

Cooper pairs in atomic nuclei

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We describe recent efforts to study Cooper pairs in atomic nuclei. We consider a self-consistent Hartree Fock mean field for the even Sm isotopes and compare results based on three treatments of pairing correlations: a BCS treatment, a number-projected BCS treatment and an exact treatment using the Richardson ansatz. Significant differences are seen in the pairing correlation energies. Furthermore, because it does not average over the properties of the fermion pairs, the Richardson solution permits a more meaningful definition of the Cooper wave function and of the fraction of pairs that are collective. Our results confirm that only a few pairs near the Fermi surface in realistic atomic nuclei are collective.

Keywords: Nuclear structure; degenerate Fermi gases; integrable systems; BCS.

Describimos los recientes esfuerzos en el estudio de pares de Cooper en el núcleo atómico. Consideramos un campo promedio autoconsistente Hartree Fock para los isótopos pares del Sm y comparamos los resultados de tres tratamientos de correlaciones de pairing: un tratamiento BCS, un tratamiento BCS con proyección de número, y un tratamiento exacto usando el ansatz de Richardson. Se encuentran diferencias significativas en las energías de correlación de pairing. Además, ya que la solución de Richardson no promedia sobre las propiedades de los pares de fermiones, permite una definición más significativa de la función de onda de Cooper y de la fracción de pares que son colectivos. Nuestros resultados confirman que solo unos pocos pares cerca de la superficie de Fermi en núcleos atómicos reales son colectivos.

Descriptores: Estructura nuclear; gases de Fermi degenerados; sistemas integrables; BCS.

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1. Introduction

After the discovery of superconductivity in 1911 [1], there followed a long history of efforts to try to explain this phenomenon. A major breakthrough occurred in 1956 with Cooper's demonstration [2] that bound pairs could be produced in the vicinity of the Fermi surface for an arbitrarily weak attractive pairing interaction. He also suggested the possibility of describing superconductivity in terms of these correlated pairs.

Soon thereafter, Bardeen, Cooper and Schrieffer [3] presented the BCS theory, whereby superconductivity was described as a number-nonconserving state of coherent pairs,

$$|\Psi_{BCS}\rangle = e^{\Gamma^\dagger} |0\rangle, \quad (1)$$

with

$$\Gamma^\dagger = \sum_k z_k c_k^\dagger c_k^\dagger$$

and z_k as variational parameters. The following year, Bohr, Mottelson and Pines [4] noted that similar physics may underly the large gaps seen in the spectra of even-even atomic nuclei, emphasizing however that finite-size effects would be

critical for a proper description of such systems. To accommodate these effects, number-projected BCS (PBCS) [5] theory was developed in 1963, based on a condensate of pairs of the form

$$|\Psi_{PBCS}\rangle = (\Gamma^\dagger)^M |0\rangle, \quad (2)$$

where M is the number of pairs and Γ^\dagger has the same form as in BCS theory.

At roughly the same time that PBCS theory was developed, Richardson [6] showed that for a pure pairing hamiltonian it is possible to *exactly* solve the Schrödinger align by following closely Cooper's original idea. More specifically, he showed that for a system with N particles, *all* solutions can be expressed as a product of distinct Cooper pairs Γ_α^\dagger , viz:

$$|\Phi\rangle = \prod_{\alpha=1}^M \Gamma_\alpha^\dagger |\nu\rangle, \quad \Gamma_\alpha^\dagger = \sum_k \frac{1}{2\epsilon_k - e_\alpha} c_k^\dagger c_k^\dagger, \quad (3)$$

where $|\nu\rangle$ represents a fully unpaired state of ν particles and $N = 2M + \nu$.

