

Accuracy of the Superconductivity Approximation for Pairing Forces in Nuclei*

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The accuracy of the superconductivity approximation for pairing forces in nuclei is studied. To this end we have exactly diagonalized the pairing force for certain nuclei and compared the results with those obtained from the approximate calculation of Kisslinger and Sorensen. When the energy is computed by use of the approximate-wave function, which is not an eigenfunction of the number operator, it is found that the excitation energies of the low-lying states with seniority one and two are correct to within 200 kev, whereas the ground-state energies are usually not given to better than 500 kev. The wave function obtained by projecting out and normalizing that part of the variational trial function that corresponds to the correct number of particles is found to agree closely with the exact energy eigenfunction. Overlap integrals greater than 98% are found in all cases considered. The expectation values of the pairing Hamiltonian with respect to these projected wave functions are therefore in excellent agreement with the exact energy eigenvalues. The variational aspects of the superconductivity approximation are also discussed briefly.

1. INTRODUCTION

KISSLINGER and Sorensen¹ have recently examined the effect of pairing forces on the structure of single-closed-shell nuclei. They use methods of approximation originally developed in studies²⁻⁴ of the superconducting state in metals, and since applied to nuclear physics by a number of authors.⁵⁻⁷ The state of a system of interacting fermions, moving in a common potential, is characterized by the probability amplitudes V_j for occupancy of the various pair states ($jm, j-m$) in the common potential. If the interaction is assumed to be a pairing force only, the energy of the system is then minimized as a function of the parameter V_j . The trial function used in this variational calculation is not an eigenstate of the particle-number operator.

In this paper we study the accuracy of Kisslinger and Sorensen's treatment of the pairing Hamiltonian. To this end we perform an exact diagonalization of the pairing Hamiltonian (Sec. 2) and compare the resulting eigenvalues and eigenfunctions with the approximate solutions of Kisslinger and Sorensen (Sec. 4). Although the nuclear ground-state energies are usually not given to better than 500 kev by the superconductivity approximation, the energies relative to the ground state

are generally accurate to within 200 kev. Remarkably large overlaps with the exact eigenfunctions are obtained by projecting out (and normalizing) that part of the Kisslinger-Sorensen wave function that corresponds to the desired number of particles. Indeed, the projected-wave functions agree more closely with the results of the exact calculation than do the energies, in spite of the fact that the projected-wave function usually constitutes no more than 60% of the original trial function. This circumstance is a survival from the situation wherein all single-particle levels are degenerate. In this special case, for which analytical solutions can be written down, (Sec. 3), the exact and projected eigenfunctions are found to be identical, although there are finite errors in the eigenvalues.

We conclude that the best procedure is to adopt the projected-wave function of the variational calculation as an approximation to the energy eigenfunction. Matrix elements of physical quantities should ideally be calculated with the aid of this projected-wave function rather than with the full trial-wave function. In particular, expectation values of the pairing Hamiltonian are found to be in excellent agreement with the exact energy eigenvalues.

Kisslinger and Sorensen¹ make a number of additional approximations in solving the sets of coupled equations that determine the optimum values of the parameters V_j . We examine these approximations in Sec. 5, concluding that the errors introduced are small.

2. DIAGONALIZATION OF THE PAIRING HAMILTONIAN

We consider the pairing Hamiltonian⁸

$$H = \sum_{j,m} \epsilon_j a_{jm}^\dagger a_{jm} - \frac{1}{4} G \sum_{j,m,j',m'} (-1)^{j-m} \times a_{jm}^\dagger a_{j-m}^\dagger (-1)^{j'-m'} a_{j'-m'} a_{j'm'}, \quad (1)$$

⁸ Since our interest here is confined to the superconductivity

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¹ L. S. Kisslinger and R. A. Sorensen, Kgl. Danske Videnskab, Selskab, Mat.-fys. Medd. **32**, (9) (1960).

² J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

³ N. N. Bogolubov, Soviet Phys.—JETP **34**, 58, 73 (1958); Nuovo cimento **7**, 794 (1958).

⁴ J. G. Valatin, Nuovo cimento **7**, 843 (1958).

⁵ B. R. Mottelson, *The Many-Body Problem* (Dunod, Paris, France, 1959), pp. 283-315.

⁶ S. T. Belyaev, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **31**, 11 (1959).

