The nuclear pairing problem: new perspectives

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The overview of the Exact Pairing technique based on the quasispin symmetry is presented. Extensions of this method are discussed in relation to mean field, quadrupole collectivity, electromagnetic transitions, and many-body level density. Realistic calculations compared with experimental data are used to support the methods as well as to emphasize the manifestations of pairing correlations in nuclear many-body systems.

1. Introduction

The pairing forces are known to be one of the main ingredients of the residual interaction between the nucleons inside the nucleus. Superconducting pairing correlations significantly influence all nuclear properties. The role of pairing correlations increases for weakly bound nuclei far from stability, and some nuclei turn out to be bound only due to the pairing. However, the traditional methods of solving the pairing problem borrowed from macroscopic physics are insufficient for the correct description of the pairing in nuclei and other finite mesoscopic systems. Below we discuss the properties of the exact numerical solution of the pairing problem based on the seniority classification. This approach eliminates the conceptual drawbacks of the standard schemes and opens new perspectives for theoretical advances. Below we concentrate on developing new approximations for the many-body problem in heavy nuclei where the full shell model diagonalization is not feasible.

2. Standard approach and its drawbacks

The pairing is a part of the general quantum many-body problem. We consider this problem in the mean field framework. Particles are moving in the initial “bare” field that in general has both bound orbitals and continuous spectrum. The continuum will be considered elsewhere; here we assume a given set of discrete single-particle levels \(|jm\rangle\) with bare energies \(\epsilon_j\). The levels are degenerate in quantum numbers \(m\) because of rotational and time reversal invariance. The pairing interaction,

\[ H_p = \sum_{jj'} G_{jj'} P_{jj'}^{\dagger} P_{jj'}, \]  

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transfers pairs of time-conjugate partners, 

\[ P_j = \frac{1}{2} \sum_m a_{jm} a_{j\tilde{m}}, \quad (2) \]

between the orbitals. The time-reversal orbital is, in spherical basis, \( |j\tilde{m}\rangle = (-)^{j-m} |j - m\rangle \). An interaction of this type is at the core of superconductivity in condensed matter \[2\] and of pairing correlations in nuclei \[3\].

The BCS theory of macroscopic superconductivity \[2\] generalizes the mean-field approach and constructs the ground state as a self-consistent condensate of pairs with a certain distribution of pairs over the levels (plane waves in uniform superconductors) that minimizes the sum of the mean field energy and pairing energy. The condensate does not have a certain number of particles but the average number is controlled by the chemical potential \( \mu \), while fluctuations are small for macroscopic media. The nuclear analog of the BCS approach was fully developed by Belyaev \[4\]; it was shown that pairing influences all aspects of nuclear structure – binding energy, odd-even effects, occupation factors, transition and beta-decay probabilities, quasiparticle excitations, collective modes, moments of inertia and level density, see the recent review paper \[5\]. Reaction amplitudes and fission processes are also strongly sensitive to pairing.

Belyaev also pointed out the shortcomings of the BCS approximation for finite systems. The particle number violation can be critical for small systems, especially on the edge of stability. There exist vast literature devoted to the corresponding corrections \[6\]. Another drawback is related to the mean field character of the BCS solution. As a signature of the developed pairing, the quasiparticle spectrum acquires the gap, \( \epsilon_j - \epsilon_j' = \sqrt{(\epsilon_j - \mu)^2 + \Delta_j^2} \), which is determined by the BCS equation

\[ \Delta_j = \sum_{j'} G_{jj'} \frac{\Delta_{j'}}{2\epsilon_{j'}}. \quad (3) \]

In a large system with a continuous single-particle spectrum, eq. (3) always has a non-trivial solution (Cooper effect), although at weak interaction the gap is exponentially small. Contrary to that, in a finite system with a discrete spectrum \( \epsilon_j \), the non-zero solution appears only if typical pairing matrix elements \( G_{jj'} \) exceed a critical value of the order of the single-particle level spacing. Otherwise, the gap disappears revealing a sharp phase transition to the normal phase as a function of the pairing strength. As seen in large-scale shell model calculations, pairing correlations in a nucleus do not vanish momentarily but smoothly decrease. Similarly, the thermal phase transition is extended, and a long high-temperature tail of pairing correlations was observed in shell model simulations \[7\] as well as in experiments with small superconducting particles \[8\]. The HFB method \[9\], making a step beyond the BCS in the direction of accounting for the interplay between the mean field and pairing effects, does not cure the mentioned drawbacks.

