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Microscopic description of average level spacing in even-even nuclei

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Abstract. A microscopic theoretical approach to the average level spacing at the neutron binding energy in even-even nuclei is proposed. The approach is derived based on the Bardeen-Cooper-Schrieffer (BCS) theory at finite temperature and projection M of the total angular momentum J, which is often used to describe the superfluid properties of hot rotating nuclei. The exact relation of the J-dependent total level density to the M-dependent state densities, based on which the average level spacing is calculated, was employed. The numerical calculations carried out for several even-even nuclei have shown that in order to reproduce the experimental average level spacing, the M-dependent pairing gaps as well as the exact relation of the J-dependent total level density formula should be simultaneously used.

1. Introduction

Knowledge of the average level spacing between resonances of a compound nucleus has an important role in the calculation of the nuclear level density (NLD). The latter, which is defined as the number of excited levels per unit of excitation energy E^*, has major contribution in the study of nuclear structure and low-energy reaction. This average level spacing has been extensively studied within a number of theoretical models including both phenomenological and microscopic ones (see e.g., Refs. [1, 2, 3] and references therein). The phenomenological models are often derived based on the Bethe formula of NLD [4], in which several phenomenological parameters are introduced and their values are found from the fitting to the experimental data. The microscopic models are usually constructed based on the statistical nuclear thermodynamic theories such as the Bardeen-Cooper-Schrieffer (BCS) theory at finite temperature (FTBCS) [5] or finite temperature Hartree-Fock-Bogoliubov (FTHFB) [6], in which the effects of superfulid pairing, deformation, vibration, rotation and shell structure, which are important for the description of NLD, are microscopically or empirically included. However, within the FTBCS and FTHFB, the angular-momentum dependent total NLD is calculated approximately from the state density by assuming that the distribution of nuclear spins can be approximated with the Gaussian function [7]. In fact, the angular-momentum dependent total NLD can be calculated directly from the angular-momentum dependent state densities via its exact relation (see e.g., Eq. (56) of Ref. [7]), which can be obtained within the BCS theory at finite temperature and

angular momentum (FTABCS). The goal of the present paper is to employ the FTABCS theory to calculate the angular-momentum dependent total NLD using this exact relation. The results obtained will be used to calculate the average level spacing at the neutron binding energy. The numerical calculations are restricted to even-even nuclei, whereas the extension to odd-even and odd-odd cases is still going on.

2. Formalism

2.1. BCS theory at finite temperature and finite angular momentum (FTABCS)

The FTABCS equations are derived based on the grand-canonical ensemble average of the nuclear Hamiltonian, which consists of the one-body mean field and two-body monopole pairing interaction with the rotational field acted on the projection M of the total angular momentum J as an external field. The derivation of the FTABCS equations for the pairing gap Δ, particle number N, and angular momentum M has been reported in a number of papers [7, 8, 9, 10], so we report here only their final forms, which are given as

$$\begin{aligned} \Delta &= G\sum_k u_k v_k(1-n_k^+-n_k^-)\ , \\ N &= 2\sum_k\left[(1-n_k^+-n_k^-)v_k^2+\frac{1}{2}(n_k^++n_k^-)\right]\ , \\ M &= \sum_k m_k(n_k^+-n_k^-)\ , \end{aligned} \tag{1}$$

where

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left(1+\frac{\epsilon_k-\lambda}{E_k}\right), \quad v_k^2=1-u_k^2\ , \\ E_k &= \sqrt{(\epsilon_k-\lambda)^2+\Delta_k^2}\ , \quad n_k^\pm=\frac{1}{1+e^{(E_k\mp\gamma m_k)/T}}\ . \end{aligned}$$

Here ϵ_k are energies of the single-particle levels k written in the deformed basis and λ, γ, G, and T are respectively chemical potential, rotational velocity (frequency), pairing interaction parameter, and temperature of the nuclear system, which corresponds to a given excitation energy of the compound nucleus.

