

# Strong-coupling expansion for the pairing Hamiltonian for small superconducting metallic grains

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The paper is devoted to the study of the effects due to superconducting pairing in small metallic grains. We explicitly determine the low-energy spectrum of the problem at strong superconducting coupling and in the limit of large Thouless conductance. We start with the strong-coupling limit and develop a systematic expansion in powers of the inverse coupling constant for the many-particle spectrum of the system. The strong-coupling expansion is based on the formal exact solution of the Richardson model and converges for realistic values of the coupling constant. We use this expansion to study the low-energy excitations of the system, in particular energy and spin gaps in the many-body spectrum.

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## I. INTRODUCTION

Since the mid-1990's, when Ralph, Black, and Tinkham succeeded in resolving the discrete excitation spectrum of nanoscale superconducting metallic grains,<sup>1</sup> there has been considerable effort to describe theoretically superconducting correlations in such grains (see, e.g., Ref. 2 for a review). However, very few explicit analytical results relevant for the low-energy physics of superconducting grains have been obtained, since, in contrast to bulk materials, the discreteness of single-electron levels plays an important role. In this paper we address this problem in the regime of well-developed superconducting correlations.

The electron-electron interactions in weakly disordered grains with negligible spin-orbit interaction are described by a simple Hamiltonian,<sup>3</sup>

$$H_{\text{univ}} = H_{BCS} - JS(S+1), \quad (1)$$

$$H_{BCS} = \sum_{i,\sigma} \epsilon_i c_{i\sigma}^\dagger c_{i\sigma} - \lambda d \sum_{i,j=1}^N c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}, \quad (2)$$

where  $\epsilon_i$  are single-electron energy levels,  $d$  is the mean level spacing,  $c_{i\sigma}^\dagger$  and  $c_{i\sigma}$  are creation and annihilation operators for an electron on level  $i$ , and  $S$  and  $N$  are the total spin and number of levels, respectively. There are only two sample-dependent coupling constants:  $\lambda$  and  $J$ , which correspond to superconducting correlations and spin-exchange interactions, respectively. Throughout the present paper, for the sake of brevity, we consider only the less trivial case of ferromagnetic exchange,  $J > 0$ .

Although Hamiltonian (1) is integrable<sup>4,5</sup> and solvable by Bethe's *Ansatz*, the exact solution<sup>6</sup> yields a complicated set of coupled polynomial equations [see Eq. (3) below]. As a consequence, very few explicit results have been derived and most studies resorted to numerics based on the exact solution. The purpose of the present paper is to remedy this situation and to build a simple and intuitive picture of the low-energy physics of isolated grains in the superconducting phase.

It is well known that physical observables of a superconductor are nonanalytic in the coupling constant  $\lambda$  at  $\lambda = 0$ . On the other hand, the opposite limit of large  $\lambda$  turns out to

be regular and relatively simple. Here we use the exact solution to obtain an explicit expansion in powers of  $1/\lambda$  for the ground state and low-lying excitation energies.

We will distinguish between two types of excitations: ones that preserve the number of Cooper pairs (the number of doubly occupied orbitals) and ones that do not. Only the latter excitations are capable of carrying nonzero spin. It turns out that for  $J=0$  to the lowest order in  $1/\lambda$  both types of excitations are gapped with the same gap  $\lambda Nd$ . We compute explicitly the two gaps to the next nonzero order in  $1/\lambda$  and find the gap for pair-breaking excitations to be larger. The difference between the two gaps turns out to be of the order of  $d^2/\Delta$ , where  $d$  is the mean single-particle level spacing and  $\Delta$  is the BCS energy gap, i.e., the difference vanishes in the thermodynamical limit. We were not able to determine the convergence criteria for the strong-coupling expansion exactly; however, we present evidence that the expansion converges up to realistic values of  $\lambda$  between  $\lambda_{c1} \approx 1$  and  $\lambda_{c2} \approx 1/\pi$ .

The Hamiltonian (2) was studied extensively in 1960s in the context of pair correlations in nuclear matter (see, e.g., Ref. 7). A straightforward but important observation was that singly occupied levels do not participate in pair scattering.<sup>8</sup> Hence, the labels of these levels are good quantum numbers and their contribution to the total energy is only through the kinetic and the spin-exchange terms in Eq. (1). Due to this "blocking effect" the problem of diagonalizing the full Hamiltonian (1) reduces to finding the spectrum of the BCS Hamiltonian (2) on the subspace of either empty or doubly occupied ("unblocked") orbitals. The latter problem turns out to be solvable<sup>6</sup> by Bethe's *Ansatz*. The spectrum is obtained from the following set of algebraic equations for unknown parameters  $E_i$ :

$$-\frac{1}{\lambda d} + \sum_{j=1}^m \frac{2}{E_i - E_j} = \sum_{k=1}^n \frac{1}{E_i - 2\epsilon_k}, \quad i = 1, \dots, m \quad (3)$$

where  $m$  is the number of pairs and  $n$  is the number of unblocked orbitals  $\epsilon_k$ . Bethe's *Ansatz* equations (3) for the BCS Hamiltonian (2) are commonly referred to as Richardson's equations. The eigenvalues of the full Hamiltonian (1) are known to be related to Richardson parameters,  $E_i$ , via

$$E = \sum_{i=1}^m E_i + \sum_B \epsilon_B - JS(S+1), \quad (4)$$

where  $\sum_B \epsilon_B$  is a sum over singly occupied (“blocked”) orbitals and  $S$  is the total spin of blocked orbitals (i.e., the total spin of the system).