⁷ M. Baranger, Phys. Rev. **120**, 957 (1960).

where the a 's are fermion creation and annihilation operators, the ϵ_j are single-particle energies, and G measures the strength of the pairing interaction. Only identical nucleons (all neutrons or all protons) are considered. To diagonalize H we define the "quasi-spin" operators^{9,10}

$$S_+ = \sum_j S_+^j = \sum_{j,m>0} (-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger, \quad (2a)$$

$$S_- = (S_+)^{\dagger} = \sum_{j,m>0} (-1)^{j-m} a_{j-m} a_{jm}, \quad (2b)$$

$$S_z = \frac{1}{2} \sum_{j,m>0} \{a_{jm}^\dagger a_{jm} - a_{j-m} a_{j-m}^\dagger\}, \quad (2c)$$

which have the commutation properties of angular-momentum operators. Introducing the number operator $N^j = \sum_m a_{jm}^\dagger a_{jm}$ and the pair degeneracy $\Omega^j = (j + \frac{1}{2})$ of level j , we obtain from Eq. (2c)

$$S_z = \sum_j S_z^j = \frac{1}{2} \sum_j (N^j - \Omega^j) = \frac{1}{2} (N - \Omega). \quad (3)$$

It follows at once that

$$S^j \geq |S_0^j| = \frac{1}{2} (N^j - \Omega^j), \quad (4)$$

where S_0, S_0^j are eigenvalues of S_z, S_z^j . Thus the quasi-spin S^j attains its maximum value of $\frac{1}{2}\Omega^j$ when the j shell is empty ($S_0^j = -\frac{1}{2}\Omega^j$) or full ($S_0^j = \frac{1}{2}\Omega^j$).

Repeated application of S_+^j to any state $|S^j S_0^j\rangle$ of j^n raises S_0^j in unit steps but leaves S^j unaltered. Since S_+^j is a creation operator for a zero-coupled pair in level j , states of the same S^j differ only in the addition or removal of a number of zero-coupled pairs. This, however, is the characteristic feature of the classification of states in terms of their seniority.¹¹ The precise connection between quasi-spin S^j and seniority¹² v is, in fact,

$$v = \Omega^j - 2S^j. \quad (5)$$

The relevance of a seniority classification to the present problem becomes clear when it is realized that the pairing operator in Eq. (1) is a direct generalization for more than one j level of Racah's¹² seniority operator Q . It is both convenient and in accordance with the physical ideas underlying the concept of seniority to proceed further with this generalization and to refer to the quantum number $\sum_j (\Omega^j - 2S^j)$ as the seniority. In other words the seniority of a state is simply the number of unpaired particles it contains.

We now use Eqs. (2) to rewrite the Hamiltonian in terms of the S operators as

$$H = -GS_+S_- + 2 \sum_j \epsilon_j S_z^j + \sum_j \epsilon_j \Omega^j. \quad (6)$$

approximation for pairing forces, we omit the long-range quadrupole force in Kisslinger and Sorensen's Hamiltonian (reference 1). We also remark on a minor error in Eq. (2) of reference 1, where the pairing operator differs from the one in our Eq. (1) by replacement $G/4 \rightarrow G/2$. The numerical results given in reference 1 correspond to the Hamiltonian of Eq. (1) above.

⁹ A. K. Kerman, Ann. Phys. (N. Y.) **12**, 300 (1961).

¹⁰ P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

¹¹ The connection between quasi spin and seniority is discussed in more detail in reference 9.

¹² G. Racah, Phys. Rev. **62**, 438 (1942).

To diagonalize H we introduce a representation based on the eigenstates $|xSS_0\rangle$ of the pairing operator

$$GS_+S_-|xSS_0\rangle = G[S(S+1) - S_0(S_0-1)]|xSS_0\rangle, \quad (7)$$

where x symbolizes a set of additional quantum numbers chosen in some suitable fashion to complete the specification of the state.

