PHYSICAL REVIEW C **69**, 061303(R) (2004)

Solving the Richardson equations for fermions

S. Rombouts and D. Van Neck
Universiteit Gent, Vakgroep Subatomaire en Stralingsfysica, Proeftuinstraat 86, B-9000 Gent, Belgium

J. Dukelsky
Instituto de Estructura de la Materia, CSIC, Serrano 123, 28006 Madrid, Spain
(Received 18 December 2003; published 11 June 2004)

Forty years ago Richardson showed that the eigenstates of the pairing Hamiltonian with constant interaction strength can be calculated by solving a set of nonlinear coupled equations. However, in the case of fermions these equations lead to singularities which made them very hard to solve. This paper 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.

DOI: 10.1103/PhysRevC.69.061303 PACS number(s): 21.60.−n, 71.10.Li, 74.20.Fg, 02.30.Ik

Exactly solvable models serve as a guideline for understanding the properties of correlated many-body systems. Already in the 1960s, Richardson solved the eigenproblem of a constant pairing interaction in a set nondegenerate 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 nanometallic grains [6] (for a review see Ref. [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 $N \sim Z$ nuclei and high-T_c superconductivity, suffer from the same kind of singularities.

This paper show how the Richardson equations can be solved numerically, avoiding the singularities, through an appropriate change of variables. This procedure provides a fast and 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 nonlinear equations of the Richardson type.

The exactly solvable pairing Hamiltonian has the following form:

$$H = \sum_{j,m} e_j a^\dagger_{jm} a_{jm} - \frac{g}{4} \sum_{j,m,j',m'} a^\dagger_{jm} a^\dagger_{j\bar{m}} a_{j'\bar{m}'} a_{j'm'} \qquad (1)$$

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

$$\prod_{\alpha=1}^{N} \left[\sum_{j,m} \frac{1}{2e_j - x_\alpha} a^\dagger_{jm} a^\dagger_{j\bar{m}} \right] |0\rangle, \qquad (2)$$

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

$$E(\{x\}) = \langle 0|H|0\rangle + \sum_\alpha x_\alpha. \qquad (3)$$

The complex variables x_α can be found by solving a set of nonlinear equations:

$$\sum_j \frac{d_j}{2e_j - x_\alpha} + \sum_{\beta=1,\beta\neq\alpha}^{N} \frac{1}{x_\beta - x_\alpha} + \frac{1}{2g} = 0, \qquad (4)$$

for $\alpha = 1, \ldots, N$. The parameters d_j depend on the level degeneracies and on the structure of the vacuum state $|0\rangle$. For Fermions, $d_j = \nu_j - \Omega_j/2$, where Ω_j is the pair degeneracy (for the nuclear shell model $\Omega_j = j + 1/2$), and ν_j is the seniority of the level j. Note that $d_j \leqslant 0$ because of the Pauli principle. Solving this set of nonlinear equations solves the eigenproblem for the pairing Hamiltonian, Eq. (1). 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. (4), when some of the variables x_α 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_α correspond to opposite charges. Therefore a group of variables can cluster around a single-particle level in such a way that for each of the variables the repulsive charge of the other variables is compensated for by the attractive charge of the single-particle level. These singularities occur for fermions in double or multiple degenerate levels. In the case of doubly degenerate equidistant levels these singularities can be handled for the ground state [13], but the problem arises again in the treatment of the excited states [18]. In previous