BCS results<sup>9</sup> for the energy gap, condensation energy, excitation spectrum, etc., are recovered from the exact solution (3) in the thermodynamical limit.<sup>10</sup> The proper limit is obtained by taking the number of levels,  $N$ , to infinity, so that  $Nd \rightarrow 2D = \text{const}$ ,  $m = n/2 = N/2$ , where  $D$  is an ultraviolet cutoff usually identified with Debye energy. In particular, for equally spaced levels  $\epsilon_i$ , the energy gap  $\Delta$  and the ground state energy in the thermodynamical limit are

$$\Delta(\lambda) = \frac{D}{\sinh(1/\lambda)}, \quad E_{\text{gr}}^{\text{BCS}} = -Dm \coth(1/\lambda). \quad (5)$$

Since the BCS Hamiltonian (2) contains only three energy scales:  $D$ ,  $\Delta$ , and  $d$ , there are only two independent dimensionless parameters:  $N$  and  $\lambda$ . The perturbation theory in small  $\lambda$  breaks down in the superconducting state as is already suggested by BCS formulas (5). Thus, it is natural to consider the opposite limit of large  $\lambda$  and treat the kinetic term in Hamiltonian (1) as a perturbation.

The paper is organized as follows. In Sec. II we consider the limit  $\lambda \rightarrow \infty$ , which is the zeroth order of our expansion. In this limit one can determine the spectrum straightforwardly by representing the BCS Hamiltonian (2) in terms of Anderson pseudospin operators.<sup>11</sup> In particular, one finds that at  $J=0$  excitations with nonzero spin to the lowest order in  $1/\lambda$  have the same gap (the spin gap) as spinless excitations. Next, we rederive the same results from Richardson’s equations (3) and also show that in the limit  $\lambda \rightarrow \infty$  the roots of Richardson’s equations are zeros of Laguerre polynomials.

In Sec. III Bethe’s *Ansatz* equations (3) are used to expand the ground state and low-lying excitation energies in series in  $1/\lambda$ . We write down several lowest orders explicitly and give recurrence relations that relate the  $k$ th-order term to preceding terms. These relations can be used to readily expand up to any reasonably high order in  $1/\lambda$ . Finally, we compute the spin gap to the next nontrivial order in  $1/\lambda$  and demonstrate that at  $J=0$  the first excited state always have zero spin.

## II. THE STRONG-COUPLING LIMIT

In this section we analyze the lowest order of the strong-coupling expansion. As the strength of the coupling constant  $\lambda$  increases, the spectrum of the BCS Hamiltonian (2) undergoes dramatic changes as compared to the spectrum of non-interacting Hamiltonian  $H_{\text{BCS}}(\lambda=0)$ . First, there is a region of small  $\lambda$  where the superconducting coupling causes only small perturbations in the electronic system. This region shrinks to zero in the thermodynamical limit and is roughly determined by the condition  $\Delta(\lambda) \leq d$ ,<sup>12</sup> where  $\Delta(\lambda)$  is given by Eq. (5). For larger  $\lambda$  the perturbation theory in  $\lambda$  breaks down<sup>13</sup> and strong superconducting correlations develop in the system. A representative energy level diagram is

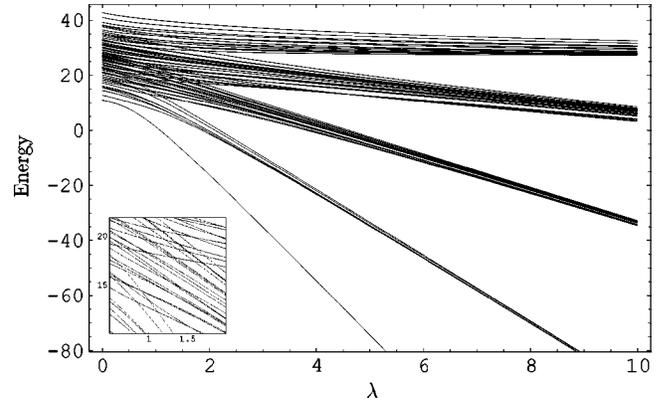


FIG. 1. Results of exact numerical diagonalization. Energies of the BCS Hamiltonian (2) for  $m=4$  pairs and  $n=8$  unblocked single-particle levels  $\epsilon_i$  versus coupling constant  $\lambda$ . All energies are measured in units of the mean level spacing  $d$ . The single-particle levels  $\epsilon_i$  are computer-generated random numbers. As the strength of the coupling  $\lambda$  increases, the levels coalesce into narrow well-separated rays (bands). The width of these bands vanishes in the limit  $\lambda \rightarrow \infty$  [see Eq. (47) and the discussion around it]. Slopes of the rays and the number of states in each ray are given by Eqs. (7), (15), and (12). The ground state is nondegenerate, while the first group of excited states contains  $n-1=7$  states. Note also the level crossings for  $\lambda \sim 1$  (see the inset on the above graph).

shown in Fig. 1. In the crossover regime the spectrum displays numerous level crossings that reflect the breakdown of perturbation theory in  $\lambda$ . The fact that the crossings occur for random single electron levels  $\epsilon_i$ , i.e., in the absence of any spatial symmetry, is a characteristic feature of quantum integrability.<sup>14</sup>

The lowest order of the strong-coupling expansion is obtained by neglecting the kinetic energy term in the BCS Hamiltonian (2). This limit can in principle be realized in a grain of an ideal regular shape.<sup>15</sup> In this case the single-electron levels are highly degenerate and if the energy distance between degenerate many-body levels is much larger than  $\lambda d$ , only the partially filled Fermi level is relevant. Then, the kinetic term in Eq. (2) is simply a constant proportional to the total number of particles and can be set to zero.

An efficient way to obtain the spectrum of Hamiltonian (1) in the strong-coupling limit is by representing the interaction term in the BCS Hamiltonian in terms of Anderson pseudospin-1/2 operators:<sup>11</sup>

$$K_i^z = \frac{c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow} - 1}{2}, \quad K_i^+ = (K_i^+)^{\dagger} = c_{i\uparrow}^\dagger c_{i\downarrow}. \quad (6)$$

The pseudospin is defined only on unblocked levels, where it has all properties of spin 1/2, i.e., proper commutation relations and definite values of  $\vec{K}_i^2 = 3/4$ .

The interaction term in the BCS Hamiltonian (2) takes a simple form in terms of  $\vec{K}_i$ :

$$H_{\text{BCS}}^{\infty} = -\lambda d K^+ K^- = -\lambda d [K(K+1) - (K^z)^2 + K^z], \quad (7)$$

where  $\vec{K} = \sum_i \vec{K}_i$  is the total pseudospin of the unblocked levels. The  $z$  projection of the total pseudospin according to Eq.

