\infty}^{\infty}d\tau_1\ldots\tau_N\prod_{j=1}^{N}u(x_j|\tau_j)\times\Phi_{\sigma_1\ldots\sigma_N}(\tau_1,\ldots,\tau_N), \tag{3a}$$

where the ''dressing'' function $u(x|\tau)$ is found to be

$$u(x|\tau)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\left(\frac{d\epsilon(k)}{dk}\right)^{1/2}\exp\{i[kx-\epsilon(k)\tau]\}. \tag{3b}$$

In the Anderson model, where $\epsilon(k)=k$, the dressing function is nothing but the Dirac delta function, $u(x|\tau)=\delta(x-\tau)$, and hence the x and τ representations coincide.

In what follows, we confine ourselves to the case of $U\to\infty$. Then, imposing periodic boundary conditions on the wave function $\Psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N)$ results in the following BA equations:

$$e^{ik_jL}\frac{\omega_j-\epsilon_d/2\Gamma-i/2}{\omega_j-\epsilon_d/2\Gamma+i/2}=\prod_{\alpha=1}^{M}\frac{\omega_j-\lambda_{\alpha}-i/2}{\omega_j-\lambda_{\alpha}+i/2}, \tag{4a}$$

$$\prod_{j=1}^{N}\frac{\lambda_{\alpha}-\omega_j-i/2}{\lambda_{\alpha}-\omega_j+i/2}=-\prod_{\beta=1}^{M}\frac{\lambda_{\alpha}-\lambda_{\beta}-i}{\lambda_{\alpha}-\lambda_{\beta}+i}, \tag{4b}$$

where M is the number of particles with spin ''down,'' $k_j\equiv k(\omega_j)$, and $\omega=\epsilon/2\Gamma$. The particle-impurity and effective particle-particle scattering amplitudes coincide with those in the Anderson model, because they are really determined only by the effective particle-impurity coupling Γ, as it is assumed in the RG approach. However, the BA equations contain also the phase factors $\exp(ik_jL)$ accounting for the spatial behavior of wave functions, which are essentially different in the metallic and toy cases. A form of the inverse dispersion $k(\omega)$ is clear to play a very important role in both further mathematical BA constructions and in the physics of the system.

As in the Anderson model, in the thermodynamic limit spin ''rapidities'' λ_{α} are grouped into bound spin complexes of size n,

$$\lambda_{\alpha}^{(n,j)}=\lambda_{\alpha}+i(n+1-2j)/2,\quad j=1,\ldots,n. \tag{5}$$

Apart from charge excitations with real charge ''rapidities'' ω_j, the spectrum of the system contains also charge complexes with complex rapidities

$$\omega_{\alpha}^{(\pm)}=\lambda_{\alpha}\pm i/2, \tag{6a}$$

provided the signs of the imaginary parts of $\omega_{\alpha}^{(\pm)}$ and corresponding momenta $k^{(\pm)}=k(\omega_{\alpha}^{(\pm)})$ are the same,

$$\text{sign}(\text{Im}\,k^{(\pm)})=\text{sign}(\text{Im}\,\omega^{(\pm)}). \tag{6b}$$

In the Anderson model, due to the linear dispersion law $k=2\Gamma\omega$ the necessary condition (NC) (6b) is obviously satisfied at an arbitrary $\lambda\in(-\infty,\infty)$. In our model, a solution of NC is governed by a form of $k(\omega)$.

To solve Eq. (6b), one has to specify first the power r in the expression for the density of states (1). Here, we consider two most important cases $r=1$ and $r=2$. At $r=2$ the inverse dispersion is found to be

$$\frac{k}{2\Gamma}=\omega-\delta\arctan\frac{\omega}{\delta}, \tag{7a}$$

where $\delta=\beta/2\Gamma$. Solving Eq. (6b), we find a critical value of the parameter δ,

$$\exp(1/\delta_{cr})=\frac{\delta_{cr}+1/2}{\delta_{cr}-1/2}. \tag{7b}$$

At $\delta<\delta_{cr}$, NC has a solution at all λ. At $\delta>\delta_{cr}$, NC has no solution on the interval $G_\Delta=(-\Delta,\Delta)$, where

$$\Delta^2=\frac{2\delta}{1-\exp(-2/\delta)}-(\delta+1/2)^2. \tag{7c}$$

Thus, in a sharp contrast to the Anderson model, the spectrum of charge complexes of the system at $\delta>\delta_{cr}$ contains a gap of size 2Δ. The gap appears at $\delta=\delta_{cr}$, and grows with increasing δ. At very large δ, $\delta\gg1$, the gap asymptotically reaches the maximal value $2\Delta_{max}=1/\sqrt{3}$.

