Integrable Model for Interacting Electrons in Metallic Grains

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(Received 9 January 2001)

We find an integrable generalization of the BCS model with nonuniform Coulomb and pairing interaction. The Hamiltonian is integrable by construction since it is a functional of commuting operators; these operators, which therefore are constants of motion of the model, contain the anisotropic Gaudin Hamiltonians. The exact solution is obtained diagonalizing them by means of Bethe ansatz. Uniform pairing and Coulomb interaction are obtained as the "isotropic limit" of the Gaudin Hamiltonians. We discuss possible applications of this model to a single grain and to a system of few interacting grains.

DOI: 10.1103/PhysRevLett.86.5759 PACS numbers: 74.20.Mn, 02.30.Ik

Introduction and summary of the results.—Progress in nanotechnology has opened up theoretical investigations on the behavior of disordered interacting systems of small size [1]. Recently, the I-V characteristic measurements of Ralph, Black, and Tinkham [2] on small Al dots stimulated the theoretical debate on how to characterize the physical properties of small metallic grains, such as superconductivity and ferromagnetism [3,4]. Because of the chaoticity of the single particle wave functions [1,3], the Hamiltonian of these systems reads

$$H_{\mathrm{grain}} = \sum_i \varepsilon_i n_{i\sigma} - g \sum_{i,j} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} + U\left(\sum_j n_{j\sigma}\right)^2 - J\left(\sum_j c_{j\sigma}^\dagger \vec{S}_{\sigma\sigma'} c_{j\sigma'}\right)^2 + \mathcal{O}(\delta E^2/E_T). \quad (1)$$

(Here and in the following, sums over spins σ, σ' are implied.) The quantum numbers i, σ label a shell of doubly degenerate single particle energy levels with energy ϵ_i and annihilation operator $c_{i\sigma}$; $n_{i\sigma} := c_{i\sigma}^\dagger c_{i\sigma}$; S^a, $a = x, y, z$, are 2×2 spin matrices; δE is the average level spacing, and E_T the Thouless energy. The *universal* part of the Hamiltonian (1) (namely the first four terms) describes the pairing attraction, the electrostatic interaction and the ferromagnetic instability, respectively.

The superconducting fluctuations [4] can be taken into account by employing the BCS model [5,6] [namely taking the first two terms in Eq. (1)]. Richardson and Sherman (RS) [7] constructed the exact solution of the BCS model by a procedure close in spirit to the coordinate Bethe ansatz (BA). The knowledge of the exact eigenstates and eigenvalues of the BCS model has been crucial to establish physically relevant observables [8]. The integrability of the model has been proved [9,10] to be deeply related to the integrability of the isotropic Gaudin magnet [11]: the BCS model can be expressed as a certain combination [see Eq. (9) below] of its integrals of motion, which contain Gaudin Hamiltonians. Relations with conformal field theory and disordered vertex models were investigated in Refs. [12,13].

Many properties of metallic grains in a normal state (negligible superconducting fluctuations) can be described by the orthodox model [1,14] [i.e., taking the first and the third terms of the Hamiltonian (1)]. This arises by assuming uniform Coulomb interaction. Magnetic phenomena like the mesoscopic Stoner instability [3] can be studied by means of the exchange contribution to the Hamiltonian [the fourth term in Eq. (1)]. The terms proportional to $\delta E^2/E_T$ correspond to nonuniform Coulomb interaction [15]. Although they lose importance with the increasing conductance of the system, these corrections gain physical relevance due to the typically low relaxation rate of the excitations in a small dot. In fact, the corrections to the orthodox model induce "fluctuations" which can explain how nonequilibrium excitations decay in the dot [16,17]. This results in the formation of clusters of resonance peaks in the tunneling spectroscopy experiments [2].

In this paper we present an integrable generalization of the BCS Hamiltonian with nonuniform pairing coupling g_{ij} and solve it exactly. Besides the nonuniform pairing, the Hamiltonian contains a nonuniform Coulomb interaction U_{ij}; g_{ij} and U_{ij} are fixed according to Eqs. (3). We shall see that the inclusion of certain $\mathcal{O}(\delta E^2/E_T)$ terms leads to our integrable model. The integrable Hamiltonian we solve is

$$H = \sum_i \varepsilon_i n_{i\sigma} - \sum_{i,j} g_{ij} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} + \sum_{i,j} U_{ij} n_{i\sigma} n_{j\sigma'} - J\left(\sum_j c_{j\sigma}^\dagger \vec{S}_{\sigma\sigma'} c_{j\sigma'}\right)^2, \quad (2)$$

