Occupation probability of harmonic-oscillator quanta for microscopic cluster-model wave functions

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We present a new and simple method of calculating the occupation probability of the number of total harmonic-oscillator quanta for a microscopic cluster model wave function. Examples of applications are given to the recent calculations including an $\alpha+n+n$ model for ^{6}He, an $\alpha+t+n+n$ model for ^{9}Li, and an $\alpha+\alpha+n$ model for ^{9}Be as well as the classical calculations of an $\alpha+p+n$ model for ^{6}Li and an $\alpha+\alpha+\alpha$ model for ^{12}C. The analysis is found to be useful for comparing various model wave functions by quantifying the amount of excitations across the major shell. [S0556-2813(96)03510-8]

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The microscopic cluster model (MCM) is a many-nucleon theory which provides a unified picture of bound-state properties of nuclei and nuclear reactions. (See, for example, [1].) It is based on the assumption that the nucleons in the nuclei form substructures, called clusters, and solves a many-nucleon Schrödinger equation with the variational method. Though the MCM is capable of describing a variety of structure, its application has mostly been limited to a two- or three-cluster system. Recent advances in the MCM have, however, enabled one to treat systems containing more than three clusters and thereby give a detailed description of light nuclei including halo nuclei [2–5]. This extension of the applicability has been made possible by the inclusion of clusters other than the α particle and by the use of the stochastic variational method [2,6].

The MCM wave function is an antisymmetrized product of the intrinsic wave functions of the clusters and the functions of relative motions. The intrinsic wave functions are usually approximated by a simple harmonic-oscillator (HO) configuration, or a linear combination of such states. The functions of relative motions are expanded in terms of some suitable functions, such as nodeless HO functions or shifted Gaussians, for example. In the latter case, an explicit angular momentum projection is necessary. As this brief description shows, a large variety of cluster models exist and in general the MCM wave functions take quite different form. These facts make it difficult to compare the wave functions in different calculations even within the family of MCM. The difficulty is further enhanced if one wants to compare the calculations which employ different cluster partitions.

The utility, understanding, and appreciation of MCM would considerably increase if its wave function and model space are easily related to other nuclear models and calculations. The MCM has relationship to the widely used nuclear shell model. Efforts have been made to relate the MCM wave function to the SU(3) [7] or symplectic [8] shell-model wave function. Such efforts were limited to the two-cluster case. It is hard to analyze a general MCM wave function in terms of shell-model configurations. Although in principle it is possible to expand the MCM wave function in shell-model terms, such a calculation would be very tedious and even the usefulness of the presumably small coefficients of the large number of shell-model configurations is unclear. We will show instead that it is easy to calculate the percentage of the HO excitations contained in the MCM wave function. This presents a useful and economic way for a comparision of MCM and shell-model wave functions, and opens the possibility of comparing different MCM wave functions as well. The new technical elements of the formalism are constructed in the spirit of MCM.

The occupation probability P_Q of a definite number of total HO quanta Q for the A-nucleon system is obtained by calculating the expectation value of the operator $\mathcal{O}$:

$$\mathcal{O}=\frac{1}{2\pi}\int_0^{2\pi} d\theta \exp\left\{ i\theta\left[\sum_{i=1}^{A} P_i\left(H_{\rm HO}(i)-\frac{3}{2}\right)-Q\right]\right\}. \quad (1)$$

Here $H_{\rm HO}(i)$ is the three-dimensional HO Hamiltonian divided by $\hbar\omega=(2\hbar^2/m)\,\gamma$ and P_i projects out either protons or neutrons. The unit operator is set when one calculates the number of total quanta occupied by both protons and neutrons.

