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Solving the Richardson equations close to the critical points

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Abstract

We study the Richardson equations close to the critical values of the pairing strength g_c, where the occurrence of divergences precludes numerical solutions. We derive a set of equations for determining the critical g values and the non-collapsing pair energies. Studying the behaviour of the solutions close to the critical points, we develop a procedure to solve numerically the Richardson equations for arbitrary coupling strength.

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1. Introduction

The exact solution of the BCS or pairing Hamiltonian was presented by Richardson in a series of papers beginning in 1963 [1, 2], just a few years after the seminal paper of Bardeen, Cooper and Schrieffer [3]. Despite the new avenues of research that it could have opened at this early stage in the development of the theory of superconductivity, the work passed almost unnoticed due to, perhaps, the technical difficulties in solving numerically the set of nonlinear equations for the spectral parameters. In recent year, the Richardson exact solution was rediscovered and applied successfully to ultrasmall metallic grains, where it was shown to be essential for the description of the soft crossover between superconductivity and the paring fluctuation regime as a function of the grain size [4]. Since then the Richardson model has been extended to a wide class of exactly-solvable models called the Richardson–Gaudin (RG) models with potential applications to several quantum many-body fermion and boson systems [5–8]. However, the numerical treatment of the exact solution for moderate to large size systems is still a cumbersome task in spite of the recent efforts to overcome this problem.

For the sake of clarity, let us begin by introducing the Richardson equations for an M-fermion pair system:

$$1 - 4g \sum_{j=1}^{L} \frac{d_j}{2\eta_j - e_\alpha} + 4g \sum_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{1}{e_\alpha - e_\beta} = 0, \tag{1}$$

where g is the pairing strength, η_j are a set of L parameters usually related to the single-particle energies, d_j are the effective degeneracies defined as $d_j = \nu_j/2 - \Omega_j/4$ with ν_j being the number of unpaired fermions in level j (seniority quantum number) and Ω_j the total degeneracy of the level j. e_α's are the M unknowns parameters called pair energies. Given the L parameters η_j, the L effective degeneracies d_j and a pairing strength g, the pair energies e_α are obtained by solving the set of M nonlinear equations (1). However, it is in general not easy to find a good initial guess that would lead directly to the appropriate solution. Instead, it is customary to begin with a given configuration in the weak coupling limit ($g \to 0$) where equations (1) can only be satisfied for $e_\alpha \to 2\eta_j$. The exact solution is then evolved step by step for increasing values of g up to the desired value [9]. In each step, one uses the solution obtained in the previous step as the input data for the numerical solver. Even if the procedure is successful, leading to the correct solution, it involves heavy numerical work. In most cases, this procedure is stopped due to the existence of singularities for some critical values g_c of the pairing strength. At $g = g_c$ a subset of pair energies e_α turn out to be equal to $2\eta_k$ for some k, giving rise to divergences in some terms of equation (1) [10]. Remarkably, these divergences cancel out and the corresponding solution (the set of e_α) is a continuous function of g in a neighbourhood of g_c. In fact, the solutions are always continuous for every value of g.

The existence of such critical points has significant consequences in the numerical solution of the equations which becomes unstable near g_c. Very slow convergence, no convergence at all or jumping to another solution are the typical problems found close to g_c. Moreover, there may be more than just one critical value in the real interval $[0, g]$, and we do not know *a priori* where g_c's are located. Those values are known only after one has already solved the equations for a large number of points surrounding g_c's and making some kind of interpolation afterward. Therefore, the localization of the critical values of g relies on heuristic procedures and is not based on any mathematical properties of the equations.

An alternative procedure to cross the critical region, based on a nonlinear transformation of the collapsing pair energies, was recently proposed [11]. However, this procedure is unable to predict the critical values of g.

In this paper, we will analyse the properties of the Richardson equations in the vicinity of critical g values. We will derive conditions that allow us to *a priori* determine all the critical values g_c associated with any 'single-particle level' η_j and provide the exact solution at these points. In addition, we will describe the asymptotic behaviour of the solution in the limit $g \to g_c$ and we will present an algorithm to solve the Richardson equations for values of g near any g_c.

2. Transforming the Richardson equations: the cluster equations

Our approach to deal with the singularities in equation (1) consists in transforming the system through a change of variables first suggested by Richardson [10] and later used by Rombouts *et al* [11] to develop a numerical algorithm for solving the equations near the critical points. We have already mentioned that for critical values of g some subset of the pair energies becomes equal to one of the values of $2\eta_k$. It can be shown [10] that the number of such pair energies is $M_k = 1 - 2d_k$. We can then characterize a critical point g_c by the condition $\lim_{g\to g_c} e_\alpha = 2\eta_k, \forall \alpha \in C_k$, where C_k stands for the subset of indices of the M_k pair energies that satisfy that limit, i.e. e_α's that cluster around the real point $2\eta_k$ in the complex plane for g near g_c (see [12] for a graphical representation of these clusters). Therefore, we will deal with two subsets of variables, the M_k e_α's with $\alpha \in C_k$ that give rise to the singularities and the remaining $(M - M_k)$ variables with $\alpha \notin C_k$, which behave smoothly close to g_c.