In this paper, we focus on the properties of Cooper pairs in atomic nuclei. We report detailed microscopic calculations

of the even Sm isotopes from ^{144}Sm through ^{158}Sm in which the pairing correlations derive from a pure pairing force. We compare the results that emerge when these pairing correlations are treated in BCS approximation, in projected BCS approximation and through exact solution using the Richardson approach. We see that both the BCS approximation and the PBCS approximation systematically miss an important piece of the pairing correlation energy when compared with Richardson's exact treatment. We also find that by making use of the exact Richardson solution we are able to get a clearer description of some important qualitative features of Cooper pairs in such finite Fermi systems. Most of the work reported here can be found in Ref. 7.

The outline of the presentation is as follows. In Sec. 2, we briefly review the Richardson solution of the pairing hamiltonian and its numerical treatment for a large number of interacting particles. We then discuss in Sec. 3 how the exact solution can be used to describe several important features of Cooper pairing and contrast this with the descriptions commonly used in BCS or BCS-like treatments. In Sec. 4, we describe the calculations we have carried out for the even Sm isotopes and discuss the results of those calculations. Finally, in Sec. 5 we briefly summarize the principal conclusions of our analysis, both for nuclear systems and for more general quantum systems.

2. Richardson's Exact solution of the Pairing Hamiltonian

We focus here on a pure pairing hamiltonian with constant strength G acting in a space of doubly-degenerate time-reversed states (k, \bar{k}) . The hamiltonian can be expressed as

$$H = \sum_k \epsilon_k c_k^\dagger c_k - \frac{G}{4} \sum_{k,k'} c_k^\dagger c_{\bar{k}}^\dagger c_{\bar{k}'} c_{k'}, \quad (4)$$

where ϵ_k are the single-particle energies for the doubly-degenerate orbits k, \bar{k} (which henceforth we refer to as orbit k).

As noted earlier, the Richardson ansatz (3) for a system with $2M$ paired particles and ν unpaired particles can be written as a product of M Cooper pair creation operators acting on an unpaired state $|\nu\rangle$,

$$|\Phi\rangle = \prod_{\alpha=1}^M \left(\sum_k \frac{1}{2\epsilon_k - e_\alpha} c_k^\dagger c_{\bar{k}}^\dagger \right) |\nu\rangle. \quad (5)$$

As Richardson showed, these are the exact eigenstates of the pairing hamiltonian if the e_α , a set of complex parameters called the pair energies, satisfy a set of M coupled non-linear equations,

$$1 + 2G \sum_k \frac{d_k}{2\epsilon_k - e_\alpha} + 2G \sum_{\beta(\neq\alpha)=1}^M \frac{1}{e_\beta - e_\alpha} = 0, \quad (6)$$

where $d_k = (\nu_k - 1)/2$ and ν_k is the number of unpaired particles in orbit k (either 0 or 1). These are usually referred

to as the Richardson equations. The energy eigenvalues of the hamiltonian can be obtained by simply summing the pair energies that result from their solution.

There are several points worth noting here. The first is that the pair energies that emerge by solving the Richardson equations are always either real or arise in complex conjugate pairs. A second is that there are as many independent solutions of these equations as there are states in the Hilbert space. Finally, all of the solutions to these equations can be readily classified in the weak-coupling $G \rightarrow 0$ limit.

The typical procedure for solving these equations is to start with the known solutions in the weak-coupling limit and then to evolve to the physical value of the pairing strength. Unfortunately, as can be seen from (5) the Richardson equations have singularities when a pair energy is real and equals twice a single-particle energy. This makes it difficult to follow the evolution of the solution for all pairs with increasing G .

A practical approach for avoiding these singularities and obtaining all solutions of the Richardson equations was presented in Ref. 7. Namely we start the numerical procedure at very weak (or alternatively very strong) coupling where the solutions are known and we add a small arbitrary imaginary component to all of the single-particle energies. We then evolve with G to the physical value, but now avoiding the singularities. Once we reach the physical value of G , we set the imaginary parts of the single-particle energies to zero and then obtain the final physical solutions. This method seems to work for any distribution of single-particle energies and any pairing strength G , enabling us to obtain all solutions to the Richardson equations for very large numbers of particles and levels.

