Exact solution of the orbit-dependent pairing Hamiltonian

1999 J. Phys. A: Math. Gen. 32 1065

(http://iopscience.iop.org/0305-4470/32/6/016)

J. Phys. A: Math. Gen. **32** (1999) 1065–1072. Printed in the UK PII: S0305-4470(99)98916-3

Exact solution of the orbit-dependent pairing Hamiltonian

Feng Pan† and J P Draayer

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA

Received 3 November 1998

Abstract. An infinite-dimensional algebraic approach is introduced to derive exact particle-number conserving solutions of the nuclear mean-field plus orbit-dependent pairing Hamiltonian. As an example, exact solutions of a model Hamiltonian for ds-shell nuclei are compared with shell-model and equal strength pairing calculations for $^{18-26}$O isotopes.

1. Introduction

Pairing, in addition to the quadrupole–quadrupole interaction, is an important interaction in nuclear physics. The concept was proposed by Racah as a seniority scheme in atomic physics [1]. Its physical significance was first realized in superconductivity studies [2]. Following the suggestions of Bohr *et al* [3], the first detailed application of pairing to nuclei was made by Belyaev [4]. The concept has since been applied to other phenomena: high T_c superconductivity [5, 6], applications using the Hubbard model [7], and pairing phenomena in liquids [8] and metal clusters [9].

In nuclear physics applications, mean-field approximations are usually supplemented with residual interactions, the short-range pairing interaction being the one most commonly used. In this case, the problem is usually handled approximately by using Bardeen–Cooper–Schrieffer (BCS) or Hartree–Fock–Bogolyubov (HFB) methods, sometimes in conjunction with correction terms evaluated within the random-phase approximation. However, when BCS or HFB methods are applied to nuclei there are some serious drawbacks. First of all, not only is the number of nucleons in a nucleus typically small, the number of valence particles ($n \sim 10$) which dominate the behaviour of low-lying states is too few to support the underlying assumptions of the approximations, specifically, $\delta n/n$ is not negligible. As a result, particle-number-nonconservation effects enter and can lead to serious difficulties, such as spurious states, nonorthogonal solutions, etc. Furthermore, an essential feature of pairing correlations are differences between neighbouring even and odd mass nuclei, which are driven mainly by Pauli blocking. It is difficult to treat even–odd differences with these methods because different quasi-particle bases must be introduced for different blocked levels. Another problem with approximate treatments of the pairing Hamiltonian is related to the fact that both the BCS and the HFB approximations break down for an important class of physical situations. A remedy in terms of particle number projection techniques complicates the algorithms considerably, and does not help to achieve a better description of the higher-excited part of the spectrum of the pairing Hamiltonian. For these reasons, a particle-number-conserving method for handling the

† On leave from the Department of Physics, Liaoning Normal University, Dalian 116029, People's Republic of China.

0305-4470/99/061065+08$19.50

pairing problem, when feasible, even if only approximate, is an appropriate way to probe the true nature of pairing effects in nuclei. Over the past few years some progress has been made in the development of better algorithms that bypass the Bogolyubov transformation and are thus free from problems related to particle number nonconservation. For instance, a particle-number-conserving method for treating the pairing problem for well-deformed nuclei was put forward in [10]. The method uses a configuration-energy truncation scheme and takes the strength of the pairing interaction to be the same for all orbitals. Unfortunately, because of the deformation, each orbital can only accommodate a single pair of particles and this limits the applicability of the theory. Very recently, a Fock-space diagonalization of the pairing Hamiltonian, also for deformed nuclei, was proposed that used some symmetry properties and a many-body Fock-space basis cut-off [11].

In the following, we will propose a new particle-number conserving method for the pairing problem. In this paper, we will mainly emphasize mathematical formalism. Further applications of this method to realistic nuclear pairing problems will be discussed elsewhere.

