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Problems in Hartree-Fock calculations of nuclear level densities

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Microscopic methods based on an effective two-body interaction, like Hartree-Fock, or Hartree-Fock-Bogoliubov approximations, give a good description of nuclear ground- and low-lying states in a wide range of the periodic table. It would be interesting to check their validity at higher excitation energies, where statistical mechanics can be applied, in order to obtain average properties, like nuclear level densities, without resorting to adjustable parameters.

An attempt was made in ref. 1 for some Sn isotopes, within the framework of the grand partition function method, by using a spherical Hartree-Fock_Bardeen-Cooper-Schrieffer formalism, without taking collective excitations into account. The theoretical level densities underestimated the experimental ones at the neutron binding energy, B_n , by a factor 20, or more.

In order to reduce this discrepancy, ref. 2 suggests that Sn isotopes could be statistically deformed at finite, but low excitation energy, of the order $E^* \simeq 8 \div 10$ MeV.

We do not comment on this possibility, which deserves further attention. Anyway, the observed level spacings for some Sn isotopes at $E^* = B_n$ are rather well reproduced in the spherical symmetry limit by microscopic calculations based on a Nilsson potential plus a simple

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pairing interaction, at the price of assuming the same average ground-state correlation function $\Delta \cong 1$ MeV for both neutrons and protons (ref.3).

The purpose of this note is to point out that a drastic underestimation of nuclear level densities for both spherical and deformed nuclei could be rather a common feature of effective interactions, which generate too weak densities of single-particle states near the chemical potential, corresponding to the Fermi energy in a Fermi gas model.

Taking ^{116}Sn as an example, we have evaluated the densities of single-particle states near the neutron and proton chemical potentials at various thermodynamic temperatures, by means of the effective D1 interaction (ref. 4; see also ref. 5 for an extensive description of its properties). The single-particle energies show a weak dependence on temperature; therefore, we can compare the ground state results with the corresponding densities of Nilsson single-particle states used in ref. 3. Fig. 1 shows that the greatest discrepancies occur if the densities are evaluated by counting the single-particle states near the Fermi energy in an interval of half-width $\Omega \simeq 1 \div 1.5$ MeV, of the order of the neutron ground-state correlation function Δ_n. Here, n-n pairing effects play an important role.

Therefore, we obtain an increase of nuclear entropies, S, and consequently of nuclear level densities, as functions of the excitation energy, E^*, much slower in the Hartree-Fock-Bogoliubov procedure than in the Nilsson-plus-pairing calculation. The functions $S(E^*)$ for ^{116}Sn, obtained through both methods with the assumption of spherical symmetry, are shown in Fig. 2.

A similar trend has been found for well deformed nuclei, too: Fig. 3 shows $S(E^*)$ for ^{158}Gd. Here, the parameters adopted in the Nilsson case to fit the experimental nuclear level spacing at $E^* = B_n$ are the same as in ref. 6. The discrepancy between the two results seems to be weaker in this case.

The present results lead us to the conclusion that self-consistent calculations of nuclear level densities would imply a preliminary improvement in the single-particle level densities near the chemical potential.

A way we would like to explore goes beyond the Hartree-Fock-Bogoliubov approximation , and implies a study of interaction of Fermions and quasibosons arising in a random phase treatment of our effective Hamiltonian. This particle-vibration coupling gives rise

to shifts in single-particle energies, which are expected to reduce the gap between occupied and unoccupied orbits in nuclear ground states (see, e. g., ref. 7). Unfortunately, a microscopic treatment of this effect involves considerable difficulties. An extensive discussion is left to a future work.

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Figure Captions

1a) ^{116}Sn: neutron level density $g(\Omega) = N(\Omega)/(2\Omega)$. $N(\Omega)$ is the number of neutron levels (degeneracy is removed) in an interval of half-width Ω centered at the Fermi energy. N: Nilsson potential (ref. 3). HF: effective D1 interaction, in Hartree-Fock approximation (ref. 5).

1b) ^{116}Sn: proton level density $g(\Omega)$. Comments as in Fig. 1a.

2) ^{116}Sn: Nuclear entropy S (in units of the Boltzmann constant) versus excitation energy E^*. NBCS: Nilsson-plus-pairing calculation; HFB: effective D1 interaction, Hartree-Fock-Bogoliubov approximation.