In a gapless Fermi system with the power $r=1$, the inverse dispersion of band states is found to be

$$\frac{k}{2\Gamma}=\omega+\delta\ln\frac{\delta-\omega}{\delta},\ \omega<0. \tag{8}$$

Solving Eq. (6b), we find no gap in the spectrum of charge complexes. Thus, the model with the power $r=1$ is qualitatively equivalent to the Anderson model. Therefore, in what follows we confine ourselves to the model with $r=2$.

The thermodynamics of the system is described by a set of basic equations for the renormalized energies of elementary excitation $\varepsilon(\omega)$, $\xi(\lambda)$, and $\kappa_n(\lambda)$, corresponding to unpaired charge excitations with real ω, charge complexes and spin complexes of size n, respectively:

$$\varepsilon(\omega)=2\Gamma\omega+a_1*F[-\xi(\omega)]-\sum_{n=1}^{\infty}a_n*F[-\kappa_n(\omega)], \tag{9a}$$

$$\xi(\lambda)=4\Gamma\lambda+a_1*F[-\varepsilon(\lambda)]+a_2*F[-\xi(\lambda)], \tag{9b}$$

$$\kappa_n(\lambda)=\sum_{m=1}^{\infty}A_{nm}*F[-\kappa_m(\lambda)]+a_n*F[-\varepsilon(\lambda)]. \tag{9c}$$

In these equations, $F[f(x)]\equiv T\ln\{1+\exp[f(x)/T]\}$, $a_n(x)=(2n/\pi)(n^2+4x^2)^{-1}$, and $A_{nm}(x)=a_{|n-m|}(x)+a_{n+m}(x)+2\sum_{k=1}^{\min(n,m)-1}a_{|n-m|+2k}(x)$. The symbol * stands for the convolution of functions, e.g.,

$$a_n*F[\xi(\lambda)]\equiv\int d\lambda' a_n(\lambda-\lambda')F[\xi(\lambda')]. \tag{10}$$

For the $U\to\infty$ Anderson model, the thermodynamic BA equations were derived by Schlottmann.[27] They also can be obtained by setting $U\to\infty$ in the thermodynamic BA equations of the general Anderson model.[15] In our case, the only difference is the appearance of the gap in the spectrum of charge complexes at $\delta>\delta_{cr}$. Therefore, the integration contour C in the integrals with the function $\xi(\lambda)$ consists of two intervals, $C=(-\infty,-\Delta)\oplus(\Delta,\infty)$.

The physical properties of the ground state of the system are governed by the gap size. At $\Delta=0$, the ground state, as in the Anderson model, is composed of charge complexes only. They occupy all states from $\lambda=-D/2\Gamma$ to $\lambda=Q$, where Q is determined by the condition $\xi(Q)=0$. In conventional metallic systems Q is a large negative value,[15] $Q=-(1/2\pi)\ln(D/\Gamma)$. The ground state of the model is not affected by the gap until the gap size does not exceed $|Q|$. When Δ exceeds $\Delta_{cr}=|Q|$, the ground state of the system is reconstructed: charge complexes with $\lambda\in(-\Delta,Q)$ decay into unbounded charge excitations and spin waves.

