Integrable Two-Band Model with Attractive and Repulsive Interactions

P. Schlottmann

Department of Physics and MARTECH, Florida State University, Tallahassee, Florida 32306

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The exact solution via Bethe's ansatz to a model consisting of two parabolic bands of electrons with local attractive and repulsive interactions is presented. Some low-temperature properties of this model are discussed as a function of the interaction strength, a magnetic field, and the crystal-field splitting between the bands. The attractive interaction leads to Cooper-pair-like bound states and a threshold magnetic field is required to overcome the binding energy. The low-T specific heat is proportional to T except at critical points where $C \propto T^{1/2}$.

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The discovery of numerous high-temperature superconductors has renewed the interest in low-dimensional systems. Although in this context the main interest is centered around two-dimensional (2D) highly correlated electron systems, it has been conjectured [1] that properties of the 1D and 2D variants of certain models have common aspects. Exact results in 1D are often more accessible than 2D ones and may provide a testing ground for approaches intended for more complex problems.

Many properties of integrable one-dimensional interacting fermion systems and quantum spin models have been derived by exact diagonalization of the Hamiltonian by means of Bethe's ansatz. The knowledge of the complete set of energy eigenvalues enables one to obtain the free energy and to study the thermodynamics of the system. In this paper we present the solution to a new integrable model consisting of two bands of electrons with local attractive and repulsive interactions. The interest in two-band models arises from the possibility that both the $3d_{x^2-y^2}$ and $3d_{z^2}$ orbitals may play a role in high-T_c cuprates. The attractive interaction leads to pairing bound states of the Cooper type and at zero temperature to no response to fields smaller than a threshold field H_c. The low-T specific heat is always proportional to T, except for band fillings very close to the one-dimensional Van Hove singularities. If the interband interaction is the attractive one, the model gives rise to exciton bands. The exciton bound states are formally analogous to the Cooper pairs if band and spin indices are interchanged.

The Hamiltonian under consideration is the following:

$$H=\sum_{m\sigma}\int dx\, c^{\dagger}_{m\sigma}(x)\left(-\frac{\partial^2}{\partial x^2}\right)c_{m\sigma}(x)+\frac{c}{L}\sum_{mm'\sigma\sigma'}\int dx_1\int dx_2\,\delta(x_1-x_2)c^{\dagger}_{m\sigma}(x_1)c^{\dagger}_{m'\sigma'}(x_2)c_{m'\sigma}(x_2)c^{\dagger}_{m\sigma'}(x_1)\,, \tag{1}$$

where $m=1,2$ labels the bands, $c^{\dagger}_{m\sigma}(x)$ creates an electron of spin σ at x in the band m, L is the length of the box, and c is the strength of the δ-function *exchange* interaction. Note that the two parabolic bands have equal masses (a necessary condition for the integrability of the model) and that the number of particles with up and down spin and the number of particles in each band are conserved quantities. This model contains as special cases the Gaudin-Yang many-body problem of N fermions interacting via a δ-function potential in 1D for both repulsive [2,3] and attractive [2,4] coupling, and its Bethe ansatz solution is topologically related to that of the *two-channel Kondo problem* [5,6].

The structure of the Bethe ansatz equations follows from the solution of the two-particle problem. The two-electron wave function can be written as a product of three factors: a coordinate wave function (referring to the positions and momenta of the particles), a spin part, and a factor involving the band labels ($m=1,2$; we will call this the orbital factor). The global wave function has to be antisymmetric under the exchange of two particles. If the spin and orbital wave functions have the same parity, the coordinate wave function has to vanish if $x_1=x_2$ and the two particles do not interact. Interacting fermions then form a spin singlet and orbital triplet (attractive interaction) or spin triplet and orbital singlet (repulsive interaction). The scattering matrix can be written as a product of spin and orbital spaces,

$$\hat{S}(k_1,k_2)=\frac{(k_1-k_2)\hat{I}_{\sigma}-ic\hat{P}_{\sigma}}{(k_1-k_2)-ic}\,\frac{(k_1-k_2)\hat{I}_{m}+ic\hat{P}_{m}}{(k_1-k_2)+ic}\,, \tag{2}$$

where $\hat{I}_{\sigma}$ ($\hat{I}_m$) and $\hat{P}_{\sigma}$ ($\hat{P}_m$) are the identity and permutation operators for the spins (band indices), respectively, and k_1 and k_2 are the momenta of the electrons. Since the scattering matrix (2) factorizes into scattering matrices for the spin and orbital channels and each of them satisfies the triangular Yang-Baxter relation [3], the model (1) is integrable.

