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ON A METHOD TO CORRECT FOR PARTICLE NUMBER FLUCTUATIONS

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It was pointed out in a publication [1] by one of the authors that the employment of the BCS wave function in the nuclear case leads to an ensemble average for the energy that is of the order of magnitude Δ_0 larger than the energy for the particular component of the wave function that corresponds to the correct number of particles. As long as one compares ensembles characterized by approximately the same mean square deviation in particle number this correction is not important. However, when in the "blocking" picture states of different seniority are compared (associated with very different σ^2) the correction for the fluctuation effect is of a similar order of magnitude as the entire "blocking" correction, it was argued in ref. 1. In this reference it was suggested that one could correct for the particle number fluctuation effect according to the following simple prescription. Consider the ensemble wave function split up according to particle number p

$$\psi(n) = \sum_p c_p(n)\, \varphi_p(n) \qquad (1)$$

where $n = \langle \hat{p} \rangle$.

Let $\mathcal{E}(n,p)$ be defined as the energy associated with the p-component. One can then employ an expansion

$$\langle \mathcal{E} \rangle = \mathcal{E}(n,n) + \tfrac{1}{2} \langle (\hat{p}-n)^2 \rangle \left\{ \frac{\partial^2 \mathcal{E}(n,p)}{\partial p^2} \right\}_{p=n} + \ldots \qquad (2)$$

It was argued in ref. 1 that $\{\partial^2 \mathcal{E}(n,p)/\partial p^2\}_{p=n}$ might be approximated by $\partial^2 \langle \mathcal{E} \rangle / \partial n^2$. Detailed computations carried out by Mang et al. [2] indicate, however, that this approximation is not very satisfactory (the average deviation in their calculations being of the order of 25%).

We have now estimated $\{\partial^2 \mathcal{E}(n,p)/\partial p^2\}_{p=n}$ by a projection method suggested by Michailov [3] (a method similar to that employed by Bayman [4]).

First, $\mathcal{E}(n,p)$ is defined by

$$\mathcal{E}(n,p) = \frac{\oint \mathrm{d}z\, \langle \psi | z^{\hat{p}-p-1} H | \psi \rangle}{\oint \mathrm{d}z\, \langle \psi | z^{\hat{p}-p-1} | \psi \rangle} \qquad (3)$$

where $|\psi\rangle$ denotes the usual BCS wave function

and $\hat{p}$ the number operator. By the transformation $z = e^{\rho}$ the path of integration is changed from a circle around the origin in the z-plane to a straight line (extending along the imaginary axis from $-i\pi$ to $+i\pi$ in the case that $p = n$).

We now take formally the derivative with respect to p and obtain

$$\left\{\frac{\partial^2 \mathcal{C}(n,p)}{\partial p^2}\right\}_{p=n} = \frac{\int \rho^2 \, d\rho \, \langle e^{\rho(\hat{p}-n)} H\rangle}{\int d\rho \, \langle e^{\rho(\hat{p}-n)}\rangle} + \\ - \frac{\int d\rho \, \langle e^{\rho(\hat{p}-n)} H\rangle \int \rho^2 \, d\rho \, \langle e^{\rho(\hat{p}-n)}\rangle}{(\int d\rho \, \langle e^{\rho(\hat{p}-n)}\rangle)^2} \quad (4)$$

Let us define

$$f(\rho) = \langle e^{\rho(\hat{p}-n)}\rangle \quad (5)$$

The saddle point of $f(\rho)$ lies at $\rho = 0$, corresponding to $f'(0) = 0$. Note also that $f(0) = 1$. We furthermore define

$$K(\rho) = H(\rho) f(\rho) = \langle e^{\rho(\hat{p}-n)} H\rangle \quad (6)$$

The integrals

$$\int f(\rho) \, d\rho, \quad \int \rho^2 f(\rho) \, d\rho, \quad \int f(\rho) H(\rho) \, d\rho \quad \text{and}$$

$$\int \rho^2 f(\rho) H(\rho) \, d\rho$$

are now evaluated using the saddle point method. As a final result we obtain

$$\left\{\frac{\partial^2 \mathcal{C}(n,p)}{\partial p^2}\right\}_{p=n} = \frac{H''(0)}{(f''(0))^2}\left\{1 - O\frac{1}{f''(0)}\right\} \quad (7)$$

For the model employed here the last term is negligible, due to the largeness of $H(0)$ the BCS energy $\langle \mathcal{C}\rangle$.

