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

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Abstract

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 $\alpha + n + n$-model for $^6\text{He}$, $\alpha + t + n + n$-model for $^9\text{Li}$, and $\alpha + \alpha + n$-model for $^9\text{Be}$ as well as the classical calculations of $\alpha + p + n$-model for $^6\text{Li}$ and $\alpha + \alpha + \alpha$-model for $^{12}\text{C}$. The analysis is found to be useful for quantifying the amount of excitations across the major shell as well as the degree of clustering. The origin of the antistretching effect is discussed.

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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. Though the MCM is capable of describing a variety of structure, its application has mostly been limited to 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 \( \alpha \)-particle and by the use of the stochastic variational method [2,6]. The MCM, as a microscopic theory, attempts to derive the nuclear properties from a many-body Hamiltonian using a fully antisymmetrized wave function. It has, therefore, some relationship to the shell model. Efforts have been made to relate the wave function of the MCM to that of the \( SU(3) \) [7] or symplectic [8] shell model. Such efforts are useful because one can compare the model space of the shell model and the MCM. It is hard to analyse a general MCM wave function in terms of shell-model configurations. We will show instead that it is easy to calculate the percentage of the harmonic-oscillator (HO) excitations involved in the MCM wave function.

The MCM wave function consists of the antisymmetrized product of the intrinsic wave functions of the clusters and the relative motion functions between the clusters. The intrinsic wave functions are usually assumed to be described with simple configurations, whereas the relative motion functions are treated flexibly enough to accommodate various types of correlations between the clusters as well as large spatial extension if necessary. The MCM wave function thus may contain a large number of HO quanta. To link it with the HO shell-model basis, it is useful to calculate the occupation probability of the number of total HO quanta. The occupation probability \( P_Q \) of a definite number of total HO quanta \( Q \) for \( A \)-nucleon system is obtained by calculating the expectation value of the operator \( \mathcal{O} \)

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

Here \( P_i \) projects out either proton or neutron. It is set the unit operator when one calculates the number of total quanta occupied by both protons and neutrons. \( H_{\text{HO}}(i) \) is the 3-dimensional HO Hamiltonian divided by \( \hbar \omega = \frac{2k^2}{m}\gamma \).

The MCM wave function is conveniently generated from the Slater determinants of the Gaussian wave-packet single-particle (sp) functions

\[
\phi_{\kappa}(s_1, ..., s_A) = A\left\{ \prod_{i=1}^{A} \varphi_{s_i\sigma_i\tau_i}^\nu(r_i) \right\} = A\left\{ \prod_{i=1}^{A} \varphi_{s_i}^\nu(r_i) \chi_{\frac{1}{2}\sigma_i} \chi_{\frac{1}{2}\tau_i} \right\},
\]

with

\[
\varphi_{s}^\nu(r) = \left( \frac{2\nu}{\pi} \right)^{3/4} e^{-\nu(r-s)^2}.
\]

Here \( A \) is the antisymmetrizer and \( \kappa = (\sigma_1\tau_1, ..., \sigma_A\tau_A) \) stands for the set of the spin-isospin quantum numbers of the nucleons. The \( s_i \) 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

$$
\langle \phi_\kappa(s_1, \ldots, s_A)| \mathcal{O} | \phi_\kappa'(s_1', \ldots, s_A') \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \exp(-iQ\theta) \det B,
$$

where the matrix $B$ is defined by $(i, j=1, \ldots, A)$

$$
B_{ij} = \langle \hat{\varphi}_\nu^{(i)} \sigma, \tau | \exp(i\theta [H_{HO} - \frac{3}{2}]) | \hat{\varphi}_\nu^{(j)} \sigma', \tau' \rangle.
$$

Since the constants, $\nu$ and $\gamma$, are in general different, the calculation of the sp matrix element of Eq. (5) may seem difficult at first sight but can be performed rather easily with the use of the following formulae

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

$$
\exp(i\theta [H_{HO} - \frac{3}{2}]) \varphi^\gamma(t) = \exp(-\gamma/2 (1 - z^2)t^2) \varphi^\gamma(z),
$$

where $z = e^{i\theta}$. One can prove Eq. (7) by noting that the function, $\varphi^\gamma(r)$, is the generating function for 3-dimensional HO functions. Using Eqs. (6) and (7) in Eq. (5) yields the needed matrix element

$$
\langle \hat{\varphi}_\nu^{(i)} \sigma, \tau | \exp(i\theta [H_{HO} - \frac{3}{2}]) | \hat{\varphi}_\nu^{(j)} \sigma', \tau' \rangle = \left( \frac{4\nu\gamma}{(\nu + \gamma)^2 - (\nu - \gamma)^2z^2} \right)^{3/2} \times \exp\left( -\nu\gamma\frac{\nu + \gamma + (\nu - \gamma)z^2}{(\nu + \gamma)^2 - (\nu - \gamma)^2z^2} \right) \delta_{\sigma,\sigma'} \delta_{\tau,\tau'},
$$

where $z = z$ or $1$ in accordance with $\langle \tau | P | \tau \rangle = 1$ or 0.