The FTABCS equations are numerically solved to obtain λ, γ, Bogoliubov transformation coefficients u_k and v_k, quasiparticle energy E_k, quasiparticle occupation numbers $n_k^\pm$, and pairing gap $\Delta_{N(Z)}$ at different values of T and M. These quantities are then used to calculate the total (internal) energy $E(T,M)$ and entropy $S(T,M)$, whose explicit forms are given as

$$E(T,M)=2\sum_k\epsilon_k\left[(1-n_k^+-n_k^-)v_k^2+\frac{1}{2}(n_k^++n_k^-)\right]-\frac{\Delta^2}{G}\ , \tag{2}$$

$$S(T,M)=-\sum_k[n_k^+\ln n_k^+ + (1-n_k^+)\ln(1-n_k^+) + n_k^-\ln n_k^- + (1-n_k^-)\ln(1-n_k^-)]\ . \tag{3}$$

As the nuclear system consists of N neutrons and Z protons, the total energy and total entropy of the nucleus should be calculated as

$$E(T,M)=E_N(T,M)+E_Z(T,M), \quad S(T,M)=S_N(T,M)+S_Z(T,M), \tag{4}$$

where $E_{N(Z)}$ and $S_{N(Z)}$ are the internal energy and entropy calculated from Eqs. (2) and (3) for neutron (proton), respectively.

2.2. Intrinsic state density and average level spacing

The intrinsic state density of an atomic nucleus at given excitation energy E^* and angular momentum M is calculated based on the inverse Laplace transform of the grand-partition function making use of the saddle-point approximation. It has the form as [7]

$$\omega(E^*, M) = \frac{e^S}{(2\pi)^2 \left|D\right|^{1/2}} \ , \tag{5}$$

where $E^*(T, M) = E(T, M) - E(T = 0, M)$ and the determinant D is given in terms of the second derivatives of the grand-partition function with respect to $\alpha = \lambda/T$ and $\mu = \gamma/T$

$$D = \begin{vmatrix} \frac{\partial^2\Omega}{\partial\alpha_N^2} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\alpha_\mu} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\alpha_\beta} \\ \frac{\partial^2\Omega}{\partial\alpha_Z\partial\alpha_N} & \frac{\partial^2\Omega}{\partial\alpha_Z^2} & \frac{\partial^2\Omega}{\partial\alpha_Z\partial\alpha_\mu} & \frac{\partial^2\Omega}{\partial\alpha_Z\partial\alpha_\beta} \\ \frac{\partial^2\Omega}{\partial\alpha_\mu\partial\alpha_N} & \frac{\partial^2\Omega}{\partial\alpha_\mu\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\alpha_\mu^2} & \frac{\partial^2\Omega}{\partial\alpha_\mu\partial\alpha_\beta} \\ \frac{\partial^2\Omega}{\partial\alpha_\beta\partial\alpha_N} & \frac{\partial^2\Omega}{\partial\alpha_\beta\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\alpha_\beta\partial\alpha_\mu} & \frac{\partial^2\Omega}{\partial\alpha_\beta^2} \end{vmatrix} \ . \tag{6}$$

In Eq. (6), the logarithm of the grand-partition function of the systems Ω is calculated as

$$\Omega = \Omega_N + \Omega_Z = S_N + S_Z + \alpha N_N + \alpha Z_Z + \mu M - \beta E \ . \tag{7}$$

The derivations of Ω with respect to α and μ can be seen explicitly in Eqs. (25)–(35) of Ref. [7].

The total NLD $\rho(E^*)$ at given excitation energy E^* is calculated as the sum of all J-dependent level densities

$$\rho(E^*) = \sum_J (2J+1)\rho(E^*, J) \ , \tag{8}$$

where $\rho(E^*, J)$ can be obtained from the difference between the state densities of the system with angular momentum $M = J$ and $M = J + 1$, namely [7]

$$\rho(E^*, J) = \omega(E^*, M = J) - \omega(E^*, M = J + 1) \ , \tag{9}$$

with $\omega(E^*, M)$ being the state density calculated from Eq. (5). It is worth noticing here that Eq. (9) is the exact relation between the total J-dependent NLD and M-dependent state densities.

