PHYSICAL REVIEW VOLUME 135, NUMBER 1B 13 JULY 1964

Conservation of Particle Number in the Nuclear Pairing Model*

KLAUS DIETRICH, HANS J. MANG, AND JEAN H. PRADAL
Lawrence Radiation Laboratory, University of California, Berkeley, California

(Received 13 January 1964; revised manuscript received 26 February 1964)

The Euler–Lagrange equations corresponding to a Bardeen–Cooper–Schrieffer state that is an eigenstate of the number operator are derived and solved numerically for a δ interaction. The errors due to the nonconservation of particle number in the usual Bardeen–Cooper–Schrieffer theory are studied as a function of particle number, level density, and strength of the pairing interaction. A proof is given that for attractive pairing interactions the lowest energy solution corresponds always to real positive probability amplitudes v_ν, u_ν.

I. INTRODUCTION

When the theory of superconductivity had been developed,[1,2] it was pointed out very early by Bohr, Mottelson, and Pines, that this theory might also be a useful tool in nuclear physics.[3] Several authors have applied the theory to heavy and medium-heavy nuclei and have obtained encouraging results on the basis of a simple constant pairing interaction.[4–8] In both formulations of the theory of superconductivity, the particle number is not conserved; only the expectation value of the number operator is kept equal to the required particle number.

One can easily project from the Bardeen-Cooper-Schrieffer (BCS) state an eigenstate of the number operator.[9] Bayman showed that starting from such an eigenstate of the number operator, we are led back to the BCS treatment as long as we evaluate the entering expectation values with the saddle-point method.[9] A crude estimate shows that the saddle-point method can be trusted as long as the number of levels that are neither empty nor fully occupied is large compared to one.[9] For applications of the theory in nuclear physics this condition is generally poorly fulfilled. Besides Bayman, Blatt considered trial wave functions of the BCS type that conserve the particle number.[10]

Kerman, Lawson, and Macfarlane compared the results of the superconductivity model with the results of an exact diagonalization assuming again a constant pairing interaction.[11] This investigation showed the results of the superconductivity model to be in remarkably good agreement with the results obtained by an exact diagonalization, even for small particle numbers. Several papers related to our topic have been published this year and have just become known to us.[12–15]

In a recent paper Högaasen-Feldman investigated the components in the ground and first excited states of the pairing model that correspond to different numbers of particles.[16] Meanwhile, various pairing-model calculations have been performed with more realistic forces such as δ forces,[17] δ plus quadrupole forces,[17] and finite range forces,[18,19] also taking into account the effect of the residual interactions on the Hartree-Fock field. In view of this increasing number of applications, it seemed worthwhile to study more widely the errors expected as a result of the nonconservation of particle number, formulating the pairing model consistently with conservation of particle number and comparing the final results with those of the BCS method.

In Sec. II, we derive the variational equations corresponding to a BCS state that conserves particle number.

In Sec. III, we generalize this treatment to odd numbers of nucleons. In Sec. IV, we show that use of the saddle-point method for the evaluation of the contour integrals leads us back to the usual superconductivity treatment. This, of course, can already be found in Bayman's paper.[9] We include the proof for the sake of completeness.

In Sec. V, we present results obtained from a numerical solution of our variational equations and compare them with the corresponding results of the BCS treatment.

---

* Work done under the auspices of the U. S. Atomic Energy Commission.

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

[2] N. N. Bogoliubov, Zh. Eksperim. i Teor. Fiz. **34**, 58 (1958) [English transl.: Soviet Phys.—JETP **7**, 41 (1958)].

[3] A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev. **110**, 936 (1958).

[4] S. T. Beliaev, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **31**, No. 11 (1958).

[5] V. G. Soloviev, Nucl. Phys. **9**, 655 (1959); Nuovo Cimento **10**, 1022 (1958).

[6] L. S. Kisslinger and R. A. Sorensen, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **32**, No. 9 (1960).

[7] N. Glendenning and J. Sawicki, Nucl. Phys. **18**, 596 (1960).

[8] S. G. Nilsson and O. Prior, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **32**, No. 16 (1961).

[9] B. F. Bayman, Nucl. Phys. **15**, 33 (1960).

[10] J. M. Blatt, Progr. Theoret. Phys. (Kyoto) **24**, 851 (1960) (with references to earlier work).

[11] A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. **124**, 162 (1961).

[12] A. Pavlikovsky and B. Rybasska, Dubna Report R–932, 1963 (unpublished).

[13] M. K. Volkov, A. Pavlikovski, B. Bybasska, and V. G. Soloviev, Dubna Report E–1154, 1963 (unpublished).

[14] S. G. Nilsson, Lund Institute of Technology (to be published).

[15] R. W. Richardson, Phys. Letters **3**, 277 (1963); **7**, 82 (1963).

[16] J. Högaasen-Feldman, Nuovo Cimento **29**, 428 (1963).

[17] H. J. Mang and J. O. Rasmussen, Bull. Am. Phys. Soc. **7**, 615 (1962).

[18] R. Arvieu, Elisabeth Baranger, M. Veneroni, M. Baranger, and V. Gillet, Phys. Letters **4**, 119 (1963).

[19] K. Dietrich, H. J. Mang, and J. Pradal, Nucl. Phys. (to be published).

The Appendix contains proof that we can restrict the variational parameters of the BCS state to real positive quantities without loss of generality.

II. THE EULER-LAGRANGE EQUATIONS CORRESPONDING TO A BCS STATE THAT CONSERVES PARTICLE NUMBER

In occupation number representation, the Hamiltonian for one sort of interacting nucleons has the form

$$H=\sum_{\pm\nu}\epsilon_\nu a_\nu{}^\dagger a_\nu+\sum_{\pm(\nu_1,\nu_2,\nu_3,\nu_4)} V_{\nu_1\nu_2\nu_3\nu_4} a_{\nu_1}{}^\dagger a_{\nu_2}{}^\dagger a_{\nu_4} a_{\nu_3}\,, \quad (2.1)$$

in which $a_\nu{}^\dagger$ and a_ν are creation and annihilation operators, respectively, of particles in state ν; ϵ_ν are single-particle energies that should contain a part of the real nucleon-nucleon (N-N) interaction;

$$V_{\nu_1\nu_2\nu_3\nu_4}=\tfrac{1}{4}\langle\nu_1\nu_2|v|\nu_3\nu_4\rangle\,,$$

where $\langle\nu_1\nu_2|v|\nu_3\nu_4\rangle$ is the matrix element of the N-N interaction between antisymmetrized and normalized products of single-particle wave functions; and ν stands for the set of quantum numbers that define a single-particle state in the chosen representation. Using the j-coupling scheme we have

$$\nu\equiv(\sigma,j,m>0)\,,$$
$$-\nu\equiv(\sigma,j,m<0)\,,$$

where j = total angular momentum, m = magnetic quantum number, σ = any additional quantum numbers that characterize the state. The distinction between states with positive and negative magnetic quantum numbers is, of course, merely a matter of convenience. We choose a representation in which the Hamiltonian without interaction is diagonal. We may think of the single-particle energies ϵ_ν as discrete energy levels of either a harmonic oscillator or a more realistic single-particle potential.

Furthermore, we use a phase convention that is particularly convenient in the BCS theory.[8] It can be related to the usual phase convention of Condon and Shortly[20] in the following way: All single-particle states with negative magnetic quantum number $m<0$ differ from the corresponding states in the Condon-Shortley (CS) convention by a factor $(-)^{j+l+m}$ (l = orbital angular momentum),

$$|jlm\rangle=(-1)^{j+l+m}|jlm\rangle_{\mathrm{CS}} \quad \text{for} \quad m<0\,, \quad (2.1')$$

$$|jlm\rangle=|jlm\rangle_{\mathrm{CS}} \quad \text{for} \quad m>0\,. \quad (2.1'')$$

We describe the system by a trial state Ψ that we obtain by projecting from the BCS state an eigenstate of the number operator N,

$$N=\textstyle\sum_{\pm\nu} a_\nu{}^\dagger a_\nu\,. \quad (2.2)$$

This state Ψ can be written in the form[9,21]

$$\Psi=C\oint d\zeta\,\zeta^{-n_0-1}\prod_\nu (u_\nu+v_\nu\zeta a_\nu{}^\dagger a_\nu{}^\dagger)\Phi_0\,, \quad (2.3)$$

where Φ_0 is the vacuum state, n_0 is the number of nucleon pairs, and C is a normalization constant that we define by requiring

$$\langle\Psi|\Psi\rangle=1\,, \quad (2.4)$$

or

$$|C|^2=1/(-4\pi^2)R_0{}^0\,.$$

[For the definition of $R_0{}^0$ see Eq. (2.8).] The contour may be any closed path around the origin.

For interactions that exhibit negative pairing-type matrix elements we obtain the lowest energy solution for real positive u_ν and v_ν. (For proof see Appendix A.) Furthermore, we may require

$$u_\nu{}^2+v_\nu{}^2=1 \quad (2.5)$$

(see Appendix A). Henceforth, we will therefore consider the u_ν and v_ν as real positive quantities, subject to condition (2.5). We wish to remark at this point that the total energy

$$E=\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle \quad (2.6)$$

remains unchanged if we multiply all the quotients v_ν/u_ν by a common factor x. Thus, even with (2.5) holding, the set of parameters u_ν, v_ν is not uniquely defined by the variational problem (see Appendix A).