The MCM wave function is conveniently generated from the Slater determinants of the Gaussian wave-packet single-particle (sp) functions, $\varphi^{\nu}_{\mathbf{s}}(\mathbf{r})=(2\nu/\pi)^{3/4}e^{-\nu(\mathbf{r}-\mathbf{s})^2}$,

$$\phi_{\kappa}(\mathbf{s}_1,\ldots,\mathbf{s}_A)=\mathcal{A}\left\{\prod_{i=1}^{A}\varphi^{\nu}_{\mathbf{s}_i}(\mathbf{r}_i)\chi_{(1/2)\,\sigma_i}\mathcal{X}_{(1/2)\,\tau_i}\right\}. \quad (2)$$

Here $\mathcal{A}$ is the antisymmetrizer and $\kappa=(\sigma_1\tau_1,\ldots,\sigma_A\tau_A)$ stands for the set of the spin-isospin quantum numbers of the nucleons. The $\mathbf{s}_i$ parameter or ''generator'' coordinate is a variational parameter in the generator coordinate method calculations or it is used in an integral transformation [6,9] to derive the matrix elements between the Gaussian basis functions [10].

The matrix element of the operator $\mathcal{O}$ between the Slater determinants is given by

$$\langle\phi_{\kappa}(\mathbf{s}_1,\ldots,\mathbf{s}_A)|\mathcal{O}|\phi_{\kappa'}(\mathbf{s}'_1,\ldots,\mathbf{s}'_A)\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\theta \exp(-iQ\theta)\det\{B\}, \quad (3)$$

where the element of the matrix B is defined by $B_{ij}=\langle\hat{\varphi}^{\nu}_{\mathbf{s}_i\sigma_i\tau_i}|\exp(i\theta P[H_{\rm HO}-3/2])|\hat{\varphi}^{\nu}_{\mathbf{s}'_j\sigma'_j\tau'_j}\rangle$ $(i,j=1,\ldots,$

A). The $\hat{\varphi}^{\nu}_{\mathbf{s}_i\sigma_i\tau_i}$ stands for $\varphi^{\nu}_{\mathbf{s}_i}\chi_{(1/2)\sigma_i}\mathcal{X}_{(1/2)\tau_i}$. Since the constants, ν and γ, are in general different, the calculation of B_{ij} may seem difficult at first sight but in fact can be easily performed with the use of the following formulas:

$$\varphi^{\nu}_{\mathbf{s}}(\mathbf{r})=\left(\frac{\nu\gamma^3}{\pi^2(\nu-\gamma)^2}\right)^{3/4}\int d\mathbf{t}\ \exp\left(-\frac{\nu\gamma}{\gamma-\nu}(\mathbf{t}-\mathbf{s})^2\right)\varphi^{\gamma}_{\mathbf{t}}(\mathbf{r}), \tag{4}$$

$$\exp\left(i\theta\left[H_{\mathrm{HO}}-\frac{3}{2}\right]\right)\varphi^{\gamma}_{\mathbf{t}}(\mathbf{r})=\exp\left(-\frac{\gamma}{2}(1-z^2)\mathbf{t}^2\right)\varphi^{\gamma}_{z\mathbf{t}}(\mathbf{r}), \tag{5}$$

where $z=e^{i\theta}$. One can prove Eq. (5) by noting that the $\varphi^{\gamma}_{\mathbf{t}}(\mathbf{r})$ is the generating function for three-dimensional HO functions. Using Eqs. (4) and (5) yields the needed matrix element

$$\begin{aligned}\left\langle\hat{\varphi}^{\nu}_{\mathbf{s}\sigma\tau}\right|&\exp\left[i\theta P\left(H_{\mathrm{HO}}-\frac{3}{2}\right)\right]\left|\hat{\varphi}^{\nu}_{\mathbf{s}'\sigma'\tau'}\right\rangle\\&=\left(\frac{4\nu\gamma}{(\nu+\gamma)^2-(\nu-\gamma)^2\overline{z^2}}\right)^{3/2}\\&\quad\times\exp\left(-\nu\gamma\frac{\nu+\gamma+(\nu-\gamma)\overline{z^2}}{(\nu+\gamma)^2-(\nu-\gamma)^2\overline{z^2}}(\mathbf{s}^2+\mathbf{s}'^2)\right.\\&\quad\left.+\frac{4\nu^2\gamma\overline{z}}{(\nu+\gamma)^2-(\nu-\gamma)^2\overline{z^2}}\mathbf{s}\cdot\mathbf{s}'\right)\delta_{\sigma,\sigma'}\delta_{\tau,\tau'},\end{aligned} \tag{6}$$

where $\overline{z}=z$ or 1 in accordance with $\langle\tau|P|\tau\rangle=1$ or 0. The value of ν is usually chosen to give an appropriate size for the cluster, while the value of γ is determined by the size of the whole nucleus. Hence the value of ν is usually larger than that of γ. The integral in Eq. (4) then does not converge, but even in this case one can show that Eq. (6) may safely be used.

