Microscopic study of spin cut-off factors of nuclear level densities

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Level densities and spin cut-off factors have been investigated within the microscopic approach based on the BCS Hamiltonian. In particular, the spin cut-off parameters have been calculated at neutron binding energies over a large range of nuclear mass using the BCS theory. The spin cut-off parameters $\sigma^2(E)$ have also been obtained from the Gilbert and Cameron expression and from rigid body calculations. The results were compared with their corresponding macroscopic values. It was found that the values of $\sigma^2(E)$ did not increase smoothly with A as expected based on macroscopic theory. Instead, the values of $\sigma^2(E)$ show structure reflecting the angular momentum of the shell model orbitals near the Fermi energy.

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I. INTRODUCTION

Nuclear level densities are important in all statistical model calculations. Analytical expressions which contain free parameters adjusted on scarce experimental data are the Bethe and constant temperature formula. They mainly differ in the low excitation energy region where pairing corrections play an important role [1,2].

Sophisticated theoretical approaches have been developed to study level densities. In particular is the microscopic approach based on the BCS Hamiltonian [3]. In all level density expressions, two parameters are of importance. The level density parameter a and the spin cut-off factor σ^2. Some authors [4,5] have calculated the level density parameter. More recently, we performed a realistic calculation that relies on the BCS theory (see Ref. [6]). The spin cut-off parameter σ^2 has also been calculated using the Fermi gas model [7,8]. So far, however, realistic calculations have never been applied to obtain the spin cut-off factor that is important in all statistical model codes. Having been shown that the BCS results agree well with experimental data for the level density $\rho(E^*)$ [9,10] and the level density parameter $a(E)$ [11,12], we extended in the present work the microscopic approach to calculate the level density and the spin cut-off parameter for a large number of nuclei. In Sec. II, the BCS model will be briefly discussed. In Sec. III, the method of calculating the level densities and spin cut-off parameters will be given; in Sec. IV, the summary and results will be presented.

II. THEORY

For a complete derivation of the formulas given in this section, see our previous publications [13,14]. On the basis of microscopic theory, the state density at excitation energy E^* is defined by

$$\omega(N, E^*) = \frac{\exp(S)}{2\pi D^{1/2}}. \tag{1}$$

Here, S is the entropy and D is a 2×2 determinant with its elements given in terms of the second derivatives of the grand partition functions of the nuclear system taken at the saddle point. At this point, the entropy is given by [14,15]

$$S = 2\sum_k \ln[1 + \exp(-\beta E_k)] + 2\beta \sum_k \frac{E_k}{1 + \exp(-\beta E_k)}, \tag{2}$$

where β is the inverse of the nuclear temperature, and $E_k = [(\varepsilon_k - \lambda)^2 + \Delta^2]^{1/2}$ is the quasiparticle energy, ε_k is the energy of the single particle k, and Δ is the gap parameter which is a measure of pairing strength.

The stationary point conditions that must be satisfied are the particle number N,

$$N = \sum_k n_k, \tag{3}$$

and its energy E,

$$E = \sum_k n_k \varepsilon_k, \tag{4}$$

with the occupational probability of level k

$$n_k = 1 - \frac{\varepsilon_k - \lambda}{E_k} \tanh\left(\frac{\beta E_k}{2}\right), \tag{5}$$

where λ is related to chemical potential. For a system with N neutrons and Z protons, the total energy is

$$E_{\text{tot}} = E_p + E_n, \tag{6}$$

and the level densities at an excitation energy $E^* = E_p^* + E_n^*$ is

$$\rho(N, Z, E^*) = \frac{\omega(N, Z, E^*)}{(2\pi\sigma^2)^{1/2}}, \tag{7}$$

where the spin cut-off factor is defined as [16]

$$\sigma^2 = \sigma_n^2 + \sigma_p^2, \tag{8}$$

with

$$\sigma_n^2 = \frac{1}{2}\sum_k m_k^2 \text{sech}^2\left(\frac{1}{2}\beta E_k\right), \tag{9}$$

and a similar equation for σ_p^2. Here, m_k is the magnetic quantum number of the single-particle level k.