Next we ask for the Euler-Lagrange equations that must be fulfilled as a necessary condition for $\langle\Psi|H|\Psi\rangle$ to be stationary. The variations of Ψ are restricted by the subsidiary conditions (2.4) and (2.5). Disposing of the restrictive condition (2.4) by the use of a Lagrangian multiplier, we have to deal with the variational problem,

$$\delta\{\langle\Psi|H|\Psi\rangle-E\langle\Psi|\Psi\rangle\}=0\,. \quad (2.7)$$

We define the following functions as residues of simple contour integrals in the complex plane:

$$R_n{}^N(\nu_1,\cdots,\nu_N)$$
$$=\frac{1}{2\pi i}\oint dz z^{-(n_0-n)-1}\textstyle\prod_{\nu\neq\nu_1,\cdots,\nu_N}(u_\nu{}^2+zv_\nu{}^2)\,. \quad (2.8)$$

In this paper we shall sometimes refer to these functions as "residuum integrals." The N states listed in parentheses are those that are to be excluded from the product $\prod_\nu(u_\nu{}^2+v_\nu{}^2z)$. For $N=0$ the product contains N_0 different factors $(u_\nu{}^2+zv_\nu{}^2)$. Physically, N_0 is the finite number of pair states $(\nu,-\nu)$ that we take into consideration in a given problem. In Appendix B, we have put together some useful mathematical properties of the functions $R_n{}^N(\nu_1,\cdots,\nu_n)$. By definition, we put

---

[20] E. V. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, New York, 1959), p. 48.

[21] If not mentioned differently the indices are always supposed to run only over positive values of the magnetic quantum number.

residuum integrals that contain any pair of equal arguments equal to zero. Using the residuum integrals (2.8), we can write the total energy E as

$$E=2\sum_{\nu}\epsilon_\nu v_\nu^2 R_1^1(\nu)/R_0^0+4\sum_{\nu}V_{\nu-\nu\nu-\nu}v_\nu^2 R_1^1(\nu)/R_0^0$$
$$+4\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}^2 v_{\nu_2}^2 R_2^2(\nu_1,\nu_2)/R_0^0$$
$$+4\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}u_{\nu_2}v_{\nu_2}R_1^2(\nu_1\nu_2)/R_0^0. \qquad (2.9)$$

In this formulation we have assumed

$$\epsilon_\nu=\epsilon_{-\nu}. \qquad (2.10)$$

The sums are extended only over states with positive magnetic quantum numbers. Variation of (2.9) with respect to v_ν and u_ν, with condition (2.5) holding, leads to the set of equations

$$(\hat{\epsilon}_\nu+\Gamma_\nu+\Lambda_\nu)u_\nu v_\nu+\Delta_\nu(u_\nu^2-v_\nu^2)=0. \qquad (2.11)$$

The quantities $\hat{\epsilon}_\nu$, Γ_ν, Λ_ν, Δ_ν are defined as follows:

$$\hat{\epsilon}_\nu=(\epsilon_\nu+2V_{\nu-\nu\nu-\nu})[R_1^1(\nu)]/R_0^0, \qquad (2.12)$$

$$\Gamma_\nu=4\sum_{\nu_1}(V_{\nu\nu_1\nu\nu_1}+V_{\nu-\nu_1\nu-\nu_1})v_{\nu_1}^2[R_2^2(\nu_1\nu)]/R_0^0, \qquad (2.13)$$

$$\Delta_\nu=2\sum_{\nu_1}V_{\nu-\nu\nu_1-\nu_1}u_{\nu_1}v_{\nu_1}[R_1^2(\nu_1\nu)]/R_0^0, \qquad (2.14)$$

$$\Lambda_\nu=\sum_{\nu_1}(\epsilon_\nu+2V_{\nu_1-\nu_1\nu_1-\nu_1})v_{\nu_1}^2\frac{R_0^1(\nu)R_2^2(\nu_1\nu)-R_1^1(\nu)R_1^2(\nu_1\nu)}{(R_0^0)^2}$$
$$+2\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}^2 v_{\nu_2}^2\frac{R_0^1(\nu)R_3^3(\nu_1\nu_2\nu)-R_1^1(\nu)R_2^3(\nu_1\nu_2\nu)}{(R_0^0)^2}$$
$$+2\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}u_{\nu_2}v_{\nu_2}\frac{R_0^1(\nu)R_2^3(\nu_1\nu_2\nu)-R_1^1(\nu)R_1^3(\nu_1\nu_2\nu)}{(R_0^0)^2}+[\hat{\epsilon}_\nu v_\nu^2+\Gamma_\nu v_\nu^2+2\Delta_\nu u_\nu v_\nu]\frac{R_0^1(\nu)-R_1^1(\nu)}{R_0^0}. \qquad (2.15)$$

The quantities Γ_ν and Δ_ν are the Hartree-Fock and pairing potentials that appear in an analogous way in the BCS method. In our formulation the term with the diagonal matrix element $V_{\nu-\nu\nu-\nu}$ is included in the single-particle energy $\hat{\epsilon}_\nu$ (see 2.12), since it contains the same residuum integral as the single-particle energies. This is merely a matter of convenience. In Sec. V we shall rearrange the terms in such a way that they immediately yield the corresponding quantities of the BCS theory when the saddle-point method is applied.

The quantity Λ_ν has no counterpart in the equations of the BCS theory, which contains instead a constant chemical potential. This potential is chosen so as to make the expectation value of the number operator equal to the required particle number. In the derivations of the Eqs. (2.11) the quantity Λ_ν arises from the differentiation of the residuum integrals with respect to v_ν and u_ν (see Appendix B). In the formulation (2.15) the recursion relations (B1) and (B2) have been used.

An equivalent formulation of Λ_ν is

$$\Lambda_\nu=\sum_{\nu_1}(\epsilon_{\nu_1}+2V_{\nu_1-\nu_1\nu_1-\nu_1})v_{\nu_1}^2\frac{R_2^2(\nu_1\nu)-R_1^2(\nu_1\nu)}{R_0^0}+2\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}^2 v_{\nu_2}^2\frac{R_3^3(\nu_1\nu_2\nu)-R_2^3(\nu_1\nu_2\nu)}{R_0^0}$$
$$+2\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}u_{\nu_2}v_{\nu_2}\frac{R_2^3(\nu_1\nu_2\nu)-R_1^3(\nu_1\nu_2\nu)}{R_0^0}-\tfrac{1}{2}E\frac{R_1^1(\nu)-R_0^1(\nu)}{R_0^0}, \qquad (2.16)$$

where E is the total energy given by (2.9).

In the usual superconductivity theory, v_ν^2 is the probability for the pair of states $(\nu, -\nu)$ being occupied, and u_ν^2 is the probability for this pair being unoccupied. This is no longer true in our treatment.

Let us call e_ν^2 the probability of occupation, f_ν^2 the probability of nonoccupation of a pair of states $(\nu, -\nu)$. Then

$$\epsilon_\nu^2=\langle\Psi|(a_\nu a_{-\nu})^\dagger a_\nu a_{-\nu}|\Psi\rangle=v_\nu^2[R_1^1(\nu)]/R_0^0, \qquad (2.17)$$

$$f_\nu^2=1-e_\nu^2=u_\nu^2[R_0^1(\nu)]/R_0^0. \qquad (2.18)$$

Of course, the sum of the occupation probabilities is equal to n_0, the number of pairs of particles

$$\sum_{\nu}^{N_0}e_\nu^2=n_0.$$

III. BLOCKING IN THE THEORY WITH CONSERVED PARTICLE NUMBER

The pairing model has been extended to systems with an odd number of particles by blocking one of the available pair states.[8,22] In our theory with conserved particle number, a system with an odd number of particles will be described by the state

$$\Psi_{\bar{\nu}}=C\oint d\zeta\zeta^{-n_0-1}a_{\bar{\nu}}^{\dagger}\prod_{\nu\neq\bar{\nu}}(u_\nu+v_\nu\zeta a_\nu^{\dagger}a_{-\nu}^{\dagger})\Phi_0. \quad (3.1)$$