(6) is  $K^z = m - n/2$ , where  $m$  and  $n$  are the total number of pairs and unblocked (either doubly occupied or empty) levels, respectively. It is simple to check that replacing a doubly occupied level with two singly occupied ones does not affect the difference  $m - n/2$ . As a result,

$$K^z = m - \frac{n}{2} = M - \frac{N}{2}, \quad (8)$$

where  $M$  is the maximum possible number of pairs and  $N$  is the total number of levels, respectively. Hence, the last two terms in Eq. (7) yield a constant independent of the number of blocked levels. This constant can be set to zero by an overall shift of all energies. Therefore, the full Hamiltonian (1) in the strong-coupling limit is

$$H_{\text{univ}}^\infty = -\lambda d K(K+1) - JS(S+1). \quad (9)$$

Since there are  $n$  pseudospin 1/2's the total pseudospin  $K$  takes values between  $|K^z|$  and  $n/2$ ,

$$\frac{n}{2} \geq K \geq \left| m - \frac{n}{2} \right|, \quad (10)$$

while the total spin  $S$  ranges from 0 (1/2) to  $M - m(M - m + 1/2)$  for even (odd) total number of electrons. For the sake of brevity, let us from now on consider only the case of even total number of electrons. Then, the sum of the total spin and pseudospin is constrained by

$$K + S \leq \frac{N}{2}. \quad (11)$$

The degree of degeneracy  $D(K, S, n)$  of each level is<sup>16</sup>

$$D(K, S) = \frac{n!(2K+1)}{(n/2+K+1)!(n/2-K)!} \times \frac{(N-n)!(2S+1)}{[(N-n)/2+S+1]![(N-n)/2-S]!}. \quad (12)$$

The ground state of Hamiltonian (9) has the maximum possible pseudospin,  $K = N/2$ , and minimal possible spin,  $S = 0$ , provided that  $\lambda d > J$  (recall that we consider only positive values of the exchange coupling  $J$ ).

There are two ways to create an elementary excitation. First, one can decrease the total pseudospin  $K$  while keeping the total number of pairs  $M$  unchanged. The second type of excitations corresponds to breaking pairs and blocking some of the single-electron levels. These excitations can contribute to the total spin of the grain  $S$ . They also affect the pseudospin since its maximal value  $K_{\text{max}} = n/2$  is determined by the number of unblocked levels. The lowest-lying excitations correspond to  $K = N/2 - 1$ , which can be achieved both with and without breaking a single Cooper pair. Therefore, we find from Eq. (9) that the pair-conserving excitations are separated by a gap  $\Delta_{\text{pair}} = N\lambda d$  while pair-breaking excitations can lower their energy by having nonzero spin  $S$ . Since the maximum value of  $S$  for two unpaired electrons is  $S = 1$ , we get  $\Delta_{\text{spin}} = N\lambda d - 2J$ . In the opposite case  $J > \lambda d$ ,

$K = 0$  and the total spin has the maximum possible value  $S = M$  in the ground state, i.e.,  $J = \lambda d$  is the threshold of Stoner instability in the strong-coupling limit.

The above results can be obtained directly from the exact solution (3). Moreover, individual parameters  $E_i$  can also be determined and, since eigenstates of the BCS Hamiltonian (2) are given in terms of  $E_i$  (see Ref. 6), this can be used to calculate various correlation functions in the strong-coupling limit.

The value of the total pseudospin  $K$  turns out to be related to the number,  $r$ , of those roots of equations (3) that diverge in the limit  $\lambda \rightarrow \infty$  (see below). To the lowest order in  $1/\lambda$  we can neglect single-electron levels  $\epsilon_i$  in Eqs. (3) for these roots

$$-\frac{1}{\lambda d} + \sum_{j=1}^r \frac{2}{E_i - E_j} = \frac{n'}{E_i}, \quad i = 1, \dots, r, \quad (13)$$

where  $n' = n + 2r - 2m$  and the summation excludes  $j = i$ . For the remaining  $m - r$  roots we have

$$\sum_{k=1}^n \frac{1}{E_i - 2\epsilon_k} = 0, \quad i = r+1, \dots, m-r. \quad (14)$$

Multiplying each equation in (13) by  $E_i$  and adding all Eqs. (13), we obtain the eigenenergies of the BCS Hamiltonian (2) for  $n$  unblocked levels and  $m$  pairs:

$$E = -\lambda dr(n - 2m + r + 1). \quad (15)$$

Comparing this to Eqs. (7) and (8), we find the relationship between  $r$  and  $K$ :

$$r = K + m - n/2. \quad (16)$$

Since the total pseudospin,  $K$ , is constrained by relation (10), the number,  $r$ , of diverging Richardson parameters,  $E_i$ , is also constrained:

$$\begin{aligned} 2m - n \leq r \leq m & \quad \text{if } n < 2m \\ 0 \leq r \leq m & \quad \text{if } n \geq 2m. \end{aligned} \quad (17)$$

Below in this section we show that Eqs. (13) have a unique solution. As a result, the degeneracy of energy levels (12) is equal to the number of solutions of Eqs. (14) for the remaining  $E_i$ . This number can be computed<sup>17,18</sup> directly from Eq. (14) and indeed coincides with Eq. (12).