3) ^{158}Gd: Nuclear entropy S versus excitation energy E^*. Comments as in Fig. 2.

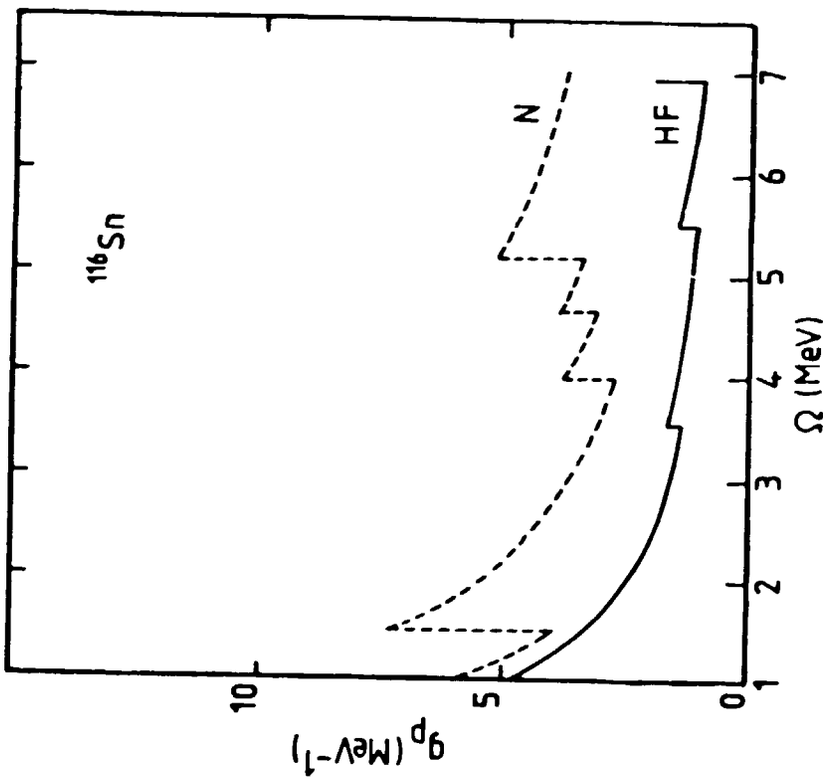
^{116}Sn
N
HF
g_p (MeV^{-1})
Ω (MeV)
0
5
10
1
2
3
4
5
6
7

Fig. 1b

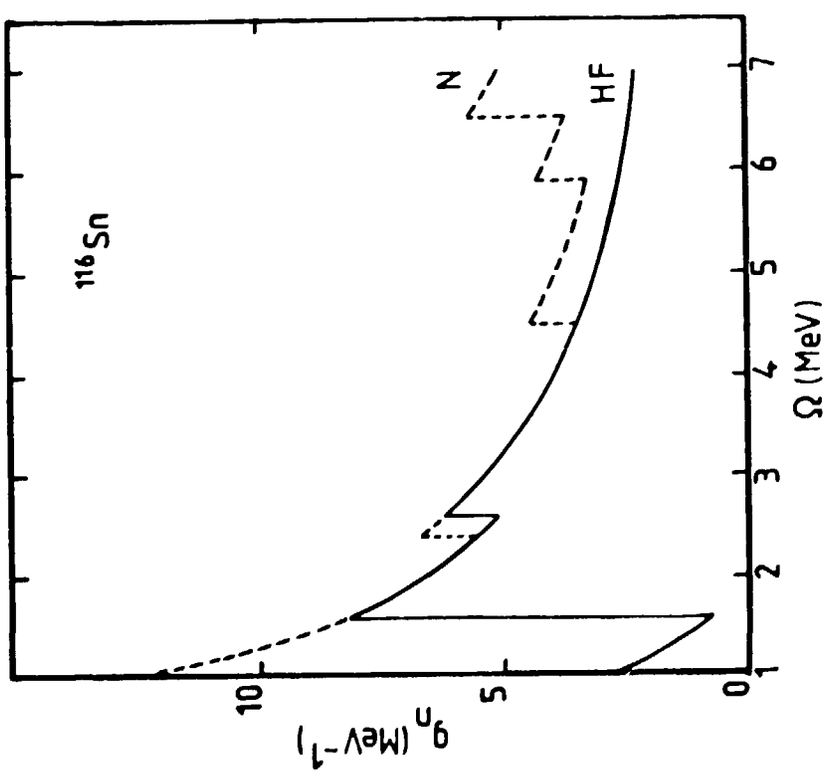
^{116}Sn
N
HF
g_n (MeV^{-1})
Ω (MeV)
0
5
10
1
2
3
4
5
6
7

