Comment on "Monte Carlo Computation of Pair Correlations in Excited Nuclei"

Recently, N.J. Cerf [1] presented a quantum Monte Carlo method for the study of thermodynamic properties of nuclear many-body systems using a monopole pairing interaction in the canonical ensemble. The author asserts that the method allows a stochastic calculation of the internal energy, the entropy, the specific heat, and the level density at finite temperature. In our opinion, the space of configurations taken into account is too limited to calculate properties at finite temperature. In the Letter [1], Monte Carlo results, starting from a model with a $(h_{11/2})^6$ configuration and with a constant pairing strength of 1 MeV, were compared to exact results obtained in the quasispin formalism. The energy levels of the system are -12 , -6 , -2 , and 0 MeV (the single-particle energy is set to 0 MeV). In the quasispin formalism, degeneracies for these levels are given by [2] $d(s) = \binom{\Omega}{s/2} - \binom{\Omega}{s/2-1}$, where s is the seniority quantum number and $\Omega = j + \frac{1}{2}$. The ground state, which has $s = 0$, has degeneracy $d(0) = 1$. These degeneracies apply only to the subspace where all particles are "accompanied" in the sense defined by Burglin and Rowley [3]. The complete Fock space contains many more states. Taking all of these states into account, one finds the same energy levels because the unpaired particles do not interact and, hence, do not contribute to the energy. But the degeneracies change dramatically for the excited levels. Instead of 1, 5, 9, and 5, respectively, one now finds 1, 65, 429, and 429 as degeneracies. We calculated the thermodynamical properties of this system with a method that is based on a Monte Carlo sampling of the Hamiltonian instead of the many-body states. The method is closely related to the shell-model quantum Monte Carlo method [4]. Canonical traces were evaluated with an algorithm that amounts to a complete summation over all states with a given number of particles [5], such that

FIG. 1. Internal energy U versus temperature T . Error bars on our Monte Carlo data were omitted because they are smaller than the symbols marking the data points.

FIG. 2. Specific heat C versus temperature T . Error bars on the Monte Carlo data represent 95% confidence intervals.

the full N -particle space is taken into account. Figure 1 shows the internal energy of the system as a function of temperature. Our Monte Carlo results are in excellent agreement with the exact results that are based on the degeneracies of the full space. They differ clearly from the results for the fully accompanied states only, with which the Monte Carlo results of Cerf coincide (his data points are not shown here). It is observed that the internal energy starts to rise at temperatures near 1 MeV. This leads to a distinct peak in the specific heat around 1.25 MeV, as is shown in Fig. 2. The curve for the fully accompanied subspace (f.a. subspace) shows a lower and broader peak at temperatures around 2 MeV. This peak was associated by Cerf with the vanishing of nucleon pair correlations. In our opinion, the breakup of pairs already at lower temperatures. This results in the stronger peak that we observe around 1.25 MeV. Though the Monte Carlo method presented in [1] offers an interesting way to study pair correlations in nuclei, we emphasize that a full treatment of the complete many-body space is required to study properties at finite temperature.

S. Rombouts and K. Heyde
Vakgroep Subatomaire en Stralingsfysica
University of Ghent Proeftuinstraat 86
B-9000 Gent, Belgium

Received 17 March 1997 [S0031-9007(97)05066-7]
PACS numbers: 21.60.Ka, 02.70.Lq, 21.10.Ma, 21.60.Cs

- [1] N. J. Cerf, Phys. Rev. Lett. **76**, 2420 (1996).
- [2] O. Burglin and N. Rowley, Nucl. Phys. **A602**, 21 (1996).
- [3] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, New York, 1980).
- [4] S. E. Koonin, D. J. Dean, and K. Langanke, Phys. Rep. **278**, 1 (1997).
- [5] S. Rombouts and K. Heyde (to be published).