Solving the Richardson equations for Fermions

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Forty years ago Richardson showed that the eigenstates of the pairing Hamiltonian with constant interaction strength can be calculated by solving a set of non-linear coupled equations. However, in the case of Fermions these equations lead to singularities which made them very hard to solve. This letter explains how these singularities can be avoided through a change of variables making the Fermionic pairing problem numerically solvable for arbitrary single particle energies and degeneracies.

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Introduction

Exactly solvable models serve as a guideline for understanding the properties of correlated many-body systems. Already in the sixties, Richardson solved the eigenvalue problem of a constant pairing interaction in a set non-degenerate single-particle levels for Fermion [1] and Boson [2] systems. However, it turned out that in the Fermion case the solutions exhibit singularities which are hard to treat numerically [3, 4]. Recently, exactly solvable pairing models have gained new attention [5], with applications to nanometric grains [6] (for a review see [7]), Bose Einstein Condensates [8] and nuclear physics [9]. It was first shown that the pairing model with non-uniform matrix elements [12] were presented. Giving rise to a large class of pairing Hamiltonians with applications to nanometric grains [7], Bose Einstein Condensates [8] and nuclear physics [9]. It was first shown that the pairing model was integrable by finding the complete set of commuting integrals of motions [10], and subsequently, three new families of fully integrable and exactly solvable models [11] giving rise to a large class of pairing Hamiltonians with non-uniform matrix elements [12] were presented. These models are exactly solvable, except for the singularities occurring in Fermion systems for some critical values of the pairing strength. This problem, in spite of some early attempts to cure it [13, 14], precluded for over forty years the use of these exactly solvable models for a wide range of applications, ranging from condensed matter to nuclear physics. Moreover, the recent developed extensions of the exact solution to pairing Hamiltonians including the isospin degree of freedom (O(5) pairing) [15] with promising applications to N ~ Z nuclei and high Tc superconductivity, suffer from the same kind of singularities.

In this letter show how the Richardson equations can be solved numerically, avoiding the singularities, through an appropriate change of variables. This procedure provides a fast an accurate way to solve the equations for a constant pairing interaction. The method can be applied as well to more general exactly solvable Hamiltonians associated with a coupled set of non-linear equations of the Richardson type.

The exactly solvable pairing Hamiltonian has the following form:

$$H = \sum_{j,m} e_j a_j^\dagger a_j - \frac{g}{4} \sum_{j,m,j',m'} a_j^\dagger a_{j'}^\dagger a_{j'} a_j$$

with $e_j$ any set of single-particle energies and $g$ the pairing interaction strength. The $N$-pair eigenstates of this Hamiltonian have the form

$$\prod_{\alpha=1}^N \left[ \sum_{j,m} \frac{1}{2e_j - x_\alpha} a_j^\dagger a_j \right] |0\rangle,$$

where $|0\rangle$ is a state without paired particles (a Racah quasiparticle vacuum state, |16⟩). The corresponding energy $E\{\{x\}\}$ is given by

$$E\{\{x\}\} = \langle 0|H|0 \rangle + \sum_\alpha x_\alpha.$$

The complex variables $x_\alpha$ can be found by solving a set of non-linear equations:

$$\sum_j \frac{d_j}{2e_j - x_\alpha} + \sum_{\beta=1, \beta \neq \alpha}^N \frac{1}{x_\beta - x_\alpha} + \frac{1}{2g} = 0,$$