Fig. 1a

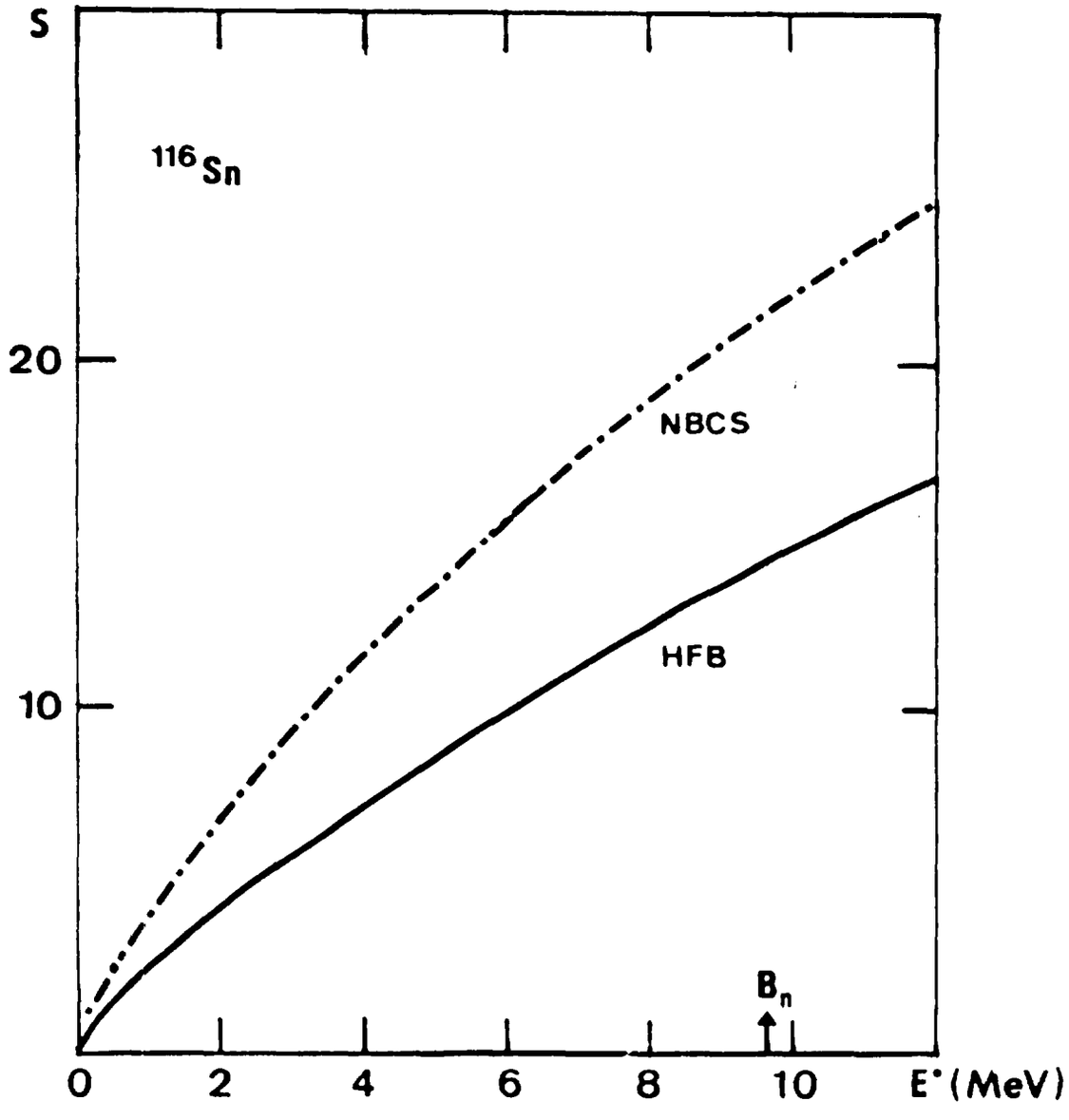