Therefore, in the continuous limit the BA equations (4) describing the ground state of the system take the form of integral equation for the ''particle,'' $\rho(\omega)$ [$\rho(\omega)=0$ at $\omega>B$], $\sigma(\lambda)$ [$\sigma(\lambda)=0$ at $\lambda>\Delta$], $\eta(\lambda)$, and ''hole,'' $\tilde{\rho}(\omega)$ [$\tilde{\rho}(\omega)=0$ at $\omega<B$], $\tilde{\sigma}(\lambda)$ [$\tilde{\sigma}(\lambda)=0$ at $\lambda<-\Delta$], densities of distributions of charge excitations, charge complexes and spin waves, respectively,

$$\frac{1}{2\pi}\frac{dk(\omega)}{d\omega}+\frac{1}{L}a_1\left(\omega-\frac{\epsilon_d}{2\Gamma}\right)=\rho(\omega)+\tilde{\rho}(\omega)+a_1*\sigma(\omega)+a_1*\eta(\omega), \tag{11a}$$

$$\frac{1}{2\pi}\frac{dq(\lambda)}{d\lambda}+\frac{1}{L}a_2\left(\lambda-\frac{\epsilon_d}{2\Gamma}\right)=\sigma(\lambda)+\tilde{\sigma}(\lambda)+a_1*\rho(\lambda)+a_2*\sigma(\lambda), \tag{11b}$$

$$a_1*\rho(\lambda)=\eta(\lambda)+a_2*\eta(\lambda), \tag{11c}$$

where $q(\lambda)=k(\lambda+i/2)+k(\lambda-i/2)$ is the momentum of the charge complexes. The ''Fermi level'' of unbounded charge excitations, B, is found from the condition

$$\frac{N}{L}=\int_{-\infty}^{B}d\omega\rho(\omega)+2\int_{-\infty}^{-\Delta}d\lambda\sigma(\lambda). \tag{12}$$

In Eqs. (11), the densities can be separated into the host and impurity parts, e.g., $\rho(\omega)=\rho_h(\omega)+L^{-1}\rho_i(\omega)$. The population of the impurity level, n_d, and the impurity spin S_i^z are then given by

$$n_d=\int_{-\infty}^{B}d\omega\rho_i(\omega)+2\int_{-\infty}^{-\Delta}d\lambda\sigma_i(\lambda), \tag{13a}$$

$$S_i^z=\frac{1}{2}\int_{-\infty}^{B}d\omega\rho_i(\omega)-\int_{-\infty}^{\infty}d\lambda\eta_i(\lambda). \tag{13b}$$

It is easy to see that Eqs. (11) and (13) are analogous to equations describing the ground state of the Anderson model in an external magnetic field $\mathcal{H}$. The latter, however, contain no spin waves, $\eta(\lambda)=0$. Therefore, the impurity spin is given by

$$S_i^z=\frac{1}{2}\int_{-\infty}^{B'}d\omega\rho_i(\omega),$$

where the limit B' is determined by the field $\mathcal{H}$. In the limit $\mathcal{H}\to0$, $B'\to-\infty$, and the impurity spin vanishes.

In our model, unbounded charge excitations and spin waves appear in the ground state of the system in the absence

of an external magnetic field due to a decay of charge complexes. However, it is easy to show from Eqs. (11c) and (13b) that their contributions to the impurity spin precisely compensate each other. Thus, the Kondo effect takes place in the toy $U\to\infty$ Anderson model with the powers $r=1$ and $r=2$ at any effective coupling Γ and gap size.

At $\Delta<|Q|$, unbounded charge excitations and spin waves disappear from the ground state, and the population of the impurity level is determined by a single function $\sigma_i(\lambda)$, $n_d=2\int_{-\infty}^{Q}d\lambda\sigma_i(\lambda)$. As in the Anderson model, the impurity population is governed by the renormalized impurity level energy $\epsilon_d^*=\epsilon_d+2\Gamma Q$. At $\Delta>|Q|$, the limit Q is replaced by $-\Delta$, and moreover a contribution of unpaired charge excitations appears in Eq. (13a). Therefore, we should expect essential changes in the behavior of the impurity population and the impurity magnetic susceptibility compared to the Anderson model.

In summary, we presented an exact BA analysis of the toy version of a model describing a $U\to\infty$ Anderson impurity embedded in a gapless Fermi system. In the RG approach, the physics of the system is assumed to be governed by an effective electron-impurity coupling only. Therefore, the toy and Anderson models should be identical to each other. The BA analysis demonstrates, however, the qualitatively different behaviors of these models.