In terms of the U and V factors one obtains for the even ground state

$$f''(0) = 4 \sum_{\nu} U_{\nu}^2 V_{\nu}^2 = \sigma^2 \quad (8)$$

and

$$H''(0) = -8G \sum_{\nu \neq \nu'} U_{\nu} V_{\nu}^3 V_{\nu'} U_{\nu'}^3 \quad (9)$$

The same expression holds in the blocked case provided, firstly, that the levels occupied by the odd particles are excluded in the sums, and secondly that U_{ν} and V_{ν} are recalculated corresponding to new Δ and λ.

To test the method employed it is of interest to evaluate $\mathcal{C}(n,n)$ directly from eq. (3).

One then finds

$$\mathcal{C}(n,n) = H(0)\left\{1 - \tfrac{1}{2}\frac{H''(0)}{(f''(0))H(0)}\right\}\ldots \simeq \\ \simeq \langle \mathcal{C}\rangle - \tfrac{1}{2}\sigma^2 \frac{H''(0)}{\sigma^4}\ldots \quad (10)$$

The correction term to the BCS energy $\langle \mathcal{C}\rangle$ is thus identical with the *first* order estimate of $-\frac{1}{2}\sigma^2 \{\partial^2 \mathcal{C}(n,p)/\partial p^2\}_{p=n}$.

For the degenerate model ($V^2 = n/2\Omega$ = const., $U^2 = 1 - n/2\Omega$ = const.) we have

$$H''(0) = 8G\Omega(\Omega - 1) U^4 V^4 \quad (11)$$

$$f''(0) = \sigma_0^2 = 4\Omega U^2 V^2 \quad (12)$$

We thus obtain

$$\left\{\frac{\partial^2 \mathcal{C}(n,p)}{\partial p^2}\right\}_{p=n} = \tfrac{1}{2} G(1 - 1/\Omega) \quad (13)$$

which, incidentally, for this case exactly equals $\partial^2 \langle \mathcal{C}\rangle^{BCS}/\partial n^2$.

However, in the other model considered in ref. 1, the so-called "continuous" or "uniform" model, consisting of equally spaced, doubly degenerate levels, extending from $-S$ to $+S$, with $S \gg \Delta$, the employment of the projection method leads to a new result. We obtain

a) for $v = 0$ case:

$$H''(0) = \frac{2\Delta_0^2}{G} - \tfrac{1}{4}\pi \rho \Delta_0 G \quad (14)$$

$$\sigma_0^2 = \pi \rho \Delta_0 \quad (15)$$

b) for the $v = 1$ case with $\epsilon_{block} = 0$:

$$H''(0) = \frac{2\Delta^2}{G} + \tfrac{1}{2} G - \tfrac{1}{4}\pi \rho \Delta G \quad (16)$$

$$\sigma^2 = \pi \rho \Delta - 1 \quad (17)$$

where Δ can be obtained from Δ_0 by the approximate relation

$$\Delta \simeq \Delta_0 \exp(-1/2\rho\Delta) \quad (18)$$

Employing $G/\Delta_0 = \frac{1}{6}$, $1/\rho\Delta_0 = \frac{1}{2}$, and $S \gg \Delta_0$ one obtains

$$\Delta \simeq 0.70\, \Delta_0 \quad (19)$$

Table 1
Six-level model

$\Delta\epsilon$	Δ	σ^2	$\langle \mathcal{C}\rangle$	$\langle \mathcal{C}\rangle - \frac{1}{2}\sigma^2 \frac{\partial^2 \mathcal{C}}{\partial p^2}$	$\langle \mathcal{C}\rangle - \frac{1}{2}\sigma^2 \frac{\partial \lambda}{\partial n}$	$\mathcal{C}^{exact}$
0.2	2.98	5.92	-8.84	-10.09	-10.35	-10.34
1	2.56	4.44	-4.65	-5.93 (-6.11)	-6.10	-6.19
2	1.65	2.13	-2.98	-4.13	-4.12	-4.40