where the couplings are

$$\begin{cases} g_{ij} = -qK(\varepsilon_i - \varepsilon_j)/\sinh q(u_i - u_j), & \\ & i \neq j \\ 4U_{ij} = A + qK(\varepsilon_i - \varepsilon_j)\coth q(u_i - u_j), & \end{cases}$$
$$g_{jj} = -\beta_j, \qquad 4U_{jj} = A + \beta_j, \quad (3)$$

where $2\beta_j = -qK\sum_{i\neq j}(\varepsilon_i - \varepsilon_j)\coth q(u_i - u_j) + C$ [18]. For generic choices of β_j, the single particle energies ε_j must be shifted by $2\beta_j + 4\sum_{i\neq j} U_{i,j}$ in order to have integrability. The parameters A, K, and C are arbitrary real constants, while q can be real or imaginary. The BCS Hamiltonian, including a tunable capacitive coupling can be obtained from (2) in the *isotropic limit* $q \to 0$. Nonuniform coupling constants are obtained for generic q, and u_j being monotonic functions of ε_j. For real q, the arising g_{ij} can be made nearly uniform for levels within an energy cutoff E_D, and exponentially suppressed otherwise; correspondingly, U_{ij} can be made nearly uniform [as specified in Eqs. (20) below].

The proof of the integrability of the Hamiltonian (2) proceeds along the two following steps. (i) First we note the factorization [19] of the eigenstates of the Hamiltonian (2): $|\Psi\rangle = |\Psi_N\rangle \otimes |\Phi_M\rangle$ with eigenvalue $E = E_N + E_M$; where $|\Psi_N\rangle$ is the eigenstate of the Hamiltonian H_N projected on the subspace with N time-reversed pairs; $|\Phi_M\rangle$ is the Fock state projected on the blocked M singly occupied levels. The solution of the corresponding Hamiltonian H_M is easily obtained [20] as $H_M|\Phi_M\rangle = [\sum_i \varepsilon_i + \sum_{ij} U_{ij} - JS(S+1)]|\Phi_M\rangle$. (ii) Then Hamiltonian (2) is integrable if and only if H_N is integrable. The Hamiltonian H_N is obtained by inverting the procedure presented in Ref. [10]: First, we modify the constants of motion (of the BCS model) to commuting operators containing the anisotropic Gaudin models (the isotropic ones being considered in [10]); then we define the Hamiltonian in terms of these operators (H_N is therefore integrable by construction). We discuss some choices of $\{u_j\}$, K, and A leading to physically relevant Hamiltonians. The exact solution of H_N is found by diagonalizing the integrals of motion through BA [11]. The exact eigenfunctions and eigenvalues Ψ_N, E_N are

$$\Psi_N = \prod_{\alpha=1}^{N} \sum_{j=1}^{\Omega} \frac{q c_{j\uparrow}^{\dagger} c_{j\downarrow}^{\dagger}}{\sinh q(\omega_\alpha - u_j)} |0\rangle, \tag{4}$$

$$E_N = qK \sum_{j=1}^{\Omega} \sum_{\alpha=1}^{N} \varepsilon_j \coth q(\omega_\alpha - u_j) + AN^2; \tag{5}$$

$|0\rangle$ is the electronic vacuum state and Ω is the number of levels. The quantities ω_α fulfill the equations

$$\frac{2}{K} - \sum_{l=1}^{\Omega} q \coth q(\omega_\alpha - u_l) + 2\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{N} q \coth q(\omega_\alpha - \omega_\beta) = 0, \qquad \alpha = 1,\ldots,N \tag{6}$$

Our results can be applied to describe a system of $\mathcal{N}$ grains, since their Hamiltonian can be written (after a suitable relabeling of the levels) in the form (2). For distinct grains g_{jk} describe Cooper pair tunneling, and U_{jk} the intergrain Coulomb interaction. We require g_{ij} to decay both with intergrain distance and level separation. This can be fulfilled with u_j fixed by Eqs. (22) and (23).

The present paper is laid out as follows. First we discuss the integrability of the model H_N; then its exact solution is presented. This will complete the study of the integrability of the Hamiltonian (2). Finally, we will explain how our model can be applied to describe single as well as many interacting grains.