III. METHOD OF CALCULATION

In the present study, the nuclear level density and the spin cut-off factor have been determined at neutron binding energies for 295 nuclei between ^{20}F and ^{251}Cf using microscopic theory. The steps necessary to calculate level density $\rho(E^*)$ and the relevant spin cut-off parameter $\sigma(E^*)$ are as follows: For a set of single-particle levels and particular choice of temperature T, the parameters λ and Δ were estimated, and a set of occupational probabilities was calculated using Eq. (5). Next, the stationary point conditions were checked for a given nucleon number using Eq. (3). If the conditions were not met, the values of λ and Δ were adjusted, and the procedure was repeated until the saddle point conditions were satisfied. Once the proper set of n_k values were computed, the entropy S_k was calculated using Eq. (2). The energy E_n was calculated by applying Eqs. (4) and (5) at particular temperature T. The excitation energy E_n^* was then determined by subtracting the energy at $T = 0$. The quantities $\sigma_n^2, \omega(N, E_n)$ were then calculated using Eqs. (1)–(9). A similar set of calculations were used to calculate E_p^* and S_p for the proton system. The total level density and spin cut-off factor were then calculated from Eqs. (7) and (8).

A systematic study of the behavior of the level density and the spin cut-off parameter across a large mass region was performed. The results for even-even nuclei are shown in Table I. Their corresponding rigid body values, $\sigma^2 = 0.0138A^{2/3}\sqrt{U/a}$, as well as their values obtained from the Gilbert and Cameron expression, $\sigma^2 = 0.0888A^{2/3}\sqrt{a(U-E_0)}$, where a is the level density parameter, U is the excitation energy, and E_0 is the back shift energy [16], are also given in Table I for comparison and are plotted in Fig. 1. Similar results for odd-odd nuclei are

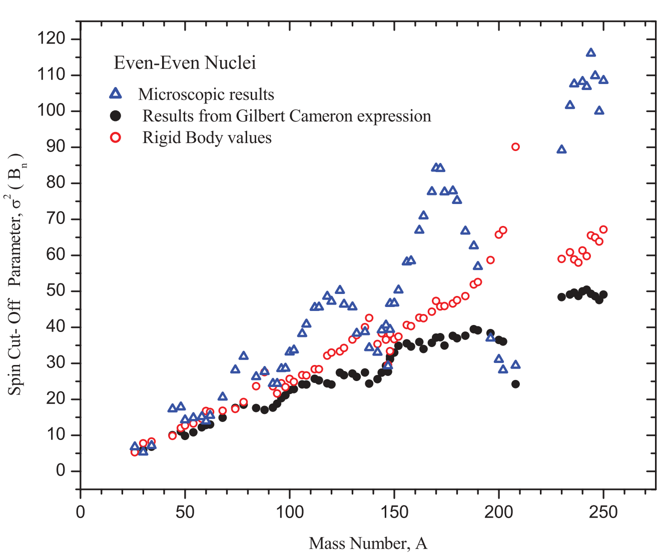

FIG. 1. (Color online) Spin cut-off parameters $\sigma^2(B_n)$ at the neutron binding energy, calculated with the microscopic theory, the Gilbert and Cameron expression, and the rigid body expression.

TABLE I. Comparison of spin cut-off parameters σ^2 from different methods for even-even nuclei: (a) Gilbert and Cameron expression, (b) rigid body approximation, and (c) microscopic theory.