Consequently, we will separately treat the M_k Richardson equations with $\alpha \in C_k$ (the cluster equations):

$$1 - 4g\frac{d_k}{2\eta_k - e_\alpha} - 4g\sum_{\substack{j=1\\(j\neq k)}}^{L}\frac{d_j}{2\eta_j - e_\alpha} + 4g\sum_{\substack{\beta\in C_k\\(\beta\neq\alpha)}}\frac{1}{e_\alpha - e_\beta} + 4g\sum_{\beta\notin C_k}\frac{1}{e_\alpha - e_\beta} = 0. \tag{2}$$

The second and fourth terms of equation (2) diverge for $g \to g_c$ since $(2\eta_k - e_\alpha)$ and $(e_\alpha - e_\beta)$ go to zero. Moreover, these quantities must approach zero at the same rate in order to cancel out. To avoid the singularities we will multiply the cluster equations by $(2\eta_k - e_\alpha)^p$ (for some $p > 0$). With this in mind we will introduce a change of variables for the pair energies in the cluster (see [10, 11]):

$$S_p = \sum_{\alpha\in C_k}(2\eta_k - e_\alpha)^p \qquad \text{for} \quad p = 1, 2, \ldots, M_k. \tag{3}$$

This is an invertible transformation and, in principle, we can always recover e_α's for any arbitrary set of S_p. Keeping in mind that we have just M_k-independent variables S_p, we will extend the definition allowing p to be any positive integer or zero (note that $S_0 = M_k$). The variables S_p behave smoothly in the vicinity of g_c, they are real and, for $p > 0$, they satisfy $\lim_{g\to g_c} S_p = 0$.

In order to transform the cluster equations (2) we first multiply them by $(2\eta_k - e_\alpha)^p$, for a generic integer power p, and then sum the resulting equations over $\alpha \in C_k$:

$$\begin{aligned} S_p + 2g(p - (1 - M_k))S_{p-1} - 2g\sum_{i=0}^{p-1}S_{p-i-1}S_i - 4g\sum_{\substack{j=1\\(j\neq k)}}^{L}\sum_{\alpha\in C_k}\frac{d_j(2\eta_k - e_\alpha)^p}{2\eta_j - e_\alpha} \\ + 4g\sum_{\beta\notin C_k}\sum_{\alpha\in C_k}\frac{(2\eta_k - e_\alpha)^p}{e_\alpha - e_\beta} = 0. \end{aligned} \tag{4}$$

Note that the last two terms on the left-hand side of the equation cannot be easily rewritten in terms of S_p if we restrict to values of $p \leqslant M_k$. To overcome this limitation, we will make a series expansion of those terms, allowing p to be any integer. We are interested in the limiting behaviour of the solution close to g_c so that our reasoning will be valid in an interval $g \in (g_c - \delta, g_c + \delta)$ for some small enough radius $\delta > 0$. Taking into account that $(2\eta_k - e_\alpha)$ is infinitesimal at g_c and that e_β in equation (4) does not belong to the cluster, we have

$$\begin{aligned} \frac{1}{2\eta_j - e_\alpha} &= \frac{1}{2\eta_j - 2\eta_k}\sum_{n=0}^{\infty}\left(\frac{2\eta_k - e_\alpha}{2\eta_k - 2\eta_j}\right)^n, \\ \frac{1}{e_\alpha - e_\beta} &= \frac{1}{2\eta_k - e_\beta}\sum_{n=0}^{\infty}\left(\frac{2\eta_k - e_\alpha}{2\eta_k - e_\beta}\right)^n. \end{aligned} \tag{5}$$

These are absolutely (and rapidly) convergent geometric series, a property that will remain valid after a finite summation over α. Introducing equation (5) in equation (4) and making the summation over α we get for $p = 1$:

$$S_1 - 4gd_kM_k - 2g\left(M_k^2 - M_k\right) + 4g\sum_{n=0}^{\infty}S_{1+n}P_n = 0, \tag{6}$$

where $\{P_n\}$ is a set of coefficients that will be defined below. Taking in (6) the limit $g \to g_c$ the second and third terms must cancel out and one gets the cluster condition $M_k = 1 - 2d_k$. Similarly, for $p > 1$ we obtain:

$$S_p - 2g(M_k + 1 - p)S_{p-1} - 2g\sum_{i=1}^{p-2} S_{p-i-1}S_i + 4g\sum_{n=0}^{\infty} S_{p+n}P_n = 0 \qquad \text{for all} \quad p > 1. \quad (7)$$

The coefficients P_n appearing in (6) and (7) are defined as

$$P_n = \sum_{\substack{j=1 \\ (j\neq k)}}^{L} \frac{d_j}{(2\eta_k - 2\eta_j)^{n+1}} + \sum_{\beta\notin C_k} \frac{1}{(2\eta_k - e_\beta)^{n+1}}. \quad (8)$$

