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CORRECTIONS TO THE BCS EXPRESSIONS FOR NUCLEAR MATRIX ELEMENTS DUE TO PARTICLE NUMBER FLUCTUATIONS

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The effect of particle-number fluctuations on matrix elements based on the BCS wave function is investigated by the employment of a saddle-point projection method. In particular, in the case of a uniform model containing 32 levels it is found that the correction is relatively small and in most cases of interest fairly well reproduced by the method discussed.

In a previous paper [1] a method was proposed to correct approximately the BCS expressions for effects of particle number fluctuations. The same method is now generalized to treat in a similar fashion matrix elements of one-body operators, involving transitions characterized by seniority quantum numbers $v_i = 0$, $v_f = 2$ and $v_i = v_f = 1$, respectively. The former types of matrix elements are involved in particular in the evaluation of the even-even moments of inertia [2], and are therefore of considerable interest.

The saddle point method [3, 4]. The BCS wave function ("unblocked" or "blocked") referring to an *average* particle number n may be decomposed according to an arbitrary particle number k as follows

$$\psi^{\mathrm{BCS}}(n) = \sum_k C_k(n)\, \varphi_k(n) \,. \qquad (1)$$

In eq. (1) the index n given in parenthesis refers to the average number of particles in terms of which the BCS coefficients U_ν and V_ν are determined. The projected matrix elements, involving only wave function components with $k = n$, of a general one-particle operator Q may be defined as

$$Q(n, n) = \langle \varphi'_n(n) \,|\, Q \,|\, \varphi''_n(n) \rangle \,. \qquad (2)$$

The projection is accomplished, as in refs. 1, 3, by the help of operator $\exp \rho(\hat{p}-n)$. One obtains

$$Q(n,n) = \int_{-i\pi}^{i\pi} K(\rho)\,d\rho \Big[\int_{-i\pi}^{i\pi} f(\rho)\,d\rho \int_{-i\pi}^{i\pi} g(\rho)\,d\rho \Big]^{-\frac{1}{2}}, \quad (3)$$

where

$$K(\rho) = \langle \psi'' | Q \exp[\rho(\hat{p}-n)] | \psi' \rangle , \quad (4)$$

and the normalization is accomplished by means of the functions

$$f(\rho) = \langle \psi' | \exp[\rho(\hat{p}-n)] | \psi' \rangle \quad (5)$$

and

$$g(\rho) = \langle \psi'' | \exp[\rho(\hat{p}-n)] | \psi'' \rangle . \quad (6)$$

The integrals (4) - (6) may be evaluated by means of a saddle-point method. Thus,

$$\int_{-i\pi}^{i\pi} K(\rho)\,d\rho \approx \tilde{K} \int_{-i\infty}^{i\infty} d\mu \, \exp\{\tfrac{1}{2}\mu^2 K''(0)/\tilde{K}\} , \quad (7)$$

where

$$\tilde{K} = K(0) - \tfrac{1}{2}[K'(0)]^2/K''(0) . \quad (8)$$

Correspondingly the integrals involving the functions f and g may be evaluated in an entirely analogous manner.

The ratio of the corrected to the uncorrected matrix element, denoted C, may now be expressed as

$$C = [\tilde{K}/K(0)]^{\frac{3}{2}} [K''(0)/K(0)]^{-\frac{1}{2}} [f''(0)\,g''(0)]^{\frac{1}{4}} [\tilde{f}\tilde{g}]^{-\frac{3}{4}} . \quad (9)$$

The actual labour is now entailed in the evaluation of the matrix elements

$$\begin{aligned} K(0) &= \langle \psi'' | Q | \psi' \rangle , \\ K'(0) &= \langle \psi'' | Q(\hat{p}-n) | \psi' \rangle , \\ K''(0) &= \langle \psi'' | Q(\hat{p}-n)^2 | \psi' \rangle , \end{aligned} \quad (10)$$

and the corresponding expressions for the functions f and g.

The even case, $\Delta v = 2$. The matrix elements involving time-reversed orbitals $\bar{\nu}$ are related to the other matrix elements through the formula

$$q_{\bar{\nu}\bar{\nu}'} = \tau q_{\nu'\nu} . \quad (11)$$

We may assume that phases such that $\tau = +1$ for $E\lambda$ and -1 for $M\lambda$ are employed. Let ψ' refer to the ground state and ψ'' to a broken-pair state with the odd particles in orbitals 1 and 2, respectively. One then obtains

$$K(0) = q_{12}(\mathring{U}_1\mathring{V}_2 + \tau\mathring{V}_1\mathring{U}_2) \prod_{\lambda\neq 1,2} (\mathring{U}_\lambda U_\lambda + \mathring{V}_\lambda V_\lambda) , \quad (12)$$

$$R' = K'(0)/K(0) = \sum_{\kappa\neq 1,2} \frac{2\mathring{V}_\kappa V_\kappa}{\mathring{U}_\kappa U_\kappa + \mathring{V}_\kappa V_\kappa} - (n-2) , \quad (13)$$

$$R'' = K''(0)/K(0) = R'^2 + \sum_{\kappa\neq 1,2} \frac{4\mathring{U}_\kappa \mathring{V}_\kappa U_\kappa V_\kappa}{(\mathring{U}_\kappa U_\kappa + \mathring{V}_\kappa V_\kappa)^2} . \quad (14)$$