The value of $\nu$ is usually chosen to give an appropriate size for the cluster, while the value of $\gamma$ is determined by the size of the whole nucleus. Hence the value of $\nu$ is usually larger than that of $\gamma$. The integral in Eq. (6) then does not converge. However, even in this case Eq. (8) may safely be used because the matrix element should be continuous at all values of $\nu$ and $\gamma$ and should have a finite value. We have confirmed the validity of Eq. (8) by comparing the occupation probability calculated by two ways for the Gaussian wave-packet, $\varphi_\nu$. One is to use Eq. (8) and to change the integration variable $\theta$ to the complex variable $z$ on a unit circle $|z| = 1$. The other is to calculate directly the overlap between $\varphi_\nu$ and 3-dimensional HO functions. Both methods have given the same result.

The sp matrix element of $H_{HO}$ itself

$$
\langle \varphi_\nu^{(i)} \sigma, \tau | [H_{HO} - \frac{3}{2}] | \varphi_\nu^{(j)} \sigma', \tau' \rangle = \left( \frac{3(\nu - \gamma)^2}{4\nu\gamma} - \frac{\nu^2 - \gamma^2}{4\gamma} (s^2 + s'^2) + \frac{\nu^2 + \gamma^2}{2\gamma} s \cdot s' \right) \times e^{-\frac{\nu}{2}(s - s')^2} \delta_{\sigma,\sigma'} \langle \tau | P | \tau' \rangle
$$

is needed 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 (cm) motion unless the wave function is free from the spurious cm motion. Though the Slater determinants of Eq. (2) contain the dependence on the cm variable, our MCM wave functions generated from them by an integral transformation turn out to be free from any problem with the spurious cm 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 \( \alpha \)-particle is constructed from the Slater determinant of a 0\(-\)particle and its relative orbital angular momentum is \( L \). \( P_Q \) is calculated by

\[
P_Q = \frac{1}{2\pi i} \oint_{|z|=1} dz \frac{f(z)}{z^{Q+1}},
\]

with

\[
f(z) = \frac{1}{e^{-2i}i_L(2d) - 4i_L(d) + 3\delta_{L,0}} \left( \frac{4\rho}{(1+\rho)^2 - (1-\rho)^2 z^2} \right)^{12} \times \exp\left( -4\rho d \frac{1+\rho}{(1+\rho)^2 - (1-\rho)^2 z^2} \right)
\times \left( i_L \left( \frac{8\rho dz}{(1+\rho)^2 - (1-\rho)^2 z^2} - 4i_L\left( \frac{4\rho dz}{(1+\rho)^2 - (1-\rho)^2 z^2} \right) + 3\delta_{L,0} \right) \right),
\]

where \( \rho = \gamma/\nu \), \( d = \nu S^2 \), and \( i_L(z) = \sqrt{\frac{\pi}{2z}} I_{L+\frac{1}{2}}(z) \) 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 in Eq. (10) 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 \( \nu = 0.25 \text{ fm}^{-2} \) and \( \gamma = 0.15 \text{ fm}^{-2} \). The \( Q \)-dependence is not the same within the \( L=0, 2, \) and \( 4 \) members but different at each \( S \) particularly in the interval of 2~4 fm, where the energy functional is known to have a minimum. A maximum of \( P_{Q=4} \) appears around \( S \sim 2.9 \text{ fm} \) in case of \( L=0 \), while it shifts to a smaller separation of \( S \sim 2.2 \text{ fm} \) in case of \( L=4 \). The diagonal energy 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 difference in the \( Q \)-dependence on \( L \) and \( S \) values accounts for the antistretching [13] that the energy functional of the cluster-model calculation shows a shrinkage of the cluster separation when \( L \) approaches the value of a band termination.