Finally, Eqs. (13) can be solved to determine parameters  $E_i$  to the lowest order in  $1/\lambda$  (see also Refs. 19 and 20). To this end it is convenient to introduce a polynomial  $f(x)$  of order  $r$  with zeros at  $x = x_i = E_i/(\lambda d)$

$$f(x) = \prod_{i=1}^r (x - x_i). \quad (18)$$

Using

$$\lim_{x \rightarrow x_i} \frac{f''(x)}{f'(x)} = \sum_{j \neq i} \frac{2}{x_i - x_j},$$

one can rewrite Eqs. (13) as

$$F(x_i)=0 \quad \text{where} \quad F(x)=xf'(x)-xf''(x)+n'f'(x). \quad (19)$$

Since  $F(x)$  and  $f(x)$  are two polynomials of the same degree  $r$  with the same roots  $x_i$ , they are proportional to each other. The coefficient of proportionality is the ratio of coefficients at  $x^r$  and, according to Eq. (19), is equal to  $r$ . Therefore,  $F(x)=rf(x)$ , or equivalently

$$xf''-(x+n')f'+rf=0. \quad (20)$$

The only polynomial solution to this equation is the Laguerre polynomial  $L_r^{-1-n'}$ . Thus, to the order  $\lambda$  the nonvanishing roots of Richardson's equations (3) in the strong-coupling limit are determined by

$$L_r^{-1-n'}\left(\frac{E_i}{\lambda d}\right)=0, \quad n'=n+2r-2m, \quad (21)$$

where  $r$  is the number of nonvanishing roots to the order  $\lambda$ . This number and the total pseudospin are related by Eq. (16). The ground state has  $r=m$ , the first degenerate group of excited states corresponds to  $r=m-1$ , etc. The constraint  $r \geq 2m-n$  in relation (17) follows from the requirement that the roots of Eq. (21) be nonvanishing.<sup>19</sup> Moreover, it can be shown<sup>19</sup> using conditions (17) that all Richardson parameters  $E_i$  are complex for even values of  $r$ , while for odd  $r$  there is a single real (negative) root. The fact that the roots of Eq. (13) are generally complex was also noted in Ref. 18 on the basis of the numerical solution of Richardson's equations.

### III. THE STRONG-COUPLING EXPANSION

Now we turn to the expansion in powers of  $1/\lambda$  around the strong-coupling limit. The evolution of energy levels with  $\lambda$  can be viewed as a motion of one-dimensional particles whose positions are the energies of the BCS Hamiltonian (2) (see, e.g., Refs. 21 and 14). Then, single-electron levels  $\epsilon_i$  determine the initial conditions at  $\lambda=0$ . As the coupling  $\lambda$  increases beyond the crossover between the weakly perturbed Fermi gas and the regime of strong superconducting correlations, the particles gradually lose the memory of their initial positions and eventually the spectrum becomes independent of  $\epsilon_i$ . In this limit, the excited levels coalesce into highly degenerate rays with a universal slope [see Fig. 1 and Eq. (15)]. In the strong-coupling expansion the system of one-dimensional particles evolves from larger to smaller  $\lambda$ . One expects this evolution to be nonsingular until we come close to the level crossings (see the beginning of the preceding section), i.e. the crossover region, where both expansions in  $\lambda$  and in  $1/\lambda$  break down.

A quantitative estimate of the convergence of the  $1/\lambda$  expansion can be obtained by considering various limiting cases. In the thermodynamical limit the ground-state energy is given by BCS expression (5). This limit is equivalent to keeping only the terms of order  $N$  in the  $1/\lambda$  expansion. We observe from BCS expressions (5) that the expansion in  $1/\lambda$  converges for  $\lambda > 1/\pi$ . In the opposite case of one pair and two levels,  $2M=N=2$ , the ground-state energy can be com-

puted exactly by, e.g., solving Eqs. (3) with the result

$$E_{\text{gr}}^2 = -d(\lambda + \sqrt{1 + \lambda^2}). \quad (22)$$

In this case the expansion of the ground-state energy (22) in  $1/\lambda$  converges for  $\lambda > 1$ . In general, we believe that strong-coupling expansion yields convergent rather than asymptotic series with the radius of convergence between  $\lambda_{c1} \approx 1$  and  $\lambda_{c2} \approx 1/\pi$ .

Later in this section we develop an efficient algorithm for calculating the low-energy spectrum to any order in  $1/\lambda$ . While the pseudospin representation detailed in the preceding section provides a simple and intuitive description of the strong-coupling limit, the usual perturbation theory becomes unmanageable beyond the first two orders in  $1/\lambda$ . An approach based on Bethe's *Ansatz* equations, on the other hand, turns out to be well suited for the purposes of systematic expansion.

#### A. The ground state

Here we expand the ground-state energy in  $1/\lambda$ . Richardson's equations (3) lead to recurrence relations for the coefficients of the expansion. From these relations the ground-state energy can be computed to any reasonably high order in  $1/\lambda$ , e.g., we write down the energy up to  $1/\lambda^7$ . As mentioned above we take the number of electrons to be even and consider only the case when  $\lambda d > J$ . As we have seen in the preceding section, this inequality ensures that in the ground state all levels are unblocked and all electrons are paired, i.e., Richardson's equations (3) should be solved at

$$m=M, \quad n=N.$$

We begin by introducing a convenient set of variables:

$$s_p \equiv \sum_{k=1}^N (2\epsilon_k)^p, \quad \sigma_p \equiv \sum_{i=1}^M \frac{1}{E_i^p}. \quad (23)$$

Variables  $\sigma_p$  can be expanded into series in the inverse coupling constant  $\lambda$ :

$$\sigma_p = \sum_{k=0}^{\infty} a_p^k \lambda^{-k-p}. \quad (24)$$

Next, we rewrite Richardson's equations (3) in a form more suitable for our purpose. We divide the equation for  $E_i$  by  $E_i^p$  with  $p \geq -1$  and add all  $M$  equations for each  $p$ . Expanding  $1/(1-2\epsilon_k/E_i)$  in  $2\epsilon_k/E_i$  and using an identity

$$\sum_{i>j} \frac{2}{E_i - E_j} \left( \frac{1}{E_i^p} - \frac{1}{E_j^p} \right) = p\sigma_{p+1} - \sum_{k=1}^p \sigma_{p-k+1}\sigma_k,$$

we obtain

$$\begin{aligned}
 E_{\text{gr}}(M, N, s_p) &= \sum_{i=1}^M E_i = -M(N-M+1)\lambda d - \sum_{k=1}^{\infty} s_k \sigma_k \\
 &= -M(N-M+1)\lambda d \\
 &\quad - d \sum_{j=0}^{\infty} \left( \sum_{k=1}^{j+1} s_k a_k^{j-k+1} \right) \lambda^{-j} \quad (25)
 \end{aligned}$$

$$\begin{aligned}
 -\frac{\sigma_p}{\lambda d} - \sum_{k=1}^p \sigma_{p-k+1} \sigma_k &= (N-p)\sigma_{p+1} + \sum_{j=1}^{\infty} s_j \sigma_{j+p+1}, \\
 p &\geq 0. \quad (26)
 \end{aligned}$$