3. Some general features of cooper pairs

Pairing is of course not limited to atomic nuclei but arises in a wide variety of strongly-correlated quantum systems. In ultra-low temperature atomic gases, for example, it has proven possible to tune the strength of the pairing interaction through the use of the Feshbach resonance [8] and in doing so to explore pairing correlations through the crossover region from BCS to BEC behavior [9]. By making use of the Richardson solution of the pure pairing hamiltonian, Ortiz and Dukelsky [10] have shown how Cooper pairs evolve in this crossover, naturally progressing from a system of pair resonances spread out across the system and free fermions to a system of spatially correlated quasibound molecules.

An interesting question for any system subject to pairing correlations is: *What fraction of the pairs are indeed strongly correlated?* This is a very difficult question to address in BCS or BCS-like theories, as there is no natural measure for this quantity, the so-called *condensate fraction*. Typically, it is defined through a prescription due to Yang [11], obtained by analyzing the Off Diagonal Long Range Order that characterizes all superconductors and superfluids. This leads to a

definition of the condensate fraction appropriate to homogeneous systems in the thermodynamic limit.

For finite Fermi systems, atomic nuclei being an example, it is necessary to modify Yang's prescription. The appropriate modification appropriate to BCS theory is to define the condensate fraction λ_{BCS} by

$$\begin{aligned}\lambda_{BCS} &= \frac{1}{M(1 - M/L)} \\ &\times \sum_{k,k'=1}^L \left[\langle c_k^\dagger c_{k'}^\dagger c_{\bar{k}'} c_{\bar{k}} \rangle - \langle c_k^\dagger c_{\bar{k}} \rangle \langle c_{k'}^\dagger c_{\bar{k}'} \rangle \right] \\ &= \frac{1}{M(1 - M/L)} \sum_{k=1}^L u_k^2 v_k^2, \quad (7)\end{aligned}$$

where L is the total number of doubly-degenerate states, M is the number of pairs and v_k and u_k are the usual BCS quasi-particle amplitudes.

The exact Richardson solution provides a more natural and more appropriate definition of the condensate fraction. From the Richardson pair wave function (3), we see that a pair for which e_α is close to a particular $2\epsilon_k$ is dominated by that particular configuration and thus is uncorrelated. In contrast, a pair energy lying sufficiently far away in the complex plane from any uncorrelated pair energy produces a correlated Cooper pair. As a practical measure we define the condensate fraction emerging from the Richardson solution as the fraction of pair energies that lie more than the mean level spacing from any unperturbed single-pair energy.

Another important question is: *What is the structure of the Cooper pairs in a system?* Once again, this is difficult to address in BCS theories and in fact there are two definitions considered. One is to look directly at the structure of the operator Γ^\dagger from which the BCS or PBCS state is built. This leads to a prescription in which the orbit k contributes v_k/u_k . However, since the operator Γ^\dagger averages over all the particles in the system, this does not provide a particularly meaningful reflection of an actual Cooper pair.

A somewhat better *average* measure is provided by the pair-correlator, for which the k content is given by

$$\langle BCS | c_{\bar{k}} c_k | BCS \rangle = u_k v_k.$$

Indeed, in several recent studies [12] that explored the spatial structure of pairing correlations in realistic nuclei, this was the measure considered.

As noted earlier, the Richardson solution provides information directly on all Cooper pairs. A given Cooper pair Γ_α^\dagger , corresponding to pair energy e_α , can be written as

$$\Gamma_\alpha^\dagger = \sum_k \frac{1}{2\epsilon_k - e_\alpha} c_k^\dagger c_{\bar{k}}^\dagger,$$

so that the orbit k contributes $1/(2\epsilon_k - e_\alpha)$ to that pair.

4. Model for the Sm isotopes

The results that we will be reporting are based on a series of self-consistent deformed Hartree Fock+BCS calculations, in which a density-dependent Skyrme force, SLy4, is used to describe the mean field correlations and a pairing force with constant strength G is used to treat the pairing correlations.