Of course, C is again the normalization constant given by

$$|C|^2=[(-4\pi^2)R_0^1(\bar{\nu})]^{-1}, \quad (3.2)$$

n_0 is the number of pairs, the total particle number being $(2n_0+1)$. The quantum state $\bar{\nu}$ is occupied by the odd nucleon. The formulas that we will obtain, starting from state (3.1) can be almost guessed without calculation: All residuum integrals will contain the additional argument $\bar{\nu}$, which means that this state is never available to any pair of particles. The interaction of a pair of particles with the odd nucleon will be represented by a special term that will modify the definitions of the quantities $\hat{\epsilon}_\nu$ and Λ_ν. The total energy E has the form

$$E=2\textstyle\sum_\nu \epsilon_\nu v_\nu^2\dfrac{R_1^2(\bar{\nu}\nu)}{R_0^1(\bar{\nu})}+\epsilon_{\bar{\nu}}+4\textstyle\sum_\nu V_{\nu-\nu\nu-\nu}v_\nu^2\dfrac{R_1^2(\bar{\nu}\nu)}{R_0^1(\bar{\nu})}$$
$$+4\textstyle\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}^2v_{\nu_2}^2\dfrac{R_2^3(\bar{\nu}\nu_1\nu_2)}{R_0^1(\bar{\nu})}$$
$$+4\textstyle\sum_{\nu_1}(V_{\bar{\nu}\nu_1\bar{\nu}\nu_1}+V_{\bar{\nu}-\nu_1\bar{\nu}-\nu_1})v_{\nu_1}^2\dfrac{R_1^2(\bar{\nu}\nu_1)}{R_0^1(\bar{\nu})}$$
$$+4\textstyle\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}u_{\nu_2}v_{\nu_2}\dfrac{R_1^3(\bar{\nu}\nu_1\nu_2)}{R_0^1(\bar{\nu})}. \quad (3.3)$$

The Euler-Lagrange equations have the form (2.11), with the coefficients

$$\hat{\epsilon}_\nu=(\epsilon_\nu+2V_{\nu-\nu\nu-\nu})R_1^2(\bar{\nu}\nu)/R_0^1(\bar{\nu})$$
$$+2(V_{\bar{\nu}\nu\bar{\nu}\nu}+V_{\bar{\nu}-\nu\bar{\nu}-\nu})R_1^2(\bar{\nu}\nu)/R_0^1(\bar{\nu}), \quad (3.4)$$

$$\Gamma_\nu=4\sum_{\nu_1}(V_{\nu\nu_1\nu\nu_1}+V_{\nu-\nu_1\nu-\nu})v_{\nu_1}^2[R_2^3(\bar{\nu}\nu_1\nu)]/R_0^1(\bar{\nu}), \quad (3.5)$$

$$\Delta_\nu=2\sum_{\nu_1}V_{\nu-\nu\nu_1-\nu_1}u_{\nu_1}v_{\nu_1}R_1^3(\bar{\nu}\nu_1\nu)/R_0^1(\bar{\nu}), \quad (3.6)$$

$$\Lambda_\nu=\sum_{\nu_1}(\epsilon_{\nu_1}+2V_{\nu_1-\nu_1\nu_1-\nu_1})v_{\nu_1}^2\frac{R_2^3(\bar{\nu}\nu_1\nu)-R_1^3(\bar{\nu}\nu_1\nu)}{R_0^1(\bar{\nu})}+2\sum_{\nu_1}(V_{\bar{\nu}\nu_1\bar{\nu}\nu_1}+V_{\bar{\nu}-\nu_1\bar{\nu}-\nu_1})v_{\nu_1}^2\frac{R_2^3(\bar{\nu}\nu_1\nu)-R_1^3(\bar{\nu}\nu_1\nu)}{R_0^1(\bar{\nu})}$$
$$+2\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}^2v_{\nu_2}^2\frac{R_3^4(\bar{\nu}\nu_1\nu_2\nu)-R_3^4(\bar{\nu}\nu_1\nu_2\nu)}{R_0^1(\bar{\nu})}$$
$$+2\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}u_{\nu_2}v_{\nu_2}\frac{R_2^4(\bar{\nu}\nu_1\nu_2\nu)-R_1^4(\bar{\nu}\nu_1\nu_2\nu)}{R_0^1(\nu)}-\frac{(E-\epsilon_{\bar{\nu}})}{2}\frac{[R_1^2(\bar{\nu}\nu)-R_0^2(\bar{\nu}\nu)]}{R_0^1(\bar{\nu})}. \quad (3.7)$$

Blocking of different states $\bar{\nu}$ will, in general, lead to different total energies E. The lowest of these energies is the ground state of the system with odd-particle number; the other ones correspond to excited states. The generalization to the case of neutrons and protons is straightforward. The results are given in a laboratory report.[23]

IV. USE OF THE SADDLE-POINT METHOD FOR THE EVALUATION OF THE RESIDUUM INTEGRALS

Bayman[9] has shown that using the saddle-point method for the evaluation of the integrals $R_n^N(\nu_1,\cdots,\nu_N)$ is equivalent to the BCS treatment. He assumes that the saddle points corresponding to different integrals R_n^N are almost equal, and he shows that this is the case for a constant level density. We reformulate his proof only for the sake of completeness, using a slightly different formulation.

We write the residuum integrals (2.8) in the following way:

$$R_n^N(\nu_1\cdots,\nu_N)=\frac{1}{2\pi i}\oint dz e^{f(z)}\chi_n^N(z), \quad (4.1)$$

where

$$f(z)=-n_0\ln z+\sum_{\nu=1}^{N_0}\ln(u_\nu^2+zv_\nu^2); \quad (4.2)$$

$$\chi_n^N(z,\nu_1\cdots\nu_N)=z^{n-1}/\textstyle\prod_{\kappa\neq\nu_1\cdots\nu_N}(u_\nu^2+zv_\nu^2). \quad (4.3)$$

$f(z)$ and $\chi_n^N(z)$ are analytic functions of z on the path of integration. The path of integration can be chosen so that it crosses the saddle point z_0 of $f(z)$ on a line of steepest descent, the saddle point being defined by

$$f'(z_0)=-\frac{n_0}{z_0}+\sum_\nu\frac{v_\nu^2}{u_\nu^2+z_0u_\nu^2}=0. \quad (4.4)$$

Thus, we can use the saddle-point method to evaluate

---

[22] V. G. Soloviev, Kgl. Danske Videnskab. Selskab, Mat. Fys. Skrifter **1**, No. 11 (1961) with references to earlier work; S. Wahlborn, Nucl. Phys. **37**, 554 (1962).

[23] K. Dietrich, H. J. Mang, and J. Pradal, Lawrence Radiation Laboratory Report UCRL-11083 (unpublished).

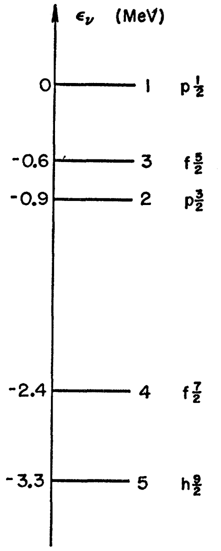

FIG. 1. Spectrum of single-particle energies for spherical nucleus.

the residuum integrals (see Appendix C). We obtain

$$R_n{}^N(\nu_1\cdots\nu_N)=\frac{1}{(2\pi)^{1/2}}\frac{e^{f(z_0)}\chi_n{}^N(z_0,\nu_1\cdots\nu_N)}{|f''(z_0)|^{1/2}}, \quad (4.5)$$

with

$$f''(z_0)=\frac{n_0}{z_0{}^2}+\sum_\nu\frac{v_\nu{}^4}{(u_\nu{}^2+z_0v_\nu{}^2)^2}. \quad (4.6)$$

The total energy E (2.9) as well as the variational equations (2.11) contain only quotients of residuum integrals. By using the saddle-point method, the total energy E will be given by

$$\begin{aligned}E=2\sum_\nu \epsilon_\nu v_\nu{}^2\chi_1{}^1(z_0,\nu)+4\sum_\nu V_{\nu-\nu\nu-\nu}v_\nu{}^2\chi_1{}^1(z_0,\nu)\\ +4\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}{}^2v_{\nu_2}{}^2\chi_2{}^2(z_0,\nu_1\nu_2)\\ +4\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}u_{\nu_2}v_{\nu_2}\chi_1{}^2(z_0,\nu_1\nu_2). \quad (4.7)\end{aligned}$$

In Appendix A we shall show that the set of v_ν and u_ν is not unique. Given a set of u_ν and v_ν that corresponds to a saddle point $z_0\neq 1$, we can always find a transformation [see (A4)] such that for the equivalent solution $\tilde{u}_\nu\tilde{v}_\nu$ of the variational equations the saddle point will be at $z_0=1$. For $z_0=1$ Eq. (4.4) is the subsidiary condition required in the theory of superconductivity

$$\sum_\nu v_\nu{}^2=\langle\Psi_{\mathrm{BCS}}|\sum_\nu a_\nu{}^\dagger a_\nu|\Psi_{\mathrm{BCS}}\rangle=n_0 \quad (4.8)$$

and (4.7) is the total energy of BCS. We can also argue in the following way: We may multiply E by z_0 and consider the variation of Ez_0, since E will be stationary if Ez_0 is stationary, and vice versa. Equation (4.4) can be written

$$n_0-\sum_\nu(z_0v_\nu{}^2)/(u_\nu{}^2+z_0v_\nu{}^2)=0. \quad (4.9)$$

We observe that Ez_0 as well as Eq. (4.9) contains z_0 only in the combination $z_0{}^{1/2}v_\nu$. Therefore, we can choose $z_0=1$ without loss of generality. This is Bayman's line of argument. Thus, it is shown that using the saddle-point method in the theory with conserved particle number is equivalent to the usual BCS treatment if we choose the saddle point at $z_0=1$. In this case all the residuum integrals become equal if they are evaluated with the saddle-point method.