Now plugging  $\sigma_p = \sum_{k=0}^{\infty} a_p^k \lambda^{-k-p}$  into the last equation and setting the coefficient at  $\lambda^{-h-p-1}$  to zero, we obtain

$$\frac{a_p^h}{d} + \sum_{k=1}^p \sum_{s=0}^h a_{p-k+1}^{h-s} a_k^s + \sum_{k=1}^h s_k a_{p+k+1}^{h-k} = -(N-p)a_{p+1}^h. \quad (27)$$

Note that from  $\sigma_0 = M$  it follows that  $a_0^0 = M$  and  $a_0^k = 0$  for  $k \geq 1$ . The values of  $a_0^k$  serve as boundary conditions for recurrence relations (27). Note also that according to Eq. (27) the coefficients  $a_p^h$  do not depend on  $\lambda$  as expected from their definition (24). Coefficients  $a_p^0$  determine  $\sigma_p$  for the ground state to the lowest nonvanishing order in  $1/\lambda$  and therefore can be expressed in terms of zeros of the Laguerre polynomial (21) with  $r = M$ . Using Eq. (21), we obtain

$$a_p^0 d^p = (-1)^p \frac{d^p}{dx^p} \ln L_M^{-1-N}(x) \Big|_{x=0}.$$

According to Eq. (25) in order to determine the ground-state energy to order  $1/\lambda^j$  one has to calculate the first  $j-p+2$  coefficients  $a_p^k$  in the expansion of  $\sigma_p$ . To do this, we first compute  $a_p^0$  for  $p \leq j+1$ , then  $a_p^1$  for  $p \leq j$ , then  $a_p^2$  for  $p \leq j-1$ , etc. In other words, we start from the  $a_1^0$  element of matrix  $a_p^h$  and use recurrence relations (27) to move down the first column of this matrix until  $a_{j+1}^0$ , then to move down the second column from  $a_1^1$  to  $a_j^1$ , etc.

While we were not able to express  $a_p^k$  in terms of  $p$  and  $k$  explicitly, the above procedure allows for an efficient calculation, e.g., using MATHEMATICA, of the ground-state energy to any given order. For example, the ground-state energy to order  $1/\lambda^2$  is

$$\begin{aligned}
 E_{\text{gr}}(M, N, s_p) &= -M(N-M+1)\lambda d + \frac{s_1 M}{N} \\
 &\quad - \left( s_2 - \frac{s_1^2}{N} \right) \frac{M(N-M)}{N^2(N-1)\lambda d} \\
 &\quad - \left( s_2 - \frac{s_1^2}{N} \right) s_1 \frac{M(N-M)(N-2M)}{N^4(N-1)(\lambda d)^2}
 \end{aligned}$$

$$+ \left( s_3 - \frac{s_1 s_2}{N} \right) \frac{M(N-M)(N-2M)}{N^3(N-1)(N-2)(\lambda d)^2}. \quad (28)$$

From Eq. (28) one can make several observations.

(1) For  $N = M$  the first two terms give the exact energy. This is seen by noting that  $N = M$  means that all levels are doubly occupied, i.e., there is only one state. Averaging Hamiltonian (1) over this state gives the exact energy of the system, which turns out to be equal to the first two terms in Eq. (28). Therefore, the remaining terms in the  $1/\lambda$  series for the ground-state energy are proportional to  $N - M$ .

(2) When  $N = 2M$ , all terms with even nonzero powers of  $1/\lambda$  vanish. This can be demonstrated, e.g., by writing the kinetic term in the BCS Hamiltonian (2) in terms of pseudospin operators (6)

$$H(\lambda = 0) = \sum_{i=1}^N 2\epsilon_i K_i^z + \frac{s_1}{2} \equiv H_0 + \frac{s_1}{2} \quad (29)$$

and noting that  $N = 2M$  correspond to the zero  $z$  projection of the total pseudospin. In this case, by Wigner-Eckart's theorem,<sup>22</sup>  $K_i^z$  has nonzero matrix elements only for transitions  $K \rightarrow K \pm 1$ , while matrix elements for transitions  $K \rightarrow K$  are equal to zero. The terms with even nonzero powers of  $1/\lambda$  vanish because they contain at least one matrix element of  $H_0$  from Eq. (29) between states with the same  $K$ . These terms are therefore proportional to  $N - 2M$ . Even terms also vanish when  $\epsilon_i$ 's are distributed symmetrically with respect to zero. Hence, they reflect an asymmetry in the distribution of  $\epsilon_i$ . For example, the ground-state energy for  $N = 2M$  and equidistant single-electron levels distributed symmetrically between  $\pm D = \pm(m - 1/2)d$  is

$$\begin{aligned}
 E_0^{2m} &= -Dm \left[ \lambda \frac{2m+2}{2m-1} + \frac{2m+1}{3(2m-1)\lambda} - \frac{16m^2+22m+7}{180(2m-1)^2\lambda^3} \right. \\
 &\quad \left. + \frac{128m^3+380m^2+344m+93}{7560(2m-1)^3\lambda^5} + O(1/\lambda^7) \right]. \quad (30)
 \end{aligned}$$

One can check that in the limit  $m \rightarrow \infty$  this expression reproduces the BCS result (5) for the ground-state energy up to terms of order  $1/\lambda^7$ , while for  $m = 1$  we recover Eq. (22). Note also that the case  $p = N$  in Eq. (27) does not seem to be problematic as at  $p = N$  the factors of  $1/(N-p)$  in Eqs. (28) and (30) are always compensated by a factor of  $(N-p)$  in the numerator of the corresponding term.