In the Anderson model, the ground state is composed of charge complexes only. The toy model with the power $r=2$ exhibits a critical value δ_{cr} of the parameter δ describing an unconventional behavior of the density of states given in Eq. (1). At $\delta>\delta_{cr}$ the spectrum of charge complexes contains a gap. If the gap is quite small, $\Delta<|Q|$, it does not affect the ground state properties, however its appearance changes the thermodynamics of the system. A large gap, $\Delta>|Q|$, not only changes the thermodynamic properties, but reconstructs also the ground state of the system, because a part of charge complexes decay into unbounded charge and spin excitations. The behavior of the impurity level population is drastically changed, however the Kondo effect takes place at any gap.

Finally, it should be emphasized that the toy versions are interesting not only as exactly solvable examples of unconventional magnetic alloys. It can be shown[28] that an exact BA solution of a model with the density of states $\rho(\epsilon)$ given in Eq. (1) and an energy independent hybridization, $t=\text{const}$, exhibits many of the qualitative features described above.

I thank S. John, V. Yudson, and M. Zhitomirsky for stimulating discussions.

*Electronic address:rupasov@physics.utoronto.ca

[1] D. Withoff and E. Fradkin, Phys. Rev. Lett. **64**, 1835 (1990).
[2] L. S. Borkowski and P. J. Hirschfeld, Phys. Rev. B **46**, 9274 (1992).
[3] C. R. Cassanello and E. Fradkin, Phys. Rev. B **53**, 15 079 (1996).
[4] K. Chen and C. Jayaprakash, J. Phys.: Condens. Matter **7**, L491 (1995).
[5] K. Ingersent, Phys. Rev. B **54**, 11 936 (1996).
[6] C. Gonzalez-Buxton and K. Ingersent, Phys. Rev. B **54**, 15 614 (1996); cond-mat/9803256 (unpublished).
[7] R. Bulla, Th. Pruschke, and A. C. Hewson, J. Phys.: Condens. Matter **9**, 10 463 (1997).
[8] T. Saso, J. Phys. Soc. Jpn. **61**, 3439 (1992).
[9] T. Saso and J. Ogura, Physica B **186-188**, 372 (1993).
[10] J. Ogura and T. Saso, J. Phys. Soc. Jpn. **62**, 4364 (1993).
[11] K. Takegahara, Y. Shimizu, and O. Sakai, J. Phys. Soc. Jpn. **61**, 3443 (1993).
[12] K. Takegahara, Y. Shimizu, N. Goto, and O. Sakai, Physica B **186-188**, 381 (1993).
[13] L. Cruz, P. Phillips, and A. H. Castro Neto, Europhys. Lett. **29**, 389 (1995).
[14] K. Chen and C. Jayaprakash, Phys. Rev. B **57**, 5225 (1998).
[15] A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983).
[16] N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983).
[17] P. Schlottmann, Phys. Rep. **181**, 1 (1989).
[18] A. C. Hewson, *The Kondo Effect to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
[19] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[20] H. R. Krishna-Murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. Lett. **35**, 1101 (1975); Phys. Rev. B **21**, 1003 (1980); **21**, 1044 (1980).
[21] A. A. Abrikosov, Physica (Amsterdam) **2**, 5 (1965).
[22] F. D. M. Haldane, Phys. Rev. Lett. **40**, 416 (1978).
[23] V. I. Rupasov, Phys. Lett. A **237**, 80 (1997).
[24] V. I. Rupasov and M. Singh, J. Phys. A **29**, L205 (1996); Phys. Rev. Lett. **77**, 338 (1996); Phys. Rev. A **54**, 3614 (1996).
[25] V. I. Rupasov, Phys. Rev. Lett. **80**, 3368 (1998).
[26] P. B. Wiegmann, Phys. Lett. **80A**, 163 (1980).
[27] P. Schlottmann, Z. Phys. B **49**, 109 (1982); **52**, 127 (1983).
[28] V. I. Rupasov, cond-mat/9810014 (unpublished).