Based on the assumption that the distribution of nuclear spin can be approximately expressed in terms of the Gaussian function, $\rho(E^*, J)$ in Eq. (8) can be calculated approximately as [5, 7]

$$\rho(E^*, J) \approx \frac{2J+1}{2\sigma^3\sqrt{2\pi}}\omega(E^*)\exp\left(-\frac{J(J+1)}{2\sigma^2}\right) \ , \tag{10}$$

where $\omega(E^*)$ is the total state density obtained from Eq. (5) with $M = 0$ and σ is the spin cut-off parameter, which is related to the nuclear moment of inertia via the relation $\sigma^2_{\perp(\parallel)} = \Im_{\perp(\parallel)}T/\hbar^2$, where $\Im_{\perp(\parallel)}$ is the moment of inertia perpendicular (parallel) to the symmetry axis of the nucleus. The perpendicular spin cut-off parameter is often calculated empirically via the limit of rigid body [11]

$$\sigma^2_\perp \approx 0.015TA^{5/3}(1 + \frac{\beta_2}{3}) \ , \tag{11}$$

where A is the nuclear mass number and β_2 is the quadrupole deformation parameter. The parallel spin cut-off parameter can be calculated microscopically within the FTBCS theory as [7]

$$\sigma^2_\parallel = \frac{1}{2}\sum_k m_k^2 \mathrm{sech}^2\frac{1}{2}\beta E_k \ . \tag{12}$$

Consequently, two approximate formulas for the J-dependent total NLD, which have been used in most theoretical models such as the FTBCS or FTHFB, are [5, 6]

$$\rho_{\rm vib}(E^*,J) \approx \frac{2J+1}{2\sigma_\parallel^3\sqrt{2\pi}}\frac{\omega(E^*)}{(1-e^{-\beta\omega_\lambda})^{2\lambda+1}}\exp\left(-\frac{J(J+1)}{2\sigma_\parallel^2}\right) , \quad (13)$$

$$\rho_{\rm rot}(E^*,J) \approx \frac{2}{2\sigma_\parallel\sqrt{2\pi}}\omega(E^*)\sum_{K=-J}^{J}\exp\left(-\frac{K^2}{2\sigma_\parallel^2}-\frac{J(J+1)-K^2}{2\sigma_\perp^2}\right) , \quad (14)$$

where ω_λ is the phonon energy of the vibrational excitation corresponding to the phonon multipolarity λ, whereas K is the projection of total angular momentum J on the symmetry axis. In these equations, Eq. (13) is used for spherical and/or slightly deformed nuclei, whose vibrational collective vibrations are significant, whereas Eq. (14) is applicable for well-deformed nuclei, whose rotational excitations are mostly important.

Knowing the J-dependent total NLD, one can easily calculate the average level spacing $\overline{D}$ at the neutron binding energy B_n based on its definition as [6]

$$\overline{D} = \frac{10^6}{\rho\left(B_n, I_t-\frac{1}{2}\right)+\rho\left(B_n, I_t+\frac{1}{2}\right)} , \quad (15)$$

where $\rho(B_n, I_t \pm 1/2)$ are the NLDs obtained at the excitation energy $E^* = B_n$ and spins $J = I_t \pm 1/2$, with I_t being the ground-state spin of the target nucleus $(Z, N-1)$.

3. Numerical results and discussion

The average level spacings are calculated within the FTABCS for several even-even nuclei from the medium ^{58}Fe to the heavy ^{250}Cf mass isotopes. The single-particle spectra ϵ_k are taken from the axially deformed Woods-Saxon (WS) potential including the spin-orbit and Coulomb interactions. The parameters of the WS potential are taken from Ref. [12]. The quadrupole β_2 and hexadecapole β_4 deformation parameters are adjusted to reproduce the experimental ground-state properties including nuclear binding energy and charge radii as well as energy of the first 2^+ state. The pairing interaction parameter $G_{N(Z)}$ is as usual adjusted so that the pairing gap $\Delta_{N(Z)}$ obtained within the FTABCS at $T = 0$ and $M = 0$ fits the experimental odd-even mass difference.