The infinite recurrence relation (7) is the fundamental equation of our formalism. In order to achieve our main goals we need to establish some important properties (lemmas 1 and 2) of the variables S_p and the series appearing in equations (6) and (7). It is easy to show that these series are bounded by their first element S_p through the condition

$$\left|\sum_{n=0}^{\infty} S_{p+n}P_n\right| \leqslant |S_p| D \frac{1}{1-x}, \quad (9)$$

where D is a positive bounded number involving η_j and e_β, and x is an upper bound for the absolute values of the geometric series ratios in equation (5) satisfying $\lim_{g\to g_c} x = 0$. On the other hand, we have that $|S_p| \leqslant \sum_{\alpha\in C_k} |2\eta_k - e_\alpha|^p$ with $(2\eta_k - e_\alpha) \to 0$ as $g \to g_c$. Therefore, we will assume in what follows that there is an integer number n_δ big enough such that we may disregard every term S_p (and related series) for $p > n_\delta$.

The next aspect we need to analyse is the order of the infinitesimal S_p in relation to the order of S_1. We will demonstrate that $S_1, S_2, S_3, \ldots, S_{M_k}$ are of the same order, implying that $\lim_{g\to g_c} S_p/S_1 = \chi_p \neq 0$ for $p \leqslant M_k$. On the other hand, S_p is of higher order than S_1 if $p > M_k$, that is $\lim_{g\to g_c} S_p/S_1 = 0$. In lemmas 1 and 2 we will demonstrate both assertions.

Lemma 1. *Assuming that* $(1 + 4gP_0) \neq 0$, *with* $g \in (g_c - \delta, g_c + \delta)$ *and* P_0 *defined in (8), the set* $\{S_2, S_3, \ldots, S_\mu\}$, *for some positive integer* μ *with* $2 \leqslant \mu \leqslant M_k$, *is infinitesimal of the same order as* S_1 *at* $g = g_c$. *In the general case* $\mu = M_k$.

Proof. Rearranging equation (7) we get

$$S_p = \frac{1}{(1+4gP_0)}\left[2g(M_k + 1 - p)S_{p-1} + 2g\sum_{i=1}^{p-2} S_{p-i-1}S_i - 4g\sum_{n=1}^{\infty} S_{p+n}P_n\right]. \quad (10)$$

To prove our statement we will apply this equation recursively starting with $p = 2$. In this case, we get

$$S_2 = \frac{2g(M_k - 1)}{(1+4gP_0)}S_1 - \frac{4g}{(1+4gP_0)}\sum_{n=1}^{\infty} S_{2+n}P_n,$$

so that S_2 is of the same order as S_1. In the next step we set $p = 3$ in equation (10), getting S_3 in terms of S_2 and S_p's with $p > 3$. Replacing S_2 with the value obtained previously and rearranging the resulting expression we get for S_3

$$S_3 = \frac{1}{(1+4gP_0)^2 + 8g^2P_1(M_k - 2)}\left[(2g)^2(M_k - 2)(M_k - 1)S_1 + 2g(1+4gP_0)S_1^2 - 4g\sum_{n=1}^{\infty}(2g(M_k - 2)P_{n+1} + (1+4gP_0)P_n)S_{3+n}\right],$$

from where we see that S_3 is of the same order as S_1. We can continue this process replacing in each step S_{p-1} in equation (10) for the expression computed in the previous step and solving again for S_p, getting for every $p > 2$ and $p \leqslant M_k$

$$S_p = B_p S_1 + \sum_{n=1}^{\infty} D_n^{(p)} S_{p+n} + \sum_{\substack{i,j \\ i+j<p}} X_{i,j}^{(p)} S_i S_j, \tag{11}$$

where the coefficients B_p, $D_n^{(p)}$ and $X_{i,j}^{(p)}$ can be calculated recursively. For intance, for the linear terms we have the recurrence relation

$$\begin{aligned} B_{p+1} &= \frac{2g(M_k - p)}{(1 + 4gP_0) - 2g(M_k - p)D_1^{(p)}} B_p, \\ D_n^{(p+1)} &= \frac{2g}{(1 + 4gP_0) - 2g(M_k - p)D_1^{(p)}} \left((M_k - p)D_{n+1}^{(p)} - 2P_n\right), \end{aligned} \tag{12}$$

starting with the known coefficiens for $p = 2$.

In this way we have shown that the local expansion of S_p has linear terms in S_1 and in S_{p+n} plus quadratic terms, thus we conclude that S_p is an infinitesimal of the same order as S_1 for $1 \leqslant p \leqslant M_k$.

Let us now consider what happens when p takes the value $M_k + 1$. In such a case the factor $(M_k + 1 - p)$ in equation (10) becomes zero and the chain of replacement is broken. The expansion of S_{M_k+1} has only linear terms of higher order and quadratic terms involving S_1. Therefore for $p > M_k$ there are no linear terms in S_1. We could have reached the same conclusion analysing the recurrence relation (12).