Z	A	Element	Spin cut-off parameter, $\sigma^2(B_n)$ (a)	(b)	(c)
12	26	Mg	5.41	5.30	6.77
14	30	Si	5.95	7.77	5.33
16	34	S	6.83	8.26	7.15
20	44	Ca	10.05	9.84	17.31
22	48	Ti	11.06	11.99	17.86
22	50	Ti	9.83	12.69	14.27
24	54	Cr	10.83	13.28	14.86
26	58	Fe	12.21	14.59	15.17
28	60	Ni	12.86	16.75	13.94
28	62	Ni	13.00	16.48	15.53
30	68	Zn	14.88	16.82	20.58
32	74	Ge	17.59	17.33	28.15
34	78	Se	18.48	19.23	31.92
36	84	Kr	17.58	23.63	26.28
38	88	Sr	17.05	27.55	27.70
40	92	Zr	17.67	23.62	24.40
40	94	Zr	18.79	21.63	24.40
42	96	Mo	20.32	24.45	28.50
42	98	Mo	21.12	23.41	28.60
44	100	Ru	22.58	25.67	33.10
44	102	Ru	22.84	24.84	33.70
46	106	Pd	24.12	26.73	38.23
46	108	Pd	24.10	26.63	40.87
48	112	Cd	25.70	28.36	45.50
48	114	Cd	25.25	28.35	45.60
50	118	Sn	24.41	32.11	48.60
50	120	Sn	24.10	32.99	47.20
52	124	Te	27.41	33.29	50.23
52	126	Te	26.68	34.27	46.40
54	130	Xe	27.14	36.59	45.66
54	132	Xe	26.22	37.80	38.35
56	136	Ba	27.45	40.03	38.75
56	138	Ba	24.37	42.59	34.34
58	142	Ce	25.59	35.35	33.05
60	144	Nd	27.39	38.32	39.27
60	146	Nd	29.30	36.56	40.61
60	147	Nd	27.66	29.56	29.27
60	148	Nd	31.86	33.36	39.41
62	148	Sm	31.13	38.12	46.62
62	152	Sm	34.86	37.40	50.32
64	156	Gd	35.53	40.65	58.12
64	158	Gd	34.63	40.32	58.44
66	162	Dy	35.92	42.68	66.95
66	164	Dy	33.95	42.53	70.93
68	168	Er	35.66	44.32	77.65
70	170	Yb	37.13	47.32	84.19
70	172	Yb	37.22	45.79	84.09
70	174	Yb	34.94	45.90	77.57
72	178	Hf	37.61	46.61	77.87
72	180	Hf	36.96	47.52	75.22
74	184	W	37.65	48.65	66.70
76	188	Os	39.46	51.89	62.61

TABLE I. (*Continued.*)

Z	A	Element	Spin cut-off parameter, $\sigma^2(B_n)$		
			(a)	(b)	(c)
76	190	Os	39.13	52.55	56.87
78	196	Pt	38.39	58.67	36.97
80	200	Hg	36.50	65.72	31.07
80	202	Hg	36.02	66.96	28.16
82	208	Pb	24.20	90.11	29.44
90	230	Th	48.37	58.98	89.21
92	234	U	49.08	60.85	101.59
92	236	U	49.62	58.85	107.58
92	238	U	48.69	57.96	–
94	240	Pu	49.99	61.33	108.24
94	242	Pu	50.44	59.78	106.88
96	244	Cm	49.30	65.51	116.09
96	246	Cm	48.63	64.97	109.86
96	248	Cm	47.57	63.83	100.03
98	250	Cf	49.09	67.15	108.55

listed in Table II and plotted in Fig. 2. The same results for odd-A nuclei are listed in Table III and plotted in Fig. 3. Examination of these figures reveals that the values of the spin cut-off factor deduced from the BCS theory did not increase smoothly with A, as expected on the basis of macroscopic theory with rigid body moment of inertia; instead, the values of $\sigma^2(E)$ showed structure reflecting the angular momentum of shell model orbitals near the Fermi energy.

We have found it worthwhile to compare our results with those obtained using the analytic expression

$$\sigma^2 = 0.0146A^{5/3}\frac{1+\sqrt{1+4a(U-E_1)}}{2a},$$

which was introduced very recently (see Ref. [7]). The σ^2 values computed from this expression for all nuclei under study

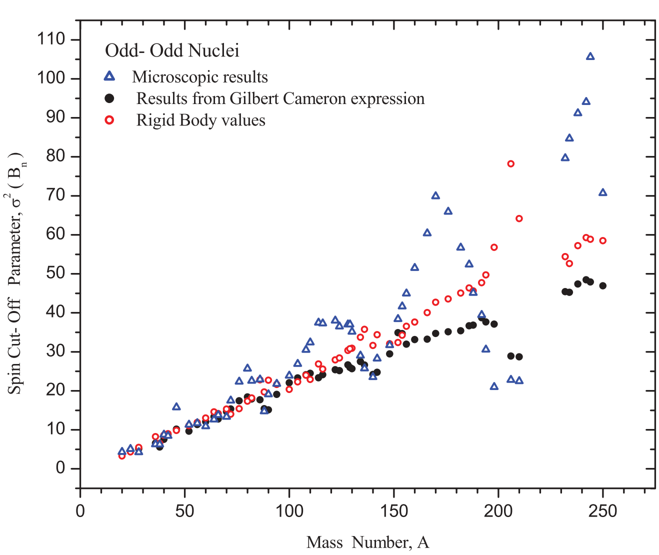

FIG. 2. (Color online) Same as Fig 1, but for odd-odd nuclei.