for $\alpha = 1, \ldots, N$. The parameters $d_j$ depend on the level degeneracies and on the structure of the vacuum state |0⟩. For Fermions, $d_j = \frac{\nu_j - \Omega_j}{2}$, where $\Omega_j$ is the pair degeneracy (for the nuclear shell model $\Omega_j = j + 1/2$), and $\nu_j$ is the seniority of the level $j$. Note that $d_j \leq 0$ because of the Pauli principle. Solving this set of nonlinear equations solves the eigenproblem for the pairing Hamiltonian Eq. [11]. Unfortunately, the algebraic solution becomes numerically unstable at certain critical values of the interaction strength [3, 4]. This is caused by singularities in the first and second terms in Eq. [16], when some of the variables $x_\alpha$ are approaching the value $2e_j$. One can understand this from the electromagnetic analogy for the exactly solvable pairing model [17]: in the Fermion case, the single-particle levels $e_j$ and the variables $x_\alpha$ correspond to opposite charges. Therefore a group of variables can cluster around a single-particle level in such a...
is evolved adiabatically up to the desired interaction weak-interaction limit (see below). Then this solution starts from an approximate solution in the case of multiply degenerate levels (see below for the singularity. No general solution method was known until now. Figure 1 illustrates the behavior of the variables in the region around different single-particle levels. By solving the equations for each cluster separately, one can obtain a solution for the whole system iteratively. A practical way to organize the clusters, is to link each variable to its nearest single-particle level $2\epsilon_k$, and to consider a cluster for each level that has variables around it.

The question now is how to solve the equations for each cluster, particularly in the case of singularities. Let us consider the set of indices $C_k$ of the $N_k$ variables that cluster around a level $2\epsilon_k$. Then one can consider the equations

$$\frac{d_{\alpha}}{2\epsilon_k - x_\alpha} + \sum_{\beta \in C_k, \beta \neq \alpha} \frac{1}{x_\beta - x_\alpha} + F_k(x_\alpha) = 0, \quad \forall \alpha \in C_k,$$

with

$$F_k(x) = \frac{1}{2g} + \sum_{\beta, \beta \neq k} \frac{d_j}{2\epsilon_j - x} + \sum_{\beta, \beta \notin C_k} \frac{1}{x_\beta - x}.$$

The function $F_k(x)$ describes the influence of the other levels and the variables of the other clusters on the variables in the cluster $C_k$. Because of the way the clusters are set up, the function $F_k(x)$ will be a smooth function in the region around $\epsilon_k$ where the variables of the cluster are located. The singularities will occur in the first two terms of Eq. (5). In the case that some of the variables in the cluster approach the value $2\epsilon_k$, the divergences in the first and the second term of Eq. (5) must cancel out. Multiplying Eq. (5) by $2\epsilon_k - x_\alpha$, and summing over the $n_k$ variables $x_\alpha$ at the singular point, leads to the condition

$$n_k = -2d_k + 1,$$

with $n_k$ the number of variables that actually converge to $2\epsilon_k$. For Fermions the value $(-2d_k)$ corresponds to the pair degeneracy of the level $\epsilon_k$; because of the Pauli principle, no more Fermion pairs can occupy the level. Trying to put more pairs in that level results in a singularity. In fact, the structure of the ground state Eq. (2) does not result in a forbidden occupation of the level. However, on expanding the wave function of Eq. (2) in terms of the pair creation operators $a_{\beta \rho}^\dagger a_{\beta \rho}^\dagger$, one finds that the leading term cancels out because of the Fermionic anti-commutation rules. This translates into the numerical difficulties encountered in the solution of the equations. For Bosons $d_k > 0$, and hence Eq. (5) shows that singularities do not occur in the Bosonic case. This can also be understood from the electrostatic analogy: Boson pairs and single-particle levels have charges of the same sign. Therefore the variables try to avoid each other at all times, and singularities do not occur.

The above procedure suggests a way to remove the singularities from the equations: multiplying Eq. (5) with $(2\epsilon_k - x_\alpha)^p$, for some power $p$, and summing over all variables $x_\alpha$ in the cluster. The resulting equations become, for $p > 1$:

$$(d_k + N_k - \frac{p}{2}) S_{p-1} + \frac{1}{2} \sum_{k=2}^{p-1} S_{k-1} S_{p-k} + R_p = 0,$$
with
\[ S_p = \sum_{\alpha \in C_k} (2e_k - x_\alpha)^p \]
\[ R_p = \sum_{\alpha \in C_k} (2e_k - x_\alpha)^p F_k(x_\alpha). \]