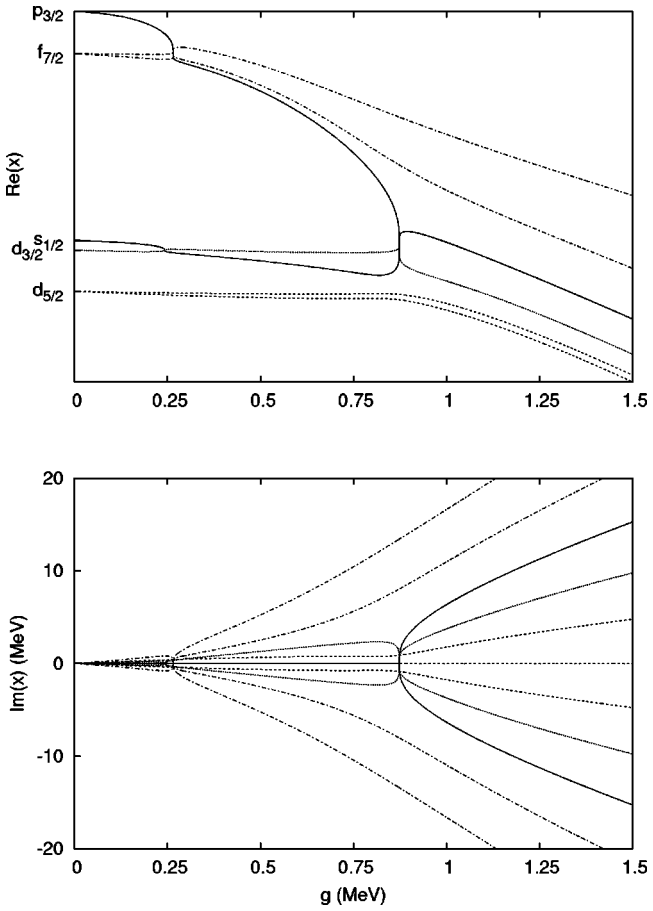

FIG. 1. Real and imaginary part of the variables x_α for the model described in the text.

calculations it was necessary to tune the solutions by hand as soon as they approach a singularity. No general solution method was known until now. Figure 1 illustrates the behavior of the variables in case of multiply degenerate levels (see below for the details of the model).

A general approach to solve the Richardson equations Eq. (4), starts from an approximate solution in the weak-interaction limit (see below). Then this solution is evolved adiabatically up to the desired interaction strength by gradually increasing the value of g. At each step in g, the previous solution has to be updated. For dealing with the singularities, it is useful to note first that the variables x_α in Eq. (4) are most sensitive to the other variables nearby. Therefore one can divide the set of variables x_α into several *clusters* of variables, grouped 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 $2e_j$, 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 $2e_k$. Then one can consider the equations

$$\frac{d_k}{2e_k - x_\alpha} + \sum_{\beta \in C_k, \beta \neq \alpha} \frac{1}{x_\beta - x_\alpha} + F_k(x_\alpha) = 0, \quad \forall\, \alpha \in C_k, \tag{5}$$

with

$$F_k(x) = \frac{1}{2g} + \sum_{j, j \neq k} \frac{d_j}{2e_j - x} + \sum_{\beta, \beta \notin C_k} \frac{1}{x_\beta - x}. \tag{6}$$

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 e_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 $2e_k$, the divergences in the first and the second term of Eq. (5) must cancel out. Multiplying Eq. (5) by $2e_k - x_\alpha$, and summing over the n_k variables x_α at the singular point, leads to the condition

$$n_k = -2d_k + 1 \tag{7}$$

with n_k the number of variables that actually converge to $2e_k$. For fermions the value $(-2d_k)$ corresponds to the pair degeneracy of the level e_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 $a^\dagger_{jm} a^\dagger_{j\bar{m}}$, one finds that the leading term cancels out because of the Fermionic anticommutation rules. This translates into the numerical difficulties encountered in the solution of the equations. For bosons $d_k > 0$, and hence Eq. (7) 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 $(2e_k - x_\alpha)^p$, for some power p, and summing over all variables x_α in the cluster. The resulting equations become, for $p > 1$:

$$\left(d_k + N_k - \frac{p}{2}\right) S_{p-1} + \frac{1}{2} \sum_{k=2}^{p-1} S_{k-1} S_{p-k} + R_p = 0 \tag{8}$$

with

$$S_p = \sum_{\alpha \in C_k} (2e_k - x_\alpha)^p \tag{9}$$

$$R_p = \sum_{\alpha \in C_k} (2e_k - x_\alpha)^p F_k(x_\alpha). \tag{10}$$

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_α. Note that given a set of variables $S_1, \ldots, S_{N_k}$, one can easily construct the polynomial whose

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

Level	Energy e_j(MeV)	Degeneracy Ω_j	Pair occupation (Ground state)	Seniority ν_j
$1d_{5/2}$	−21.5607	3	3	0
$1d_{3/2}$	−19.6359	2	2	0
$2s_{1/2}$	−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

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_α, and it is not straightforward to express them as functions of the S_p. However, for a given set of variables x_α, one can easily evaluate the values S_p and R_p. Furthermore, one can evaluate the gradient matrix G, with G_{lm} the derivative with respect to S_m of Eq. (8) for $p=l+1$,

$$G = G^S + G^R, \tag{11}$$

where

$$G^S_{lm} = \begin{cases} d_k + N_k - \dfrac{l+1}{2}, & \text{for} \quad m = l \\ S_{l-m}, & \text{for} \quad m < l \\ 0, & \text{for} \quad m > l \end{cases} \tag{12}$$

$$G^R_{lm} = \frac{dR_{l+1}}{dS_m} = \sum_{\alpha \in C_k} \frac{dR_{l+1}}{dx_\alpha} \frac{dx_\alpha}{dS_m} \tag{13}$$