TABLE II. Same as Table I, but for odd-odd nuclei.

Z	A	Element	Spin cut-off parameter, $\sigma^2(B_n)$		
			(a)	(b)	(c)
9	20	F	3.90	3.30	4.34
11	24	Na	4.70	4.35	5.10
13	28	Al	5.14	5.47	4.27
17	36	Cl	6.55	8.22	6.30
17	38	Cl	5.58	6.52	6.27
19	40	K	7.55	8.60	8.75
19	42	K	8.77	8.99	8.45
21	46	Sc	10.15	9.84	15.76
23	52	V	9.65	11.06	11.33
25	56	Mn	11.35	11.88	11.72
27	60	Co	12.05	13.02	10.91
29	64	Cu	13.35	14.60	12.65
29	66	Cu	12.77	14.17	13.79
31	70	Ga	14.65	15.33	13.34
31	72	Ga	15.34	14.01	17.52
33	76	As	17.45	15.39	22.36
35	80	Br	18.42	17.33	25.70
35	82	Br	17.89	18.16	22.58
37	86	Rb	17.69	22.82	22.90
37	88	Rb	15.42	19.71	14.75
39	90	Y	15.11	22.73	19.10
41	94	Nb	19.07	21.63	21.80
43	100	Tc	22.06	20.36	23.90
45	104	Rh	23.29	22.28	26.90
47	108	Eu	24.13	24.00	30.50
47	110	Eu	24.49	22.90	32.40
49	114	Tb	23.32	26.89	37.50
49	116	Ho	24.12	25.56	37.30
51	122	Tm	25.41	27.91	38.00
51	124	Lu	25.16	28.40	36.50
53	128	Ta	26.66	30.36	37.04
53	130	Re	25.67	30.90	35.16
54	129	Re	25.98	30.77	37.02
55	134	Ir	27.50	33.71	29.04
55	136	Ag	26.63	35.76	25.75
57	140	Ag	24.20	31.62	23.52
59	142	In	24.76	34.36	28.27
61	148	In	29.48	32.06	31.72
63	154	Sb	34.66	34.26	41.65
63	156	Sb	31.95	36.55	44.95
65	160	I	33.13	37.62	51.52
67	166	I	33.23	40.05	60.39
69	170	Xe	34.69	42.71	69.90
71	176	Cs	35.12	43.57	65.92
73	182	Cs	35.39	45.07	56.73
75	186	La	36.66	46.37	52.38
75	188	Pr	36.82	45.60	45.12
77	192	Pm	38.73	47.72	39.47
77	194	Ir	37.64	49.71	30.58
79	198	Au	37.11	56.79	20.97
81	206	Tl	28.92	78.22	22.80
83	210	Bi	28.71	64.17	22.49
91	232	Pa	45.42	54.40	79.66
91	234	Pa	45.24	52.62	84.71
93	238	Np	47.39	57.21	91.19
95	242	Am	48.48	59.26	94.08
95	244	Am	47.89	58.85	105.59
97	250	Bk	46.91	58.50	70.70

TABLE III. Same as Table I, but for odd-A nuclei.