The sp matrix element of H_{HO} itself

$$\begin{aligned}\left\langle\hat{\varphi}^{\nu}_{\mathbf{s}\sigma\tau}\right|&P\left[H_{\mathrm{HO}}-\frac{3}{2}\right]\left|\hat{\varphi}^{\nu}_{\mathbf{s}'\sigma'\tau'}\right\rangle\\&=\left(\frac{3(\nu-\gamma)^2}{4\nu\gamma}-\frac{\nu^2-\gamma^2}{4\gamma}(\mathbf{s}^2+\mathbf{s}'^2)+\frac{\nu^2+\gamma^2}{2\gamma}\mathbf{s}\cdot\mathbf{s}'\right)\\&\quad\times e^{-(\nu/2)(\mathbf{s}-\mathbf{s}')^2}\delta_{\sigma,\sigma'}\langle\tau|P|\tau'\rangle\end{aligned} \tag{7}$$

is enough to calculate the average number of total HO quanta contained in the wave function. Recently this quantity is used in Ref. [11].

The summation in the exponent of Eq. (1) runs over all the nucleons and the probability calculated with it in general contains the contribution from the center-of-mass (c.m.) motion unless the wave function is free from the spurious c.m. motion. In fact our MCM wave functions generated from the Slater determinants of Eq. (2) by an integral transformation do not contain the c.m. motion [6]. The probability calculated below is thus a purely intrinsic quantity.

A generalization to a combined occupation probability is straightforward. For example, the probability P_{Q_1,Q_2} that protons have Q_1 quanta and neutrons Q_2 quanta or spin-up nucleons have Q_1 quanta and spin-down nucleons Q_2 quanta is obtained by using Eq. (1) twice and noting the commutability of the corresponding operators.

As an illustrative example let us consider Brink's $\alpha+\alpha$ model for ^{8}Be [12]. The intrinsic wave function of the α-particle is constructed from the Slater determinant of a 0s HO function with a size parameter ν. When the two α particles are separated by S and their relative orbital angular momentum is L, P_Q is calculated by

$$\begin{aligned}P_Q&=\frac{1}{2\pi i}\oint_{|z|=1}dz\,\frac{f(z)}{z^{Q+1}},\\f(z)&=\frac{1}{e^{-2d}(i_L(2d)-4i_L(d)+3\delta_{L,0})}\\&\quad\times\left(\frac{4\rho}{(1+\rho)^2-(1-\rho)^2z^2}\right)^{12}\\&\quad\times\exp\left(-4\rho d\frac{1+\rho+(1-\rho)z^2}{(1+\rho)^2-(1-\rho)^2z^2}\right)\\&\quad\times\left[i_L\left(\frac{8\rho dz}{(1+\rho)^2-(1-\rho)^2z^2}\right)\right.\\&\quad\left.-4i_L\left(\frac{4\rho dz}{(1+\rho)^2-(1-\rho)^2z^2}\right)+3\delta_{L,0}\right],\end{aligned} \tag{8}$$

where $\rho=\gamma/\nu$, $d=\nu S^2$, and $i_L(z)=\sqrt{\pi/2z}I_{L+1/2}(z)$ are the modified spherical Bessel functions of the first kind. Since $f(z)$ is analytic in the unit circle, Cauchy's integral formula can be applied to yield $P_Q=f^{(Q)}(0)/Q!$. The function $f(z)$ has a leading term proportional to $z^{\max(L,4)}$ near $z=0$. Hence P_Q vanishes for $Q<\max(L,4)$, which is the consequence of the Pauli principle. Figure 1 shows the P_Q values ($Q=4$, 6, and 8) for $L=0$, 2, 4, and 6 as a function of S, with a choice of $\nu=0.25$ fm^{-2} and $\gamma=0.15$ fm^{-2}. The P_Q values for different L values are not the same at each S particularly in the interval of 2–4 fm. A maximum of $P_{Q=4}$ appears around $S\sim2.9$ fm in the case of $L=0$, while it shifts to a smaller separation of $S\sim2.2$ fm in case of $L=4$. The diagonal energy