The calculations are carried out in an axially symmetric harmonic oscillator space of 11 major shells, with 286 doubly-degenerate single-particle states. This basis involves oscillator parameter b_0 and axis ratio q , optimized to minimize the energy in the given space. The strength of the pairing force for protons and neutrons is chosen to reproduce the experimental pairing gaps in ^{154}Sm , and then rescaled for the other isotopes assuming a $1/A$ dependence. These calculations provide an excellent overall description of the properties of the even Sm isotopes.

We then use the results at self-consistency to define the HF mean field and consider not only the BCS approach but also the number-conserving PBCS and exact Richardson approaches to treat the pairing correlations within *this* mean field. The fact that pairing derives from a pure pairing force permits the use of the Richardson approach to obtain the exact solutions and thus to carry out the comparison of interest.

We first consider the pairing correlation energy, defined as

$$E_C = \langle \Phi_{corr} | H | \Phi_{corr} \rangle - \langle \Phi_{uncorr} | H | \Phi_{uncorr} \rangle, \quad (8)$$

where $|\Phi_{corr}\rangle$ is the correlated ground-state wave function and $|\Phi_{uncorr}\rangle$ is the uncorrelated Hartree Fock Slater determinant obtained by filling all levels up to the Fermi energy.

Table I summarizes our results for all nuclei considered. Two sets of BCS results, denoted BCS and BCS+H, respectively, are presented. The column denoted BCS does not include the v_k^4 Hartree contributions from the pairing force; the column denoted BCS+H includes this contribution. The calculations include the semi-magic nucleus ^{144}Sm , for which the BCS calculation leads to a normal solution with no pairing correlations. In contrast, the projected BCS calculation leads to substantial pairing correlations in the ground state,

TABLE I. Pairing correlation energies E_C associated with the BCS, BCS+H, PBCS and exact Richardson treatments of pairing for the even Sm isotopes. All energies are given in MeV.

Mass	<i>Exact</i>	<i>PBCS</i>	<i>BCS + H</i>	<i>BCS</i>
142	-4.146	-3.096	-1.214	-1.107
144	-2.960	-2.677	0.0	0.0
146	-4.340	-3.140	-1.444	-1.384
148	-4.221	-3.014	-1.165	-1.075
150	-3.761	-2.932	-0.471	-0.386
152	-3.922	-2.957	-0.750	-0.637
154	-3.678	-2.859	-0.479	-0.390
156	-3.716	-2.832	-0.605	-0.515
158	-3.832	-2.824	-0.816	-0.717

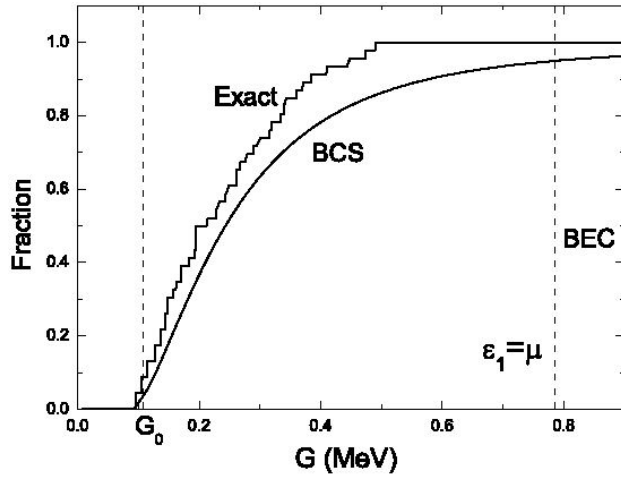


FIGURE 1. Condensate fractions appropriate to ^{154}Sm . The smooth curve gives the modified Yang prescription for the BCS treatment of pairing and the sawtooth curve gives the alternative prescription discussed in the text for the exact Richardson treatment. $G_0 = 0.106\text{MeV}$ denotes the physical value of the pairing strength and $\epsilon_1 = \mu$ denotes the strength at which the whole system binds.

consistent with results from other mean-field treatments of semi-magic nuclei [13]. The exact treatment of pairing leads to a further lowering of the energy of the ground state of the system, by 0.3 MeV.