The ground state of an even-even nucleus with the Hamiltonian (6) is one in which all nucleons are paired; the "seniority" is zero and each S^j has its maximum value of $\frac{1}{2}\Omega^j$. The specification of the states $|xSS_0\rangle$ may be completed by coupling the various S^j to a resultant S, S_0 . For more than two levels, of course, this may be done in a variety of ways, the alternative bases then being connected by simple recoupling transformations. All the relevant features of the general problem may be illustrated by the case of three levels, for which a suitable basic set of states of seniority zero is¹³

$$\begin{aligned} |(S^1 S^2) S^{12}, S^3, SS_0\rangle = & \sum_{\substack{\mu_1 \mu_2 \mu_3 \\ (\mu_1 + \mu_2 + \mu_3 = S_0)}} (S^1 S^2 \mu_1 \mu_2 | S^{12} \mu_1 + \mu_2) \\ & \times (S^{12} S^3 \mu_1 + \mu_2, \mu_3 | SS_0) \prod_{k=1}^3 (S_+^k)^{\nu_k} |0\rangle, \end{aligned} \quad (8)$$

where $\nu_k = \mu_k + \frac{1}{2}\Omega^k$, $S^k = \frac{1}{2}\Omega^k$, and $|0\rangle$ is the vacuum state of the system, with $S = -S_0 = \frac{1}{2}\Omega$. The matrix elements of the Hamiltonian (6) between such states can be calculated by straightforward Racah algebra.

The lowest states of an odd- A nucleus with the Hamiltonian (6) are those in which all nucleons but the last ($j'm'$) are paired. We refer to such states as "states of seniority one." The presence of a particle in the state ($j'm'$) has the effect of "blocking" or preventing the occupation of the corresponding-pair state. As a result [by Eq. (4)], $S^j \equiv S'$ is reduced by $\frac{1}{2}$. With this modification, a basic set of states of seniority one can be introduced as described above for seniority zero. For example, in the three-level case, Eq. (8) can again be used with the replacements

$$\begin{aligned} S' = \frac{1}{2}\Omega' & \rightarrow \frac{1}{2}(\Omega' - 1), \\ (S_+^j)^{\mu' + \frac{1}{2}\Omega'} & \rightarrow (S_+^j)^{\mu' + \frac{1}{2}(\Omega' - 1)}, \\ |0\rangle & \rightarrow a_{j'm'}^\dagger |0\rangle. \end{aligned} \quad (9)$$

Construction and diagonalization of the energy matrix now proceeds as before and states of angular momentum j' are obtained.

For an even-even nucleus, the low-lying (noncollective) excited states of the Hamiltonian (6) are those in which there are two unpaired nucleons. If these nucleons occupy different single-particle levels, the corresponding quasi spins are reduced by $\frac{1}{2}$; if they are in the same orbit the quasi-spin is reduced by 1. The total angular momentum of a state of seniority two is in general different from zero, various possibilities arising from the

¹³ For notation, see A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957), in particular Eqs. (3.5.2) and (6.1.1).

coupling of the spins of the unpaired nucleons. The eigenvalues of the pairing Hamiltonian are, however, independent of the total angular momentum.

Algebraic expressions can now be derived for the matrix elements of the pairing Hamiltonian between states of seniority zero, one, and two. Numerical calculation of the matrix elements and diagonalization of the matrices were carried out by machine. The results are presented in Sec. 4.

3. THE DEGENERATE MODEL

First let us discuss the degenerate model, wherein all single-particle energies are equal, since it can be solved exactly and is quite instructive. It is then easy to show that the difference between the exact and variational energies for states of seniority zero is^{5,14}

$$\Delta E_{\text{deg}} = -\frac{1}{2}GN \left(1 - \frac{N}{2\Omega}\right), \quad (10)$$

while for states of seniority one

$$\Delta E_{\text{deg}} \approx -\frac{1}{2}GN \left(1 - \frac{N}{2\Omega} + \frac{1}{2N}\right), \quad (11)$$

provided

$$\frac{N}{\Omega^2} \left[2 \left(\frac{N}{\Omega} - 1 \right) + \frac{N}{\Omega^2} \right] \ll 1. \quad (12)$$

With the same approximation, the energy error for states of seniority two is given by Eq. (11). In Table I, the difference ΔE_{deg} between the exact and variational energies of even-even ground states is tabulated.