The discrete Bethe ansatz equations are now derived following the standard procedure [3–6] by imposing periodic boundary conditions. Each state of the Hamiltonian is specified by one set of "charge rapidities $\{k_j\}$

representing the momenta of the electrons, one set of "spin" rapidities $\{\lambda_\alpha\}$, and one set of "orbital" rapidities $\{\omega_\beta\}$. All rapidities within a given set have to be different, leading to Fermi statistics. The rapidities are determined by

$$\exp(ik_jL)=\prod_{\alpha=1}^{M}\frac{k_j-\lambda_\alpha-\frac{1}{2}ic}{k_j-\lambda_\alpha+\frac{1}{2}ic}\prod_{\beta=1}^{m}\frac{k_j-\omega_\beta+\frac{1}{2}ic}{k_j-\omega_\beta-\frac{1}{2}ic}, \quad (3a)$$

$$j=1,\ldots,N,$$

$$\prod_{j=1}^{N}\frac{\lambda_\alpha-k_j-\frac{1}{2}ic}{\lambda_\alpha-k_j+\frac{1}{2}ic}=-\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta-ic}{\lambda_\alpha-\lambda_\beta+ic}, \quad (3b)$$

$$\alpha=1,\ldots,M,$$

$$\prod_{j=1}^{N}\frac{\omega_\beta-k_j-\frac{1}{2}ic}{\omega_\beta-k_j+\frac{1}{2}ic}=-\prod_{\alpha=1}^{m}\frac{\omega_\beta-\omega_\alpha-ic}{\omega_\beta-\omega_\alpha+ic}, \quad (3c)$$

$$\beta=1,\ldots,m,$$

and the energy and magnetization are given by

$$E=\sum_{j=1}^{N}k_j^2,\quad S_z=\tfrac{1}{2}N-M. \quad (3d)$$

$N-m$ and m are the number of electrons in the majority and minority bands, respectively. If either M or m is zero, the equations reduce to the Gaudin-Yang [2,3] many-body problem. Equations (3) are related to a variant of the two-channel Kondo model [6]. Note that the Bethe ansatz eigenfunctions are only a basis of states within the subspace of fixed N, $M\le N/2$ and $m\le N/2$, but they are not a complete set of eigenstates of the Hamiltonian [7].

Each eigenstate of the Hamiltonian is specified by sets of rapidities which have to satisfy the Bethe ansatz equations (3). In the thermodynamic limit the solutions to Eqs. (3) are given by strings [8] and can be classified as follows [4,6]: (i) $N-2\tilde{M}$ *real* charge rapidities k representing unpaired electrons; (ii) $\tilde{M}$ *pairs* of complex-conjugated charge rapidities corresponding to bound states of the Cooper type; (iii) M_n' *strings* of length n, associated with excited spin states, of the form

$$\lambda=\lambda_n'+\tfrac{1}{2}ic(n+1-2p),\quad p=1,\ldots,n; \quad (4a)$$

and (iv) m_n *strings* of length n forming interband bound states of the type

$$\omega=\omega_n'+\tfrac{1}{2}ic(n+1-2p),\quad p=1,\ldots,n. \quad (4b)$$

Here λ_n' and ω_n' are real parameters, and the integers M, $\tilde{M}$, m, M_n', and m_n satisfy the following relations:

$$M'=M-\tilde{M}=\sum_{n=1}^{\infty}nM_n',\quad m=\sum_{n=1}^{\infty}nm_n. \quad (4c)$$

The above solutions are inserted into the discrete Bethe ansatz equations and integral equations relating the densities of states of the different classes of rapidities are obtained. We now proceed to calculate the free energy of the system following standard methods [4,5,9,10]. Since all rapidities within one class have to be different, their occupation follows Fermi statistics and is conveniently described in terms of energy bands. We denote these energy bands with $\epsilon(k)$ for the real charge rapidities, $\psi(\lambda)$ for the paired charge rapidities, $\varphi_n(\lambda)$ for the λ strings, and $\kappa_n(\omega)$ for the ω strings of length n ($n=1,2,3,\ldots$), respectively. These thermodynamic energy potentials satisfy the following set of nonlinear integral equations:

$$\epsilon(k)=k^2-\mu-\tfrac{1}{2}H-\Delta+Ta_1*\ln(1+e^{-\psi/T})-T\sum_n a_n*\ln[(1+e^{-\varphi_n/T})(1+e^{-\kappa_n/T})], \quad (5a)$$

$$\psi(\lambda)=2(\lambda^2-\tfrac{1}{4}c^2-\mu-\Delta)+Ta_2*\ln(1+e^{-\psi/T})+Ta_1*\ln(1+e^{-\epsilon/T})-T\sum_n[a_{n-1}+a_{n+1}]*\ln(1+e^{-\kappa_n/T}), \quad (5b)$$