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 multidimensional 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

$$G^S_{ll} = d_k + N_k - \frac{l+1}{2} \tag{14}$$

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 $N_k \geqslant -2d_k+1$, 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_{l_s} cannot be determined accurately from the set of equations, Eq. (8). 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_α. 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. (8) for the last value, $p=N_k+1$, by a similar equation obtained using $p=0$:

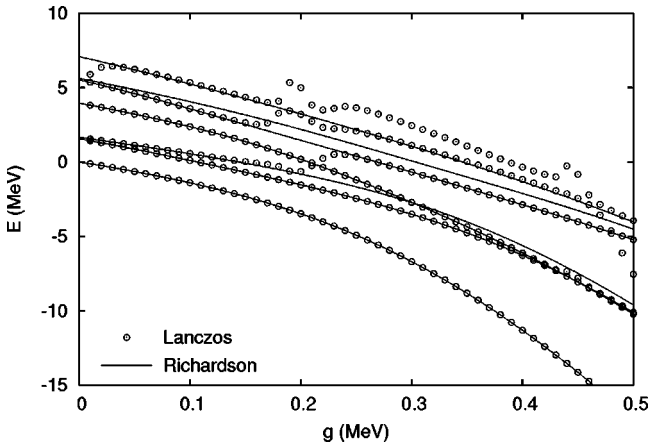

FIG. 2. Lanczos and Richardson results for the energies of the lowest zero-seniority states, relative to the non-interacting ground-state energy.

$$d_k g S_{-1} + g R_0 = 0 \tag{15}$$

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

For weak-interaction strengths the function $F_k(x_\alpha)$ is dominated by the constant term $1/2g$, see Eq. (6). In the weak-interaction limit one can take F_k to be a constant. The resulting functions R_p take the simple form

$$R_p = \frac{S_p}{2g}. \tag{16}$$

Now the equations, Eqs. (8) and (15), can be solved straightforwardly to yield the variables S_l, from which one can construct the polynomial that gives a unique set of variables x_α. 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 noninteracting 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 first case, 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_i 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_α passing through a singularity can change from real to complex or vice versa. At the same time the variables S_l 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_l, because they vary smoothly through the singularities and they remain real all the time. Assume that converged solutions x'_α and x''_α were obtained for values g' and g'' of the interaction strength. The variables x''_α 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 diagonalisation 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 14 894. 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 $g \simeq 0.2$. 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 as a function of g. In Fig. 4 one can see that the corresponding variables S_l behave much more smoothly. More singularities occur around other levels at higher interaction strengths, as is shown in Fig. 1. The solution of the Richardson equations is faster than the Lanczos method and requires much less computer memory. It is accurate for *all* eigenstates, not just for the lowest lying eigenvalues. Moreover, the procedure can deal with much larger systems, well beyond the limits of large-scale exact diagonalizations: our largest run sofar for a system with multiply degenerate levels has been for 100 pairs distributed over 40 levels. The limiting factor is the size of the pair clusters around one single-particle level, which is directly related to the degeneracy of the levels. The present implementation (in 64-bit precision) becomes unstable when clusters get as large as 60–80 pairs. The reason is that switching from the S to the x variables requires finding all roots of a polynomial equation with high enough accuracy.

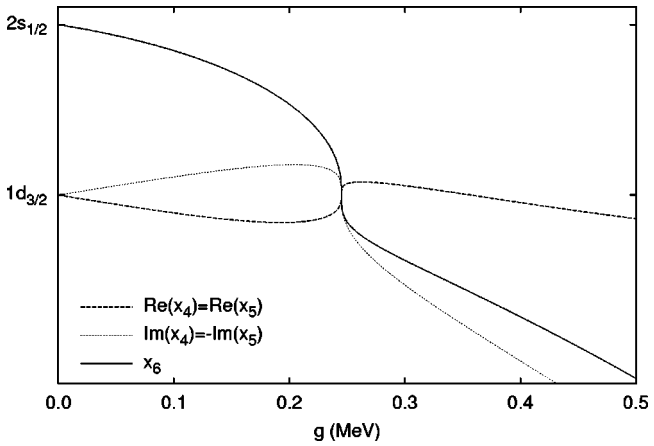

FIG. 3. Behavior of the variables near the singularity around the $2d_{3/2}$ level. Variables x_4 and x_5 are complex conjugates, x_6 is real over the whole range of g values.

This work shows that the exactly solvable pairing models are indeed solvable in practice, even for fermions with multiple degeneracies. It opens up a whole new range of applications for these models. Furthermore, similar techniques might be useful to solve the nonlinear equations for other exactly-solvable pairing and spin models [11,15,23,24].