Z	A	Element	Spin cut-off parameter, $\sigma^2(B_n)$		
			(a)	(b)	(c)
12	25	Mg	4.99	4.62	5.39
12	27	Mg	4.65	4.33	3.96
14	29	Si	4.76	5.93	4.13
14	31	Si	4.67	5.54	3.62
15	33	P	5.40	6.55	4.78
16	33	S	6.05	7.10	4.61
16	35	S	5.61	6.61	4.16
18	41	Ar	7.25	6.73	8.89
20	41	Ca	7.73	8.40	10.24
20	43	Ca	8.98	8.29	12.46
20	45	Ca	8.82	8.48	12.47
22	47	Ti	10.12	10.69	15.91
22	49	Ti	9.39	10.30	13.24
22	51	Ti	6.66	10.24	8.06
23	51	V	11.18	13.22	16.02
24	51	Cr	10.8	12.04	16.65
24	53	Cr	9.74	12.11	13.05
24	55	Cr	9.56	10.61	10.19
26	55	Fe	10.81	13.85	13.04
26	57	Fe	11.33	12.56	11.48
26	59	Fe	10.99	11.55	10.86
28	59	Ni	11.98	14.67	10.34
28	61	Ni	11.86	13.62	10.61
28	63	Ni	11.40	12.78	11.18
28	65	Ni	11.08	12.24	12.15
29	64	Cu	13.35	14.60	12.65
30	65	Zn	13.78	14.00	12.44
30	67	Zn	13.87	13.29	13.57
30	69	Zn	13.56	13.02	15.16
30	71	Zn	12.58	12.54	16.39
32	71	Ge	16.13	13.79	16.61
32	73	Ge	16.25	13.65	17.82
32	75	Ge	15.59	14.29	19.81
32	77	Ge	15.12	14.32	20.36
34	75	Se	17.78	15.34	21.56
34	77	Se	17.32	15.38	22.30
34	79	Se	16.93	16.11	22.31
34	81	Se	15.77	16.15	19.98
34	83	Se	15.96	15.56	13.42
36	79	Kr	18.60	17.04	26.28
36	81	Kr	18.67	16.83	26.25
36	85	Kr	17.75	17.70	18.23
38	85	Sr	19.49	19.71	28.09
38	87	Sr	17.10	22.71	23.53
38	89	Sr	14.10	20.94	16.50
40	91	Zr	15.92	22.13	20.80
40	93	Zr	16.61	20.83	19.75
40	95	Zr	16.35	20.60	19.10
40	97	Zr	14.37	20.31	17.80
42	93	Mo	17.52	24.25	26.60
42	95	Mo	18.74	22.11	23.10
42	97	Mo	19.50	20.97	22.70
42	99	Mo	20.20	18.90	20.80
42	101	Mo	21.15	17.61	20.00
44	103	Ru	22.11	20.40	24.40
44	105	Ru	22.58	19.34	24.90
46	105	Pd	22.72	22.76	26.30
46	107	Pd	22.58	21.83	27.70
46	109	Pd	23.82	20.78	29.60
46	111	Pd	23.77	19.85	30.20
48	107	Cd	23.09	25.30	27.60
48	109	Cd	23.25	24.03	24.50
48	111	Cd	23.87	23.91	33.30
48	113	Cd	23.69	23.37	33.40
48	115	Cd	23.25	22.87	34.90
48	117	Cd	23.59	22.73	33.60
50	113	Sn	22.95	27.17	36.60
50	115	Sn	21.83	28.09	38.80
50	117	Sn	22.16	27.09	38.70
50	119	Sn	22.31	26.40	38.60
50	121	Sn	20.92	27.43	37.40
50	123	Sn	22.23	27.17	34.60
50	125	Sn	20.78	29.02	31.80
52	123	Te	25.43	27.74	40.66
52	125	Te	25.25	27.53	37.90
52	127	Te	24.29	28.62	33.90
52	129	Te	24.39	28.89	29.50
52	131	Te	23.20	30.03	22.90
54	129	Xe	25.98	30.77	37.02
54	131	Xe	26.13	30.14	31.08
54	133	Xe	24.64	31.99	27.03
54	135	Xe	22.85	33.86	21.73
55	135	Cs	26.81	39.97	35.35
56	131	Ba	28.06	31.71	41.74
56	133	Ba	27.65	32.20	37.42
56	135	Ba	26.13	34.02	32.21
56	137	Ba	23.43	36.69	28.13
56	139	Ba	20.18	31.10	19.73
57	139	La	26.36	43.23	37.03
58	137	Ce	28.80	33.76	37.01
58	141	Ce	22.20	32.34	27.20
58	143	Ce	24.16	29.61	24.88
60	143	Nd	23.95	34.44	32.02
60	145	Nd	26.23	32.07	30.46
60	147	Nd	27.66	29.56	29.27
60	149	Nd	29.89	27.89	28.39
60	151	Nd	29.94	30.19	30.63
62	145	Sm	24.82	38.13	37.74
62	149	Sm	29.69	31.62	34.07
62	151	Sm	32.77	29.72	33.99
62	153	Sm	32.90	31.82	36.87
62	155	Sm	30.68	33.53	41.46
63	153	Eu	36.29	40.66	51.80
63	155	Eu	34.84	40.47	54.22
64	153	Gd	34.49	31.96	39.22
64	155	Gd	34.61	33.63	42.66
64	157	Gd	33.70	35.06	49.36
64	159	Gd	32.18	35.12	45.36
64	161	Gd	30.52	35.57	50.54
66	157	Dy	36.17	35.35	46.53
66	159	Dy	34.31	37.78	50.30
66	163	Dy	33.67	37.96	57.77