2. Separable strength pairing Hamiltonian

The general pairing Hamiltonian for spherical nuclei can be written as

$$\hat{H} = \sum_{jm} \varepsilon_j a^\dagger_{jm} a_{jm} - \sum_{jj'} c_{jj'} S^+(j) S^-(j') \tag{1}$$

where the ε_j are single-particle energies and $S^\pm(j)$ and $S^0(j)$ are the pairing operators for a single-j shell defined by

$$\begin{aligned} S^+(j) &= \sum_{m>0} (-)^{j-m} a^\dagger_{jm} a^\dagger_{j-m} \\ S^-(j) &= \sum_{m>0} (-)^{j-m} a_{j-m} a_{jm} \\ S^0(j) &= \tfrac{1}{2} \sum_{m>0} (a^\dagger_{jm} a_{jm} + a^\dagger_{j-m} a_{j-m} - 1) = \tfrac{1}{2}(\hat{N}_j - \Omega_j). \end{aligned} \tag{2}$$

In (2), $\Omega_j \equiv j + \frac{1}{2}$ is the maximum number of pairs in the jth shell, $\hat{N}_j$ is the particle number operator for the jth shell, and $c_{jj'}$ is the strength of the pairing interaction between the j and j' shells.

In general, for k pairs, Hamiltonian (1) can be diagonalized in bases states that are products of the single-j shell pairing wavefunctions:

$$|k\rangle = \sum_{k_i} B_{k_1 k_2 \cdots k_p} S^{+k_1}(j_1) S^{+k_2}(j_2) S^{+k_3}(j_3) \ldots S^{+k_p}(j_p)|0\rangle \tag{3}$$

where the summation is restricted by

$$\sum_{i=1}^{p} k_i = k \tag{4}$$

p is the total number of orbitals, the $B_{k_1 k_2 \cdots k_p}$ are expansion coefficients that need to be determined, and $|0\rangle$ is the pairing vacuum state which satisfies the condition

$$S^-(j)|0\rangle = 0 \qquad \text{for all} \quad j. \tag{5}$$

Though simple to formulate, this problem is algebraically intractable because there are no analytic expressions or recursion relations for determining the $B_{k_1 k_2 \cdots k_p}$ coefficients. Furthermore, the number of single j-shell basis vectors included in (3) has to be fixed on a case-by-case basis because of the Pauli principle.

As an approximation to the general theory, we assume a separable strength pairing (SSP) interaction, $c_{jj'} = c_j c_{j'}^*$. Though strong, this assumption is physically motivated because it links the pair–pair interaction strength to the individual pair formation probability. In this case, $|c_j|^2/\sum_{j'}|c_{j'}|^2$ gives the percentage of single-j shell pairing in the Hamiltonian. Furthermore, it is expected to be better than the equal strength pairing approximation for which $c_{jj'} = |G|$ for all orbitals. The equal strength pairing (ESP) approximation has been commonly used in many applications because it is much simpler than the general case.

To diagonalize the SSP Hamiltonian, we need to introduce the following two-parameter algebra generated by $\{S_{mn}^{\mu};\ \mu = 0, +, -;\ m, n = 0,\ 1,\ 2, \ldots\}$ with

$$\begin{aligned} S_{mn}^{+} &= \sum_j \varepsilon_j^m |c_j|^{2n} c_j S^{+}(j) \\ S_{mn}^{-} &= \sum_j \varepsilon_j^m |c_j|^{2n} c_j^* S^{-}(j) \\ S_{mn}^{0} &= \sum_j \varepsilon_j^m |c_j|^{2n} S^{0}(j). \end{aligned} \tag{6}$$

It is easy to show that these generators satisfy the following commutation relations:

$$\begin{aligned} [S_{mn}^{+}, S_{m'n'}^{-}] &= 2S_{m+m'n+n'+1}^{0} \\ [S_{mn}^{0}, S_{m'n'}^{\pm}] &= \pm S_{m+m'n+n'}^{\pm}. \end{aligned} \tag{7}$$

Therefore, the S_{mn}^{μ} form an infinite-dimensional algebra, which is a Lie algebra of the two-parameter affine type without central extension. The Hamiltonian (1) with $c_{jj'} = c_j c_{j'}^*$ can be written in terms of the S_{mn}^{μ} operators as

$$\hat{H} = \sum_j \varepsilon_j \Omega_j + 2S_{10}^{0} - S_{00}^{+} S_{00}^{-}. \tag{8}$$