In the Euler-Lagrange equations (2.11), the term $\hat{\epsilon}_\nu u_\nu v_\nu$ contains the diagonal matrix element $V_{\nu-\nu\nu-\nu}$ in the form

$$2V_{\nu-\nu\nu-\nu}u_\nu v_\nu[R_1{}^1(\nu)]/R_0{}^0.$$

We can write this term as

$$\begin{aligned}2V_{\nu-\nu\nu-\nu}[R_1{}^1(\nu)/R_0{}^0]u_\nu v_\nu\\ =4V_{\nu-\nu\nu-\nu}[R_1{}^1(\nu)/R_0{}^0]v_\nu{}^2u_\nu v_\nu+2V_{\nu-\nu\nu-\nu}\\ \times[R_1{}^1(\nu)/R_0{}^0]u_\nu v_\nu(u_\nu{}^2-v_\nu{}^2). \quad (4.10)\end{aligned}$$

So, if we define $\hat{\epsilon}_\nu$, Γ_ν, Δ_ν as

$$\hat{\epsilon}_\nu=\epsilon_\nu[R_1{}^1(\nu)/R_0{}^0], \quad (4.11)$$

$$\begin{aligned}\Gamma_\nu=4\sum_\nu(V_{\nu\nu_1\nu\nu_1}+V_{\nu-\nu_1\nu-\nu_1})v_{\nu_1}{}^2\frac{R_2{}^2(\nu_1\nu)}{R_0{}^0}\\ +4V_{\nu-\nu\nu-\nu}v_\nu{}^2\frac{R_1{}^1(\nu)}{R_0{}^0}, \quad (4.12)\end{aligned}$$

and

$$\begin{aligned}\Delta_\nu=2\sum_{\nu_1}V_{\nu-\nu\nu_1-\nu_1}u_{\nu_1}v_{\nu_1}\frac{R_1{}^2(\nu_1\nu)}{R_0{}^0}\\ +2V_{\nu-\nu\nu-\nu}u_\nu v_\nu\frac{R_1{}^1(\nu)}{R_0{}^0}, \quad (4.13)\end{aligned}$$

these quantities go over into the corresponding quan-

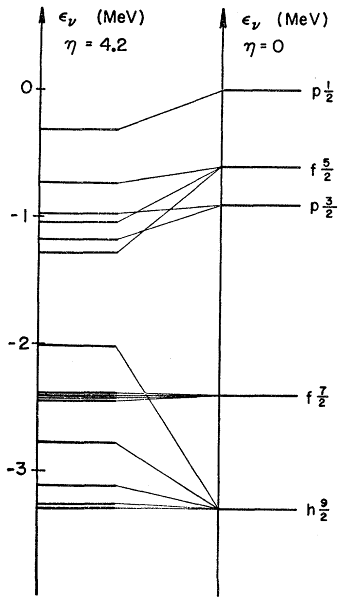

FIG. 2. Spectrum of single-particle energies for deformed nucleus ($\eta_{\mathrm{Nilsson}}\approx 4.2$).

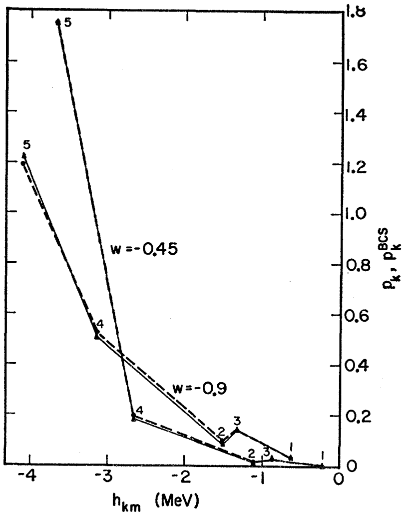

FIG. 3. Level occupation p_k as a function of the (self) energies h_{km} for two pairs ($n_0=2$) and different interaction strength. ▲ solid line, theory with conserved-particle number; ● dashed line, BCS theory.

tities of the BCS theory if the saddle-point method is applied.

V. NUMERICAL RESULTS

We wish to study the differences between the BCS theory and the results of the theory with conserved particle number as a function of (a) the particle number, (b) the strength of the pairing type interaction, and (c) the level spectrum. For this we use the special case of a level system with 15 pair states and an attractive δ function potential of strength constant w. We consider separately the case of a level spectrum that corresponds to a spherically symmetric nucleus (see Fig. 1) and one that corresponds to an axially symmetric, rather strongly deformed nucleus (see Fig. 2, deformation parameter η of Nilsson[24] ≈ 4.2).

In this publication, we only study the errors due to the nonconservation of the particle number.

The results of the BCS theory with conservation of particle number will be compared to the results of an exact diagonalization in a forthcoming paper of Rasmussen and Rho.

We have also performed some calculations with more complicated forces such as delta-plus quadrupole and finite-range forces and have found the expected result that the errors due to nonconservation of particle number do not depend much upon the special type of forces but mainly on the relative strength of the attractive short-range part of the force compared to the average level spacing. Thus, it is sufficient to study the question of nonconservation of particle number in the special example mentioned above.

In Figs. 3–15 we plot on the abscissa the quantities

$$h_\nu \equiv \epsilon_\nu + \Gamma_\nu^{\mathrm{BCS}}, \tag{5.1}$$

where ϵ_ν are the single-particle energies and $\Gamma_\nu^{\mathrm{BCS}}$ is the Hartree-Fock potential Γ_ν in the BCS theory, i.e.,

$$\Gamma_\nu^{\mathrm{BCS}} = 4 \sum_{\nu_1} (V_{\nu\nu_1\nu\nu_1} + V_{\nu-\nu_1\nu-\nu_1}) v_{\nu_1}^2 . \tag{5.2}$$

In the case of our spherical nucleus, $\nu \equiv$ (angular momentum k, magnetic quantum number m). Physically, h_ν is the average field acting on a particle in state ν. It depends, of course, on the interaction strength w and on the number of particles.

We call the pairing interaction strong if the pairing potential $\Delta_\nu^{\mathrm{BCS}}$ in the BCS treatment is larger in absolute value than the experimental odd-even mass differences where

$$\Delta_\nu^{\mathrm{BCS}} = 4 \sum_{\nu_1} V_{\nu-\nu\nu_1-\nu_1} u_{\nu_1} v_{\nu_1} . \tag{5.3}$$

[The factor of 4 used in Eq. (5.3) is a different convention than the factor of 2 used in Eq. (2.14).] The level spectrum we have chosen corresponds to a nuclear situation in the Pb^{208} region where the odd-even mass differences are known to be of the order of 1.0 MeV. This means that $w=-1$ must be regarded as a strong pairing interaction, $w=-0.9$ is still slightly stronger than realistic, $w=-0.45$ is slightly weaker than realistic, and $w=-0.2$ is extremely weak.

In the case of the spherically symmetric nucleus the levels are degenerate. For this case, we define quantities p_k as the sum of occupation probabilities for all the degenerate magnetic substates of the level with angular momentum k,

$$p_k = \sum_m e_{km}^2 , \tag{5.4}$$

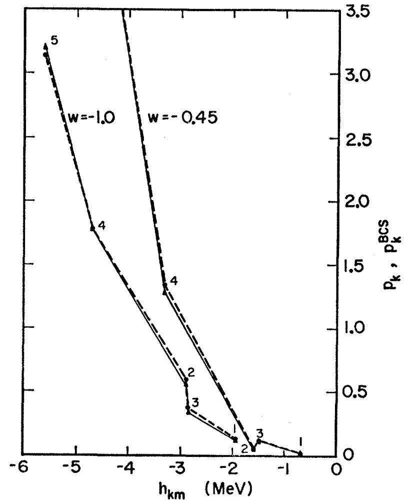

FIG. 4. Level occupation p_k as a function of the (self) energies h_{km} for six pairs ($n_0=6$) and different interaction strength.

---

[24] S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 29, No. 16 (1955).

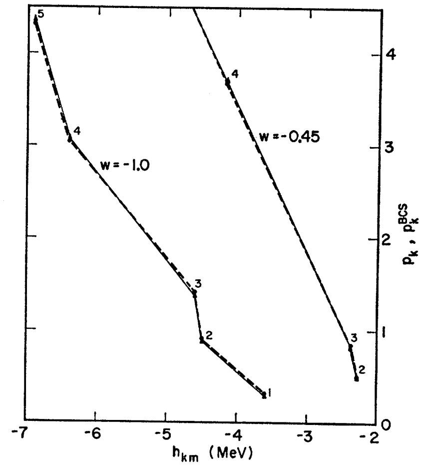

FIG. 5. Level occupation p_k as a function of the (self) energies h_{km} for ten pairs ($n_0=10$).

and p_k^{BCS} is the corresponding quantity in the BCS theory,

$$p_k^{\mathrm{BCS}}=\sum_m v_{km}^2, \tag{5.5}$$

Figs. 3, 4, and 5 show p_k and p_k^{BCS} as a function of h_{km} for pairing interactions of different strength and for different pair numbers n_0.

Besides realizing that the agreement between the results of the BCS theory and the theory with conserved particle number is good, rather independently of the number of pairs, we mention that for strong and moderately strong pairing interaction, the BCS theory overestimates the dissolution of the Fermi surface; for weak pairing interactions it underestimates it.