TABLE III. (*Continued.*)

Z	A	Element	Spin cut-off parameter, $\sigma^2(B_n)$		
			(a)	(b)	(c)
66	165	Dy	32.14	36.95	55.57
68	163	Er	36.36	37.99	55.85
68	165	Er	35.48	38.97	59.17
68	167	Er	34.53	39.54	62.79
68	169	Er	32.96	39.44	62.18
68	171	Er	32.59	38.84	60.93
69	171	Tm	36.03	44.98	76.50
70	169	Yb	36.93	40.05	66.55
70	171	Yb	35.02	41.87	69.19
70	173	Yb	34.07	42.57	67.86
70	175	Yb	32.65	41.43	61.24
70	177	Yb	32.76	40.68	56.92
71	177	Lu	36.24	46.21	72.47
72	175	Hf	36.56	42.86	68.96
72	177	Hf	35.98	42.55	65.88
72	179	Hf	35.32	42.72	62.38
72	181	Hf	33.04	41.69	54.49
73	181	Ta	37.72	47.45	71.88
73	183	Ta	36.25	47.84	62.23
74	181	W	36.78	45.25	66.18
74	183	W	35.49	44.98	56.95
74	185	W	35.66	42.99	47.56
74	187	W	35.52	42.01	43.25
76	187	Os	37.82	45.75	52.86
76	189	Os	37.29	44.87	42.95
76	191	Os	37.38	45.24	36.26
76	193	Os	35.93	45.73	29.29
77	193	Ir	41.14	54.69	42.87
78	193	Pt	39.50	47.25	37.34
78	195	Pt	36.40	51.95	31.22
78	197	Pt	35.31	52.09	25.89
78	199	Pt	33.94	50.49	21.19
80	199	Hg	37.23	56.52	27.48
80	201	Hg	32.71	58.88	24.16
82	205	Pb	32.65	69.17	25.19
82	207	Pb	24.92	82.30	25.25
82	209	Pb	21.22	61.59	15.74
88	227	Ra	43.47	45.82	55.33
90	229	Th	47.49	49.14	63.04
90	231	Th	45.86	50.05	71.77
90	233	Th	45.29	48.69	71.55
92	233	U	47.09	55.02	85.40
92	235	U	46.48	53.69	81.65
92	237	U	46.20	53.22	86.22
92	239	U	45.74	51.42	82.94
93	239	Np	50.72	59.77	104.1
94	239	Pu	47.33	57.96	94.37
94	241	Pu	47.63	55.41	90.55
94	243	Pu	47.38	54.18	82.27
94	245	Pu	45.97	52.12	79.74
95	243	Am	50.23	64.20	104.45
96	243	Cm	45.26	61.11	96.84
96	245	Cm	48.05	59.69	97.53
96	247	Cm	46.04	58.95	86.75
98	251	Cf	48.10	57.60	72.85