For non-semi-magic nuclei, the effect of an exact treatment on the pairing correlation energy is even greater. While PBCS gives a significant lowering of the energy due to number projection, it misses about 1 MeV of the exact correlation energy. Considering the extensive recent efforts to carry out systematic microscopic calculations of nuclear masses using mean-field methods [14], we feel that this is an important conclusion. While renormalization of G could accommodate these corrections, it might not be possible to adopt a simple renormalization recipe when dealing with more general effective interactions, such as the Gogny force, for which the particle-hole and particle-particle interactions derive from the same force.

Next we compare results for the condensate fraction appropriate to ^{154}Sm , obtained from the BCS solution using the modified Yang prescription and from the Richardson solution using the prescription based on the distance of the associated pair energy from the various unperturbed single-pair energies. The results are plotted in Fig. 1 as a function of the pairing strength G , with the physical value appropriate to ^{154}Sm being $G_0 = 0.106\text{ MeV}$.

To see how the exact results emerge, we show in Fig. 2 the associated pair energies in ^{154}Sm for four values of G , ranging from the physical value of $G = 0.106\text{ MeV}$ to a fairly strong pairing strength of $G = 0.4\text{ MeV}$. In ^{154}Sm the mean level spacing between the Hartree Fock single-particle levels is roughly 0.5 MeV. For $G = 0.106\text{ MeV}$, most of the pair energies lie very near the real axis and quite close to at least one unperturbed single-pair energy, $2\epsilon_k$. Two of them

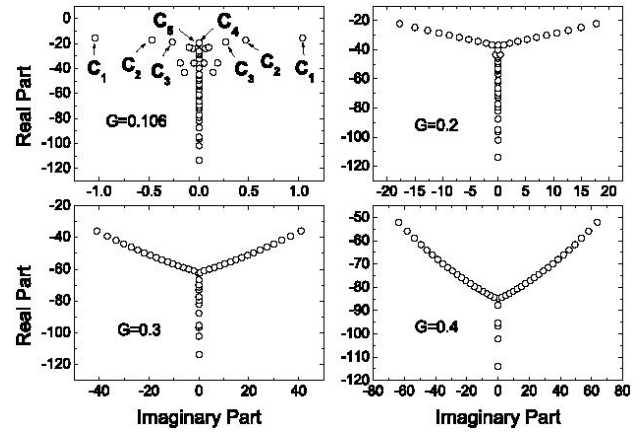


FIGURE 2. Pair energies (in MeV) for the exact Cooper pairs that emerge from four calculations of the ^{154}Sm isotope. $G = 0.106\text{ MeV}$ is the physical value of the pairing strength. In that panel, we denote the most collective pairs as C_i , for subsequent notational purposes.

(which form a complex conjugate pair) are about 1 MeV away from the real axis, and thus are clearly collective. Another two are marginally collective, lying roughly 0.5 MeV from the closest $2\epsilon_k$. The two most collective pairs, denoted C_1 in the figure, each have a real energy of -15.55 MeV , which is roughly twice the energy of the single-particle levels just below the Fermi surface. This suggests that the first pairs that become collective are those involving the valence orbits. As G increases, we see a gradual increase in the number of collective pairs, which form an arc in the complex plane. As can be seen from Fig. 1, by a pairing strength of roughly 0.5 MeV all of the pairs of the system are correlated giving a condensate fraction of 1, even though the BEC regime has not yet been reached. The BEC limit is realized when the chemical potential μ crosses the lowest single-particle energy ϵ_1 , which for ^{154}Sm occurs at $G = 0.788\text{ MeV}$. At this point all pairs are bound. Note, however, that the revised Yang prescription (7) fails to predict a complete condensate at this point, as it likewise failed to in the homogeneous case [10].