Finally and for the sake of completeness, let us mention that after replacing S_{p-1} in equation (10) the terms involving S_p on both sides of the equation might cancel out. It would be equivalent to the cancellation of the denominators in the recurrence relation (12). In such a case our process of replacement is interrupted and ends for $p = \mu < M_k$. □

So far, we have shown that first S_p's are of the same order as S_1. At the same time, it was suggested that S_p is of higher order if $p > M_k$. In the next lemma we will proof this statement.

Lemma 2. *The set of variables* $\{S_p\}$ *for* $p > M_k$ *are infinitesimal of higher order than* S_1 *at* $g = g_c$.

Proof. In this case we proceed in the reverse way as we have done in lemma 1. We will begin with an S_p for a large value of p and carry out the replacement in backward direction. Once again we start rewriting equation (7) to obtain

$$S_p = \frac{1}{(M_k - p)} \left[\frac{(1 + 4gP_0)}{2g} S_{p+1} + 2 \sum_{n=1}^{\infty} S_{p+1+n} P_n - \sum_{i=1}^{p-1} S_{p-i} S_i \right]. \tag{13}$$

We will now take, for $g \in (g_c - \delta, g_c + \delta)$, an integer number n_δ large enough such that we may disregard every term S_p for $p > n_\delta$. We start making $p = n_\delta$ in equation (13). After removing the negligible terms it leads us to

$$S_{n_\delta} = \frac{1}{(M_k - n_\delta)} \sum_{i=1}^{n_\delta - 1} S_{n_\delta - i} S_i.$$

In the second step we make $p = n_\delta - 1$ in equation (13) and replace the value of S_{n_δ} computed before. Repeating the same operation for $p = n_\delta - 2, n_\delta - 3, \ldots, M_k + 1$ and

replacing, in each case, the linear term for its value computed in the previous step, eventually we get the following quadratic expression for every $p > M_k$:

$$S_p = \sum_{\substack{i,j \\ i+j \geqslant p}} Y_{i,j}^{(p)} S_i S_j. \tag{14}$$

In this equation, the coefficients $Y_{i,j}^{(p)}$ can be calculated recursively and the indices i, j take values starting from 1 but keeping the condition $i + j \geqslant p$. As only quadratic terms are retained we conclude that S_p for $p > M_k$ are infinitesimal of higher order than $S_1, S_2, \ldots, S_{M_k}$. Note once again that the chain of replacement cannot be continued for $p \leqslant M_k$. □

So far we have shown some essential properties of the variables S_p and the related series that are required to develop our formalism. In the next section, we will derive the equations that allow us to calculate the values of g_c associated with any single-particle level η_k.

3. Critical values of g and the solution of the Richardson equations

In this section, we will derive a set of equations suitable to compute all the values of g_c for any single-particle level η_k. Furthermore, we will obtain, at the same time, the solution of the Richardson equation at g_c, namely, the values of the unknowns e_β for $\beta \notin C_k$, assuming that the variables in the cluster reach their limiting value $e_\alpha = 2\eta_k$ ($e_\alpha \in C_k$). We summarize our results in the following theorem:

Theorem 1. *All critical g values of the Richardson equations (1) associated with the single-particle level η_k and the corresponding values of the non-collapsing pair energies e_β ($\beta \notin C_k$) are the solutions of the following system of equations:*

$$\begin{vmatrix} (1+4gP_0) & 4gP_1 & 4gP_2 & \cdots & 4gP_{M_k-1} \\ -2g(M_k-1) & (1+4gP_0) & 4gP_1 & \cdots & 4gP_{M_k-2} \\ 0 & -2g(M_k-2) & (1+4gP_0) & \cdots & 4gP_{M_k-3} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & -2g & (1+4gP_0) \end{vmatrix} = 0, \tag{15a}$$

$$1 - 4g \sum_{j=1}^{L} \frac{d_j}{2\eta_j - e_\alpha} + 4gM_k \frac{1}{e_\alpha - 2\eta_k} + 4g \sum_{\substack{\beta \notin C_k \\ (\beta \neq \alpha)}} \frac{1}{e_\alpha - e_\beta} = 0 \qquad \text{for all} \quad \alpha \notin C_k. \tag{15b}$$