$$\ln(1+e^{\varphi_n(\lambda)/T})=nH/T+\sum_{n'}A_{nn'}*\ln(1+e^{-\varphi_{n'}/T})+a_n*\ln(1+e^{-\epsilon/T}), \quad (5c)$$

$$\ln(1+e^{\kappa_n(\omega)/T})=2n\Delta/T+\sum_{n'}A_{nn'}*\ln(1+e^{-\kappa_{n'}/T})-a_n*\ln(1+e^{-\epsilon/T})-[a_{n-1}+a_{n+1}]*\ln(1+e^{-\psi/T}), \quad (5d)$$

where the asterisk denotes convolution and μ, H, and Δ are the Lagrange multipliers for the conservation of the number of particles, the spin, and the relative band population, i.e., the chemical potential, the magnetic field, and the crystalline-field splitting. Here a_n ($n>0$) and $A_{nn'}$ are the Fourier transforms of

$$e^{-cn|x|/2},$$

$$\coth(c|x|/2)[e^{-|n-n'|c|x|/2}-e^{-(n+n')c|x|/2}],$$

respectively. The free energy of the system is given by

$$\frac{F}{L}=-T\int\frac{dk}{2\pi}\ln(1+e^{-\epsilon/T})-T\int\frac{d\lambda}{\pi}\ln(1+e^{-\psi/T}). \quad (6)$$

The solution of the above integral equations yields the thermodynamic properties of the model as a function of c, T, μ, H, and Δ. In the limit $\Delta\to\infty$ (keeping $\mu+\Delta$ finite) the potentials κ_n are very large and it is straightforward to verify that these equations reduce to those for the one-band model with an attractive potential [4]. Similarly, for $H\to\infty$ (with $\mu+\frac{1}{2}H$ kept finite) the potentials ψ and φ_n become very large so that those states cannot be occupied and Eqs. (5) reduce to those of the one-band problem with repulsive interaction [4]. The structure of Eqs. (5) (but not the driving terms) is also similar to the thermodynamic Bethe ansatz equations of a variant of the two-channel Kondo problem [10].

We now restrict ourselves to analyze the low-temperature properties of the model. It follows from Eq. (5c) that $\varphi_n(\lambda)>0$ for all λ and n. Similarly one obtains after some transformation of Eq. (5d) that $\kappa_n(\omega)>0$ for all ω if $n>2$. In view of the Fermi statistics obeyed by the rapidities a positive potential implies that the state is empty at low T, while rapidity values for which the energy potential is negative correspond to occupied states. Hence, the low-T physics is completely determined by the potentials $\epsilon(k)$, $\psi(\lambda)$, $\kappa_1(\omega)$, and $\kappa_2(\omega)$. All four potentials are symmetric functions of their argument and vary monotonically with $|k|$, $|\Lambda|$, or $|\omega|$. The respective "Fermi surfaces" are obtained by the conditions

$$\epsilon(\pm Q)=0,\quad \psi(\pm B)=0,\qquad \kappa_1(\pm A_1)=0,\quad \kappa_2(\pm A_2)=0. \tag{7}$$

Here Q, B, A_1, and A_2 are determined by μ, H, and Δ. It is usual to separate $\epsilon(k)=\epsilon^-(k)+\epsilon^+(k)$, $\psi(\lambda)=\psi^-(\lambda)+\psi^+(\lambda)$, and $\kappa_i(\omega)=\kappa_i^-(\omega)+\kappa_i^+(\omega)$, $i=1,2$, where the index $+$ $(-)$ denotes the positive (negative) part of the function. Renormalizing $\mu\to\mu+\Delta$ the ground-state integral equations can be written as

$$\epsilon^+(k)+\epsilon^-(k)=k^2-\mu-\tfrac{1}{2}H+a_2*\kappa_2^- -a_1*[\psi^- -\kappa_1^-], \tag{8a}$$

$$\psi^+(\lambda)+\psi^-(\lambda)-2(\lambda^2-\tfrac{1}{4}c^2-\mu)=-a_2*[\psi^- -\kappa_1^-]-a_1*\epsilon^- +[a_3+a_1]*\kappa_2^- =-[\kappa_1^+(\lambda)+\kappa_1^-(\lambda)-2\Delta], \tag{8b}$$

$$\kappa_2^+(\lambda)+\kappa_2^-(\lambda)=4\Delta-[2a_2+a_4]*\kappa_2^- +a_2*\epsilon^- +[a_3+a_1]*[\psi^- -\kappa_1^-]. \tag{8c}$$