The compact form of Eq. (8) suggests that it might be advantageous to solve them for the new variables \( S_p \) instead of the original variables \( x_\alpha \). Note that given a set of variables \( S_1, \ldots, S_{N_k} \), one can easily construct the polynomial whose roots correspond to the values \( 2e_k - x_\alpha \). Hence one can switch from one set of variables to the other. The problem comes with the quantities \( R_p \): these are functions of the \( x_\alpha \), and it is not straightforward to express them as functions of the \( S_p \). However, for a given set of variables \( x_\alpha \), one can easily evaluate the values \( S_p \) and \( R_p \). Furthermore, one can obtain the gradient matrix \( G \), with \( G_{lm} \) the derivative with respect to \( S_m \) of Eq. (5) for \( p = l + 1 \),

\[ G = G^S + G^R, \]

where
\[ G^S_{lm} = \begin{cases} \frac{d_k + N_k - \frac{l+1}{2}}{S_{l-m}}, & \text{for } m = l \\ S_{l-m}, & \text{for } m < l \\ 0, & \text{for } m > l \end{cases} \]
\[ G^R_{lm} = \frac{dR_{l+1}}{dS_m} = \sum_{\alpha \in C_k} \frac{dR_{l+1}}{dx_\alpha} \frac{dx_\alpha}{dS_m}, \]

for \( l, m = 1, \ldots, N_k \). \( G^R \) can be evaluated accurately using a special inversion algorithm for Vandermonde matrices [19]. Therefore one can solve the new set of equations, Eq. (8) for \( p = 2, \ldots, N_k + 1 \), in the new variables \( S_1, \ldots, S_{N_k} \) using a standard gradient technique such as the multi-dimensional Newton-Raphson method [20]. However, in the case of a singularity, the gradient matrix becomes ill-conditioned: the diagonal elements of the gradient matrix are given by

\[ G^S_{ll} = d_k + N_k - \frac{l+1}{2}, \]

for \( l = 1, \ldots, N_k \). The diagonal element will vanish for the index \( l_s = 2(d_k + N_k) - 1 \). This will occur as soon as \( N_k \geq -2d_k + 1 \), which matches the value for which singularities can occur, see Eq. (7). In such a case the lower-triangular matrix \( G^S \) becomes singular. The other part of the gradient matrix, \( G^R \), is derived from the smooth function \( F_k \). A series expansion of \( F_k(x) \) in \( x \) will be dominated by the lowest orders. Therefore the elements of \( G^R_{lm} \) are very small for larger values of \( m \). As a result, the value of \( S_1 \) can not be determined accurately from the set of equations Eq. (5). One can avoid this problem by limiting the cluster sizes to at most the critical value \( N_k = n_k = -2d_k + 1 \), and by using \( gS_{-1} \) as an unknown variable instead of \( S_{N_k} \). If more variables are found near to the same single-particle level, one can always divide the cluster into smaller, well-separated clusters, because at most \( n_k \) of the variables can approach the single-particle level closely. Knowing \( S_{-1} \) and \( S_1, \ldots, S_{N_k-1} \), one can still straightforwardly construct the polynomial whose roots give the corresponding values \( x_\alpha \). Therefore one can easily switch between the two sets of variables. Furthermore \( gS_{-1} \) behaves smoothly, even at a singularity. To set up an efficient gradient method, it is useful to replace Eq. (5) for the last value, \( p = N_k + 1 \), by a similar equation obtained using \( p = 0 \):

\[ d_k gS_{-1} + gR_0 = 0, \]

with \( R_0 = \sum_{\alpha \in C_k} F_k(x_\alpha) \).

For weak interaction strengths the function \( F_k(x_\alpha) \) is dominated by the constant term \( \frac{1}{2g} \), see Eq. (9). In the weak interaction limit one can take \( F_k \) to be a constant. The resulting functions \( R_p \) take the simple form

\[ R_p = \frac{S_p}{2g} \]

Now the equations Eq. (5) and Eq. (15) can be solved straightforwardly to yield the variables \( S_1 \), from which one can construct the polynomial that gives a unique set of variables \( x_\alpha \). The resulting eigenstate will depend on the size of the cluster for each of the single-particle levels. This establishes a one-to-one correlation between the eigenstates of the non-interacting system \((g = 0)\) and the eigenstates of the weakly-interacting system. One can conclude that the Richardson equations are complete: their solutions generate all eigenstates, and there are no spurious solutions.