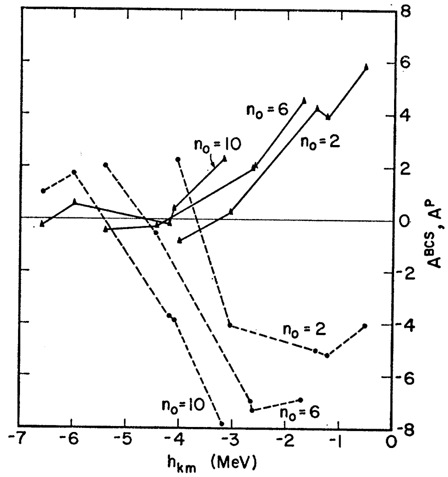

FIG. 6. Accuracy of occupation probabilities in methods without conservation of particles for different pair numbers and strength constant $W=-0.9$. ▲ solid line, BCS method with subsequent projection; ● dashed line, BCS method.

Furthermore, we observe from Fig. 3 that there may be cases in which a level of higher energy is more strongly occupied than a neighboring one with lower energy. This happens if the gain in pairing energy is larger than the loss in single-particle energies. This phenomenon is well known since the early days of the shell model.[25]

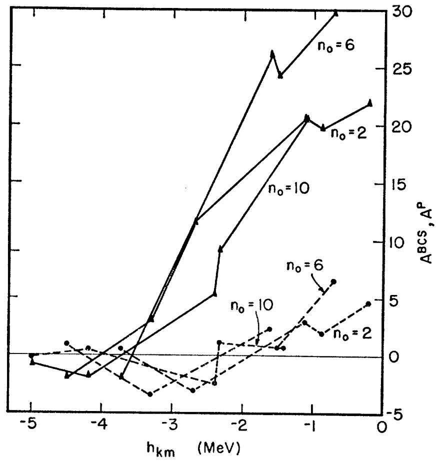

FIG. 7. Accuracy of occupation probabilities in methods without conservation of particles for different pair numbers and strength constant $W=-0.45$.

A clearer picture of the errors connected with nonconservation of particle number can be obtained from Figs. 6, 7, and 8.

A procedure that is frequently used to improve the result of a BCS treatment consists in first solving the BCS equations and then projecting from the obtained BCS state the required eigenstate of the number operator. In this case, a new set of occupation proba-

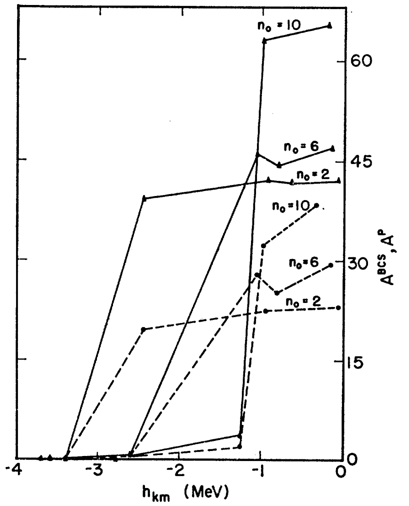

FIG. 8. Accuracy of occupation probabilities in methods without conservation of particles for different pair numbers and strength constant $W=-0.2$.

---

[25] M. Goeppert-Meyer, J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure* (John Wiley & Sons, New York, 1955), p. 8.

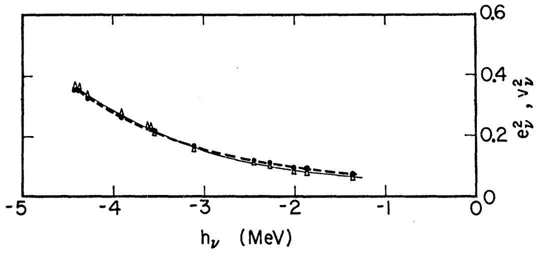

FIG. 9. Occupation probabilities for deformed nucleus ($\eta_{\text{Nilsson}} \approx 4.2$), pair number $n_0=3$; strength constant $W=-1.0$. △ solid line, theory with conserved particle number; ● dashed line, BCS theory.

bilities e_ν^{P2} is calculated according to (2.17) from the set of v_ν^2 that has been obtained as a solution of the BCS equations.

In order to measure the accuracy of the BCS solution and of the solution obtained from it by projection, we define the quantities

$$A^{\text{BCS}}=[(e_\nu^2-v_\nu^{\text{BCS}2})/e_\nu^2]\times 100 \qquad (5.6)$$

and

$$A_\nu^P=[(e_\nu^2-e_\nu^{P2})/e_\nu^2]\times 100 \qquad (5.7)$$

and plot them against h_ν for different pair numbers n_0 and different strength constants w. This is done in Figs. 6, 7, and 8 for the case of spherical nuclei. We can learn several things from these diagrams:

(1) The smaller the occupation probabilities in question, the larger the deviations of the BCS and projection results from the ones with conservation of particle number.

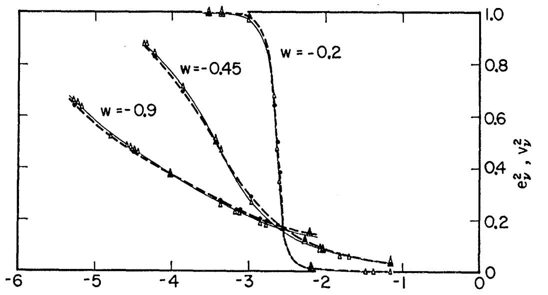

FIG. 10. Occupation probabilities for deformed nucleus ($\eta_{\text{Nilsson}} \approx 4.2$), pair number $n_0=6$ and different strength constants.

(2) The weaker the pairing type interactions the larger the deviations of the BCS and projection results from the ones of our method. In this connection, we stress that the projected solution is only nearer to the solution with conservation of particle number, if the pairing interaction is not too weak.

(3) In all the cases considered, the solution obtained by projection yielded too small occupation probabilities for the weakly occupied levels. In other words, the projected solution generally underestimates the smearing out of the Fermi surface.

Figures 9 to 12 show the corresponding plots in the case of a level scheme corresponding to a deformed nucleus. Figures 9 and 10 show the occupation probabilities as a function of the single-particle energies h_ν. The distributions of energy levels are very smooth now, and no shell effects are discernible. Figures 11 and 12 again show the fractional errors of the BCS treatment and of the BCS calculation with subsequent projection. Evidently, the statements we have made for the case of the spherical nucleus remain correct also for the

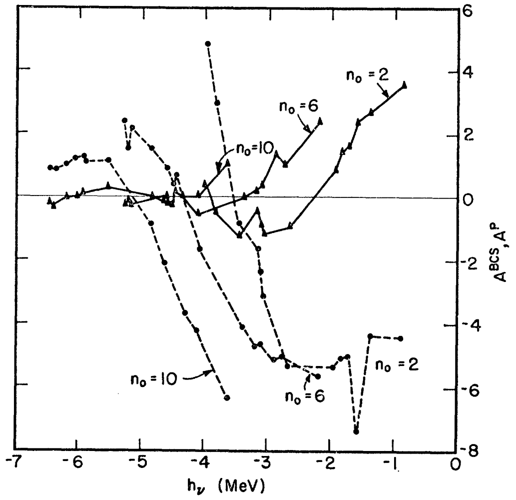

FIG. 11. Accuracy of occupation probabilities in methods without conservation of particles for deformed nucleus ($\eta_{\text{Nilsson}} \approx 4.2$), strength constant $w=-0.9$.

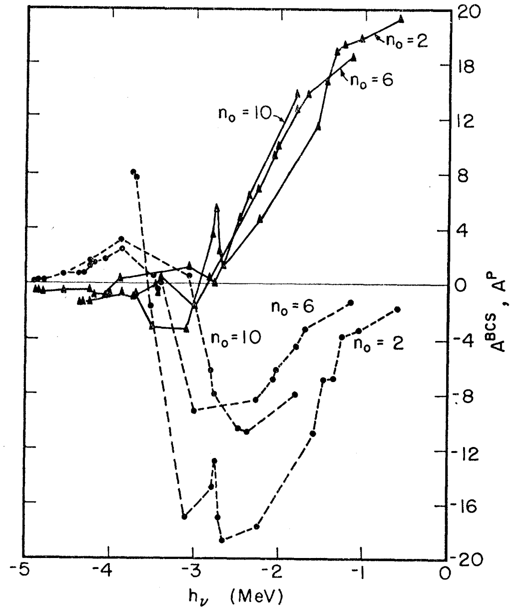

FIG. 12. Accuracy of occupation probabilities in methods without conservation of particles for deformed nucleus ($\eta_{\text{Nilsson}} \approx 4.2$), strength constant $W=-0.45$.

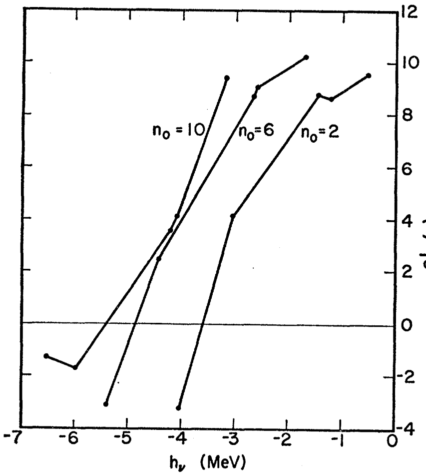

FIG. 13. Accuracy of the saddle-point method for different pair numbers and spherical nucleus-strength constant $W=-0.9$.

deformed nucleus. For the case of a strong pairing-type force the projected solution becomes a very good approximation.