(3) Richardson's equations (3) remain invariant if single-electron levels  $\epsilon_k$  are shifted by  $\delta$  and parameters  $E_i$  are shifted by  $2\delta$ . The total energy  $E = \sum_{i=1}^M E_i$  then shifts by  $2M\delta$ . Note that this shift is entirely contained in the second term of expansion (28). Thus, the remaining combinations of  $s_k$  at each power of  $1/\lambda$  are "shiftless." For example,

$$s_2 - \frac{s_1^2}{N} \rightarrow s_2 + 2\delta s_1 + N\delta^2 - (s_1^2 + 2N\delta s_1 + N^2\delta^2)/N$$

$$= s_2 - \frac{s_1^2}{N}.$$

### B. Excited states

Let us now expand energies of low-lying excitations in  $1/\lambda$ . These expansions turn out to be analogous to that for the ground-state energy. We begin with the excitations that conserve the number of pairs and then turn to the simpler case of pair-breaking excitations.

It was demonstrated in Sec. II that for  $\lambda d > J$  lowest pair-conserving excitations correspond to total pseudospin  $K = N/2 - 1$  and total spin  $S = 0$ , where  $N$  is the total number of single-particle levels. The number of such states according to degeneracy formula (12) is  $N - 1$  and their energy is  $-\lambda d K(K + 1)$  according to Eq. (9). We also know from Sec. II that for these states one of the parameters  $E_i$  (say  $E_M$ ) remains finite as  $\lambda \rightarrow \infty$ , while all others diverge in this limit.

To distinguish  $E_M$  from the rest of parameters  $E_i$ , we denote it by  $\eta$ . Richardson's equations (3) read

$$-\frac{1}{\lambda d} + \sum_{j=1}^{M-1} \frac{2}{E_i - E_j} = \sum_{k=1}^N \frac{1}{E_i - 2\epsilon_k} - \frac{2}{E_i - \eta}, \quad i < M \quad (31)$$

$$-\frac{1}{\lambda d} - \sum_{j=1}^{M-1} \frac{2}{E_j - \eta} = \sum_{k=1}^N \frac{1}{\eta - 2\epsilon_k}, \quad i = M. \quad (32)$$

Expanding the left-hand side (LHS) of Eqs. (31) in  $2\epsilon_k/E_i$  and  $\eta/E_i$  and performing the same manipulations that lead to Eqs. (25) and (26) for the ground state, we obtain

$$\sum_{i=1}^{M-1} E_i = -(M-1)(N-M)\lambda d - \sum_{k=1}^{\infty} (s_k - 2\eta^k)\sigma_k, \quad (33)$$

$$-\frac{\sigma_p}{\lambda d} - \sum_{k=1}^p \sigma_{p-k+1}\sigma_k$$

$$= (N-p-2)\sigma_{p+1} + \sum_{j=1}^{\infty} (s_j - 2\eta^j)\sigma_{j+p+1}, \quad p \geq 0 \quad (34)$$

where now  $\sigma_p = \sum_{i=1}^{M-1} 1/E_i^p$ . We see that replacements

$$M \rightarrow M-1, \quad N \rightarrow N-2, \quad s_p \rightarrow s_p - 2\eta^p \quad (35)$$

transform Eqs. (33) and (34) into Eqs. (25) and (26) for the ground state. Thus, energies of the first  $N-1$  excited states are

$$E_{\text{pair}} = \sum_{i=1}^{M-1} E_i + E_M = E_{\text{gr}}(M-1, N-2, s_p - 2\eta^p) + \eta. \quad (36)$$

Let us also rewrite Eq. (32) for  $\eta$  as

$$\sum_{k=1}^N \frac{1}{\eta - 2\epsilon_k} = -\frac{1}{\lambda d} - 2\sigma_1 - 2\eta\sigma_2 - 2\eta^2\sigma_3 - \dots \quad (37)$$

One can see [by, e.g., sketching the LHS of Eq. (37)] that this equation has  $N-1$  roots with the  $k$ th root lying between  $2\epsilon_k$  and  $2\epsilon_{k+1}$ . To the lowest order in  $1/\lambda$  this equation reads

$$\sum_{k=1}^N \frac{1}{\eta_0 - 2\epsilon_k} = 0. \quad (38)$$

Equations (34) and (37) are to be solved iteratively order by order in  $1/\lambda$ . The procedure is similar to that for the ground state, e.g., recurrent relations analogous to Eq. (27) can also be derived. The only difference is that the coefficients at powers of  $1/\lambda$  now depend also on  $\eta_0$ , which has to be obtained from Eq. (38). For example, the excitation energies (36) to the first two orders in  $1/\lambda$  are

$$E_{\text{pair}} = -(M-1)(N-M)\lambda d + \frac{(s_1 - 2\eta_0)(M-1)}{N-2} + \eta_0, \quad (39)$$

$$E_{\text{pair}} - E_{\text{gr}} = N\lambda d + \eta_0(1 - 2f), \quad (40)$$

where

$$f = (M-1)/(N-1) \approx M/N \quad (41)$$

is the filling ratio.

Energies of higher excitations can be computed in the same way by solving 2,3,4, ... coupled equations of the type (38). For instance, energies of the next group of excited levels to the first two orders in  $1/\lambda$  are determined by solutions of the system

$$\sum_{k=1}^n \frac{1}{\eta_1 - 2\epsilon_k} = \frac{2}{\eta_1 - \eta_2}, \quad \sum_{k=1}^n \frac{1}{\eta_2 - 2\epsilon_k} = -\frac{2}{\eta_1 - \eta_2}.$$

Now let us consider pair-breaking excitations. For  $\lambda d > J$  low-energy excitations of this sort correspond to breaking a single pair of electrons thereby decreasing the number of pairs by 1 and the number of unblocked levels by 2. Let the single-electron levels occupied by two unpaired electrons have energies  $\epsilon_a$  and  $\epsilon_b$ . Since the lowest energy is achieved by having the unpaired electrons in a triplet state (recall that  $J > 0$  corresponds to the ferromagnetic exchange), the energy of lowest pair-breaking excitations according to Eq. (4) is

$$E_{\text{spin}} = \epsilon_a + \epsilon_b - 2J + E_{\text{gr}}(N-2, M-1, s_p - (2\epsilon_a)^p - (2\epsilon_b)^p). \quad (42)$$