In the following, we assume that the parameters ε_j and c_j are all different for different j values, that is, we only consider the nondegenerate case. The situations are different for the degenerate and other simpler cases and these will be discussed later. For the nondegenerate case, the unique lowest-weight state is simply the product of the single-j shell pairing vacua with arbitrary seniority quantum numbers. Therefore, it suffices to consider the total seniority zero case. The lowest-weight state satisfies

$$S_{mn}^{-}|0\rangle = 0 \qquad \forall\, m, n. \tag{9}$$

It seems that a two-parameter Bethe ansatz wavefunction might be needed in this case. However, a careful analysis shows that the following one-parameter Bethe ansatz suffices to diagonalize the Hamiltonian (8):

$$|k\rangle = \mathcal{N} S^{+}(x_1) S^{+}(x_2) \ldots S^{+}(x_k)|0\rangle \tag{10}$$

where $\mathcal{N}$ is the normalization constant. It is assumed that $S^{+}(x_i)$ can be expanded in terms of S_{m0}^{+} near the $x_i \sim 0$ region as

$$S^{+}(x_i) = \sum_n x_i^n a_n S_{n0}^{+} \tag{11}$$

where $a_{n_i} S_{n_i 0}^{+}$ are Fourier–Laurent coefficients in the expansion of $S^{+}(x_i)$, namely,

$$a_{n_i} S_{n_i 0}^{+} = \frac{1}{2\pi \mathrm{i}} \oint_0 \mathrm{d}x_i\, x_i^{n_i} S^{+}(x_i). \tag{12}$$

The wavefunctions given by (10) are similar to the algebraic Bethe ansatz [12] which has been proven to be a very useful and powerful tool for solving various spin-chain models and one-dimensional many-body problems [13].

To determine the operators $S^+(x_i)$ and the c-number variables $\{x_i; i = 1, 2, \ldots, k\}$, we first expand (10) in terms of the x_i around $x_i = 0$,

$$|k\rangle = \sum_{n_i} x_1^{n_1} x_2^{n_2} \ldots x_k^{n_k} a_{n_1} a_{n_2} \ldots a_{n_k} S^+_{n_1 0} S^+_{n_2 0} \ldots S^+_{n_k 0} |0\rangle. \tag{13}$$

However, when one applies $\hat{H}$ on (13), the result will not only consist of vectors spanned by a linear combination of products of $S^+_{n_i 0}$, but also consist of those of $S^+_{n_i 1}$. It can also be proved that the results will no longer be algebraically closed, if the whole family of the generators S^+_{mn} given by (6) is used instead of only $\{S^+_{n0}\}$ assumed in (13). Though in both cases the basis vectors spanned by S^+_{n0} and S^+_{n1} are within the same Hilbert subspace, of which both can be expanded in terms of single-j pairing operators $S^+(j)$, the parametrization of S^+_{n0} and S^+_{n1} is different, namely

$$S^+_{n0} = \sum_j \varepsilon_j^n c_j S^+(j) \tag{14a}$$

while

$$S^+_{n1} = \sum_j \varepsilon_j^n |c_j|^2 c_j S^+(j). \tag{14b}$$

However, this difficulty can be overcome if the parameters $|c_j|^2$ can be expressed in terms of a simple analytical function of ε_j. Therefore, there is freedom to choose a simpler relation between $|c_j|^2$ and ε_j. We found that the following auxiliary relations are not only possible, but also convenient:

$$\sum_{i=1}^{p} \frac{b_i}{1 - \varepsilon_j z_i} = |c_j|^2 \qquad j = 1, 2, \ldots, p \tag{15}$$

where $\{b_i, z_i; i = 1, 2, \ldots, p\}$ are c-numbers that need to be determined. Because we have assumed the ε_j and c_j are all different for different j values, (15) is always valid. However, it should be stated that the choice of condition (15) is not unique. Different choices will lead to different versions of the Bethe equations. Of course, the final results for the eigenvalues must be the same, and the corresponding eigenvectors should be equivalent up to a normalization factor. As is well known, the Bethe ansatz consists of two parts. One is proportional to the Bethe wavefunction (13), while the other part will contain k terms not having the initial Bethe form, which are the so-called unwanted terms. The condition of cancellation of these terms imposes some special conditions, which are commonly known as Bethe ansatz equations. The choice of (15) has been made in order to derive the Bethe ansatz equations from those unwanted terms uniformly. Using (13)–(15) and commutation relations (7), one can prove that a_n is an n-independent factor, and x_i, b_j, and z_j, must satisfy the following relations:

$$E_k = \sum_{i=1}^{k} \frac{2}{x_i} \tag{16a}$$

$$\frac{2}{x_i} = \sum_{j'} \frac{\Omega_{j'} |c_{j'}|^2}{\varepsilon_{j'} x_i - 1} + 2 \sum_{j \neq i} \left(\sum_m \frac{b_m x_j}{x_j - z_m} + 1 \right) x_j / (x_j - x_i) \tag{16b}$$