As a function of the band energy potentials, the ground-state energy, the total number of electrons, the magnetization, and the minority band occupation are given by, respectively,

$$\frac{E}{L}=\int\frac{dk}{2\pi}\epsilon^-(k)+\int\frac{d\lambda}{\pi}\psi^-(\lambda),\quad N=-\frac{\partial E}{\partial\mu},$$

$$\frac{S_z}{L}=-\int\frac{dk}{4\pi}\frac{\partial\epsilon^-(k)}{\partial\mu},\quad \frac{m}{L}=-\int\frac{d\omega}{2\pi}\frac{\partial\kappa_1^-(\omega)}{\partial\mu}-\int\frac{d\omega}{\pi}\frac{\partial\kappa_2^-(\omega)}{\partial\mu}. \tag{8d}$$

In the absence of a magnetic field all electrons are paired in Cooper-like spin-singlet bound states and the band of unpaired electrons is empty, i.e., $Q=0$. Although bosons form the symmetry of the wave function and their spin, these Cooper pairs must have all different quantum numbers, i.e., they have a Fermi surface. They are hard-core bosons and do not undergo a condensation (analogous to spin waves in the antiferromagnetic Heisenberg chain); i.e., the system has no long-range order. The particle-hole excitations of these hard-core bosons form a continuum spectrum with energies vanishing for small momentum transfer and for excitations across the Fermi surface. A magnetic field H larger than a critical value

$$H_c=-2\mu-2\int d\lambda[a_1(\lambda)\psi^-(\lambda)-a_1(\lambda)\kappa_1^-(\lambda)-a_2(\lambda)\kappa_2^-(\lambda)] \tag{9}$$

is needed to overcome the binding energy of the Cooper pairs. In other words, there is no response to a field smaller than H_c. The depaired electrons for $H>H_c$ occupy the unpaired-electron band, $\epsilon(k)$, and give rise to a magnetization [11,12]. Hence, if $H_c>H$ the $\epsilon(k)$ band has a finite excitation energy of H_c-H; on the other hand, if $H>H_c$ also this band has a Fermi surface and a continuum spectrum of electron-hole excitations.

Assume that the field is incremented by a small amount from H_c to H. The magnetization then changes from 0 to a value proportional to $2Q$, i.e., the "Fermi momentum" of the unpaired electron band. For small k, the dispersion of this band is parabolic [see Eq. (8a)], so that $H-H_c\propto Q^2$ and $M\propto Q\propto(H-H_c)^{1/2}$ [12]. The susceptibility is then proportional to $(H-H_c)^{-1/2}$, as a consequence of the 1D Van Hove singularity, and the critical exponent is $\delta=2$, characteristic of a Prokovsky-Talapov [13] level-crossing transition.

The ground-state integral equations simplify in three limiting cases. (i) If Δ is very large and $H=0$ only one band is occupied and Eqs. (8) reduce to one integral equation for ψ. (ii) If $\Delta=0$ the two bands are degenerate and the ω strings for $n=1$ and 2 fill the real axis, so that $\kappa_1^+(\omega)$ and $\kappa_2^+(\omega)$ vanish identically. Fourier transforming, the ω strings can be eliminated from the set of equations and again the problem reduces to one integral equation if $H=0$. (iii) The integral equations can be solved in the limit $c\to 0$, yielding (a) $H_c=0$, as expected, (b) an empty κ_1 band, and (c) a partially occupied κ_2 band only if $\Delta<\mu/2$.

As already noted in the introduction, if either the sign of c is changed or the spin and band indices are interchanged, the interband interaction is attractive. The bound states can then be interpreted as excitons, H corresponds to the interband splitting, and Δ is the Zeeman energy.

The low-temperature specific heat can be obtained using the Sommerfeld expansion. One obtains that $C\propto T$ for all parameters except when the Fermi level is at a Van Hove singularity, where it is proportional to $T^{1/2}$ in analogy to the Prokovsky-Talapov level crossing [13].

Note that the Cooper-pair bound states do not cease to exist at finite T ($T_c=0$) and are still the dominant states if the temperature is low. At $T\neq 0$ the system responds to a small magnetic field, but the susceptibility is exponentially small as $T\rightarrow 0$.

Finally, we briefly discuss the one-particle and two-particle correlation functions as a function of distance at $T=0$. Since the spin excitations have a gap for $H<H_c$ and it is necessary to unpair a Cooper pair if one electron is withdrawn from the system, the one-particle Green's function must fall off exponentially with distance, the correlation length being inversely proportional to $H-H_c$. If the field is larger than H_c, this correlation function will fall off as a power law, typical of one-dimensional conductors. Correlations between Cooper pairs, on the other hand, just fall off with distance as a power law, since the excitation spectrum is a continuum.

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