Note that, unlike  $\eta$  in Eq. (36), single-electron energies  $\epsilon_a$  and  $\epsilon_b$  do not depend on  $\lambda$ . Therefore, to compute the energy of pair-breaking excitations we need only recursion relations (27) for the ground state with  $N' = N-2$ ,  $M' = M-1$ , and  $s'_p = s_p - \epsilon_a^p - \epsilon_b^p$ . In particular, to the first two orders in  $1/\lambda$  we get from Eq. (28)

$$E_{\text{spin}} = -(M-1)(N-M)g + \frac{(s_1 - 2\epsilon_a - 2\epsilon_b)(M-1)}{N-2} + \epsilon_a + \epsilon_b - 2J, \quad (43)$$

$$E_{\text{spin}} - E_{\text{gr}} \approx N\lambda d + (\epsilon_a + \epsilon_b)(1-2f) - 2J.$$

It is instructive to compare the above results with the BCS theory.<sup>9</sup> For this purpose let us write the energies of the pair-conserving excitations for large  $M$  and  $N$  up to the order  $1/\lambda$ .

$$E_{\text{pair}} - E_{\text{gr}} \approx 2D\lambda + \eta_k(1-2f) + \eta_k^2 \frac{f(1-f)}{D\lambda}, \quad (44)$$

where  $D = Nd$ ,  $f$  is the filling ratio (41), and  $\eta_k$  is the  $k$ th root of Eq. (37). In deriving the above equation from Eqs. (40) and (28) we shifted the single-electron levels so that  $\bar{\epsilon}_i = (\sum_{i=1}^N \epsilon_i)/N = 0$ . In BCS theory (i.e., in the limit  $N, M \rightarrow \infty$ ) pair-conserving excitation energies are<sup>10</sup>

$$2\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}, \quad (45)$$

where  $\mu$  is the chemical potential and  $\Delta$  is the gap. In the strong-coupling regime both  $\mu$  and  $\Delta$  are of order  $\lambda$ . Expanding the square root in expression (45) in small  $\epsilon_k$  up to  $\epsilon_k^2$ , we see that term (45) and relation (44) coincide to this order if we identify

$$\eta_k = 2\epsilon_k \quad \Delta = D\lambda \sqrt{4f(1-f)}, \quad \mu = (2f-1)D\lambda.$$

The first of these equations follows from Eq. (37) in the limit of large  $N$ , while the remaining two can be derived from the BCS equation for the gap and chemical potential (see, e.g., Ref. 10). Similarly one can check that pair-breaking excitations (42) correspond to two Bogoliubov quasiparticles with total energy

$$\sqrt{(\epsilon_a - \mu)^2 + \Delta^2} + \sqrt{(\epsilon_b - \mu)^2 + \Delta^2}. \quad (46)$$

Note that in the BCS limit the difference between pair-breaking and pair-conserving excitations disappears and expression (45) simply corresponds to two quasiparticles in a singlet state, each having the energy  $\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$ .

We have seen in Sec. II (see also Fig. 1) that in the strong-coupling limit many-particle energy levels of the BCS Hamiltonian (2) coalesce into narrow well-separated bands. Expression (44) can be used to estimate the ratio of the width of the first band,  $W_1$ , to the single-particle bandwidth  $D = Nd$ :

$$\frac{W_1}{D} \approx 2(1-2f) + \frac{f(1-f)}{\lambda}, \quad (47)$$

where  $W_1$  is the width. Note that at half filling,  $f = 1/2$ , the width of the first band goes to zero as  $\lambda \rightarrow \infty$ . In general, it follows from the Wigner-Eckart theorem<sup>22</sup> [see the discussion in item (2) under the ground-state formula (28)] that at half-filling widths of higher bands also vanish as  $\lambda \rightarrow \infty$ .

According to the BCS equations for the excitation energies (44) and (46) the gaps  $\Delta_{\text{spin}} = [E_{\text{spin}} - E_{\text{gr}}]_{\text{min}}$  and  $\Delta_{\text{pair}} = [E_{\text{pair}} - E_{\text{gr}}]_{\text{min}}$  for the two types of excitations coincide in the thermodynamical limit. We have also seen in Sec. II [see the discussion below degeneracy formula (12)] that when

$0 < J < \lambda d$  and  $J/(\lambda d)$  remains finite as  $\lambda \rightarrow \infty$ , spin-1 excitations have lower energy as compared to pair-conserving excitations. If, however,  $J \sim d$  or smaller, keeping  $J$  to the lowest order in  $1/\lambda$  in excitation energy (42) is not justified. In this case the two gaps are the same to this order. Therefore, it is interesting to set  $J = 0$  and evaluate the gaps to the next nonzero order.

Depending on the filling ratio  $f$  [see Eq. (41)] we can distinguish two different cases.

(1)  $f \neq 1/2$ . Lowest-lying excitations correspond to smallest or largest possible values of  $\eta_0$  and  $\epsilon_a + \epsilon_b$  depending on the sign of  $(1-2f)$ . To determine the maximal and minimal  $\eta_0$ , note that the  $k$ th root of Eq. (38) lies between  $2\epsilon_k$  and  $2\epsilon_{k+1}$ . If  $N$  is large and  $\epsilon_k - \epsilon_{k+1} \rightarrow 0$  as  $N \rightarrow \infty$ , the smallest and largest solutions of Eq. (38) are  $\eta_0^{\text{min}} \approx 2\epsilon_1$  and  $\eta_0^{\text{max}} \approx 2\epsilon_n$  respectively. We have from relations (40) and (43)

$$\Delta_{\text{spin}} - \Delta_{\text{pair}} = d|1-2f| > 0, \quad (48)$$

where we have used  $\epsilon_n - \epsilon_{n-1} \approx \epsilon_2 - \epsilon_1 \approx d$  and  $d$  is the mean level spacing.