for $i = 1, 2, \ldots, k$, where E_k is the k-pair excitation energy, under the conditions

$$\sum_{i=1}^{p} \frac{b_i}{1 - \varepsilon_j z_i} \sum_{r>q} \frac{z_i^2}{(x_r - z_i)(x_q - z_i)} = \sum_{r>q} \frac{1}{(1 - \varepsilon_j x_r)(1 - \varepsilon_j x_q)} \tag{17}$$

for $j = 1, 2, \ldots, p$. Though these relations were derived for $x_i \approx 0$, they are valid in the entire complex plane. Therefore, the coefficients x_i ($i = 1, 2, \ldots, k$), z_j, b_j ($j = 1, 2, \ldots, p$),

and eigenvalues of the pairing energy are simultaneously determined by the system of equations (15)–(17).

Let

$$U_{ji} = \frac{b_i}{1-\varepsilon_j z_i} \qquad W_i = \sum_{r>q} \frac{z_i^2}{(x_r - z_i)(x_q - z_i)} \qquad V_j = \sum_{r>q} \frac{1}{(1-\varepsilon_j x_r)(1-\varepsilon_j x_q)}. \tag{18}$$

Then the auxiliary conditions (15) are just unity conditions for the transformation matrix U,

$$\sum_i \frac{U_{ji}}{|c_j|^2} = 1 \qquad \text{for} \quad j = 1, 2, \ldots, p \tag{19}$$

and (17) is a 'linear transformation' from vector W to V,

$$\sum_i U_{ji} W_i = V_j \qquad \text{for} \quad j = 1, 2, \ldots, p. \tag{20}$$

It can easily be seen that equations (15)–(17) are necessary and sufficient conditions for solving the eigenvalue problem. Finally, the operator $S^+(x_i)$ can now be written explicitly as

$$S^+(x_i) = \sum_j \frac{c_j}{1-\varepsilon_j x_i} S_j^+. \tag{21}$$

If the parameters $\{c_j\}$ are all real, one can define the following operators:

$$\begin{aligned} S_n^+(x_i) &= \sum_j \frac{c_j^n}{1-\varepsilon_j x_i} S_j^+ \\ S_n^-(x) &= (S_n^+(x))^\dagger \qquad S_n^0(x) = \sum_j \frac{c_j^n}{1-\varepsilon_j x} S_j^0. \end{aligned} \tag{22}$$

These operators generate a nonlinear algebra $\mathcal{G}(SU_2)$, which is an infinite-dimensional extension to the Gaudin algebra given in [18]. The commutation relations of the generators given in (22) are

$$\begin{aligned} [S_m^+(x), S_n^-(y)] &= \frac{2}{x-y}(x S_{m+n}^0(x) - y S_{m+n}^0(y)) \\ [S_m^0(x), S_n^\pm(y)] &= \pm\frac{1}{x-y}(x S_{m+n}^\pm(x) - y S_{m+n}^\pm(y)). \end{aligned} \tag{23}$$

These relations together with the auxiliary relations (15) can be used to verify that the Bethe ansatz equations (16) and (17) are indeed valid, which justifies that the Bethe ansatz equations are valid in the entire complex plane. (23) can also be used to calculate matrix elements of physical quantities in the model.

So far we have assumed that the ε_j and c_j are all different for different j values. When the ε_j are all the same or the c_j are all the same the situation is greatly simplified [14]. These special cases can be regarded as limiting cases of the Hamiltonian (8). It should be pointed out that the exact solutions for the equal strength pairing limit case with $c_{jj'} = |G|$, which is a special case of the SSP model, was studied by Richardson [15, 16] in terms of boson mappings including the effect of the Pauli principle. That result can now be obtained more simply and directly by using the infinite-dimensional algebraic approach.