On the other hand, the component in the trial-wave function of the degenerate model corresponding to the correct number of particles, is identical (after normalization) to the exact wave function. Thus the errors ΔE_{deg}

TABLE I. Difference between the exact energy and variational energy for the lowest seniority-zero state. N is the number of particles, ΔE_{deg} is the error when the single-particle levels are all degenerate, and $G=0.331$ Mev for nickel, 0.187 Mev for tin, and 0.111 Mev for lead. ΔE represents the error, for the same values of G , when the states are not degenerate. For nickel the energies of the single-particle levels are taken to be $\epsilon(p_{3/2})=0$, $\epsilon(f_{5/2})=0.78$ Mev, $\epsilon(p_{1/2})=1.56$ Mev, and $\epsilon(g_{9/2})=4.52$ Mev; for tin $\epsilon(d_{5/2})=0$, $\epsilon(g_{7/2})=0.22$ Mev, $\epsilon(s_{1/2})=1.90$ Mev, $\epsilon(d_{3/2})=2.20$ Mev, and $\epsilon(h_{11/2})=2.80$ Mev; and for lead the energies of the hole states are $\epsilon(p_{1/2})=0$, $\epsilon(f_{5/2})=0.57$ Mev, $\epsilon(p_{3/2})=0.90$ Mev, $\epsilon(i_{13/2})=1.634$ Mev, and $\epsilon(f_{7/2})=2.35$ Mev.

N	Nickel		Tin		Lead	
	ΔE (Mev)	ΔE_{deg} (Mev)	ΔE (Mev)	ΔE_{deg} (Mev)	ΔE (Mev)	ΔE_{deg} (Mev)
± 2	-0.367	-0.301			-0.187	-0.108
± 4	-0.601	-0.542	-0.313	-0.327	-0.205	-0.209
± 6	-0.645	-0.722	-0.382	-0.456	-0.295	-0.304
± 8	-0.752	-0.843	-0.691	-0.561	-0.342	-0.392
± 10	-0.781	-0.903	-0.693	-0.643	-0.260	-0.473

¹⁴ B. F. Bayman, Nuclear Phys. **15**, 33 (1960).

are due entirely to the presence in the trial wave function of components with the wrong number of particles.

4. COMPARISON OF EXACT AND APPROXIMATE SOLUTIONS

We now compare the exact solutions of the pairing Hamiltonian with the results of an approximate calculation¹ which seeks to replace the original interacting particles by noninteracting "quasi-particles." These quasi-particles (normal modes of the system) are introduced by a canonical transformation whose parameters are determined, in principle, by minimizing the energy.¹⁵ The seniority-zero ground state of an even-even nucleus is then identified with the quasi-particle vacuum $|\phi_0\rangle$ whose wave function and energy are

$$|\phi_0\rangle = \prod_{j,m>0} [(1 - V_j^2)^{\frac{1}{2}} + V_j S_+^{jm}] |0\rangle, \quad (13)$$

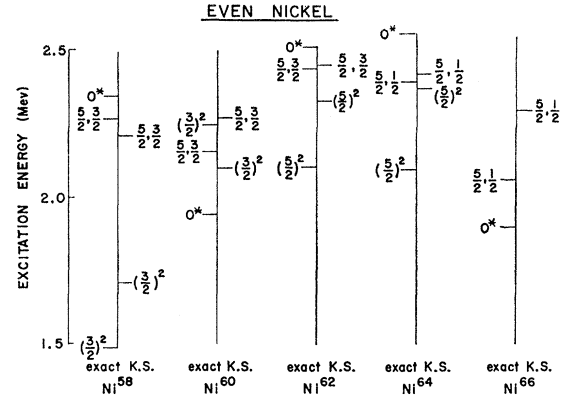


FIG. 1. Low-lying excited states in the even-even nickel isotopes. The notation $(\frac{5}{2})_2$, etc. denotes the single-particle levels occupied by the unpaired particles, while 0^+ labels the first excited seniority-zero state. The columns labeled "exact" are those obtained from diagonalizing the energy matrices. The entries above K. S. are those determined from the calculations of Kisslinger and Sorensen. The coupling constant G was taken to be 0.331 Mev and the positions of the single-particle levels were chosen as $\epsilon(p_{3/2})=0$, $\epsilon(f_{5/2})=0.78$ Mev, $\epsilon(p_{1/2})=1.56$ Mev, and $\epsilon(g_{9/2})=4.52$ Mev.

and

$$E_0 = 2 \sum_j \Omega^j \epsilon_j V_j^2 - \frac{1}{G} \Delta^2 - G \sum_j \Omega^j V_j^4, \quad (14)$$

the probability amplitudes V_j being given by

$$V_j^2 = \frac{1}{2} \{ 1 - (\epsilon_j - \lambda) [(\epsilon_j - \lambda)^2 + \Delta^2]^{-\frac{1}{2}} \}. \quad (15)$$