Proof. Let us consider the transformed Richardson equations according to the change of variables defined in equation (3). This system is formed by the $(M - M_k)$ Richardson equations (1) for $\alpha \notin C_k$ together with equation (6) and the subset of equations (7) for $p = 2, 3, \ldots, M_k$. It is a set of M-independent equations equivalent to the original ones. In fact, we can consider the unknowns $S_1, S_2, \ldots, S_{M_k}$ as independent variables together with $\{e_\beta\}$ for $\beta \notin C_k$. The variables $\{e_\alpha\}$ for $\alpha \in C_k$, that still appear in the equations, and S_p for $p > M_k$ are formally functions of $S_1, S_2, \ldots, S_{M_k}$ computable through the inverse of transformation (3). At this point we are ready to analyse the M_k cluster equations (6 and 7 for $p \leqslant M_k$) in the limit $g \to g_c$, keeping the lower order terms. According to lemmas 1 and 2 we can discard terms with $p > M_k$ and terms involving the products $S_i S_j$, since they are of

higher order than $S_1, S_2, \ldots, S_{M_k}$, thus we get the system of equations

$$\begin{cases} (1+4gP_0)S_1 + 4gP_1S_2 + 4gP_2S_3 + \cdots + 4gP_{M_k-1}S_{M_k} = 0 \\ -2g(M_k-1)S_1 + (1+4gP_0)S_2 + 4gP_1S_3 + \cdots + 4gP_{M_k-2}S_{M_k} = 0 \\ -2g(M_k-2)S_2 + (1+4gP_0)S_3 + \cdots + 4gP_{M_k-3}S_{M_k} = 0 \\ \cdots \qquad\qquad\qquad \cdots \\ -2gS_{M_k-1} + (1+4gP_0)S_{M_k} = 0. \end{cases} \tag{16}$$

This is a linear homogeneous system with the trivial solution $S_1 = 0, S_2 = 0, \ldots, S_{M_k} = 0$, and indeed the variables S_p vanish for $g = g_c$. Since we are looking for nontrivial solutions that are continuous functions of g also valid in the vicinity of g_c where $S_p \neq 0$, the condition for such solutions to exist is the cancellation of the determinant of the linear system (shown in equation (15*a*)). As the coefficients of the system are functions of the variables e_α not belonging to the cluster, we have to resort to the $(M - M_k)$ remaining Richardson equations (1) with $\alpha \notin C_k$. After realizing the limit $g \to g_c$, we obtain the system of equations (15) introduced by the theorem. □

As we have already stated, the numerical solutions of the nonlinear system of equations (15) provide all the critical values g_c for the single-particle level η_k that has been previously selected. In addition, for each solution, we get the complete set of pairs energies e_α defining the wavefunction of the quantum many-body system.

With respect to the possible complex g_c solutions, they may be still interpreted as critical values for non-Hermitian integrable Hamiltonians, but we will not analyse these cases in the present paper.

Once we have the numerical solution of equations (15) we can use the values of g_c and e_α's ($\alpha \notin C_k$) to compute the coefficients of the homogeneous linear system (16). Solving this linear system yields (after normalizing to $S_1 = 1$) the limit ratio $\chi_p = \lim_{g\to g_c} \frac{S_p}{S_1}$. As $S_p = 0$ at $g = g_c$ for all $p \geqslant 1$, we can obtain from equations (16) the derivatives

$$\chi_p = \left.\frac{\mathrm{d}S_p}{\mathrm{d}S_1}\right|_{g=g_c}. \tag{17}$$

4. Solving the Richardson equations near g_c

So far we have shown how to compute the solution at $g = g_c$. We will now derive a method to approach the solution at a value g_0 close to the critical point g_c. The main issue in the numerical solution of the Richardson equations is to determine a good initial guess for the pair energies, specially in the vicinity of g_c, where the equations become unstable. With that initial guess, the solution at $g = g_0$ is obtained with standard numerical techniques. Once we have the solution for this specific value g_0, we can reach a more distant value of g, by increasing (or decreasing) g, step by step, using the solution of the previous step as the starting guess for the next one.

An appropriate set of starting values at $g_0 = g_c + \delta g$ can be obtained by means of a linear approximation for the parameters S_p and e_α:

$$\begin{aligned} &S_1(g_0) \approx \left(\frac{\mathrm{d}S_1}{\mathrm{d}g}\right)_{g=g_c} \delta g, \qquad S_p(g_0) \approx \left(\frac{\mathrm{d}S_1}{\mathrm{d}g}\right)_{g=g_c} \chi_p\, \delta g \quad (p > 1), \\ &e_\alpha(g_0) \approx e_\alpha(g_c) + \left(\frac{\mathrm{d}e_\alpha}{\mathrm{d}g}\right)_{g=g_c} \delta g \quad (\alpha \notin C_k), \end{aligned} \tag{18}$$

these approximate values will be the initial guess to solve the Richardson equations.

