Interaction Strengths for the Fock-Space Formulation of the Nuclear Pairing Problem

J. Dudek\textsuperscript{1}, K. Mazurek\textsuperscript{1,2} and B. Nerlo-Pomorska\textsuperscript{2}
\textsuperscript{1}Institut de Recherches Subatomiques, IN2P3-CNRS/Université Louis Pasteur F-67037 Strasbourg Cedex 2, France
\textsuperscript{2}Katedra Fizyki Teoretycznej, Uniwersytet Marii Curie-Skłodowskiej, PL-20031 Lublin, Poland

9th November 2018

Abstract

A realistic nuclear mean-field hamiltonian with pairing has been diagonalized using Fock space representation that allows for nearly exact treatment of the problem. Calculations were performed for all the even-even nuclei with $Z \in (20, 100)$, whose pairing gaps were possible to extract out of the experimental masses. The optimal values of the pairing strength constants for the protons and neutrons have been found.

PACS: 21.30.Fe, 21.60.-n, 71.10.Li

In the large scale microscopic calculations of the nuclear total-energy surfaces the method of Strutinsky plays an important role allowing for fast and fully automatic calculations related to the equilibrium deformations, shape coexistence, fission probabilities and many other mechanisms and phenomena. In the related formalism the calculation of shell- and pairing-energies plays a decisive role, the latter obtained so far with the help of the Bogolyubov transformation and the associated Bardeen-Cooper-Schrieffer approximate method. The new method proposed in Ref. [1] allows to obtain the exact (in some cases nearly exact) solutions of the pairing problem using realistic hamiltonians - in particular those with the state-dependent pairing hamiltonian. The new method is based on the direct solution of the many-body problem in Fock space; it employs techniques similar to those used in the nuclear shell-model, including the Lanchos diagonalisation scheme. The hamiltonian in question has the form:

$$\hat{H} = \hat{H}_{mf} + \sum_{\alpha, \beta} G_{\alpha, \beta} c_\alpha^\dagger c_\beta^\dagger c_\beta c_\alpha ,$$

This work has been partly supported by the Polish Committee for Scientific Research under Contract No. 2P 03B 115 19 and the collaboration between IN2P3 and Polish Laboratories nr. 99-95
where $\hat{H}_{mf}$ denotes any mean-field Hamiltonian e.g. the one with deformed Woods-Saxon potential and matrix $G_{\alpha,\beta}$, in general non-diagonal in its indices, defines the state-dependent pairing Hamiltonian. Owing to three exact symmetries obeyed by Hamiltonians of the above general form, cf. Ref. [1] for details, the corresponding matrix written down using a Fock space basis can be block-diagonalized analytically, thus reducing the problem of diagonalisation of huge-size matrices to much smaller ones that can be treated easily with the help of the Lanczos methods.

In this article we report on the results of an introductory large-scale test that consists in fitting the coupling constants of the simplest (monopole-pairing) version of pairing Hamiltonian in (1), i.e. $G_{\alpha,\beta} = G_{\delta,\alpha,\beta}$. Pairing calculations were performed within Fock space defined by 24 particles placed on 24 double-degenerate single-particle energy levels in the 'pairing window'. The corresponding full Hamiltonian matrix has the size of $N_{\text{ham}} = 32\,247\,603\,683\,100$, while the sizes of Hamiltonian blocks, after applying the formalism of Ref. [1], are: $N_{s=0} = 2\,704\,156$ in the seniority-zero and $N_{s=2} = 705\,432$ in seniority-two blocks. In both cases we have applied a basis cut-off reducing the sizes of the effectively diagonalized matrices to $N'_{s=0} = 27\,703$ and $N'_{s=2} = 26\,263$. We have verified by comparison with the results of the exactly soluble method of Richardson that the basis cut-off that reduces the matrix sizes by roughly two orders of magnitude induces errors of $\sim 2\%$ only.

We have diagonalized the Fock-space Hamiltonian matrix corresponding to (1) and we obtained the ground-state energy (seniority-zero) and the lowest-energy seniority-two states. The difference between the two energies has been interpreted as corresponding approximately to twice the 'pairing gap', the latter obtained from the mass-difference expression

$$
\Delta^{(3)}_{s}(N) = \frac{\pi N}{2} (B(N) + B(N + 2) - 2B(N + 1)),
$$

as discussed recently in detail in Ref. [4]. Above, $\pi_N = (-1)^N$, $B(N)$ are (negative) binding energies of nuclei, for the fixed $Z$-number. To obtain the proton 'pairing gap' one has to replace $N$ with $Z$ and fix the neutron number $N$. The resulting proton and neutron pairing gaps for even-even nuclei are illustrated in Fig. 1 top, in function of the mass number $A$; the $\Delta^{(3)}$-values with the experimental errors exceeding 250 keV were not taken into account.