The Lagrange multiplier λ and the "gap" parameter Δ are obtained from the equations

$$2 \sum_j \Omega^j V_j^2 = n, \quad (16)$$

$$\frac{1}{2} G \sum_j \{ \Omega^j / [(\epsilon_j - \lambda)^2 + \Delta^2]^{\frac{1}{2}} \} = 1. \quad (17)$$

The seniority-one states, which lie lowest in odd- A nuclei, are described in the approximate calculation by

¹⁵ The variational aspects of the approximate calculation of Kisslinger and Sorensen (reference 1) are discussed in Sec. 5.

exciting a single quasi-particle. If the unpaired nucleon is in level j , the energy of such a state is

$$E_1 = E_0 + E_j, \quad (18)$$

where E_j , the excitation energy of a quasi-particle, is given by

$$E_j = [(\epsilon_j - \lambda)^2 + \Delta^2]^{1/2}. \quad (19)$$

Kisslinger and Sorensen again obtain λ and Δ from Eqs. (16) and (17), with the appropriate (odd) value in Eq. (16) for n , the number of particles in the levels under consideration. (See Sec. 5.)

Seniority-two excited states of even-even nuclei are approximated by exciting two quasi-particles. If the unpaired nucleons are in levels j_1 and j_2 , the energy of such a state is

$$E_2 = E_0 + E_{j_1} + E_{j_2}, \quad (20)$$

with the values of λ and Δ determined for the ground-state configuration.

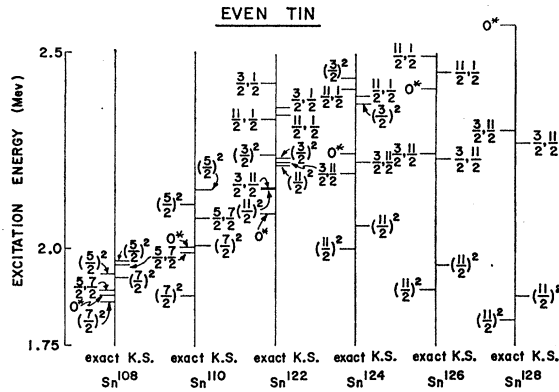


FIG. 2. Low-lying excited states in the even-even tin isotopes deduced from Kisslinger and Sorensen's calculation (K. S.) and the exact calculation. The coupling constant G is 0.187 Mev and the energies of the single-particle levels were taken as $\epsilon(d_{5/2})=0$, $\epsilon(g_{7/2})=0.22$ Mev, $\epsilon(s_{1/2})=1.90$ Mev, $\epsilon(d_{3/2})=2.20$ Mev, and $\epsilon(h_{11/2})=2.80$ Mev.

The exact and approximate solutions for many of the isotopes of Ni, Sn, and Pb have been compared. We now discuss this comparison, starting with the even-even nuclei.

In Table I we have listed the errors ΔE in the energy of the even-even ground states. It will be seen that these differ very little from the energy errors ΔE_{deg} of the degenerate model. Figures 1-3 show the exact and approximate excitation energies of states of seniority two, the corresponding absolute energies¹⁶ involving errors no more than 200 kev larger than those given in Table I. It is clear that Kisslinger and Sorensen's calculation provides a fairly close approximation to the

¹⁶ For some of the more highly excited states the approximate energy is actually less than the exact energy. This merely reflects the fact that for states of two- (and one-) quasi particles, the calculation of Kisslinger and Sorensen is only approximately variational.

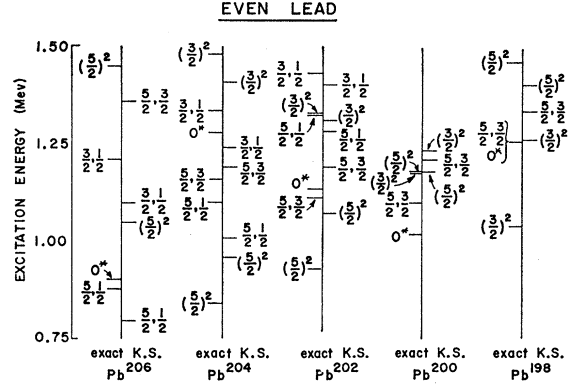


FIG. 3. Low-lying excited states in the even-even lead isotopes. The columns labeled "exact" are the excitation energies obtained from this calculation, while those marked K. S. are the results of the Kisslinger-Sorensen theory. The coupling constant G was taken to be 0.111 Mev and the energies of the hole states are $\epsilon(p_{1/2})=0$, $\epsilon(f_{5/2})=0.57$ Mev, $\epsilon(p_{3/2})=0.90$ Mev, $\epsilon(i_{13/2})=1.634$ Mev, and $\epsilon(f_{7/2})=2.35$ Mev.

order and to the excitation energies of low-lying states of seniority two.