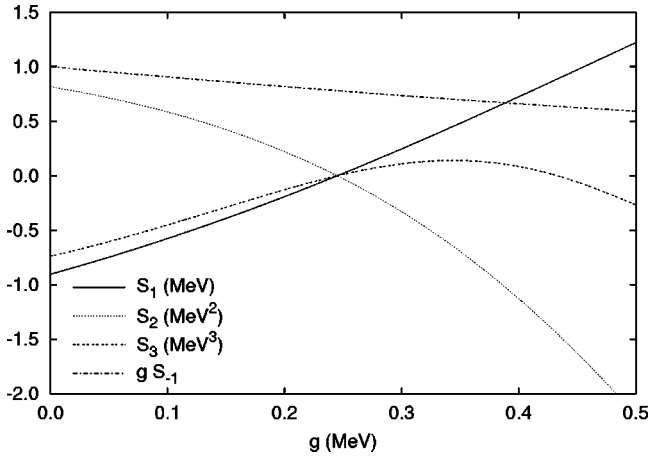

FIG. 4. Smooth behavior of the new variables near the $2d_{3/2}$ singularity.

We wish to thank R. Richardson, S. Pittel, J. Draayer, F. Pan, and K. Heyde for the interesting discussions and suggestions. This work was supported by the Fund for Scientific Research - Flanders (Belgium), the Research Board of Ghent University and by the Spanish DGI Grant No. BFM2003-05316-C02-02.

[1] R. W. Richardson, Phys. Lett. **3**, 277 (1963); R. W. Richardson and N. Sherman, Nucl. Phys. **52**, 221 (1964).
[2] R. W. Richardson, J. Math. Phys. **9**, 1327 (1968).
[3] R. W. Richardson and N. Sherman, Nucl. Phys. **52**, 253 (1964).
[4] R. W. Richardson, J. Math. Phys. **6**, 1034 (1965).
[5] M. Heritier, Nature (London) **414**, 6859 (2001).
[6] G. Sierra, J. Dukelsky, G. G. Dussel, J. von Delft, and F. Braun, Phys. Rev. B **61**, R11890 (2000).
[7] J. von Delft and D. C. Ralph, Phys. Rep. **345**, 61 (2001).
[8] J. Dukelsky and P. Schuck, Phys. Rev. Lett. **86**, 4207 (2001).
[9] J. Dukelsky and S. Pittel, Phys. Rev. Lett. **86**, 4791 (2001); J. Dukelsky, C. Esebbag, and S. Pittel, *ibid.* **88**, 062501 (2002); M. Hasegawa and K. Kaneko, Phys. Rev. C **67**, 024304 (2003).
[10] M. C. Cambiaggio, A. M. F. Rivas, and M. Saraceno, Nucl. Phys. **A624**, 157 (1997).
[11] J. Dukelsky, C. Esebbag, and P. Schuck, Phys. Rev. Lett. **87**, 066403 (2001).
[12] J. Dukelsky, J. M. Román, and G. Sierra, Phys. Rev. Lett. **90**, 249803 (2003).
[13] R. W. Richardson, Phys. Rev. **141**, 949 (1966).
[14] M. Hasegawa and S. Tazaki, Phys. Rev. C **35**, 1508 (1987).
[15] F. Pan and J. P. Draayer, Phys. Rev. C **66**, 044314 (2002); J. Links, H.-Q. Zhou, M. D. Gould, and R. H. McKenzie, J. Phys. A **35**, 6459 (2002).
[16] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, Berlin, 1980), Chap. 6.
[17] J. Dukelsky, C. Esebbag, and S. Pittel, Phys. Rev. Lett. **88**, 062501 (2002).
[18] J. M. Román, G. Sierra, and J. Dukelsky, Phys. Rev. B **67**, 064510 (2003).
[19] G. H. Golub and C. F. Van Loan, *Matrix Computations* (The Johns Hopkins University Press, London, 1989), Chap. 4.
[20] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in Fortran* (Cambridge University Press, Cambridge, 1992), Chap. 9.
[21] S. Rombouts, K. Heyde, and N. Jachowicz, Phys. Rev. C **58**, 3295 (1998).
[22] A. Volya, B. A. Brown, and V. Zelevinsky, Phys. Lett. B **509**, 37 (2001).
[23] F. Pan, J. P. Draayer, and W. E. Ormand, Phys. Lett. B **422**, 1 (1998).
[24] A. Dhar and B. S. Shastry, Phys. Rev. Lett. **85**, 2813 (2000).