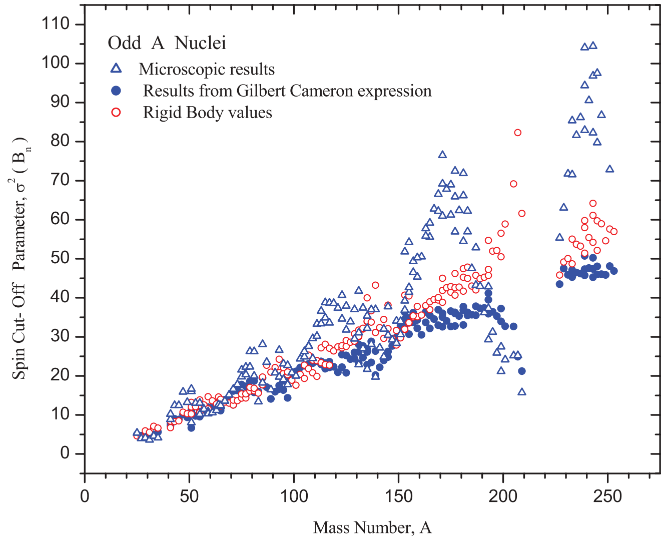

FIG. 3. (Color online) Same as Fig 1, but for odd-A nuclei.

at neutron binding energy ($U = B_n$) using the parameters in Table I of Ref. [6] are plotted in Fig 4. The corresponding values of σ^2 from the microscopic theory are also shown in this figure for comparison. Although the results from both methods are in general agreement with each other, they differ for nuclei near the major shells; in particular, this difference is very large for nuclei near the doubly magic nuclei $A \approx 206$. This may be accounted for by the fact that the microscopic theory uses the realistic single-particle orbitals, whereas the analytic expression ignores them.

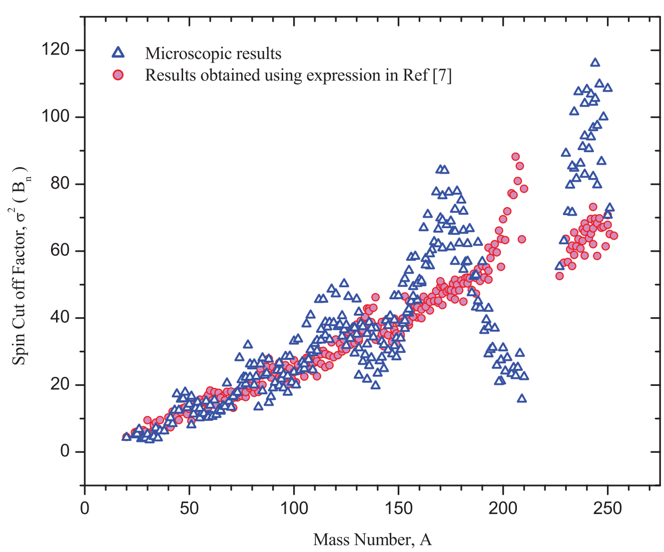

FIG. 4. (Color online) Spin cut-off parameters $\sigma^2(B_n)$ at the neutron binding energy, calculated using the microscopic theory and the analytic expression of Ref. [7].

IV. SUMMARY AND RESULTS

The spin cut-off parameter, which is an important parameter in all statistical model codes, has been computed for the first time using the microscopic approach. The spin cut-off parameter has been computed for a large range of nuclear mass by including a balanced number of even-even, odd-A, and odd-odd, light, medium, and heavy, and spherical and deformed nuclei. Our results indicate that the σ^2 values at B_n show structure reflecting the angular momentum of the shell model orbitals near the Fermi energy. For example, there are four strong peaks in Fig. 1 where the difference between the current and the rigid body calculations is great. The same results can be seen in Figs. 2 and 3. Examination of the single-particle level schemes for nuclei in these mass regions indicates that the orbitals with large angular momentum are responsible for these differences. In particular, the $1f_{5/2}$,$1g_{7/2}$, $2d_{5/2}$, and $1i_{11/2}$ proton orbitals and $1g_{9/2}$, $1h_{9/2}$, $1h_{11/2}$, and $1i_{13/2}$ neutron orbitals play an important role in the $\sigma^2(B_n)$ values. This finding is not consistent with the results obtained from the macroscopic approach.

In summary, in this paper we have presented more realistic calculations of the spin cut-off parameter for a wide atomic mass region and have shown that the values of $\sigma^2(B_n)$ obtained from the macroscopic methods are approximate. Moreover, they are completely inadequate near the magic nuclei, since significant shell and pairing effects appear for these nuclei.

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