One can obtain the solutions for strong interaction strengths by solving the weakly interacting case first, and then gradually increasing the interaction strength. At each step one can use the gradient method outlined above in order to update the solution to the new interaction strength. It is useful to adapt the stepsize in interaction strength to the convergence of the iterative procedure by taking smaller steps in \( g \) when the convergence of the Newton-Raphson method for the variables \( S_1 \) becomes slower, which typically occurs around the critical \( g \) values. One more ingredient is needed to avoid problems with the singularities: when the interaction strength passes through a critical value, the variables \( x_\alpha \) passing through a singularity can change from real to complex or vice versa. At the same time the variables \( S_1 \) will become very small, except for \( l = -1 \). Even using the new variables, the gradient method does not lead to the right solution when it has to pass through critical values of the interaction strength. One can avoid this problem by including an extrapolation step based upon the previous solutions. This extrapolation has to be done in the variables \( S_1 \), because they vary smoothly through the singularities and they remain real all the time. Assume that converged solutions \( x_\alpha' \) and \( x_\alpha'' \) were obtained for values \( g' \) and \( g'' \) of the interaction strength. The variables \( x_\alpha '' \) are grouped into clusters. For each cluster, one evaluates...
the variables $S_p'$ and $S_p''$. Because the variables $S_p$ behave smoothly, even near a singularity, one can estimate the variables $S_p$ for the new interaction strength $g$ by linear extrapolation:

$$S_p = \frac{(g - g')S_p'' - (g - g'')S_p'}{g'' - g'} \tag{17}$$

The resulting values of $S_p$ can then be updated using the Newton-Raphson method or another gradient method. The extrapolation step avoids the problems with the singularities and greatly improves the convergence of the method.

As an example, consider the level scheme listed in Table I, together with a constant pairing interaction. This model describes neutrons in $^{56}$Fe; its ground state and finite-temperature properties have been studied using a Quantum Monte Carlo method [21]. The eigenstates can also be found through the solution of Richardson’s equations, Eq.(4), or through Lanczos diagonalization in a seniority basis [22]. The full many-body space has a dimension of the order of $10^{15}$, while the zero-seniority basis has dimension 14894. In Fig. 2, the lowest zero-seniority eigenvalues for this model are shown as a function of the interaction strength, calculated using the Lanczos method and using the method explained above (only 50 Lanczos iterations were used). To calculate the ground state, a straightforward implementation of the Newton-Raphson method for the original equations, Eq.(4), works well up to an interaction strength of $g \approx 0.2$. It turns out that a singularity occurs around the $1d_{3/2}$ level at a value of $g = 0.245$. A Fortran-95 computer program was written based upon the procedure outlined above. It was able to solve the equations for all interaction strengths in a matter of seconds. Figure 3 shows the behavior of the three $x$ variables that cluster around the $1d_{3/2}$ level. Variables $x_4$ and $x_5$ are complex conjugates, $x_6$ is real over the whole range of $g$ values.

**TABLE I: Woods-Saxon single-particle levels [21].**

| level      | energy  | degeneracy | pair occupation | seniority |
|------------|---------|------------|-----------------|-----------|
| $1d_{3/2}$ | -21.5607| 3          | 3               | 0         |
| $1d_{3/2}$ | -19.6359| 2          | 2               | 0         |
| $1f_{7/2}$ | -19.1840| 1          | 1               | 0         |
| $1f_{7/2}$ | -10.4576| 4          | 4               | 0         |
| $2p_{3/2}$ | -8.4804 | 2          | 1               | 0         |
| $1f_{5/2}$ | -7.7003 | 3          | 0               | 0         |
| $2p_{1/2}$ | -7.6512 | 1          | 0               | 0         |
| $3s_{1/2}$ | -0.3861 | 1          | 0               | 0         |
| $2d_{5/2}$ | 0.2225  | 3          | 0               | 0         |
| $1g_{9/2}$ | 0.5631  | 5          | 0               | 0         |

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FIG. 4: Smooth behavior of the new variables near the $2d_{3/2}$ singularity.

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