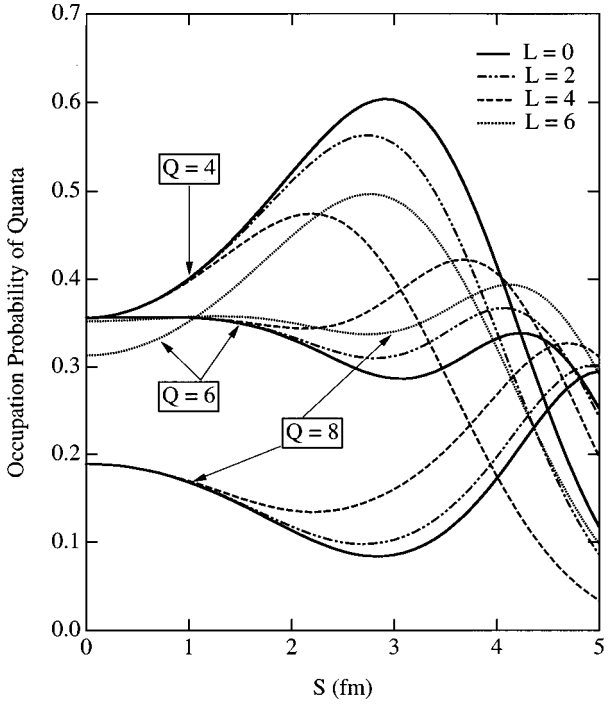

FIG. 1. The occupation probability of the number of oscillator quanta Q for the $L=0-6$ states of ^{8}Be. The wave functions of ^{8}Be are assumed to be given by Brink's 2α model [12] with a mean separation S.

TABLE I. The occupation probability of the number of harmonic-oscillator quanta for microscopic multicluster model wave functions. The probabilities for nucleons, protons, and neutrons are given in percentages in the upper, middle, and lower rows, respectively, as a function of oscillator excitations. When the probability for neutrons is the same as that for protons, only the proton case is shown. An asterisk indicates the probability of less than 1% and dashed line represents the vanishing probability. The average number of oscillator excitations is given in the column labeled $\langle Q_{\rm exc}\rangle$. The details of the wave functions are referred to Ref. [4(b)] for ^{6}He and ^{6}Li, to Ref. [5] for ^{7}Li, ^{8}Li, ^{9}Li, and ^{9}C, and to Ref. [14] for ^{9}Be.