Table 2
Sixteen-level model

No. of levels	No. of particles	No. of blocked levels	Δ	σ^2	$\langle\mathcal{C}\rangle$	$\langle\mathcal{C}\rangle - \frac{1}{2}\sigma^2 \frac{\partial^2\mathcal{C}}{\partial p^2}$	$\langle\mathcal{C}\rangle - \frac{1}{2}\sigma^2 \frac{\partial\lambda}{\partial n}$	Wahlborn's results
16	16	0	4.42	5.75	-11.19	-14.43 (-14.47)	-14.17	-14.37
17*	17*	1	3.50	3.78	-8.67	-11.82	-11.43	-12.42
17*	17*	0	4.69	6.11	-12.71	-16.16	-15.87	-
16	16	2	0.96	0.35	-6.93	-9.41	-9.02	-9.63
16	16	$\mathcal{C}(2) - \mathcal{C}(0)$			4.26	5.03	4.65	4.74
17	17	$\mathcal{C}(1) - \mathcal{C}(0)$			3.04	4.34	4.45	-

* Note the different number of levels and particles for this case.

The quantity $\frac{1}{2}\sigma^2\{\partial^2\mathcal{C}(n,p)/\partial p^2\}_{p=n}$ assumes the value 0.94 Δ_0 in the even case and 0.85 Δ_0 in the odd case. The theoretical odd-even mass difference should thus from here receive a correction of +0.09 Δ_0. The corresponding corrections are 0.79 Δ_0, 0.53 Δ_0 and +0.26 Δ_0, respectively if the estimate $\{\partial^2\mathcal{C}(n,p)/\partial p^2\}_{p=n} \approx \partial\lambda/\partial n$ is employed. Thus, the correction for particle number fluctuations in determining odd-even mass differences for the uniform model is less important than previously believed (cf., however, table 2, valid for a finite case).

Finally we have tested the model on a few other numerical examples. In table I we compare the results based on eq. (2) with those of an exact diagonalization for the case of six equally spaced levels with the level separation energy $\Delta\epsilon = 0.2$, 1, and $2G$, respectively. Energies are given in units of G and measured with respect to the $G = 0$ case. The term $\{\partial^2\mathcal{C}/\partial p^2\}_{p=n}$ is evaluated only to leading order. It is found in this case that 80-85% of the discrepancy with the exact result is eliminated by the simple procedure suggested. It is also found that the replacement of $\partial^2\mathcal{C}/\partial p^2$ with $\partial\lambda/\partial n$ does not significantly alter the result. As in this case there are altogether only 64 terms in the BCS wave function, of which 20 correspond to the correct particle number, it is amazing that the method of steepest decent on the whole gives so good a result. A more detailed comparison of $\partial^2\mathcal{C}/\partial p^2$ and $\partial\lambda/\partial n$ should not be made for this case.

A more realistic example may be provided by the sixteen-level model of table 2 with $\Delta\epsilon = 2G$. As no exact results are available, we compare with the results obtained by Wahlborn based on a variational method (last column of table). The energies are given in units of G and with reference to the case $G = 0$. In the case $v = 0$ (seniority zero) we obtain a value very near to Wahlborn's. In column seven the value in parenthesis corresponds to a redetermination of U_ν and V_ν to make $\mathcal{C}^{\mathrm{corr}}$ rather than $\langle\mathcal{C}\rangle$ minimum, as suggested in ref. 1, eq. (34). (Note the missing factor 2 in eqs. (35) and (36a). Thus, K should equal $G - 2\partial^2\mathcal{C}/\partial p^2$.) It appears that for this larger system containing 2^{16} terms in the BCS wave function, the suggested estimate of $\partial^2\mathcal{C}/\partial p^2$ gives a result significantly improved compared to that based on $\partial\lambda/\partial n$. Note that the odd-even mass difference $\mathcal{C}(1) - \mathcal{C}(0)$ comes out nearly the same in the two cases and close to Δ_0.

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