Generally speaking, the errors due to nonconservation of particle number are appreciable only for the small components of the wave function. These small components of the BCS state will usually differ from the corresponding components of the exact solution by amounts of the same order of magnitude. Preliminary calculations show that for rather weak, but not too weak, pairing interactions, conservation of particle number improves the BCS results appreciably as compared to the exact solution.[26] At this point we would like to mention that once one has decided on solving the BCS equations with the help of a fast computer it is not much more difficult to solve the equations given in this paper. The residuum integrals R_n^N can be calculated from recursion relation (B1). Since this recursion relation is very well suited for numerical calculation, a solution of Eqs. (2.11) is even not excessively more time consuming than a solution of the BCS equations, the time depending sensitively on the number of states N_0 taken into account.

Figures 13 and 14 are supposed to show the accuracy of the saddle-point method for the case of individual integrals R_n^N. We define the quantity $Q_1^1(\nu)$ as

$$Q_1^1(\nu)=[[R_1^1(\nu)-R_0^0]/R_0^0]\times 100. \tag{5.8}$$

The quantities $Q_1^1(\nu)$ are evaluated as a function of the set of v_ν^2 that is obtained from a solution of the BCS equations. Hence, if the saddle-point method were correct, the quantities $Q_1^1(\nu)$ should be zero according to what has been said in Sec. V. The $Q_1^1(\nu)$ can also be written

$$Q_1^1(\nu)=(e_\nu^{P2}-v^{\mathrm{BCS}^2})/(v_\nu^{\mathrm{BCS}^2})\times 100, \tag{5.9}$$

i.e., the differences between the occupation probabilities $v_\nu^{\mathrm{BCS}^2}$ of the BCS theory and the occupation probabilities e_ν^{P2} obtained by subsequent projection give a direct measure of the accuracy of the saddle-point method. For physical pairing interactions the true occupation probabilities e_ν^2 usually lie between the quantities e_ν^{P2} and $v_\nu^{\mathrm{BCS}^2}$. This means that for these cases the BCS theory is more reliable than one would expect from considering the accuracy of the saddle-point method.

In the case of odd nuclei we obtain different nuclear states by putting the unpaired nucleon into different orbitals. The state of lowest energy is the ground state of the odd nucleus; the others represent excited states. These states are calculated in different approximations in the literature. If we do not conserve the particle number in the pairing model, we write the wave function $\Phi_{\bar\nu}$ of an odd nucleus with the unpaired nucleon being in state $\bar\nu$ as

$$\phi_{\bar\nu}=a_{\bar\nu}^\dagger \textstyle\prod_{\nu\neq\bar\nu}(u_\nu+v_\nu a_\nu^\dagger a_{-\nu}^\dagger)\phi_0, \tag{5.10}$$

and we obtain the excitation energy $E_{\bar\nu}$ from

$$E_{\bar\nu}=(\phi_{\bar\nu}|H|\phi_{\bar\nu})-E_0, \tag{5.11}$$

where E_0 is the ground-state energy of the odd nucleus. In crudest approximation (approximation Q in Fig. 15), the variational equations corresponding to an ordinary BCS state

$$\phi=\prod_\nu(u_\nu+v_\nu a_\nu^\dagger a_{-\nu})\phi_0 \tag{5.12}$$

are solved, and the expectation value of the number operator is kept equal to the required odd-particle number. The set of u_ν and v_ν thus obtained is used to calculate $E_{\bar\nu}$ according to (6.11). A better approximation (approximation B in Fig. 15) consists in solving the Euler-Lagrange equations corresponding to the trial state (6.10). One can hope to improve this latter approximation by projecting from solution B the correct eigenstate of the number operator (approximation BP in Fig. 15).

In Fig. 15, results of these three methods are com-

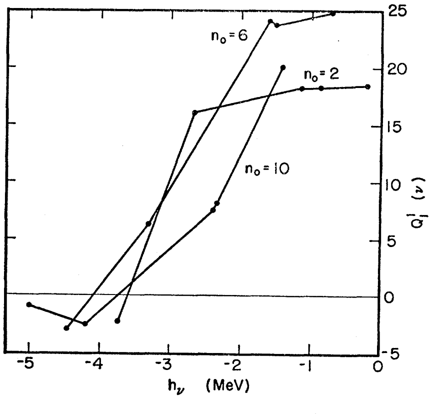

FIG. 14. Accuracy of the saddle-point method for different pair numbers and spherical nucleus-strength constant $W=-0.45$.

---

[26] J. Rasmussen and M. Rho (private communication).

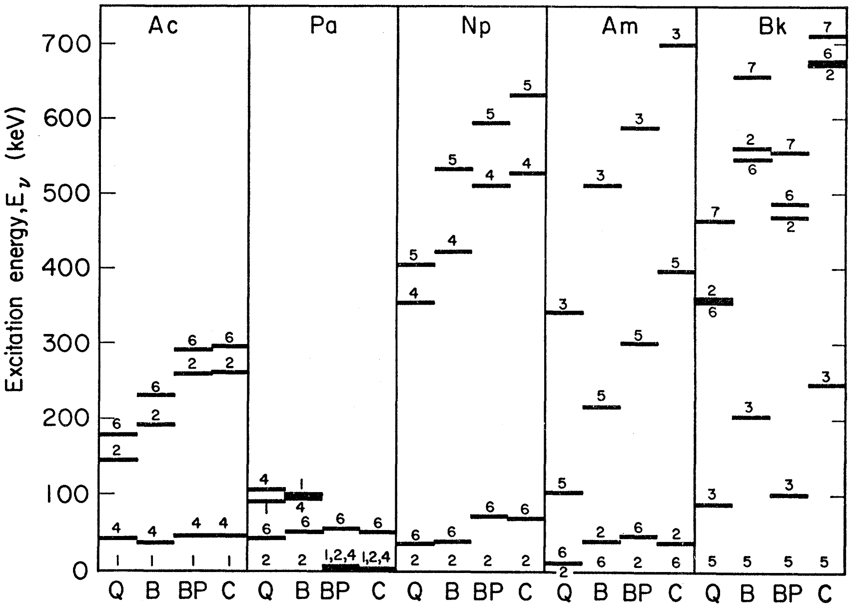

FIG. 15. Excitation energies of odd nuclei calculated with different approximations (see text). The level numbers signify the following Nilsson orbitals: $\frac{3}{2}$ 651=1; $\frac{5}{2}$ 642 =2; $\frac{7}{2}$ 633=3; $\frac{1}{2}$ 530=4; $\frac{3}{2}$ 521=5; $\frac{5}{2}$ 523=6; $\frac{7}{2}$ 514=7.

pared with the result of the theory with conserved particle number (method C).

The cases of 13, 15, 17, 19, and 21 nucleons in 25 Nilsson orbitals are considered. Again, a δ force is used as pairing interaction. The orbitals correspond to the actinide region and the nuclei successively to Ac, Pa, Np, Am, Bk. Having neglected the neutron-proton interaction, we do not put any emphasis upon obtaining agreement with experiment. Nevertheless, the ground-state spins come out correctly. We are interested only in the comparison of results of the different methods.

Approximation *Q* in almost all cases, differs the most from the results with conservation of particle numbers. The excitation energies differ usually by more than 100% from the values obtained with the theory with conserved particle number.

The blocking calculations (B) give relatively better results. However, there are still errors up to more than 100 keV for excitation energies ranging from a few keV up to 700 keV, and neighboring levels sometimes come out in the wrong order.

Subsequent projection (BP) improves the blocking calculations for the case of Ac, Pa, and Np, where the pairing interaction is relatively strong compared to the average level distance. In the spectrum of Am this procedure brings the levels 2 and 6 into wrong order. In the case of Bk the solution obtained by subsequent projection is definitely of poorer accuracy than the simple blocking calculation. In this case, the pairing interaction is weak relative to the average level distance. Thus, we find again that subsequent projection does not improve the BCS results if the pairing interaction is relatively weak.

It should be mentioned that conserving the nucleon number generally leads to a smaller level density near the ground state as compared with all other methods. The only exception is the case of Pa where there is an accidental near degeneracy of three levels one of which is the ground state.

Generally speaking, the errors due to nonconservation of particle number are larger for the excitation energies than for the occupation probabilities. Furthermore, these errors are usually of different magnitude for neighboring even-even and odd-even nuclei. This question is studied in detail in a forthcoming paper by Nilsson.[14]

Last but not least, it should be mentioned that the total energy *E* as obtained from the BCS theory, from the BCS theory with subsequent projection, or finally from our formulation with rigorous conservation of particle number differ usually only by fractions of a percent. The reason is that the main contributions to the total energy originate from strongly occupied levels. As we have seen before the occupation probabilities for strongly occupied levels are by far more accurate than the ones corresponding to weakly occupied levels.