In order to determine the derivative dS_1/dg at $g = g_c$, we will consider up to second-order terms in equations (6) and (7) and substitute the variables S_p in terms of the quadratic expression $S_p \approx \chi_p S_1 + a_p S_1^2$, where $\chi_p = 0$ for $p > M_k$, $\chi_1 = 1$ and $a_1 = 0$. From equation (14) we can see that S_p has quadratic terms in S_1 only for $p \leqslant 2M_k$, while for greater values of p the order in S_1 is higher due to the condition $i + j \geqslant p$. Therefore, we will retain just the first $2M_k$ variables S_p and deal with a system of $2M_k$ equations. Computing the derivative with respect to g of the resulting system, and after making some simple algebraic manipulations, we get for $p = 1$

$$4g \sum_{n=1}^{2M_k} [(\chi_n + a_n S_1) P'_{n-1} + (a_n P_{n-1}) S'_1] = \frac{1}{g} \tag{19}$$

and for $1 < p \leqslant 2M_k$

$$S'_1 \left[a_p - 2g(M_k + 1 - p) a_{p-1} - 2g \sum_{i=1}^{p-2} (\chi_{p-i-1} \chi_i) \right] + 4g \sum_{n=0}^{2M_k - p} [(\chi_{n+p} + a_{n+p} S_1) P'_n + a_{n+p} P_n S'_1] = \frac{\chi_p + a_p S_1}{g}, \tag{20}$$

where the primes stand for the derivatives with respect to g and, according to definition (8), we have

$$P'_n = \sum_{\beta \notin C_k} \frac{(n+1)}{(2\eta_k - e_\beta)^{n+2}} \left(\frac{de_\beta}{dg} \right). \tag{21}$$

Taking the limit $g \to g_c$ and reordering the equations in a convenient way, we obtain

$$\left(-\frac{1}{g_c} + 4g_c \sum_{n=1}^{M_k} \chi_n P'_{n-1} \right) + \sum_{n=2}^{2M_k} (4P_{n-1})(a_n S'_1) = 0, \tag{22}$$

for $p = 1$, and

$$\left(-\frac{\chi_p}{g_c} - 2g_c S'_1 \sum_{i=1}^{p-2} (\chi_{p-i-1} \chi_i) + 4g_c \sum_{n=0}^{M_k - p} \chi_{n+p} P'_n \right) - 2g_c (M_k + 1 - p) a_{p-1} S'_1 + (1 + 4g_c P_0) a_p S'_1 + \sum_{j=p+1}^{2M_k} (4g_c P_{j-p})(a_j S'_1) = 0, \tag{23}$$

for $1 < p \leqslant 2M_k$. This is a non-homogeneous system of $2M_k$ equations with a set of $2M_k + (M - M_k)$ unknowns: $S'_1, a_2, a_3, \ldots, a_{2M_k}$ joined with the derivatives (de_β/dg), for $\beta \notin C_k$.

The system of equations (23) is nonlinear because of the products $a_j S'_1$. However, we can obtain a linear system for the derivatives with a unique solution by defining a matrix $\mathbf{B}$ as

$$B_{p,1} = \left(-\frac{\chi_p}{g_c} - 2g_c S'_1 \sum_{i=1}^{p-2} (\chi_{p-i-1} \chi_i) + 4g_c \sum_{n=0}^{M_k - p} \chi_{n+p} P'_n \right),$$

$$B_{p,p-1} = -2g_c (M_k + 1 - p), \qquad B_{p,p} = (1 + 4g_c P_0) \qquad (p > 1),$$

$$B_{p,j} = 4g_c P_{j-p} \qquad (j > p), \qquad B_{p,j} = 0 \qquad (1 < j < p - 1),$$

and the non-null vector $\mathbf{v}$ as

$$\mathbf{v} = \left(1, a_2 \frac{dS_1}{dg}, a_3 \frac{dS_1}{dg}, \ldots, a_{2M_k} \frac{dS_1}{dg} \right).$$

Using these definitions, equations (23) can be rewritten as

$$\mathbf{B}\cdot\mathbf{v}=\mathbf{0},$$

such that the following condition must be satisfied:

$$\det(\mathbf{B})=0. \tag{24}$$

Since the derivatives appear just in the first column of the matrix $\mathbf{B}$, (24) is a linear equation in $\frac{\mathrm{d}S_1}{\mathrm{d}g}$ and in the $(M-M_k)$ derivatives $\frac{\mathrm{d}e_\beta}{\mathrm{d}g}$ (for $\beta\notin C_k$) that does not include the unknown coefficients a_p. A set of $(M-M_k)$ equations is required to complete the system. In order to get the necessary equations we will compute the derivatives of the Richardson equations out of the cluster:

$$1-4g\sum_{j=1}^{L}\frac{d_j}{2\eta_j-e_\alpha}+4g\sum_{\substack{\beta\notin C_k\\(\beta\neq\alpha)}}\frac{1}{e_\alpha-e_\beta}+4g\sum_{\beta\in C_k}\frac{1}{e_\alpha-e_\beta}=0\qquad(\alpha\notin C_k). \tag{25}$$

Expanding the last term in the variables S_p, we obtain

$$1-4g\sum_{j=1}^{L}\frac{d_j}{2\eta_j-e_\alpha}+4g\sum_{\substack{\beta\notin C_k\\(\beta\neq\alpha)}}\frac{1}{e_\alpha-e_\beta}-4g\sum_{n=0}^{\infty}\frac{1}{(2\eta_k-e_\alpha)^{n+1}}S_n=0. \tag{26}$$