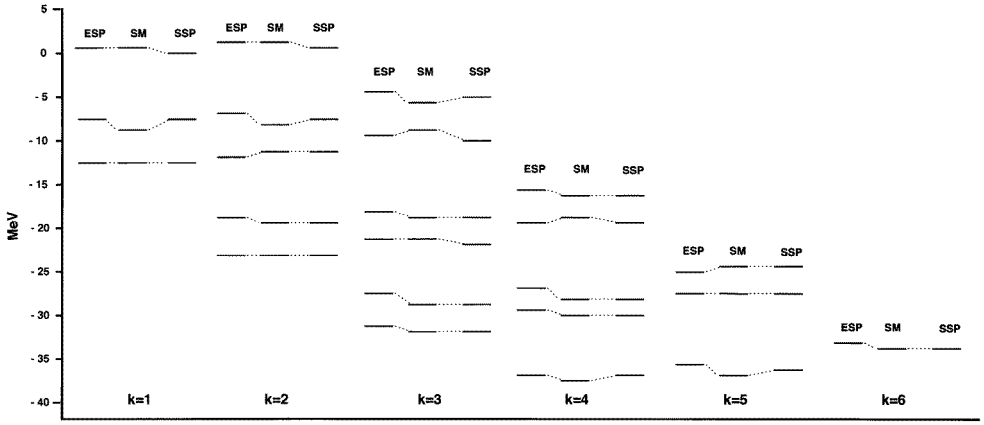

Figure 1. Comparison of realistic shell-model results and spectra of the SSP and ESP Hamiltonians as a function of the number of neutron pairs in the ds-shell.

3. Applications for ds-shell nuclei

To demonstrate the effectiveness of the theory as well as the accuracy of the SSP assumption we considered the case of neutrons in the nuclear ds-shell with the $0d_{5/2}$, $0d_{3/2}$, and $1s_{1/2}$ orbitals all active, which can be used to describe oxygen isotopes $^{16-26}$O. The neutron single-particle energies ε_j were taken from the energy spectra of ^{17}O ($\varepsilon_{1/2} = -3.273$ MeV, $\varepsilon_{3/2} = 0.941$ MeV, and $\varepsilon_{5/2} = -4.143$ MeV). These values are all relative to the binding energy of ^{16}O, which was taken to be zero. The two-body terms of the general pairing Hamiltonian (1) were obtained from the $J = 0$ two-body matrix elements of the universal ds-shell Hamiltonian of Wildenthal [17]. Thus, the $c_{jj'}$ parameters (in MeV) in the shell model (SM) are $c_{\frac{1}{2}\frac{1}{2}} = 2.125$, $c_{\frac{3}{2}\frac{3}{2}} = 1.092$, $c_{\frac{5}{2}\frac{5}{2}} = 0.940$, $c_{\frac{1}{2}\frac{3}{2}} = 0.766$, $c_{\frac{1}{2}\frac{5}{2}} = 0.765$, $c_{\frac{3}{2}\frac{5}{2}} = 1.301$. While in (8) the single-particle energies are taken to be the same as those of the SM, the parameter c_j in the SSP were adjusted to give a best fit to experimental data, which gives $c_{\frac{1}{2}} = 0.70$ MeV$^{\frac{1}{2}}$, $c_{\frac{3}{2}} = 1.15$ MeV$^{\frac{1}{2}}$, $c_{\frac{5}{2}} = 1.048$ MeV$^{\frac{1}{2}}$. We also calculated energy levels in the ESP approximation, with the single-particle energies also taken to be the same as those of the SM, the parameter $|G|$ was adjusted to give the best fit. The quality of the fits are indicated by the quantity

$$\sigma = \left(\frac{1}{N} \sum_{i,total} |E_{SM}(i) - E_{cal}|^2 \right)^{1/2} \tag{24}$$

where N is the total number of the energy levels included in the fit. Because only the $J = 0$ pairing interaction is considered, even the SM results show deviations from experimental data. This is due to missing residual interactions which could, presumably, be treated by perturbation theory. The real test is how well SSP reproduces the SM results. Therefore, only seniority zero 0^+ levels calculated by using SM, SSP, and ESP are shown in figure 1. The calculation results yielded $\sigma = 0.631$ MeV for SSP and $\sigma = 0.824$ MeV for ESP. The results show that the SSP assumption is a rather good approximation, better than the ESP approximation. The binding energies of $^{18-26}$O are also calculated by using SM, SSP, and ESP. These calculated results and the corresponding experimental values are shown in table 1. From the SM results, it can be seen that the residual interaction has a little effect on ground states of the oxygen isotopes. It is very clear that for all measures the SSP results are close to those of the SM, closer than those of the ESP limit.

Table 1. Binding energies (in MeV) of $^{18-26}$O.