The coefficients $\mathring{U}_\kappa$ and $\mathring{V}_\kappa$ refer to the ground state, U_κ and V_κ to the excited state where the levels 1 and 2 are "blocked". One may thus evaluate the correction factor C of eq. (9) by the help of eqs. (12) - (14) in the "blocked" case.

In the "unblocked" case, on the other hand, we obtain the following simple expression

$$C \approx 1 + \sigma_0^{-2}\Big[-\frac{5}{8}\Big(\frac{\epsilon_1}{E_1} + \frac{\epsilon_2}{E_2}\Big)^2 + \frac{1}{4}\Big(\frac{\Delta^2}{E_1^2} + \frac{\Delta^2}{E_2^2}\Big)\Big] . \quad (15)$$

The character of the saddle-point method as an expansion in σ_0^{-2} is clearly born out by eq. (15).

The odd case, $\Delta v = 0$. The procedure in the $v_i = 1$, $v_f = 1$ odd case is analogous to the even case. However, for $\Delta v = 0$ one can no longer introduce *one* simple correction factor as was done in the $\Delta v = 2$ case. Instead one finds (with "blocking" included)

$$Q(n,n) = q_{21} \prod_{\lambda\neq 1,2} (U''_\lambda U'_\lambda + V''_\lambda V'_\lambda) \times \quad (16)$$
$$\times [U''_1 U'_2 C_a - \tau V''_1 V'_2 C_b] ,$$

where the correction factors C_a and C_b are given in ref. 5. Some representative values are listed in figs. 2.

For the "unblocked" case one may give simple explicit expansion formulae for C_a and C_b, resembling eq. (15)

$$C_{\binom{a}{b}} = 1 + \sigma_0^{-2}\Big[-\frac{5}{4}\Big(\frac{\epsilon_1}{E_1} + \frac{\epsilon_2}{E_2} \mp 1\Big)^2 + \quad (17)$$
$$+ \frac{5}{8}\Big(\frac{\epsilon_1^2}{E_1^2} + \frac{\epsilon_2^2}{E_2^2}\Big) + \frac{1}{4}\Big(\frac{\Delta^2}{E_1^2} + \frac{\Delta^2}{E_2^2}\Big)\Big] .$$

One should observe that for the case of $\tau = +1$ and $\epsilon_1 = -\epsilon_2$, i.e., when $U''_1 = V'_2$, $V''_2 = U'_1$, C_a and C_b become equal. Hence, also the corrected matrix elements vanish under the particular conditions cited.

We have compared the approximate, saddle-point projection method with an exact projection [5-7] as obtained with the help of a computer program in close analogy to that of ref. 6. The following conclusions may be reached from a comparison of correction factors (see figs. 1 and 2). In general, the corrections are unexpectedly small for matrix elements moderately near to the