Computing the derivative with respect to g and taking the limit $g\to g_c$, we finally get

$$\begin{aligned}-\frac{1}{g_c}-4g_c\sum_{j=1}^{L}\frac{d_j}{(2\eta_j-e_\alpha)^2}\left(\frac{\mathrm{d}e_\alpha}{\mathrm{d}g}\right)_{g=g_c}&\\+4g_c\sum_{\substack{\beta\notin C_k\\(\beta\neq\alpha)}}\frac{1}{(e_\alpha-e_\beta)^2}\left(\frac{\mathrm{d}e_\beta}{\mathrm{d}g}-\frac{\mathrm{d}e_\alpha}{\mathrm{d}g}\right)_{g=g_c}-4g_c\frac{M_k}{(2\eta_k-e_\alpha)^2}\left(\frac{\mathrm{d}e_\alpha}{\mathrm{d}g}\right)_{g=g_c}&\\-4g_c\left(\sum_{n=1}^{M_k}\frac{\chi_n}{(2\eta_k-e_\alpha)^{n+1}}\right)\frac{\mathrm{d}S_1}{\mathrm{d}g}=0\qquad(\alpha\notin C_k).&\end{aligned} \tag{27}$$

Equations (24) and (27) constitute a non-homogeneous linear system with a unique solution for the desire derivatives.

5. A numerical example: fermions in a two-dimensional lattice

In this section, we will apply our formalism to a pairing model of fermions in a 2D square lattice of $N\times N$ sites with periodic boundary conditions. This example was previously treated in [5] for the ground state with a repulsive pairing interaction ($g>0$). We will now analyse the model using the methodology developed here, focusing on the critical g values and in the behaviour of the solutions in their vicinities.

We will consider a 6×6 lattice with 36 fermions (half filling, $M=18$). The pairing Hamiltonian in momentum space is

$$H_P=\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+\frac{g}{2}\sum_{\substack{\mathbf{k}\\\mathbf{k}'}}a^\dagger_{\mathbf{k}}a^\dagger_{\bar{\mathbf{k}}}a_{\bar{\mathbf{k}}'}a_{\mathbf{k}'},$$

where $\mathbf{k}\equiv[k_x,k_y]$ and $\varepsilon_{\mathbf{k}}=-2[\cos(k_x)+\cos(k_y)]=\eta_{\mathbf{k}}$, and $\bar{\mathbf{k}}$ is the time reversal of $\mathbf{k}$. The single fermion energies ε_j and the corresponding degeneracies Ω_j for the 6×6 lattice are displayed in table 1. In the limit $g=0$, the ground state is obtained by distributing the $M=18$ pairs in the lowest possible states. In this numerical example, we will work within

Table 1. Single fermion energies and degeneracies for the 6×6 lattice.

j	1	2	3	4	5	6	7	8	9
ε_j	−4	−3	−2	−1	0	1	2	3	4
Ω_j	2	8	8	8	20	8	8	8	2

Table 2. First critical g values for the cluster collapsing at $2\varepsilon_4 = -2$.

g_c	Energy
−0.038 4565	−47.6184
−0.039 1412	−49.5405
−0.039 4719	−53.3549
−0.040 4240	−55.5262
−0.041 2922	−57.4106
−0.041 3245	−62.5795

Table 3. Critical g values for the ground state

	$2\varepsilon_4 = -2$	$2\varepsilon_3 = -4$	$2\varepsilon_2 = -6$	$2\varepsilon_1 = -8$
g_c (negative)	−0.041 3245	−0.063 5021	−0.087 7434	−0.131 927
g_c (positive)	0.598 232	0.240 579	0.170 878	–

the fully paired subspace containing the ground state ($v_j = 0, d_j = -\Omega_j/4$). Consequently, the excited states to which we will refer to in this example are within the seniority 0 subspace.

We will begin solving the system of equations (15) for a specific single-particle level, for instance, $j = 4$ and $\varepsilon_4 = -1$ (see table 1). The degeneracy of this level is 8 and the number of pair energies in the cluster that collapses at $2\varepsilon_4 = -2$ is given by the cluster condition $M_4 = 1 - 2d_4 = 5$, one more than the value allowed by the Pauli exclusion principle. The solution of the system (15) provides all the information concerning the many-body state at each specific critical value of g. In table 2 we show, for $j = 4$, the first negative g_c's together with the corresponding energy eigenvalues.

A different kind of analysis is presented in table 3, where we show the first critical g values for the ground state. In this case, the clusters collapse at different single-particle levels for each g_c as indicated. All the clusters are formed by five pair energies except for $j = 1$ where $M_1 = 3$. In order to have a global vision of the results in figure 1 we show the real part of the pair energies for the ground-state solution of the Richardson equations (1) for positive and negative g values. The full lines are the pair energies e_α and the horizontal dotted lines correspond to $2\varepsilon_j$. The critical points of table 3 can be seen in the figure at the crossing point of each cluster with twice the corresponding single-particle energy.