State	rms radius	$Q_{\rm exc}$															$\langle Q_{\rm exc}\rangle$
(model)	(fm)	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	
^{6}He(0^+)	$r_m=2.51$	60	—	14	—	12	—	5	—	3	—	2	—	1	—	*	2.2
($\alpha+n+n$)	$r_p=1.87$	74	10	11	2	1	*	*	*	*	*	*	*	*	*	*	0.5
	$r_n=2.78$	67	3	8	5	7	2	2	1	1	*	*	*	*	*	*	1.7
^{6}Li(1^+)	$r_m=2.44$	62	—	16	—	10	—	5	—	3	—	2	—	*	—	*	1.9
($\alpha+p+n$)	$r_p=2.44$	69	8	10	4	4	2	1	*	*	*	*	*	*	*	*	1.0
^{7}Li($3/2^-$)	$r_m=2.34$	63	—	20	—	9	—	4	—	2	—	*	—	*	—	*	1.4
($\alpha+t$)	$r_p=2.28$	77	2	16	*	4	*	*	*	*	*	*	*	*	*	*	0.6
	$r_n=2.38$	73	1	17	*	5	*	1	*	*	*	*	*	*	*	*	0.8
^{8}Li(2^+)	$r_m=2.45$	61	—	18	—	11	—	4	—	2	—	1	—	*	—	*	1.7
($\alpha+t+n$)	$r_p=2.19$	79	6	11	1	2	*	*	*	*	*	*	*	*	*	*	0.4
	$r_n=2.60$	67	3	14	2	7	1	2	*	1	*	*	*	*	*	*	1.3
^{8}Be(0^+)	$r_m=3.27$	36	—	18	—	12	—	7	—	5	—	4	—	3	—	2	7.6
($\alpha+\alpha$)	$r_p=3.27$	47	—	21	—	11	—	6	—	4	—	3	—	2	—	1	3.8
^{9}Li($3/2^-$)	$r_m=2.40$	66	—	17	—	11	—	4	—	2	—	*	—	*	—	*	1.3
($\alpha+t+n+n$)	$r_p=2.10$	82	6	9	1	1	*	*	*	*	*	*	*	*	*	*	0.4
	$r_n=2.54$	71	3	12	2	6	1	2	*	*	*	*	*	*	*	*	1.0
^{9}C($3/2^-$)	$r_m=2.52$	60	—	17	—	12	—	5	—	3	—	1	—	*	—	*	1.8
($\alpha+h+p+p$)	$r_p=2.68$	65	4	12	3	7	1	2	*	1	*	*	*	*	*	*	1.4
	$r_n=2.16$	79	8	9	2	1	*	*	*	*	*	*	*	*	*	*	0.4
^{9}Be($3/2^-$)	$r_m=2.50$	54	—	21	—	12	—	5	—	3	—	2	—	*	—	*	2.1
($\alpha+\alpha+n$)	$r_p=2.39$	71	3	17	1	5	*	1	*	*	*	*	*	*	*	*	0.8
	$r_n=2.58$	65	2	18	1	8	*	3	*	1	*	*	*	*	*	*	1.3
^{12}C(0_1^+)	$r_m=2.20$	54	—	30	—	11	—	3	—	*	—	*	—	*	—	*	1.4
($\alpha+\alpha+\alpha$)	$r_p=2.20$	70	5	19	1	4	*	*	*	*	*	*	*	*	*	*	0.7
^{12}C(0_2^+)	$r_m=3.75$	*	—	11	—	12	—	12	—	10	—	8	—	7	—	6	16.1
($\alpha+\alpha+\alpha$)	$r_p=3.75$	5	7	15	7	11	6	8	5	6	4	4	3	3	2	2	8.2

curve of ^{8}Be as a function of S is expected to have a local minimum around the point where $P_{Q=4}$ reaches a maximum. Then the behavior of the P_Q values with respect to L and S is in accord with the antistretching [13] that the minimum of the diagonal energy curve appears at a smaller cluster separation as L increases to the value of a band termination.

Table I lists the P_Q values in percentages for nucleons, protons, and neutrons for some of the wave functions obtained in our recent MCM calculations [4,5,14] using the Minnesota potential [15]. A common value of $\nu=0.26$ fm^{-2} is used to describe the intrinsic wave functions of α, t, and h clusters. The choice of γ has some influence on the probability. It is set 0.17 fm^{-2} ($\hbar\omega=14.4$ MeV), a standard value used in a shell model calculation for p-shell nuclei. For the sake of reference the calculated root-mean-square (rms) radii for nucleons (matters), protons, and neutrons are included in the table. The P_Q values are given as a function of $Q_{\rm exc}=Q-Q_{\rm min}$, where $Q_{\rm min}$ is the minimum number of HO quanta for the lowest Pauli-allowed configuration. The lowest $0\hbar\omega$ component is around 50–60 % for most cases and the sum of 0, 2, and $4\hbar\omega$ components accumulates to about 90%. The admixtures of higher components than $Q_{\rm exc}=4$ are significant in the ground states of ^{6}Li and ^{9}Be and also in the ground state of ^{6}He corresponding to its extended halo structure [4(b)]. The probability distribution spreads out to a very large number of HO quanta in ^{8}Be and the 0_2^+ state of ^{12}C, well-known cluster states. They are described as a bound state in a large basis. Our wave functions for ^{12}C are similar to those of Ref. [16], which reproduces many properties of ^{12}C in the 3α model. The parameter u of the Minnesota potential is set $u=0.95$ to reproduce the energy of the 0_2^+ state. The ground state energy becomes then about 4.5 MeV lower than experiment. The calculated monopole matrix element is 4.0 fm^2, which reasonably agrees with the experimental value of 5.4 ± 0.2 fm^2. It is noted that no component is dominant in the 0_2^+ state of ^{12}C. Of course it would be possible to maximize the probability with lower Q by choosing an appropriate value of γ. However, the probability distribution would then spread to higher HO quanta in the ground state of ^{12}C. It is also noted that the components with odd $Q_{\rm exc}$ values for protons or neutrons are generally smaller. For example, in ^{6}He $P_{Q_{\rm exc}(p)=1,Q_{\rm exc}(n)=1}$ is about 3%, whereas $P_{0,2}$ and $P_{2,0}$ are 5