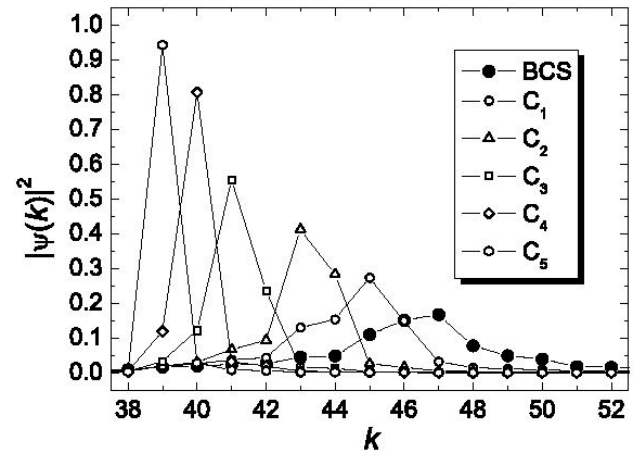


FIGURE 3. Square of the wave function of the most collective Cooper pairs in ^{154}Sm (denoted C_1 , C_2 , C_3 , C_4 , and C_5) and the pair correlator (BCS) versus the single-particle levels.

Next we focus on the structure of the Cooper pairs, which as noted earlier can be obtained exactly from the Richardson solutions. In Fig. 3, we compare the square of the wave function for the most correlated Cooper pairs in ^{154}Sm , *i.e.* those whose pair energies lie farthest from any unperturbed single-pair energy, with the square of the pair correlator wave function obtained from the BCS solution. As noted earlier, this is the most meaningful measure of pair correlations in BCS approximation. All wave functions are plotted versus the order of the single-particle states to make clear the relevant mixing of configurations in each pair. The pair labels in the figure (C_1 through C_5) refer to corresponding labels in the upper left panel of Fig. 2. C_1 refers to the two most collective pairs, namely those that are farthest from any unperturbed single-particle pair. Being complex conjugate pairs, both have exactly the same absolute square of their wave function and thus we only show one in the figure. C_2 refers to the next two most collective pairs, which as noted earlier are marginally collective according to our prescription. C_3 refers to the next two most collective pairs after C_2 , which according to the prescription given above involve perturbative mixing of configurations and are thus not truly collective. C_4 and C_5 , the following pairs in descending collective order, have real pair energies and involve almost pure single-particle configurations.

From the figure, we see that the pair correlator wave function is spread over several single-particle configurations and peaked at the 47^{th} single-particle level, just beyond the Fermi energy (^{154}Sm has 46 neutron pairs). In contrast, the most highly correlated Cooper pair wave function is somewhat narrower (less collective) and is peaked slightly within the Fermi sphere. The less-collective Cooper pairs are peaked progressively further inside the Fermi sphere and are progressively narrower. These results suggest that the size of even the most collective Cooper pairs in coordinate space will be larger than the size of the pair correlator. Investigations [12] on the size of the pair correlator in spherical nuclei concluded that it is unexpectedly small in the nuclear surface ($2 - 3 \text{ fm}$). The

present calculations would suggest that the actual size of the few highly collective Cooper pairs is larger than the typical size of the pair correlations in the nuclear medium.

5. Summary

In this paper, we described recent work carried out to address pairing properties of atomic nuclei. We considered a realistic description of the even Sm isotopes with their mean field properties described in Skyrme Hartree Fock approximation and their pairing properties treated at various levels of approximation. We found that even a projected BCS treatment of pairing misses a sizable component of the pairing correlation energy, which could have important implications in fully microscopic efforts to describe nuclear masses. We also confirmed that very few of the nucleons in a realistic nucleus coherently pair, and that they typically involve strong admixtures of the outermost valence orbits only. Furthermore, the associated collective Cooper pairs are slightly larger in spatial extent than the corresponding BCS pair correlator.

We also addressed several general issues on pairing in strongly-correlated quantum systems, showing that when the Richardson exact solution can be obtained it provides a more meaningful definition of both the condensate fraction (the fraction of pairs that are strongly correlated) and the structure of the associated Cooper pairs.

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