(2)  $f = 1/2$ . To the first two orders in  $1/\lambda$ ,  $\Delta_{\text{spin}} - \Delta_{\text{pair}} = 0$ . In the next order we obtain from Eqs. (28), (36), and (42)

$$\Delta_{\text{pair}} - \Delta_{\text{spin}} = \frac{\eta_0^2 - 2\epsilon_a^2 - 2\epsilon_b^2}{2N\lambda d}, \quad (49)$$

where we shifted single electron levels so that  $\bar{\epsilon}_i = (\sum_{i=1}^N \epsilon_i)/N = 0$ . We show in the Appendix using Eq. (38) for  $\eta_0$  that the minimal value of  $\eta_0^2$  is always smaller than that of  $2(\epsilon_a^2 + \epsilon_b^2)$ . Therefore,  $\Delta_{\text{spin}} > \Delta_{\text{pair}}$ .

Thus, at  $J = 0$  the pair-breaking excitations always have a larger gap in the strong-coupling limit. Note that for  $\lambda = 0$  the situation is opposite as it always costs less energy to move one of the two electrons on the highest occupied single-electron levels to the next available level. Since according to BCS expression (5) the energy gap in the strong-coupling limit is  $2\Delta \approx 2D\lambda = N\lambda d$ , we see from Eq. (49) that at half-filling  $\Delta_{\text{pair}} - \Delta_{\text{spin}} \approx d^2/\Delta$ , i.e., the difference between the two gaps vanishes in the thermodynamical limit.

#### IV. CONCLUSION

We determined the spectrum of the universal Hamiltonian (1) in the strong superconducting coupling ( $\lambda \geq 1$ ) limit [Eqs. (9), (12), and (21)] and developed a systematic expansion in  $1/\lambda$  around this limit [Eqs. (27), (28), (36), and (42)] for the ground state and low-lying excitation energies. We detailed an algorithm by which these energies can be explicitly evaluated up to arbitrary high order in  $1/\lambda$  and estimated that the expansion converges for  $\lambda > \lambda_c$ , where  $\lambda_c$  lies between  $\lambda_{c1} \approx 1$  and  $\lambda_{c2} \approx 1/\pi$ . Technically, this expansion is based on the existence of the exact solution<sup>6</sup> of the BCS Hamiltonian (2). We found that in the strong-coupling limit Richardson parameters are zeros of appropriate Laguerre polynomials (21) and analyzed their behavior at large enough but finite  $\lambda$ .

We found that it is important to distinguish between two types of excitations in the problem: those that conserve the

total number of paired electrons and those that do not. We determined the energy gaps for both types and found that at zero spin-exchange constant,  $J=0$ , in contrast to the weak superconducting coupling limit, the gap for pair-breaking excitations is always larger [Eqs. (48) and (49)].

We believe there are two physically motivated questions within the scope of validity (see Ref. 3) of the universal Hamiltonian (1) that still need further clarification. The first problem is to develop a quantitative description of the crossover between a perturbed Fermi gas and the region of strong superconducting correlations (see Ref. 13 and the discussion in the beginning of Secs. II and III). The second problem is to study analytically the interplay between superconducting correlations and spin exchange (see, e.g., Ref. 23).

### APPENDIX

We show here using Eq. (38) for  $\eta_0$  that the minimal value of  $\eta_0^2$  is always smaller than that of  $2(\epsilon_a^2 + \epsilon_b^2)$ , i.e.,

$$x_0^2 < 2(a^2 + b^2), \quad (\text{A1})$$

where  $x_0$  is the smallest in the absolute value solution of [Eq. (38)],  $a$  and  $b$  are the two smallest in absolute value single-electron levels  $\epsilon_i$ , and  $|a| \leq |b|$ . Indeed, consider a function

$$g(x) = \sum_{k=1}^N \frac{1}{x - 2\epsilon_k}. \quad (\text{A2})$$

To prove relation (A1) we need to show that  $g(x)$  has a zero on the interval  $(-c, c)$ , where

$$c = \sqrt{2(a^2 + b^2)}.$$

For  $N=2$  there is only one zero,  $x_0 = \epsilon_1 + \epsilon_2$ , and relation (A1) clearly holds. Consider  $N > 2$ .

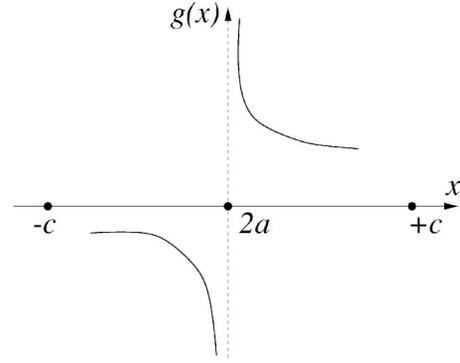


FIG. 2. A schematic plot of the function  $g(x) = \sum_{k=1}^N [1/(x - 2\epsilon_k)]$  on the interval from  $-c$  to  $c$ , where  $c = \sqrt{2(a^2 + b^2)}$ ,  $a$  and  $b$  are the two smallest in absolute value single-electron levels  $\epsilon_i$ , and  $|a| \leq |b|$ . Note that since  $2|b| > c$  there is only one pole on this interval. In the vicinity of  $2a$  we have  $g(x) \approx 1/(x - 2a)$  and therefore  $g(x)$  is positive on the immediate right of  $x = 2a$  and negative on the left.

First, note that  $g(x)$  has a single pole at  $x = a$  on this interval from  $-c$  to  $c$ , and  $g(a+) > 0$ , while  $g(a-) < 0$ . (See Fig. 2.) Hence, there is a zero between  $c$  and  $-c$  if either  $g(c) < 0$  or  $g(-c) > 0$ . To show that this is the case it is sufficient to demonstrate that  $g(c) - g(-c) < 0$ . We have

$$g(c) - g(-c) = \sum_{i=1}^N \frac{2c}{c^2 - 4\epsilon_i^2} = \sum_{\epsilon_i \neq a, b} \frac{2c}{c^2 - 4\epsilon_i^2},$$

which is indeed negative since  $c^2 < 4\epsilon_i^2$  for all  $\epsilon_i$  except  $\epsilon_i = a, b$ .

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