and 6%, respectively, and, among the probability of 12% for $4\hbar\omega$ excitations, the probability with $Q_{\rm exc}(p) = 1$ or 3 is only about 4%.

Comparing the results for $^{7-9}$Li, we see that the probability for neutrons has a larger change in the isotopes than that for protons. The change follows that of the neutron radius, which is consistent with the change of the neutron separation energy. In fact the nucleus ^{8}Li has the smallest neutron separation energy among the three. Since the MCM consistently predicts the largest neutron rms radius for ^{8}Li [17], its average number of oscillator excitations, $\langle Q_{\rm exc}\rangle$, for neutrons is largest among the three. A comparison of our result with that of Ref. [11] indicates that the latter wave functions, giving generally much smaller $\langle Q_{\rm exc}\rangle$ values, are rather close to simple shell model configurations; e.g., $\langle Q_{\rm exc}\rangle$ for neutrons is about 0.1 for ^{9}Li and 0.5 even for ^{8}Be. This may not be surprising because the model of Ref. [11] uses basically a single Slater determinant of Eq. (2).

It is interesting to compare those wave functions which are obtained in different MCM calculations. As an example we generate the ground state wave function of ^{7}Li in an $\alpha+p+n+n$ four-body model. This model may be considered equivalent to a kind of shell-model calculation where three valence nucleons outside the ^{4}He core are allowed to be excited to any orbits and where no spurious c.m. problem is nevertheless involved. The u parameter is kept the same as the one used in [5] which treated ^{7}Li in a simpler $\alpha+t$ model. The ground state energy becomes slightly overbound, but its radius hardly changes from the previous result. The resulting wave function is decomposed to

$$66\%|0\hbar\omega\rangle+17\%|2\hbar\omega\rangle+10\%|4\hbar\omega\rangle+4\%|6\hbar\omega\rangle +2\%|8\hbar\omega\rangle+\cdots. \quad (9)$$

The $\langle Q_{\rm exc}\rangle$ value is 1.4. This distribution is very similar to that of the $\alpha+t$ two-body model, as seen from Table I. This indicates that the t cluster can be regarded as a useful substructure.

The calculational method developed here has nothing to do with the assumption of the existence of clusters and can be applied to those precise wave functions for a few-nucleon system which are obtained with a sophisticated technique [6]. As an example we analyze the solution for the ground state of ^{4}He which is obtained in a $p+p+n+n$ four-body calculation with the Minnesota potential. For the sake of comparison with a recent large-basis shell-model calculation [18], we expand the solution in the HO basis with $\hbar\omega = 14$ MeV. The result is

$$68\%|0\hbar\omega\rangle+19\%|2\hbar\omega\rangle+8\%|4\hbar\omega\rangle+3\%|6\hbar\omega\rangle +0.9\%|8\hbar\omega\rangle+\cdots. \quad (10)$$

The $\langle Q_{\rm exc}\rangle$ value becomes 1.1. It is remarkable that our wave function gives percentages similar to those of Ref. [18] that uses the G matrices calculated from the Nijmegen potential.

In summary, we have presented a new and simple method of calculating the occupation probability of the number of harmonic-oscillator quanta. It has been applied to the analysis of some of the wave functions obtained in a microscopic multicluster model calculation. The analysis is found to be useful for comparing various wave functions by quantifying the amount of excitations across the major shell.

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