Fig. 2

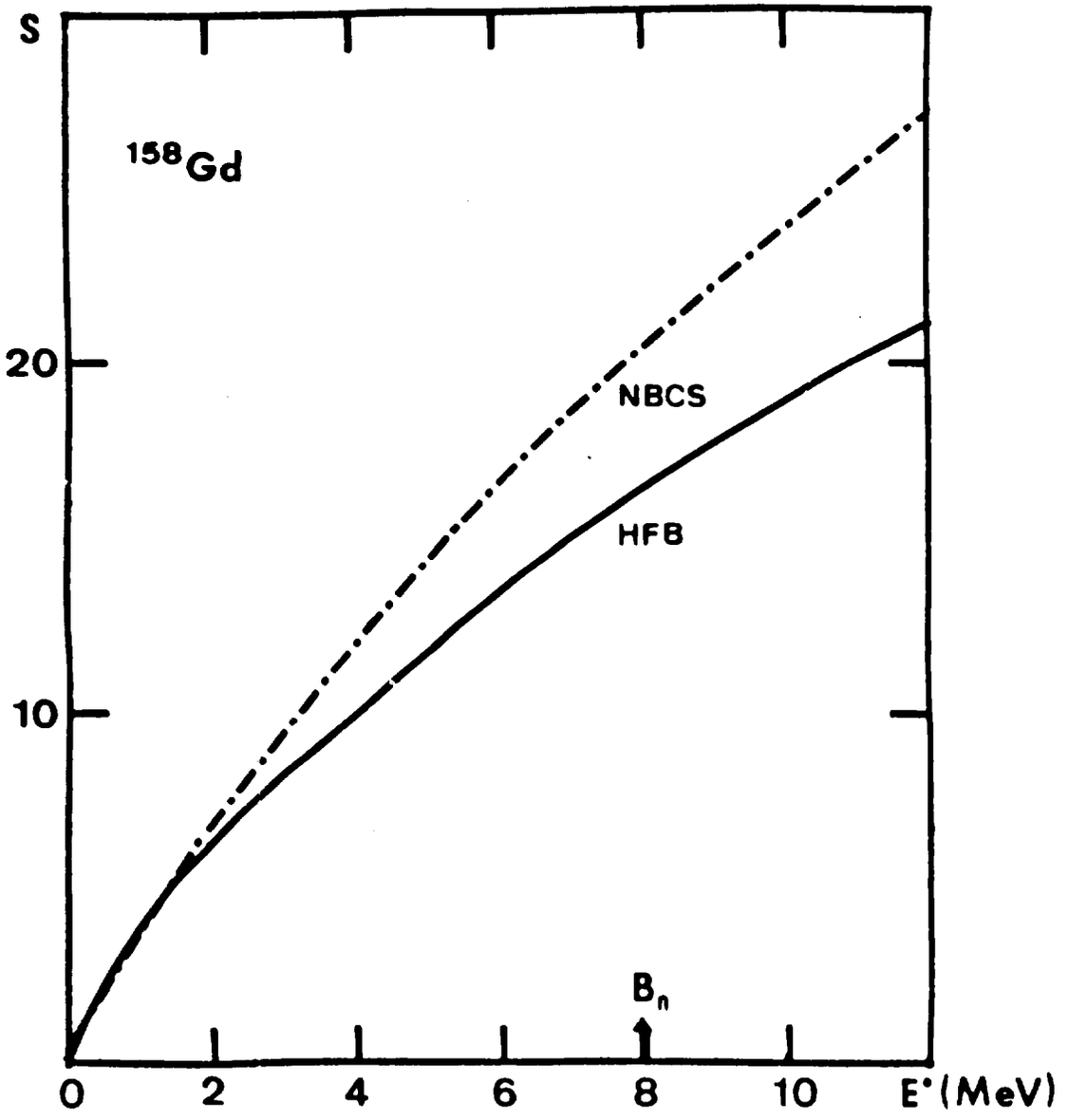

Fig. 3