Integrability.—The BCS Hamiltonian can be written in terms of the spin-1/2 realization of $su(2)$:

$$H_{\mathrm{BCS}} = \sum_j 2\varepsilon_j S_j^z - g \sum_{j,k} S_j^+ S_k^-,$$

where

$$S_j^- := c_{j\downarrow} c_{j\uparrow}, \qquad S_j^+ := (S_j^-)^\dagger = c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger,$$
$$S_j^z := \frac{1}{2}(c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow} - 1), \tag{7}$$

obeying $[S_j^z, S_k^\pm] = \pm\delta_{jk} S_k^\pm$, $[S_j^+, S_k^-] = 2\delta_{jk} S_k^z$. Its constants of motion are written in terms of isotropic Gaudin Hamiltonians $\tilde{\Xi}_j$,

$$\tilde{\tau}_j = S_j^z - g\tilde{\Xi}_j; \qquad \tilde{\Xi}_j = \sum_{\substack{k=1\\ k\neq j}}^{\Omega} \frac{\mathbf{S}_j \cdot \mathbf{S}_k}{\varepsilon_j - \varepsilon_k}. \tag{8}$$

The $\tilde{\tau}_j$ mutually commute and we have $[\tilde{\tau}_j, \tilde{\tau}_k] = [H, \tilde{\tau}_j] = 0$ for all $i, j \in \{1, \ldots, \Omega\}$, because the BCS Hamiltonian can be written in terms of the $\tilde{\tau}_j$ only:

$$H_{\mathrm{BCS}} = \sum_j 2\varepsilon_j \tilde{\tau}_j + g \sum_{j,k} \tilde{\tau}_j \tilde{\tau}_k. \tag{9}$$

Our approach is now to modify the integrals of motion (8) and then to construct an integrable BCS-like model (which turns out to be characterized by a nonuniform pairing) following formula (9):

$$H_N := \sum_j 2\varepsilon_j \tau_j + A \sum_{j,k} \tau_j \tau_k + \text{const.} \tag{10}$$

The ansatz for the modified integrals τ_j is

$$\tau_j = S_j^z + \Xi_j; \qquad \Xi_j = \sum_{\substack{k=1\\ k\neq j}}^{\Omega} w_{jk}^\alpha S_j^\alpha S_k^\alpha, \tag{11}$$

where the operators Ξ_j are anisotropic Gaudin Hamiltonians (the isotropic case corresponding to $w_{ij}^x = w_{ij}^y = w_{ij}^z$). These operators mutually commute if

$$w_{ij}^\alpha w_{jk}^\gamma + w_{ji}^\beta w_{ik}^\gamma = w_{ik}^\alpha w_{jk}^\beta, \tag{12}$$

$$w_{ij}^x = -w_{ji}^y, \tag{13}$$

where (12) emerges from imposing $[\Xi_i, \Xi_j] = 0$ [11]. The other condition arises from $[S_i^z, \Xi_j] + [\Xi_i, S_j^z] = 0$. We furthermore postulate particle number conservation, which in the spin picture means $[\sum_{i=1}^{\Omega} S_i^z, \Xi_j] = 0$ for all $j \in \{1, \ldots, \Omega\}$, leading to another condition

$$w_{ij}^x = w_{ij}^y \overset{\text{Eq.(13)}}{=} -w_{ji}^x =: w_{ij} = -w_{ji}. \tag{14}$$

The last equation reduces the anisotropy to the XXZ-type and Eqs. (12) finally become

$$w_{ij} v_{jk} + w_{ji} v_{ik} = w_{ik} w_{jk}, \qquad v_{ij} := w_{ij}^z. \tag{15}$$

The solution of Eqs. (15) (see Ref. [11]) is

$$v_{jk} = qK \coth q(u_j - u_k),$$
$$w_{jk} = \frac{qK}{\sinh q(u_j - u_k)}, \quad (16)$$

where u_j are arbitrary complex parameters such that v_{jk}, w_{jk} are real. The transition from hyperbolic to trigonometric functions in the solution (16) is gained through the choice $q = i$, with real K, u_j. The cubic and quartic terms in S_j^α [obtained from formula (10)] vanish for the antisymmetry of v_{jk}. We finally obtain

$$H_N = \sum_j 2\varepsilon_j S_j^z - \sum_{j,k} g_{jk} S_j^+ S_k^- + 4\sum_{j,k} U_{jk} S_j^z S_k^z, \quad (17)$$

where the couplings are given in Eqs. (3). Up to a constant, the Hamiltonian (2) (projected on doubly occupied states) is recovered writing back the spin operators in terms of creation and annihilation operators.