3. Exact solution of the pairing problem

The exact algebraic solution of the pairing problem was developed by Richardson in the series of papers, see \[10\] and references therein. Unfortunately, this formalism turns out to be numerically quite complicated and works only for specific choices of the matrix
elements $G_{jj'}$. We suggested [11] a direct method of a simple numerical solution of the pairing problem based on the quasispin algebra. The operators $P_j, P_j^\dagger$ and the occupancy of the level $j$, $N_j = \sum_m a_{jm}^\dagger a_{jm}$, obey the commutation relation of the $SU(2)$ algebra forming the partial quasispin vector $L_j$. This formalism is known long ago [12,13] to give the simple and exact solution for a degenerate limit.

In a general many-level case, the pairing interaction does not involve unpaired particles, and therefore their number on each $j$-level, the partial seniority $s_j$, is preserved. For the quasispin quantum number $\Lambda_j$ we have

$$L_j^2 = \Lambda_j(\Lambda_j + 1), \quad s_j = \frac{\Omega_j}{2} - 2\Lambda_j,$$

where $\Omega_j$ is the capacity of the $j$-level ($2j + 1$ in the spherical shell model). A given set of partial seniorities $s_j$, or quasispins $\Lambda_j$, defines a class of states closed with respect to the pairing interaction, regardless of the values of matrix elements $G_{jj'}$. The states with different total spin $J$ within a class are degenerate in the absence of other types of interaction. The ground state of an even-even nucleus with $J = 0$ belongs to the class with all $s_j = 0$. The dimensions of the classes are never exceedingly large, and, with a sparse pairing Hamiltonian matrix, the numerical solution is very fast.

Already at this stage, one can compare the results of the exact solution with those of the BCS approximation for the same pairing matrix elements and single-particle energies (long ago such a comparison for simple examples on the existed level of accuracy was considered [14] as an argument in favor of the BCS approach). The detailed comparison for a typical spherical nucleus $^{114}\text{Sn}$ within the space of $g_{7/2}, d_{5/2}, d_{3/2}, s_{1/2}$, and $h_{11/2}$ neutron orbitals was made in Ref. [15]. This case, with the filled $g_{7/2}$ and $d_{5/2}$ levels, is not the most favorable for the BCS method. Nevertheless, with 14 neutrons above the double-magic $^{100}\text{Sn}$, the results of the BCS and exact solution are reasonably close. While in the BCS theory the occupation numbers in the ground state are expressed in terms of the coherence factors of the Bogoliubov transformation,

$$N_j = v_j^2 = 1 - u_j^2,$$

in the exact solution one needs to distinguish between these three numbers since the coherence factors are certain matrix elements between the states $|N, s\rangle$ of different nuclei,

$$v_j(N) = \langle N - 1, s_j = 1|a_j|N, 0\rangle, \quad u_j(N) = \langle N + 1, s_j = 1|a_j^\dagger|N, 0\rangle.$$  (5)

Typical differences for $^{114}\text{Sn}$ are on the level of 10%. The effect is more pronounced for the pair transfer amplitudes $\langle N + 2, 0|P_j^\dagger|n, 0\rangle$ and $\langle N, 0|P_j|N - 2, 0\rangle$ which differ on the level of 20%, whereas the BCS result is around their mean value.

As discussed in Ref. [16], the situation is quite different for nuclei as $^{48}\text{Ca}$, Fig. 1. Here the BCS approximation results in a trivial solution because of the complete filling of the $0f_{7/2}$ orbital. The exact solution predicts a noticeable correlation energy close to 2 MeV. A quenching of pairing effects is expected in the BCS theory for $^{52}\text{Ca}$, where the orbital $1p_{3/2}$ is filled; the exact solution again differs by almost 2 MeV. Thus, the BCS theory is unreliable for many practically important cases, especially outside of the valley of stability, where the structure and the very existence of nuclei are very sensitive to magic
numbers, and the latter can be different from the region of stability being determined by the details of the mean field and interaction that, in turn, includes pairing.

The pairing solution in a given seniority sector gives, along with the ground state, many excited states with the same quantum numbers. In the class of $s = 0$, all these states are built without unpaired particles, and we can consider them as progressively worsened copies of the pair condensate with a different pair distribution over the orbitals. In the pure BCS approach, we have only quasiparticle excitations. Adding the quasiparticle random phase approximation as the next step beyond BCS, one obtains, see [17] and references therein, the so-called pair vibrations with excitation energies $\omega$ as the roots of the secular equation for the amplitudes $A_j$,

$$A_j = \sum_{j'} G_{jj'} \frac{2e_{j'}^2 A_{j'}}{4e_{j'}^2 - \omega^2}. \quad (7)$$

This equation has the solution $\omega = 0$, when $A_j$ coincide with the condensate amplitudes $\Delta_j$ of eq. (3), plus other roots above pair breaking threshold $2\Delta$. As excitation energy grows, the abundant states found with the exact solution have gradually decreasing collectivity that can be measured with the off-diagonal matrix elements of the operators $N_j$. (It is known that many nuclei have unexplained $0^+$ levels in the region above the gap.) In the upper part of the spectrum one can see signatures of chaotic mixing [18] with no random interactions included. Moreover, the exponential convergence of the numerical results as a function of truncated dimension [19] confirms the onset of chaoticity at high level density in the pure pairing problem. The further studies in this direction are promising.