ACKNOWLEDGMENTS

We thank K. Poggenburg for carrying out the calculations that correspond to Fig. 16. One of the authors (K.D.) wishes to express his gratitude to the Bundesministerium für wissenschaftliche Forschung for a fellowship and to the Fulbright Commission for a travel grant. K. D. and J. P. are very grateful to Professor Perlman and Professor Rasmussen for the kind hospitality extended to them at the Radiation Laboratory.

APPENDIX A: DISCUSSION OF THE SOLUTION OF THE VARIATIONAL EQUATIONS

We can write the trial state in the form

$$\Psi=C\Big[\prod_{\nu} u_{\nu}\Big]\oint\frac{d\zeta}{\zeta^{n_0+1}}\prod_{\nu}\left(1+\frac{v_{\nu}}{u_{\nu}}\zeta a_{\nu}{}^{\dagger}a_{-\nu}{}^{\dagger}\right)\Phi_0$$

$$=C'\oint\frac{d\zeta}{\zeta^{n_0+1}}\prod_{\nu}\left(1+\frac{v_{\nu}}{u_{\nu}}\zeta a_{\nu}{}^{\dagger}a_{-\nu}{}^{\dagger}\right)\Phi_0. \qquad \text{(A1)}$$

From this it follows that only the quotient v_{ν}/u_{ν} will be defined by the variational equations. We may, of course, retain the redundant parameters and impose as many conditions as there are superfluous parameters. We choose the conditions

$$u_{\nu}{}^{*}u_{\nu}+v_{\nu}{}^{*}v_{\nu}=1. \qquad \text{(A2)}$$

The normalization coefficient C is given by

$$\langle\Psi|\Psi\rangle=1. \qquad \text{(A3)}$$

The numerator and denominator on the right side of Eq. (A1) are sums of terms each containing a product of n_0 factors v_{ν}/u_{ν}. Thus, if we multiply all quotients v_{ν}/u_{ν} with a common factor X, this factor cancels in (A1). This means that even with the restrictive conditions (A2), the set of u_{ν}, v_{ν} is determined only up to the following transformation between equivalent sets of u_{ν}, v_{ν}:

$$\tilde{v}_{\nu}=Xv_{\nu}/(u_{\nu}{}^2+X^2v_{\nu}{}^2)^{1/2};\quad \tilde{u}_{\nu}=u_{\nu}/(u_{\nu}{}^2+X^2v_{\nu}{}^2)^{1/2}. \qquad \text{(A4)}$$

Physically meaningful quantities like the probabilities of occupation $e_{\nu}{}^2$ or the total energy E are invariant under the transformation (A4). This ambiguity of the solutions does not exist in the BCS theory. Next, we wish to show that we may assume the v_{ν} and u_{ν} to be real without loss of generality.

In the case of complex coefficients v_{ν} and u_{ν}, the total energy E is given by

$$E=2\sum_{\nu}\epsilon_{\nu}v_{\nu}{}^{*}v_{\nu}\frac{R_1{}^1(\nu)}{R_0{}^0}+4\sum_{\nu}V_{\nu-\nu\nu-\nu}v_{\nu}{}^{*}v_{\nu}\frac{R_1{}^1(\nu)}{R_0{}^0}$$

$$+4\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})v_{\nu_1}{}^{*}v_{\nu_1}v_{\nu_2}{}^{*}v_{\nu_2}\frac{R_2{}^2(\nu_1\nu_2)}{R_0{}^0}$$

$$+4\sum_{\nu_1\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}u_{\nu_1}v_{\nu_1}{}^{*}u_{\nu_2}{}^{*}v_{\nu_2}\frac{R_1{}^2(\nu_1\nu_2)}{R_0{}^0}. \qquad \text{(A5)}$$

We can write the u_{ν} and v_{ν} as

$$v_{\nu}=|v_{\nu}|\exp(i\arg v_{\nu});\quad u_{\nu}=|u_{\nu}|\exp(i\arg u_{\nu}). \qquad \text{(A6)}$$

From (A1) we infer that we may put

$$\arg u_{\nu}=0 \qquad \text{(A7)}$$

without loss of generality.

We choose the representation so that the matrix elements of the nucleon-nucleon interaction are all real. Then we have the symmetry condition

$$V_{\nu_1-\nu_1\nu_2-\nu_2}=V_{\nu_2-\nu_2\nu_1-\nu_1}, \qquad \text{(A8)}$$

and with the aid of (A6) and (A7), we may write the energy as

$$E=2\sum_{\nu}\epsilon_{\nu}|v_{\nu}|^2\frac{R_1{}^1(\nu)}{R_0{}^0}+4\sum V_{\nu-\nu\nu-\nu}|v_{\nu}|^2\frac{R_1{}^1(\nu)}{R_0{}^0}$$

$$+4\sum_{\nu_1\nu_2}(V_{\nu_1\nu_2\nu_1\nu_2}+V_{\nu_1-\nu_2\nu_1-\nu_2})|v_{\nu_1}|^2|v_{\nu_2}|^2\frac{R_2{}^2(\nu_1\nu_2)}{R_0{}^0}$$

$$+8\sum_{\nu_1<\nu_2}V_{\nu_1-\nu_1\nu_2-\nu_2}|u_{\nu_1}||u_{\nu_2}||v_{\nu_1}||v_{\nu_2}|$$

$$\times\cos[\arg v_{\nu_2}-\arg v_{\nu_1}]\,\frac{R_1{}^2(\nu_1\nu_2)}{R_0{}^0}. \qquad \text{(A9)}$$

The < sign at the last sum means that any couple of quantum states (ν_1,ν_2) should appear only once, not also in the reversed order (ν_2,ν_1). The residuum integrals are all independent of the phases.

Variation with regard to the quantities $|u_{\nu}|$ and $|v_{\nu}|$ leads to the set of equations that we have derived in Sec. II, the only difference being that all pairing-type matrix elements are multiplied by $\cos[\arg v_{\nu_2}-\arg v_{\nu_1}]$. Variation with respect to the phases leads to the following equations:

$$\sum_{\nu_2}V_{\nu-\nu\nu_2-\nu_2}|u_{\nu_2}||v_{\nu_2}|[\sin[\arg v_{\nu_2}-\arg v_{\nu}]]$$

$$\times R_1{}^2(\nu\nu_2)/R_0{}^0. \qquad \text{(A10)}$$

Equation (A10) has the trivial solution

$$\arg v_{\nu}=\text{const}. \qquad \text{(A11)}$$

Since a common phase factor of all parameters v_{ν} can be immediately replaced by $+1$, (A11) corresponds to a solution with real, positive coefficients v_{ν} and u_{ν}, the one considered in Sec. II.

We assert that this solution corresponds to the lowest energy E, if the pairing-type matrix elements are all negative. This is the case for an attractive interaction and the phase convention defined in (2.1′), and (2.1″). *Proof:* Suppose we have found a solution of the Euler-Lagrange equations (A10) and (2.11) [(2.11) being modified by the phases in the above-mentioned way] with a set of phases $\arg v_{\nu}\neq\text{const}$, and E_0 being the energy corresponding to this solution. Then we can certainly find a lower energy $E_1<E_0$ by replacing all the cosine factors by 1. Since the set of $|u_{\nu}|$, $|v_{\nu}|$ is consistent only with the set of nonconstant phases, E_1 does not correspond to a solution of the variational problem. But we can now determine the minimum of E_1 by variation of $|v_{\nu}|$ and $|u_{\nu}|$ keeping

$$|u_{\nu}|^2+|v_{\nu}|^2=1. \qquad \text{(A12)}$$

This variation leads to the set of equations (2.11) and to a total energy E_2 that is lower or equal to E_1,

$$E_2 \leqslant E_1 < E_0\,, \qquad \text{(A13)}$$

if the second variation of $\langle\Psi|H|\Psi\rangle$ is positive in the neighborhood of our solution. This must be the case for any physically reasonable solution.

APPENDIX B: SOME PROPERTIES OF THE RESIDUUM INTEGRALS

From definition (2.8) of the residuum integral we can easily infer the following recursion relations:

$$\begin{aligned} R_{n+1}{}^{N+1}(\nu_1\cdots\nu_N\nu)v_\nu{}^2+R_n{}^{N+1}(\nu_1\cdots\nu_N\nu)u_\nu{}^2& \\ =R_n{}^N(\nu_1\cdots\nu_N)\,, &\quad \text{(B1)}\end{aligned}$$

$$\begin{aligned} R_n{}^{N+1}(\nu_1\cdots\nu_N\nu)R_{n+1}{}^{N+1}(\nu_1\cdots\nu_N\nu')-R_n{}^N(\nu_1\cdots\nu_N)& \\ \times R_{n+1}{}^{N+2}(\nu_1\cdots\nu_N\nu\nu')=v_\nu{}^2[R_n{}^{N+1}(\nu_1\cdots\nu_N\nu)& \\ \times R_{n+2}{}^{N+2}(\nu_1\cdots\nu_N\nu\nu')-R_{n+1}{}^{N+1}(\nu_1\cdots\nu_N\nu)& \\ \times R_{n+1}{}^{N+2}(\nu_1\cdots\nu_N\nu\nu')]. &\quad \text{(B2)}\end{aligned}$$

Relation (B1) is useful for numerical computation of the residuum integrals. In the limit of the saddle-point method (with saddle point at $z_0=1$) relation (B1) becomes the normalization condition

$$u_\nu{}^2+v_\nu{}^2=1$$

of the usual superconductivity theory. Furthermore, we see from (B1) that all the residuum integrals will have values between 0 and +1 if the u_ν and v_ν fulfill condition (2.5).