Figures 1-3 also show the position of the lowest-excited state of seniority zero, concerning which the approximate calculation can say nothing. Such states might lie sufficiently low to destroy the gap in the spectrum of intrinsic excitations, whose prediction has been the chief physical argument in favor of the pairing Hamiltonian.⁵ Figures 1-3 show that no such attribution of the energy gap occurs. Although the lowest-excited state of seniority zero is sometimes below all states of seniority two,¹⁷ a gap is clearly in evidence in each of the exact excitation spectra and, furthermore the magnitude of this gap is quite close to 2Δ .

For the energies of seniority-one states in odd- A nuclei, agreement is again satisfactory (Figs. 4-6). In particular, the approximate calculation gives the correct ordering of the levels, except in a few cases (for example, in Ni^{61} , Ni^{65} , Pb^{203} , and Pb^{205}) in which it inverts pairs of states that are nearly degenerate in the exact calculation.

In the typical cases, only about 40% of the trial-wave function of Eq. (13) (or its appropriate modification for states of seniority one or two) describes a system with the desired number of particles. To compare the exact and approximate eigenfunctions, we therefore project out that part of the trial wave function that corresponds to the correct number of particles and normalize to unity. The resulting wave functions for the seniority-one states of Ni^{59} are given in Table II. The similarity between the exact and approximate eigenfunctions is striking, with overlap integrals greater than 0.99 in each

¹⁷ The first excited seniority-zero state is particularly low when a subshell is filled. To understand this, consider two levels j_1 and j_2 , with $\epsilon_{j_1} < \epsilon_{j_2}$. We simulate the relationship between the two lowest states of seniority zero by considering $j_1^{n_1} j_2^{n_2}$ and $j_1^{n_1-2} j_2^{n_2+2}$. The separation of these states and also the interaction matrix element between them is smallest when $n_2=0$ and $n_1=2j_1+1$ so that there is a subshell effect of the kind under consideration.

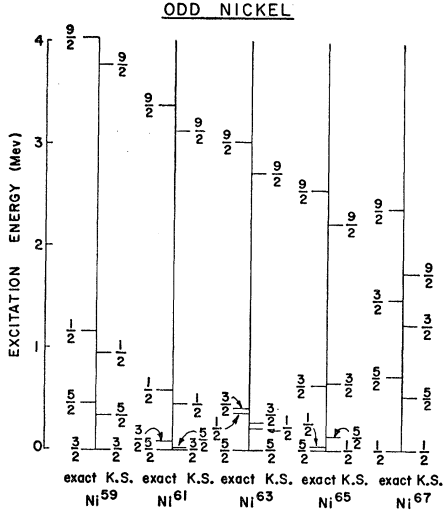


FIG. 4. The seniority-one states in the odd nickel isotopes. The notation $5/2^-$, etc., represents the spin of the state. The columns labeled "exact" are those obtained from diagonalizing the energy matrices, and the entries above K. S. are the states determined from Kisslinger and Sorensen's calculation. The coupling constant G and the single-particle energies are the same as used in constructing Fig. 1.

case. Similar excellent agreement is obtained for the ground states of even-even nuclei and also for the excited states of seniority two. For example, the two quasi-particle excited states of Ni^{60} with the largest and smallest energy errors are, respectively, the $(5/2, 3/2)$ and the $(9/2, 1/2)$ states. For the former, the overlap integral between exact and approximate wave functions is 0.982, for the latter it is 0.999.

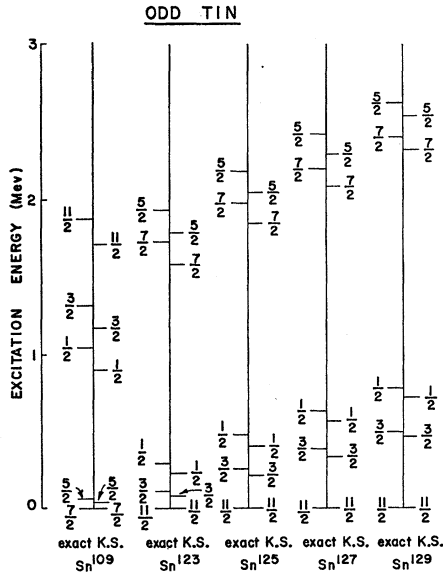


FIG. 5. The seniority-one states in the odd tin isotopes deduced from Kisslinger and Sorensen's calculation (K. S.) and the exact calculation. The coupling constant G and the single-particle energies are the same as used in constructing Fig. 2.