It is found that the pairing gap $\Delta_{N(Z)}$ decreases with increasing both T and M and collapses at given $T = T_c$ and $M = M_c$ values, which are defined as the critical temperature and critical angular momentum, respectively (See e.g., Figs. 2 and 3 of Ref. [8]). This change of the pairing gaps is known to affect the state density (5) as well as level density (9) at low E^* and M. Consequently, one can see in Table 1 the average level spacings $\overline{D}$ obtained within the FTABCS using Eq. (15) with $\rho(E^*, J)$ being calculated from its exact relation (9) are in quite good agreement with the experimental data of all nuclei under consideration. It is also seen in this Table 1 that the results obtained within the FTBCS by Maino [5] and FTHFB by Goriely [6] are far from the measured data, especially for nuclei with large ground-state spins such as ^{68}Zn($I_t = 5/2$), ^{88}Sr($I_t = 9/2$), ^{98}Mo($I_t = 5/2$), ^{144}Nd($I_t = 7/2$), ^{150}Sm($I_t = 7/2$), ^{162}Dy($I_t = 5/2$), ^{168}Er($I_t = 7/2$), ^{248}Cm($I_t = 9/2$), and ^{250}Cf($I_t = 9/2$). One of the reasons of the discrepancy between the results obtained within the FTBCS and FTHFB approaches and the experimental data is that the pairing gaps obtained within these theoretical models depend only on $T(E^*)$, whereas in reality the pairing gaps should depend on not only $T(E^*)$ but also $M(J)$. Other reason is certainly due to the use of the approximate formulas (13) and (14) within the FTBCS (FTHFB) instead of the exact relation (9) for $\rho(E^*, J)$.

Compound Nucleus	I_t	B_n	$\overline{D}_{exp}$	$\overline{D}_{Maino}$	$\overline{D}_{Goriely}$	$\overline{D}_{FTABCS}$
^{58}Fe	$\frac{1}{2}$	10.044	7050 ± 700		3440	6889
^{68}Zn	$\frac{5}{2}$	10.198	370 ± 20		235	365.7
^{78}Se	$\frac{1}{2}$	10.498	120 ± 15		409	122.6
^{88}Sr	$\frac{9}{2}$	11.112	290 ± 80		160	285.1
^{98}Mo	$\frac{5}{2}$	8.643	60 ± 10	30.3	42	59.96
^{112}Cd	$\frac{1}{2}$	9.394	27 ± 2	23.9	14.1	26.86
^{118}Sn	$\frac{1}{2}$	9.324	61 ± 7	76.7	38.1	68.58
^{126}Te	$\frac{1}{2}$	9.113	43 ± 3	49.0	20.8	47.14
^{132}Xe	$\frac{3}{2}$	8.935	49 ± 8	52.2	34.1	48.11
^{144}Nd	$\frac{7}{2}$	7.817	38 ± 2	30.1	25.4	34.49
^{150}Sm	$\frac{7}{2}$	7.987	2.4 ± 0.2	1.56	1.94	2.486
^{162}Dy	$\frac{5}{2}$	8.197	2.4 ± 0.2	2.67	1.48	2.464
^{168}Er	$\frac{7}{2}$	7.771	4.2 ± 0.3	4.61	2.7	3.987
^{180}Hf	$\frac{9}{2}$	7.380	4.6 ± 0.3	3.73	3.56	6.768
^{202}Hg	$\frac{3}{2}$	7.754	90 ± 30		36.4	86.75
^{248}Cm	$\frac{9}{2}$	6.21	1.27 ± 0.19	1.48	1.28	1.242
^{250}Cf	$\frac{9}{2}$	6.62	0.79 ± 0.12	0.73	0.426	0.7738

Table 1. Average level spacings of even-even nuclei at the neutron binding energy (B_n) and the ground-state spin (I_t) of the target nucleus obtained within the FTABCS ($\overline{D}_{FTABCS}$) in comparison with the experimental data ($\overline{D}_{exp}$) [14] as well as the FTBCS given by Maino ($\overline{D}_{Maino}$) [5] and FTHFB given by Goriely ($\overline{D}_{Goriely}$) [6].

4. Conclusions

Present paper applies the BCS theory at finite temperature and angular momentum (FTABCS) to describe the average level spacings of several even-even nuclei. Within the FTABCS, the neutron and proton pairing gaps and total state densities, which depend on both temperature (excitation energy) and angular momentum, are microscopically calculated. The average level spacings are then obtained based on the exact relation of the angular-momentum dependent total level density to the state densities instead of the approximate formulas, which are often used in previously proposed theoretical approaches. The results obtained within the FTABCS are in good agreement with the experimental data, especially for nuclei having large ground-state spins, whose angular-momentum dependent pairing correlations are important. Present paper is restricted to even-even nuclei. The extension of this method will be studied and the results will be reported in the forthcoming papers.

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