The solutions near the critical points g_c were obtained following the approach described in section 4. With the solution for the first g_c next to $g = 0$ (negative or positive depending on the case), i.e e_β for $\beta \notin C_k$ and value of g_c itself, we solve the linear system of equations (24) and (27) to obtain the derivatives $(\mathrm{d}S_1/\mathrm{d}g)$ and $(\mathrm{d}e_\beta/\mathrm{d}g)$ at the critical point. In addition, we solve the linear system (16) to get the coefficients χ_p. With all this information we determine a good initial guess at some g_0 near g_c by means of the linear approximation (18). Next we solve the Richardson equations at g_0, a process that rapidly converges to an accurate numerical solution. With the solution at g_0 as a starting point we move to the next value of $g = g_0 + \Delta g$. Proceeding in this way and updating the starting values at each step we compute all the desired points in the curves. We repeat the process for each critical g. The pair energies obtained from the solutions for $g \approx 0$ smoothly connect with those obtained near the first g_c. The same smooth behaviour is observed between two consecutive critical values.

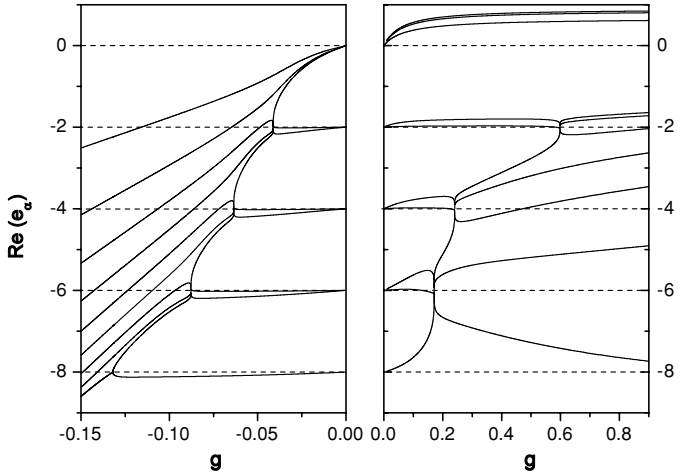

Figure 1. Real part of the pair energies e_α for attractive ($g < 0$) and repulsive ($g > 0$) pairing in a 6×6 lattice.

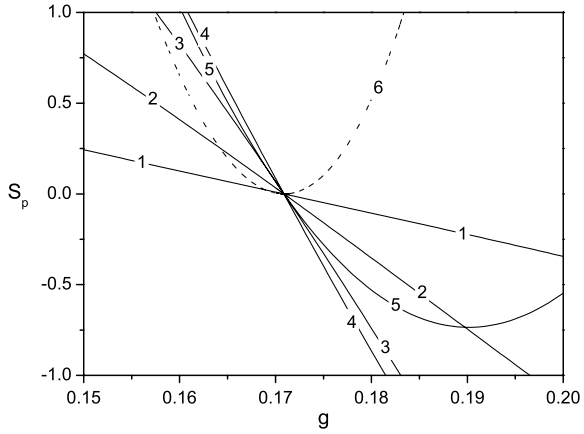

Figure 2. Variables S_p close to the collapse at $g_c = 0.170\,878$. The first five S_p's are displayed by solid lines while S_6 is shown by the dashed line.

The good quality of the initial guess near g_c is due to the smooth behaviour of the variables S_p and e_β ($\beta \notin C_k$) that allows us to use the linear approximation (18). For e_β's this fact can be appreciated in figure 1. In figure 2, we show a graphical representation of the first S_p's in a range of g around $g_c = 0.170\,878$ corresponding to the collapse at the single-particle level $j = 2$, $2\varepsilon_2 = -6$, of a cluster of $M_2 = 5$ pair energies. We can we see in the figure the linearity of S_p's for $1 \leqslant p \leqslant 5$ confirming that S_p is an infinitesimal of the same order as S_1 for $2 \leqslant p \leqslant M_2$. In addition, we have plotted the results for S_6, which clearly shows that it is an infinitesimal of a higher order.

6. Conclusions

In this work, we have studied the solution of the Richardson equations close to the critical values of the coupling constant g. We have derived a set of well-behaved equations to determine

the actual critical values g_c associated with any single-particle energy ε_k and the complete set of pair energies defining the exact eigenstate of the system. In addition, we studied the behaviour of the solutions close to the critical points, obtaining a linear approximation for the pair energies that serves as a good initial guess in the critical region. With this formalism, one can solve numerically the Richardson equations around the critical points, overcoming the numerical instabilities that usually arise. The knowledge of the critical values of the coupling constant greatly simplifies the numerical treatment of the equations. To illustrate the formalism, we have analysed the pairing Hamiltonian in a 6×6 square lattice at half filling for repulsive and attractive pairing strength. Making use of our approach we have located g_c's for the ground state and several excited states in the seniority 0 subspace. The numerical solution between consecutive values of g_c's can be easily carried out by solving the original Richardson equations (1). With this new approach we hope to be able to solve exactly large systems with arbitrary single-particle energies and degeneracies.

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