Exact solution.—The exact solution of the anisotropic Gaudin model for w_{ij} and v_{ij} fixed by Eqs. (16) was obtained in Ref. [11]. The same procedure can be applied to diagonalize τ_j. The eigenfunctions of τ_j defined in Eq. (11) are written in the form

$$|\Psi_j\rangle = \sum_{j_1 \le \cdots \le j_M}{}' c(j_1, \ldots, j_M) S_{j_1}^+ \cdots S_{j_M}^+ |0\rangle + \sum_{j_1 \le \cdots \le j_{M-1}}{}' e(j_1, \ldots, j_{M-1}) S_{j_1}^+ \cdots S_{j_{M-1}}^+ S_j^+ |0\rangle. \quad (18)$$

The vacuum $|0\rangle$ corresponds to $|\downarrow, \ldots, \downarrow\rangle$; the prime on the sums means the indices run in the range $\{1, \ldots, \Omega\}\setminus\{j\}$. Imposing that $|\Psi_j\rangle$ is an eigenstate of τ_j we find a set of equations which $c(\{j_i\})$ and $e(\{j_i\})$ must fulfill. For a suitable change of variables these conditions are transformed in Eqs. (6). The quantities τ_j have the following eigenvalues:

$$\tau_j |\Psi_j\rangle = \frac{1}{2}(h_j - 1)|\Psi_j\rangle,$$
$$\frac{1}{K} h_j = \frac{1}{2} \sum_{l=1}^{\Omega}{}' q \coth q(u_j - u_l) - \sum_{\alpha=1}^{N} q \coth q(u_j - \omega_\alpha). \quad (19)$$

The parameters ω_α are determined by Eq. (6). The eigenvalues of H_N immediately follow from formula (10). Together with the eigenfunctions they are given in Eqs. (4) and (5).

Single grain.—We discuss how our results can be applied to describe the physics of a single grain. The isotropic limit $q \to 0$ of Eqs. (3) gives the BCS Hamiltonian plus a tunable capacitive coupling $A + g$, with $K = g/E_D$, $\beta_i = -g$, $u_j = -\varepsilon_j/[E_D \Theta(|\varepsilon_j - E_F| - E_D)]$, where E_F is the Fermi level, and Θ is the Heaviside function [$\Theta(x) = 1$ if $x < 0$, $\Theta(x) = 0$ if $x > 0$], setting sharp cutoffs at the Debye energy [21]; the diagonal elements U_{jj} and g_{jj} can be independently set to arbitrary values (since they would renormalize ε_j). Choosing $A = -g$ gives the "pure" BCS model. In this limit, the eigenstates and eigenvalues Eqs. (5) and (4) coincide with those of the BCS model and Eq. (6) reduces to the RS equations [7].

We now discuss the case corresponding to $q = 1$:

$$K = g/E_D, \qquad \beta_i = -g,$$
$$A \gg (g/E_D) \max_{j,k}\{\varepsilon_j - \varepsilon_k\}, \qquad u_j = -\varepsilon_j/E_D. \quad (20)$$

We can identify three regimes depending on the value of E_D: (i) $E_D < \delta E$, g_{ij} is nearly zero, while $U_{ij} \simeq A - g$; (ii) $E_D \sim \delta E$, the pairing interaction decays on the scale $E_D \sim \delta E$, while U_{ij} is slowly modulated by the energy separation; (iii) $E_D > \max_{i,j}(\varepsilon_i - \varepsilon_j)$ both g_{ij} and U_{ij} are nearly uniform.

Application to many interacting grains.—We now discuss applications of the model (2) to interacting dots. The Hamiltonian (2) can be reinterpreted as follows: the set $I = \{1, \ldots, \Omega\}$ can be split into the (disjoint) sets I_a, $a = 1, \ldots, \mathcal{N}$ containing the levels of the ath grain: $I = \bigcup_a I_a$; $\Omega = \sum_{a=1}^{\mathcal{N}} \Omega_a$, where $\Omega_a = |I_a|$. Thus the Hamiltonian H_N is equivalent to the following one:

$$H_{\mathcal{N}} = \sum_{a=1}^{\mathcal{N}} \sum_{i_a} \varepsilon_{i_a}^{(a)} c_{a,i_a\sigma}^\dagger c_{a,i_a\sigma} - \sum_{a,b=1}^{\mathcal{N}} \sum_{i_a,j_b} g_{i_a j_b}^{(a,b)} c_{a,i_a\uparrow}^\dagger c_{a,i_a\downarrow}^\dagger c_{b,j_b\downarrow} c_{b,j_b\uparrow} + \sum_{a,b=1}^{\mathcal{N}} \sum_{i_a,j_b} U_{i_a j_b}^{(a,b)} n_{a,i_a\sigma} n_{b,j_b\sigma'}, \quad (21)$$

where $i_a = 1, \ldots, \Omega_a$ label the elements of I_a and $c_{a,i_a\sigma}$ annihilates an electron with spin σ in the i_ath level of the ath grain. For $a \neq b$, $g^{(a,b)}$ describe tunneling of Cooper pairs; in terms of (2), $g_{i_a j_b}^{(a,b)} = g_{ij}$, where i is the i_ath element of I_a, and j the j_bth element of I_b; $U^{(a,b)}$ describe a Coulomb-like coupling between grains a and b, and is written in terms of U_{ij} analogously to $g^{(a,b)}$. Couplings $g^{(a,a)}$ and $U^{(a,a)}$ describe pairing and Coulomb intragrain interactions, respectively. We fix the couplings as in (20) with the exception that

$$u_j = \Phi_a - \varepsilon_j/E_D, \qquad \text{when } j \in I_a. \quad (22)$$

Now we impose

$$\Phi_{a+1} - \Phi_a \gg \max_{j,k \in I_a}\{(\varepsilon_j - \varepsilon_k)/E_D\} \quad (23)$$

to make the tunneling amplitude exponentially suppressed with the *spatial* distance between the grains. The pairing interaction is nearly uniform for levels within E_D in the same grain. The intragrain Coulomb interaction is also nearly uniform $U_{jk} \simeq A$, while the intergrain Coulomb interaction is modulated by the corresponding energy separation.

Conclusions.—We found a class of integrable Hamiltonians, which are a generalization of the BCS Hamiltonian characterized by nonuniform coupling constants. To our knowledge, this is the first exact solution for nonuniform pairing interaction. The strategy we have adopted consists in generalizing the procedure of Ref. [10], namely constructing the Hamiltonian of the system in terms of anisotropic Gaudin Hamiltonians. By means of the integrability and the exact solvability of the latter we obtain the integrability and the exact solution of the model Eqs. (2) and (3). In this sense, our procedure is close in spirit to the quantum inverse scattering method [22]. The isotropic limit $q \to 0$ of the Gaudin Hamiltonians corresponds to uniform couplings. For arbitrary A, the Hamiltonian is the sum of the BCS and the orthodox model. For $A = g$ the BCS Hamiltonian is obtained; the same isotropic limit of the exact solution Eqs. (4)–(6) coincides with the RS solution.

This class of models might be useful for applications to the physics of metallic grains. The nonuniformity [23] of the coupling constants (3) corresponds to include certain $\mathcal{O}(\delta E^2/E_T)$ terms [15] in the Hamiltonian (1). In fact, we recover the fluctuations of the Coulomb interaction of the Ref. [15] identifying $\delta U_H \equiv U_{ij} - U_{ij'}$. The integrable model presented here might be applied as a starting point for suitable perturbation schemes leading to the explanation of the tunneling phenomena.

The present model can be applied to systems of few interacting dots, since our capacitivelike intergrain interaction does not decay with spatial distance.

In a recent paper (Ref. [24]) a nonuniform coupling for bosonic systems was studied. The Hamiltonian was constructed from the bosonic analog of formulas (10) and (11), where the S^a are generators of $su(1,1)$ [instead of $su(2)$]. This algebraic difference does not affect the equations which w_{ij}, v_{ij} have to fulfill to ensure the commutativity of the (bosonic) τ_j. The coupling constants of this bosonic model can be obtained in the isotropic limit of our Eqs. (3) with $u_j \propto \varepsilon_j^d$ and $A = 0$. This shows that the bosonic Hamiltonian in Ref. [24] can be obtained by the limit $q \to 0$ of anisotropic $su(1,1)$ Gaudin models. Work is in progress along this direction.

This line of research was suggested by G. Falci whose invaluable help is a pleasure to acknowledge. We thank R. Fazio for constant support, fruitful discussions, and critical reading of the manuscript. We acknowledge R. W. Richardson for critical discussions on our work. We also thank A. Mastellone for useful discussions.

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