Nucleus	Experiment	SM	SSP	ESP
^{18}O	139.81	140.22	140.35	140.20
^{19}O	143.76	143.20	143.18	143.15
^{20}O	151.37	150.77	150.63	150.60
^{21}O	155.18	152.60	153.00	152.28
^{22}O	162.03	158.82	158.63	158.71
^{23}O	164.75	159.45	159.47	158.74
^{24}O	168.48	165.55	164.37	164.27
^{25}O	168.38	167.86	166.76	166.09
^{26}O	168.43	165.44	164.60	164.06
		$\sigma = 2.66$	$\sigma = 2.97$	$\sigma = 3.31$

4. Conclusions

In summary, an exact particle-number-conserving solution to the SSP Hamiltonian has been derived with the help of a two-parameter $SU(2)$ affine Lie algebra without central extension. An infinite-dimensional nonlinear algebra generated by the building blocks of the wavefunctions for the pairing Hamiltonian is reported. This nonlinear algebra is an infinite-dimensional extension of the Gaudin algebra [18]. The method can be used to obtain exact values for the eigenenergies as well as the exact number of the excited levels, both being consistent with restrictions on the number of excited levels allowed by the Pauli principle. A comparison with realistic shell-model results, figure 1, shows that the SSP assumption is a good approximation. Indeed, for the ds-shell case considered the absolute deviations of the eigenenergies of the SSP Hamiltonian from those of the realistic shell-model calculation are small, showing that the assumption is reasonable. The present solution, together with those given in [14], means the general pairing Hamiltonian (1) has exact solutions in three special cases: the SSP limit, $c_{jj'} = c_j c_{j'}^*$, with nondegenerate single-particle energies; the SSP limit, $c_{jj'} = c_j c_{j'}^*$, with degenerate single-particle energies; and the ESP case, $c_{jj'} = |G|\mathrm{e}^{\mathrm{i}(\delta_j - \delta_{j'})}$, where δ_j is an orbital dependent phase. It needs to be pointed out that the ESP approximation is also a good approximation for the ds-shell system studied. It should also be clear from the analysis that there may be other many-body problems that are exactly solvable using infinite-dimensional algebraic techniques. Further applications of this procedure to realistic nuclear systems will be published elsewhere.

Acknowledgments

FP is grateful to Dr W E Ormand and others in the nuclear theory group at Louisiana State University for helpful discussions and critical comments. This work was supported by the National Science Foundation through Grant no 9603006 and Cooperative Agreement no 9550481 which includes matching from the Louisiana Board of Regents Support Fund.

References

[1] Racah G 1942 *Phys. Rev.* **62** 438
[2] Bardeen J, Cooper L N and Schrieffer J R 1957 *Phys. Rev.* **108** 1175
[3] Bohr A, Mottelson B R and Pines D 1958 *Phys. Rev.* **110** 936
[4] Belyaev S T 1959 *Mat.-Fys. Medd. K. Dan. Vidensk. Selsk.* **31** 11

[5] Randeria M, Duan J M and Shieh L Y 1989 *Phys. Rev. Lett.* **62** 981
[6] Schmitt-Rink S, Verma C M and Ruckenstein A E 1989 *Phys. Rev. Lett.* **63** 455
[7] Yang C N 1989 *Phys. Rev. Lett.* **63** 2144
[8] Cooper D W, Batchlder J S and Taubenblatt M A 1991 *J. Colloid Interface Sci.* **144** 201
[9] Barranco M, Hernandez S and Lombard R J 1992 *Z. Phys.* D **22** 659
[10] Zeng J Y and Cheng C S 1983 *Nucl. Phys.* A **405** 1
Zeng J Y and Cheng C S 1984 *Nucl. Phys.* A **411** 49
Zeng J Y and Cheng C S 1984 *Nucl. Phys.* A **414** 253
[11] Molique H and Dudek J 1997 *Phys. Rev.* C **56** 1795
[12] Bethe H A 1931 *Z. Phys.* **71** 205
[13] Yang C N 1967 *Phys. Rev. Lett.* **19** 1312
[14] Feng Pan, Draayer J P and Ormand W E 1998 *Phys. Lett.* B **422** 1
[15] Richardson R W 1965 *J. Math. Phys.* **6** 1034
[16] Richardson R W 1965 *Phys. Lett.* **14** 324
[17] Wildenthal B H 1984 *Prog. Part. Nucl. Phys.* **11** 5
[18] Gaudin M 1976 *J. Physique* **37** 1087