In the derivation of the Euler-Lagrange equations, we have to evaluate variational derivatives of the residuum integrals $\delta R_n{}^N(\nu_1\cdots\nu_N)/\delta v_\nu$:

$$\frac{\delta R_n{}^N(\nu_1\cdots\nu_N)}{\delta v_\nu}=\left[\frac{\partial}{\partial v_\nu}-\frac{v_\nu}{u_\nu}\frac{\partial}{\partial u_\nu}\right]R_n{}^N(\nu_1\cdots\nu_N).$$

From definition (2.8) of the residuum integral we can immediately see that the following relation holds:

$$\begin{aligned}\frac{\delta R_n{}^N(\nu_1\cdots\nu_N)}{\delta v_\nu}=2v_\nu[R_{n+1}{}^{N+1}(\nu_1\cdots\nu_N,\nu)& \\ -R_n{}^{N+1}(\nu_1\cdots\nu_N)]. &\quad \text{(B3)}\end{aligned}$$

From (B3) it becomes apparent how the term Λ [see (2.16)] comes to exist.

APPENDIX C: USE OF THE SADDLE-POINT METHOD

Integrals of the type

$$I=\int_A^B e^{tf(z)}\chi(z)dz\,, \qquad \text{(C1)}$$

where t is real and positive and $f(z)$, $\chi(z)$ are analytic on the path of integration, can be approximated by the method of steepest descent (see, for instance, Ref. 27). If $f(z)$ exhibits a saddle-point z_0 somewhere between A and B, the path of integration should be chosen so as to cross the saddle point on a line of steepest descent. In this case the integral I can be approximated by (see Ref. 27)

$$I\approx[e^{tf(z_0)}\chi(z_0)(2\pi)^{1/2}e^{i\alpha}]/|tf''(z_0)|^{1/2}. \qquad \text{(C2)}$$

In (C2) α is the angle between the positive real axis and the direction of the path in z_0. If $f''(z_0)\neq 0$, $f(z)$ can be expanded near z_0 in the form

$$f(z)=f(z_0)+\tfrac{1}{2}(z-z_0)^2 f''(z_0)+\cdots\,; \qquad \text{(C3)}$$

the direction of the path in z_0 has to be such that $(z-z_0)^2f''(z_0)$ is real and negative.[27]

Equation (C2) represents the first term of an asymptotic expansion (see Ref. 27, p. 502). The higher order terms of this expansion are, in general, difficult to obtain. Therefore, it is difficult to obtain a reliable estimate of the accuracy of formula (C2). The error will certainly be small if the dominant contributions to the integral come from the immediate vicinity of the saddle point.

In the case of our residuum integrals the saddle point is at $z_0=1$ and we integrate over the unit circle. The quantities $f(z)$, $\chi(z)$ are defined in (4.2) and (4.3). Let ψ be the angle where the exponential $e^{f(z)}$ has dropped to $1/e$ of its value at $z_0=1$. The equation for ψ is given by

$$\psi=\frac{\sqrt{2}}{|f''(z_0)|^{1/2}}=\frac{\sqrt{2}}{|n_0-\sum v_\nu{}^4|^{1/2}}=\frac{\sqrt{2}}{|\sum_\nu u_\nu{}^2v_\nu{}^2|^{1/2}}. \qquad \text{(C4)}$$

For the saddle-point method to be applicable, 2ψ should be small compared to the total path length 2π, or

$$(\sum_\nu u_\nu{}^2v_\nu{}^2)^{1/2} \gg \sqrt{2}/\pi\approx\tfrac{1}{2}. \qquad \text{(C5)}$$

The product $u_\nu v_\nu$ is different from zero only if v_ν as well as u_ν is substantially different from 0, i.e., only in the region II, where $v_\nu{}^2$ drops from ≈ 1 to almost 0 (see Fig. 16). Bayman[9] uses the approximation

$$\sum_\nu u_\nu{}^2v_\nu{}^2\approx\tfrac{1}{4}\Omega\,, \qquad \text{(C6)}$$

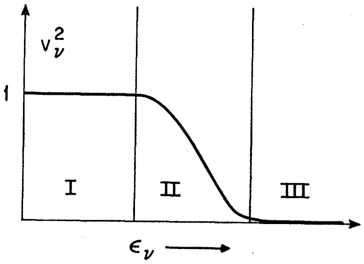

FIG. 16. Occupation probabilities as a function of the energy levels.

---

[27] H. and B. S. Jeffreys, *Methods of Mathematical Physics* (Cambridge University Press, New York, 1956), Chap. 17.

where Ω is the number of states ν in region II. With this we obtain the criterion

$$\sqrt{\Omega}\gg 1. \tag{C7}$$

The larger Ω is, the more reliable the saddle-point method should be. Large Ω is favored by strong pairing interactions. On the other hand, the BCS state conserves particle number in the case of a sharp Fermi surface. Thus, it is to be expected that in the limit of very small Ω the errors connected with the nonconservation of particle number should be small too,[9] whereas the saddle-point method can be substantially wrong in this case. This is borne out by our numerical results (see Sec. V).

PHYSICAL REVIEW VOLUME 135, NUMBER 1B 13 JULY 1964

Separability of Center-of-Mass Motion in the Nuclear Shell Model

M. A. NAGARAJAN
Case Institute of Technology, Cleveland, Ohio

(Received 13 February 1964)

It is shown that one can find an orthogonal transformation that will enable one to split the motion of a many-body system to a center-of-mass motion and an internal motion. A particular orthogonal transformation has been chosen which retains the independent-particle aspect of a harmonic-oscillator shell-model Hamiltonian. It is suggested that one could easily study and eliminate the states with spurious motions of the center of mass by a direct transformation of the shell-model wave function into the new coordinate system.

1. INTRODUCTION

IN calculations of nuclear structure using shell-model wave functions, the shell-model wave functions are constructed from independent-particle wave functions. These independent-particle wave functions describe the motion of a particle moving in a potential fixed in space. Because of the assumption of a potential fixed in space, the shell-model wave functions so obtained are not translationally invariant. It has been recognized that the neglect of the center-of-mass motion will cause errors in the calculations of energies and transition matrix elements. But the extraction of the center-of-mass motion leaves us only (A−1) degrees of freedom and the internal coordinates cannot be treated symmetrically; therefore, the construction of antisymmetric states becomes very cumbersome.

It was first shown by Bethe and Rose[1] that the antisymmetrized shell-model wave function for the lowest states in a harmonic-oscillator potential are always translationally invariant. However, some of the excited states of the nucleus could be describing a system whose center of mass is in motion. These "spurious states" were first recognized by Elliott and Skyrme.[2] They pointed out that when two or more unclosed shells are involved, one has to investigate that the state has the proper center-of-mass motion. Their prescription is to form suitable linear combinations of shell-model wave functions to describe the proper center-of-mass motion.

In our investigations, we have tried to find a coordinate transformation such that the total kinetic-energy operator of the many-body Hamiltonian splits up into the center-of-mass kinetic energy and the remaining kinetic energy of relative motion. This has been done for the case of two degrees of freedom by Talmi[3] and Theiberger.[4] In the particular case of the harmonic-oscillator potential, our choice of orthogonal transformation separates the center-of-mass part of the potential energy for a general n-body problem.

2. THE COORDINATE TRANSFORMATION

We shall designate the original A-independent set of coordinates by $(\gamma_1,\gamma_2\cdots,\gamma_A)$, and the transformed coordinates by $(\xi_0,\xi_1\cdots\xi_{A-1})$. The transformation[5] is given by[6]

$$\xi_i=\gamma_i-\frac{1}{A-i}\sum_{j=i+1}^{A}\gamma_j \quad i=0,1\cdots A-1 \tag{2.1}$$

$$\gamma_0=0.$$

The inverse transformation is given by

$$\gamma_i=\xi_i-\xi_0-\sum_{j=1}^{i}\frac{1}{(A-j+1)}\xi_j \quad i=1\cdots A \tag{2.2}$$

$$\xi_A=0.$$

---

[1] H. A. Bethe and M. E. Rose, Phys. Rev. **51**, 283 (1937).

[2] J. P. Elliott and T. H. R. Skyrme, Proc. Roy. Soc. (London) **A232**, 561 (1955).

[3] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

[4] R. Thieberger, Nucl. Phys. **2**, 533 (1956).

[5] Note that our first coordinate is $\xi_0=-\mathbf{R}$, and is thus different from the corresponding one of Lipperheide. Our choice makes the transformation orthogonal.

[6] R. Lipperheide, Ann. Phys. (N. Y.) **17**, 114 (1962); S. Hochberg, H. S. W. Massey, and L. H. Underhill, Proc. Phys. Soc. (London) **A67**, 957 (1959).