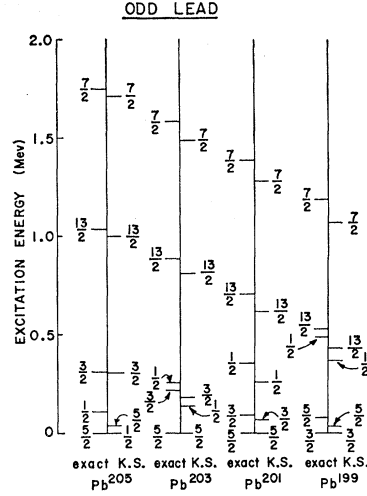


FIG. 6. The seniority-one states in the odd lead isotopes. The columns labeled "exact" list the states obtained from this calculation, while those marked K. S. are the results of the Kisslinger-Sorensen theory. The coupling constant G and the hole energies are the same as used in constructing Fig. 3.

Since the projected-wave functions are almost identical to the true energy eigenfunctions, it is clear that if we use them to evaluate expectation values of the Hamiltonian, the resulting approximation to the energies will be very much better than that provided by the original trial-wave function. As an illustration we have done this calculation for Ni^{59} . The results are given in Table III, where it is seen that the exact- and quasi-particle energies are almost identical. Thus, to calculate matrix elements of physical quantities, we should use the wave functions obtained by projecting out and normalizing the parts of the original trial-wave functions corresponding to the correct number of particles. This procedure has already been suggested by Bayman,¹⁴ and is in accordance with the general theorem that a trial-wave function can always be improved by projecting from it the parts containing known good quantum numbers.

5. VARIATIONAL ASPECTS OF THE SUPERCONDUCTIVITY APPROXIMATION

As is well known, the superconductivity approximation for states of seniority zero consists in selecting the wave function $|\phi_0\rangle$ of Eq. (13) as a trial function and minimizing $\langle\phi_0|H|\phi_0\rangle$ as a function of the parameters V_j , subject to the constraint

$$\langle\phi_0|N|\phi_0\rangle = n. \quad (21)$$

By introducing a Lagrange multiplier λ , the solution of this variational problem is obtained from Eq. (21) and the set of equations

$$\frac{\partial}{\partial V_j} \langle\phi_0|H - \lambda N|\phi_0\rangle = 0. \quad (22)$$

This leads directly to Eqs. (15) and (16).¹⁸

¹⁸ Strictly $\epsilon_j \rightarrow \epsilon_j - GV_j^2$ in Eqs. (15)–(17), and (19). Although the additional term $-GV_j^2$ has an appreciable effect on λ and Δ , its influence on energies and wave functions is negligible.

TABLE II. The amplitudes of the various components in the seniority-one wave functions in Ni⁵⁹. The last column is the overlap integral between the quasi-particle and exact wave functions. In the notation used, the exact wave function of, for example, the 3/2 state is $0.812 (p_{3/2})_{3/2} + 0.526 (f_{5/2})_0 p_{3/2} + 0.187 (p_{1/2})_0 p_{3/2} + 0.170 (g_{9/2})_0 p_{3/2}$.

	State	$(p_{3/2})^2$	$(f_{5/2})^2$	$(p_{1/2})^2$	$(g_{9/2})^2$	Overlap
$p_{3/2}$	Exact	0.812	0.526	0.187	0.170	0.993
	Quasi-particle	0.737	0.614	0.216	0.183	
$f_{5/2}$	Exact	0.885	0.394	0.179	0.170	0.999
	Quasi-particle	0.876	0.421	0.181	0.153	
$p_{1/2}$	Exact	0.858	0.484		0.174	0.999
	Quasi-particle	0.852	0.501		0.149	
$g_{9/2}$	Exact	0.837	0.488	0.185	0.161	0.999
	Quasi-particle	0.841	0.495	0.174	0.132	