Figure 1. Pairing correlation energy along the chain of Ca isotopes.
4. On the way to the full interaction

The exact solution for pairing (EP) is merely the first step in the nuclear many-body problem. Even in the cases, such as Sn isotopes, where pairing is the predominant part of the residual interaction, one cannot ignore the presence of other parts. Since our entire discussion assumes that the full shell model solution in the required single-particle space is not feasible or too time-consuming, we can try to develop intermediate approximations based on the exact pairing solution as a starting point.

First of all, the monopole part (a combination of all particle-particle interactions, except for exactly treated pairing, transformed to the particle-hole channel) is necessary in order to account for the smooth change of the mean field along with the change of occupation. This “EP + monopole” approximation works well for global quantities, especially if we are interested in the evolution of those quantities with the mass number. In fact, this part was taken into account in the calculation of correlational energy in Fig. 1.

At the next step, we move to the analog of the HFB method, where the pairing and the mean field, including the deformation effects, become mutually interrelated. The EP solution determines the occupation numbers $N_j$ in the ground state. Similar to what is used at nonzero temperature, we build the Hartree-Fock approximation on those occupation numbers instead of the Slater determinant. In the new mean field (possibly, deformed) we can solve a new the pairing problem and repeat these cycles up to convergence. Fig. 2 shows the neutron separation energies for the longest chain of tin isotopes calculated in this approximation [20]. A popular model “pairing + quadrupole-quadrupole interaction” was analyzed from this viewpoint in Ref. [21]. The model is usually treated as an interpolation picking up the most important interaction parts in both channels. Being considered literally, this model reveals strong pairing effects coming from the usually ignored exchange terms from the quadrupole interaction [15].

Currently, there exists a strong interest to the behavior of electromagnetic transition probabilities $B(E2; 2^+ \rightarrow 0^+)$ from the first excited quadrupole states to the ground state in the chain of even-even tin isotopes [22]. The $2^+$ energies are known to be approximately constant for all non-magic isotopes from $^{102}$Sn to $^{130}$Sn, Fig. 3, right panel. This can be considered as absence of considerable deformation effects usually attributed to the interaction between valence neutrons and protons. Meanwhile, the experimental $B(E2)$ values measured for $A \geq 112$ display a non-trivial $A$-dependence shown on the left panel in Fig. 3. The comparison of different types of calculations shown in Fig. 3 reveals the important role of collective correlations beyond pairing. EP + monopole calculations, although quite accurate for the ground state and lowest pair vibration states, are insufficient once there are unpaired particles in the system; the residual interactions beyond pairing become crucial. In Fig. 4, the full shell model calculation agrees reasonably well with available data for both $B(E2; 2^+_1 \rightarrow 0^+_1)$ and energy of the lowest $2^+$ state. The exact EP + monopole calculation that ignores all other interactions still reproduces the total ground state energy within 0.4 MeV error; but the results are poor for the $2^+$ excited state that is treated as a seniority $s = 2$ state. Indeed, gross underestimates of $B(E2; 2^+_1 \rightarrow 0^+_1)$, and $E(2^+)$ being almost a factor of 2 high indicate a substantial lack of collectivity. The quadrupole collectivity increases significantly when states with unpaired particles are allowed to interact breaking seniority. The calculation of $B(E2)$ values for
Figure 2. One-neutron separation energies for Sn isotopes, including those beyond $^{132}$Sn. Single-particle energies were obtained from the fully self-consistent spherically symmetric solution of HF equations, using the SKX interaction [23], with the EP solution based on the renormalized G-matrix interaction from Ref. [24].

Figure 3. The transition probabilities $B(E2;2^+_1 \rightarrow 0^+_1)$, see the text.
the most quadrupole-coherent superposition of seniority \(s = 2\) states is shown on left panel in Fig. 3 with stars. The remaining discrepancy supposedly comes from the admixture of states with \(s > 2\) and from breaking the proton closed shell. In this situation, the results of the planned at the NSCL experiment for measuring \(B(E2)\) for lighter Sn isotopes are of significant interest.