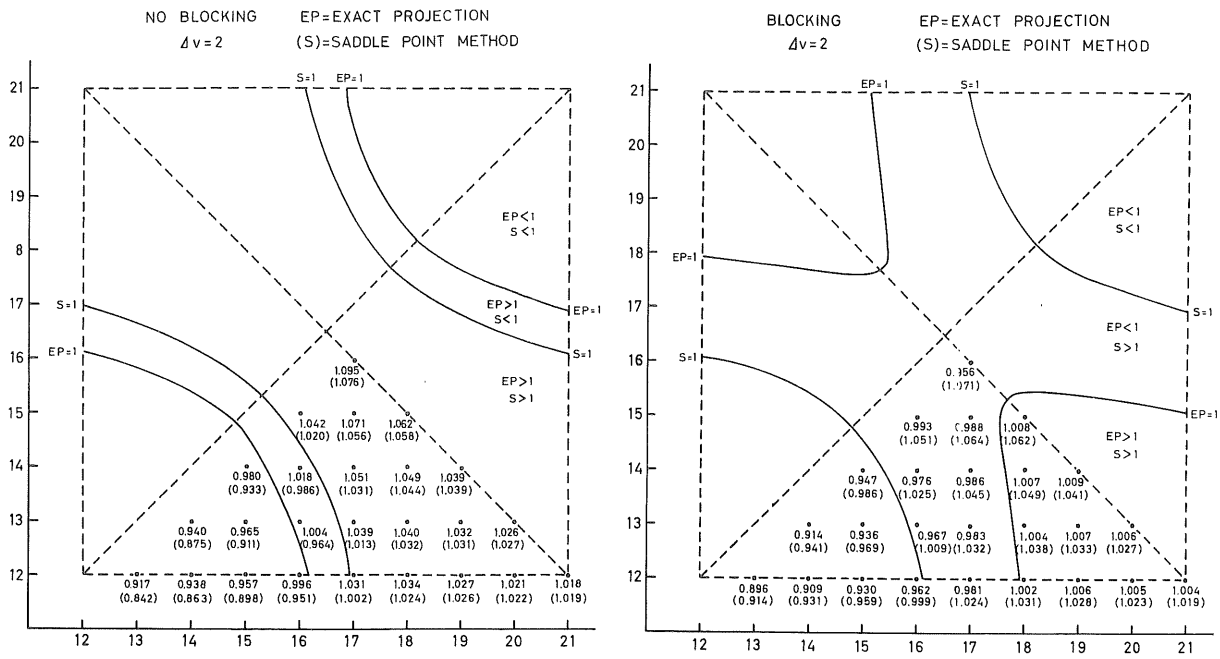

Fig. 1. Correction factor C for single-particle matrix elements between $v_i = 0$ and $v_f = 2$ states without and with "blocking". Numbers given in parenthesis are obtained by the approximate (saddle-point) method described in the text. These should be compared with the numbers given just above obtained by an exact projection method. The numbers on the axis refer to the levels of an equally spaced doubly degenerate single-particle model consisting of 32 levels, in which 16 pairs are accomodated. Thus, in the $v = 0$ ground state the chemical potential falls half-way between levels number 16 and 17, which defines a point of symmetry in the figure.

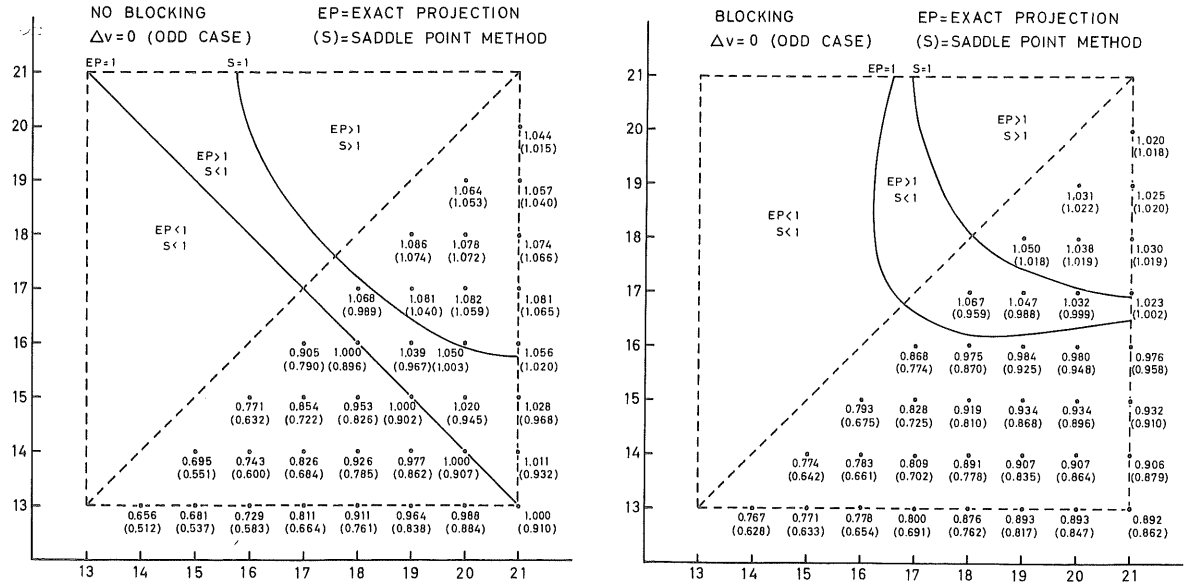

Fig. 2. Correction factor C_a (see text) for $v_i = v_f = 1$, without and with "blocking". (The model is here modified to 33 levels and 33 particles.) The other correction factor C_b can also be read from a mirror reflexion of this figure through the diagonal extending from the upper left to the lower right corner.

Fermi surface in the case treated, which should be considered fairly realistic (32 equidistant energy levels, $G = 0.4\ \Delta\epsilon$). This holds both for the "blocked" and the "unblocked" cases.

For $\Delta v = 0$, "blocked" and "unblocked", and for $\Delta v = 2$, "unblocked", the saddle-point method is fairly successful in reproducing the very small corrections in question. For the $\Delta v = 2$ "blocked" case, on the other hand, the method appears unreliable.

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