In considering states of seniority one, Kisslinger and Sorensen determine the energies from Eqs. (18) and (19), obtaining the parameters λ and Δ from the *same equations*¹⁹ [Eqs. (16) and (17)] as are used for states of seniority zero. Strictly, a fresh variation calculation should be carried out, the appropriate modification of Eq. (13) being

$$|\psi_{j_1 m_1}\rangle = \prod'_{j, m > 0} [(1 - V_j^2)^{\frac{1}{2}} + V_j S_+^{j m}] a_{j_1 m_1}^\dagger |0\rangle, \quad (23)$$

where \prod' indicates a product over all j, m with the exception of $j_1 m_1$. Carrying out this variational calculation, we find that for $j \neq j_1$, V_j^2 is again given by Eq. (15). For $j = j_1$, we have instead

$$V_{j_1}^2 = \frac{1}{2} \{1 - (\bar{\epsilon}_{j_1} - \lambda) [(\bar{\epsilon}_{j_1} - \lambda)^2 + \Delta^2]^{-\frac{1}{2}}\}, \quad (24)$$

with

$$\bar{\epsilon}_{j_1} = \epsilon_{j_1} + \frac{1}{2} G - 2 G V_{j_1}^2. \quad (25)$$

The parameters λ and Δ (we now have different ones for each level j) are obtained from Eq. (16) and the appropriate modification of Eq. (17) is,

$$2 \sum_j \Omega_j V_j^2 + (1 - 2 V_{j_1}^2) = n. \quad (26)$$

In the special case $j_1 = \frac{1}{2}$, the energy is independent of V_{j_1} as is obvious from the fact that the trial function [Eq. (23)] then does not involve V_{j_1} . We have in fact

$$E_{\frac{1}{2}} = 2 \sum_j' \Omega_j \epsilon_j V_j^2 - (1/G) \Delta'^2 - G \sum_j' \Omega_j V_j^4, \quad (27)$$

where the primes indicate that all relevant summations are to be carried out as if the $j = \frac{1}{2}$ level did not exist.

The variational calculation for states of seniority one is much more laborious than it was for seniority zero,

¹⁹ This involves, for example, the neglect of additional one-quasi-particle contributions to the number operator.

TABLE III. The energies of the various seniority-one states in Ni⁵⁹ calculated exactly, by the quasi-particle theory, by a variational procedure, and by projecting out (and normalizing) that part of the approximate-wave function that corresponds to the desired number of particles. The single-particle energies were taken to be $\epsilon(p_{3/2}) = 0$, $\epsilon(f_{5/2}) = 0.78$ Mev, $\epsilon(p_{1/2}) = 1.56$ Mev, and $\epsilon(g_{9/2}) = 4.52$ Mev, and $G = 0.331$ Mev.

State	Exact energy (Mev)	Quasi-particle energy (Mev)	Variational energy (Mev)	Projected energy (Mev)
$p_{3/2}$	-0.93	-0.48	-0.54	-0.91
$f_{5/2}$	-0.47	-0.14	-0.13	-0.47
$p_{1/2}$	0.23	0.47	0.56	0.24
$g_{9/2}$	3.10	3.28	3.32	3.13

since there is now a different value of λ and of Δ for each level. Table III lists the variational and Kisslinger-Sorensen energies of seniority-one states in Ni⁵⁹. It is clear that the differences are too small to be of any practical importance. The corresponding wave functions also agree closely.²⁰ We may therefore regard the procedure of Kisslinger and Sorensen as a numerically simpler and satisfactorily accurate way of performing a variational calculation for states of seniority one. It also seems likely that the simplified procedure provides an adequate treatment of states of seniority two.

6. CONCLUSIONS

Recent work on the theory of superconductivity has suggested that pairing forces between identical nucleons might profitably be studied by a variational procedure, with a trial-wave function that is not an eigenstate of the particle-number operator. We have studied the accuracy of such variational calculations and have shown that projecting out and normalizing that part of the trial-wave function that corresponds to the correct number of particles yields a remarkably close approximation to the true energy eigenfunction. It is therefore clear that the projected-wave function should be used to calculate the matrix elements of operators of physical interest. In particular, the expectation values of the pairing Hamiltonian are found to agree closely with the exact energy eigenvalues.

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²⁰ The values of λ and Δ , however, vary considerably from level to level, and differ appreciably from the values obtained by Kisslinger and Sorensen.