5. Density of states in paired systems

Pairing correlations leave their footprints far beyond few low-lying states. Recently developed new experimental techniques allow for determination of the level density \([25]\) up to neutron separation energy. The experimental density of states in \(^{116}\)Sn is shown in Fig. 4, where the solid line shows the density of states computed with the EP+monopole technique. The calculated curve is significantly lower than the experiment. The absent in this approximation interactions of unpaired particles broaden the density of states \([7]\) and bring specific high-lying states lower. The same phenomenon is responsible for the lowering of the \(2^+\) state discussed in Sec. 4.

Despite poor general agreement between the data and calculations in the EP+monopole approximation, the full density of states exhibits bumps that can be traced to the prominent seniority peaks obtained in the model. In the calculations with pure pairing, and large degeneracy within a given seniority class, the opening of a new class with higher seniority brings in a large enhancement of the level density. The peaks have to be considerably, or maybe even completely, washed out by other types of interactions lifting degeneracies. This can be noted by examining Fig. 4(b), where presence of peaks is clear in both experiment and theory, but in order to fit the scale of the peaks observed in experiment a reduction factor of 2.5 is needed for the theoretical curve.

The role of pair breaking in creating peaks in density of states can be seen in Fig. 5 for the case of \(^{106}\)Sn. Although the complete experimental data are not available for this system, the relatively small valence space allows here for the exact shell model diagonalization shown with the solid curve. The EP+monopole calculations, dashed line, exhibit large peaks, similar to those in Fig. 4. The peaks coming from pairing can be still well recognized in the full calculation with all interactions included. To see the relation of these peaks to seniority we show the density of \(s = 2\) states with the dotted line. The dashed and dotted curves coincide at low energies, but seniority \(s = 2\) subspace gets exhausted by the time energy reaches -36 MeV (this is relative to the \(^{100}\)Sn core and equivalent to about 6 MeV excitation energy). Then another pair has to be broken, and a large peak in the dashed line corresponding to \(s = 4\) follows, while the dotted \(s = 2\) line goes to zero. The related discussions, other experimental results, and model studies can be found in the review \([5]\). We have to mention recent theoretical suggestions for calculating the shell model level density avoiding the full diagonalization \([26]\).

6. Conclusions

The crucial importance of pairing correlations in nuclear structure has been identified more than half a century ago, and it is remarkable that today this topic is as fresh as ever before. New theoretical and experimental techniques allow us to uncover yet more and more bright manifestations of these correlations. This paper is centered around just
Figure 4. Density of states measured in $^{116}\text{Sn}$, courtesy of U. Agvaanluvsan. The solid curves show the density of states computed for the same system with just pairing+monopole interactions. In panel (a) full density of states from the experiment is compared to the theoretical calculation. To emphasize the oscillations, panel (b) displays the same comparison with the level density plotted as a ratio to the fitted curve defined as $\rho_{\text{fit}}(E) = A \exp(BE)$ with $A$ and $B$ being parameters of the fit. For theoretical curve the amplitude of oscillations is scaled down by a factor of $1/2.5$. 

\[\begin{align*}
\text{(a)} & \quad \text{Density of states measured in } ^{116}\text{Sn} \\
\text{(b)} & \quad \text{Density of states compared to theoretical calculation, ratio to fitted curve}
\end{align*}\]
Figure 5. Density of positive parity states calculated for $^{106}$Sn.: full shell model calculation, solid line; EP+monopole calculation, dashed line; the contribution from seniority $s = 2$ states in the EP+monopole calculation.

one of the new theoretical methods. Using algebraic simplicity of the pairing interaction, we can drastically extend the applicability of the nuclear shell model and eliminate all shortcomings of the conventional treatment borrowed from macroscopic physics. The same approach should be useful for other mesoscopic Fermi-systems with superfluid or superconducting correlations.

The interactions beyond pairing can be incorporated in the perturbative manner which would allow one to study transitions from small systems to superconducting media. We discussed the role of pairing and other interactions in electromagnetic transitions, and quadrupole collectivity. The ability of the EP method to generate all many-body states was crucial. Our study of density of states reaffirmed that even at relatively high excitation energy, and with all non-pairing interactions present, pairing correlations are still an important part of the nuclear many-body dynamics. Along with the realization of vibrational and rotational states on top of the EP, as well as of details of the quenched phase transition to a normal state, where we suggested invariant correlational entropy as a signature of phase transformations [27], this should be a subject of future research. We did not discuss here the continuum effects and the bridge to the reaction theory, where the role of pairing is also crucial [28,29].

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