The best average fit in terms of the $\alpha/\sqrt{A}$ one-parameter dependence for all the nuclei is $\Delta^{(3)}_{n} = 10.85/\sqrt{A}$ and $\Delta^{(3)}_{p} = 10.02/\sqrt{A}$ (solid lines in Fig. 1 top). The fitted $\alpha$-values are smaller than those obtained in [3] from the liquid drop model formula, the corresponding curves denoted in Fig. 1 with the dashed lines. One can also use alternative one-parameter expressions similar to those in Ref. [4]; the results of the fit are

$$
\Delta_{n} = 23/(\sqrt{A})^{3} \quad \text{and} \quad \Delta_{p} = 21/(\sqrt{A})^{3},
$$

or

$$
\Delta_{n} = 4.66/A^{1/3} \quad \text{and} \quad \Delta_{p} = 4.18/A^{1/3},
$$

but the fit precision remains similar to that with the $\alpha/\sqrt{A}$-type dependence.
To avoid the undesired type of variation in pairing delta, characteristic for spherical (especially doubly magic) nuclei, the nuclei with available experimental masses have been arbitrarily divided into 5 regions: (I) with \( Z \in (32, 38) \) and \( N \in (32, 44) \); (II) with \( Z \in (40, 46) \) and \( N \in (56, 72) \); (III) with \( Z \in (54, 66) \) and \( N \in (58, 76) \); (IV) with \( Z \in (60, 82) \) and \( N \in (88, 104) \) and (V) with \( Z \in (90, 100) \) and \( N \in (142, 156) \); there the doubly-magic nuclei have been eliminated. Within those regions the \( \Delta \)-values were extracted and, as the next step, the \( G \)-constants found that reproduce the extracted \( \Delta \) values exactly for each of the studied nuclei at the calculated in advance equilibrium deformations. The mean field hamiltonian used is the same as in Ref. [6] (see also references there). The irregular behavior of \( \Delta^{(3)} \) in function of \( A \) suggests that the resulting \( G \) values will also vary in a relatively irregular fashion and as a consequence we have tried 'a few parameter' fits in terms of \( A \) and \( I \equiv (N - Z)/(N + Z) \) and possibly some powers of those variables:

\[
G_{p(n)} = \rho_{p(n)}(A^s) \left( \rho_0 + \rho_1 I + \rho_2 I^2 \right) \quad \text{where} \quad s = 1/2, 2/3 ,
\]

(5)
In Fig. 1, frames C) and D), the products \( G_{p(n)} \cdot A \) are shown in function of the isospin factor \( I \) while the corresponding average behavior is shown with the help of the solid lines. In frames E) and F) the quantities \( G_{p(n)} \cdot A^{2/3} \) are illustrated. The dependence in terms of \( I \) obtained here is nearly constant.

Table 1: Pairing strength constants in terms of the approximating expressions for neutrons and protons for 5 regions considered.

| Region | \( a/A + bI \) | \( (c + d I)/A^{2/3} \) | \( (c' + d' I + eI^2)/A^{2/3} \) |
|--------|----------------|-----------------|----------------|
|        | \( a \) | \( b \) | \( c \) | \( d \) | \( c' \) | \( d' \) | \( e \) |
| all \( n \) | 24.872 | -0.147 | 6.517 | -5.921 | 5.657 | 10.96 | -64.18 |
| I | 24.230 | -0.001 | 5.887 | -1.438 | 5.657 | 7.43 | -65.63 |
| II | 27.177 | -0.165 | 6.230 | -6.453 | 5.657 | 0.67 | -21.39 |
| III | 33.129 | -0.214 | 7.097 | -10.298 | 5.657 | 19.60 | -152.21 |
| IV | 56.170 | -0.849 | 11.457 | -33.690 | 5.657 | 36.46 | -206.93 |
| V | 38.548 | -0.144 | 6.315 | -6.408 | 5.657 | -0.29 | -13.35 |
| all \( p \) | 26.861 | -0.331 | 7.100 | -2.905 | 6.529 | 2.65 | -3.51 |
| I | 24.548 | 0.018 | 5.934 | 4.493 | 6.529 | -9.13 | 103.58 |
| II | 45.893 | -0.750 | 7.249 | -2.892 | 6.529 | 1.74 | -3.91 |
| III | 39.296 | -0.481 | 7.178 | -3.700 | 6.529 | 4.55 | -7.60 |
| IV | 54.546 | -0.608 | 7.289 | -3.327 | 6.529 | 1.88 | -4.47 |
| V | 78.763 | -0.635 | 8.333 | -4.289 | 6.529 | 6.18 | -8.67 |

Results in Table 1 give the overall r.m.s. deviations that are rather small. The variations obtained, based on the experimental data concerning a broad range of nuclei, show more structure than the simple parametrisations tested can take care of. In particular, strong variations in parameter \( e \) from one nuclear range to another, cf. column 8 in the Table, indicates that the \( I^2 \) fluctuations are too rapid to allow deducing any systematic trends in this context.

The parametrisations summarized in the Table are ‘ready to use’ in conjunction with the Fock-space diagonalisation method of Ref. [1].

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