Table I lists the \( P_Q \) values in % 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 \( \nu=0.26 \text{ fm}^{-2} \) is used to describe the intrinsic wave functions of \( \alpha, t, \) and \( h \) clusters. The choice of \( \gamma \) has some influence on the probability. It is set 0.17
\( f m^{-2} \) (\( \hbar \omega = 14.4 \text{ MeV} \)), a standard value used in a shell-model calculation for \( p \)-shell nuclei. The value is, however, reduced to 0.13 and 0.14 \( f m^{-2} \) for \( ^{6}\text{He} \) and \( ^{6}\text{Li} \), respectively, to take into account their significantly large sizes. For the sake of reference the calculated root-mean-square (rms) radii for nucleons (maters), protons, and neutrons are included in the table. The \( P_Q \) values are given as a function of \( Q_{\text{exc}} = Q - Q_{\text{min}} \), where \( Q_{\text{min}} \) 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 \( Q_{\text{exc}} = 4 \) are significant in the ground states of \( ^{6}\text{Li} \) and \( ^{9}\text{Be} \) and even larger in the ground state of \( ^{6}\text{He} \) corresponding to its extended halo structure [4(b)]. The probability distribution spreads out to a very large number of HO quanta in \( ^{8}\text{Be} \) and the \( 0^+_2 \) state of \( ^{12}\text{C} \), well-known cluster states. They are described as a bound state in a large basis. Our wave functions for \( ^{12}\text{C} \) are similar to those of Ref. [16], which reproduces many properties of \( ^{12}\text{C} \) in the \( 3\alpha \)-model. The probability of the Minnesota potential is set 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 \( f m^2 \), which is in reasonable agreement with the experimental value of 5.4±0.2 \( f m^2 \). It is noted that no component is dominant in the \( 0^+_2 \) state of \( ^{12}\text{C} \). Of course it would be possible to maximize the probability with lower \( Q \) by choosing a smaller value of \( \gamma \). However, the probability distribution would then spread to higher HO quanta in the ground state of \( ^{12}\text{C} \). A recent large-basis shell-model calculation [17] also suggests that the low-lying states in light nuclei from \( ^{4}\text{He} \) to \( ^{7}\text{Li} \) have significant admixtures of large HO quanta. Since the calculation seems promising, it is interesting to see how the \( 0^+_2 \) state of \( ^{12}\text{C} \) is incorporated in its framework. It is also noted that the components with odd \( Q_{\text{exc}} \) values for protons or neutrons are generally smaller. For example, in \( ^{6}\text{He} \) \( P_{Q_{\text{exc}}(p)=1,Q_{\text{exc}}(n)=1} \) is about 3 \%, whereas \( P_{0,2} \) and \( P_{2,0} \) are 9 and 11 \%, respectively, and, among the probability of 16 \% for \( 4\hbar \omega \) excitations, the probability with \( Q_{\text{exc}}(p) \ (Q_{\text{exc}}(n)) =1 \) or 3 is less than 4 \%.

Comparing the results for \( ^{7}\text{−}^{9}\text{Li} \), 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 \( ^{8}\text{Li} \) has the smallest neutron separation energy among the three. Since the MCM consistently predicts the largest neutron rms radius for \( ^{8}\text{Li} \) [18], its average value, \( <Q_{\text{exc}}> \), 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 \( <Q_{\text{exc}}> \) values, are rather close to simple shell-model configurations; e.g., \( <Q_{\text{exc}}> \) for neutrons in their paper is about 0.1 for \( ^{9}\text{Li} \) and 0.5 even for \( ^{8}\text{Be} \). This may not be surprising because they use a single Slater determinant of the Gaussian wave-packets sp functions.

The calculational method developed here has nothing to do with the assumption of the existence of clusters and can obviously be applied to those precise wave functions for few-nucleon system which are obtained with a sophisticated technique. For example, it will be interesting to analyse some of the wave functions obtained in Ref. [6].

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 multichuster-model calculation. The analysis is found to be useful for clarifying the difference from the shell-model truncation made on the basis of a major shell as well as quantifying the degree of clustering or spa-
tial extension. The origin of the antistretching effect is discussed from the change of the occupation probability in the rotational band.

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REFERENCES


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 % 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. Asterisk indicates the probability of less than 1 % and dashed line represents vanishing probability. The average number of oscillator excitations is given in the column labeled $<Q_{exc}>$.

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.

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<th>$r_m$</th>
<th>$r_p$</th>
<th>$r_n$</th>
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<td>21</td>
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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 2$\alpha$-model [12] with a mean separation $S$. 