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Multi-particle and Multi-hole State Densities Based on the Harmonic Oscillator Model

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On the premise of considering the Pauli exclusion principle strictly, we have obtained an exact general formula of multi-particle and multi-hole state densities for any single-particle Hamiltonian. Besides, by using the semi-classical Thomas-Fermi approximation, we have calculated the state densities for three-dimensional linear oscillators and the state densities of $1p$--$10p$, $1h$--$7h$ and $1p1h$--$6p6h$. We have also discussed the effect of the Pauli exclusion principle and made comparisons with the state densities of the equi-interval model generally used in the exciton model. The results indicate that the equi-interval single-particle density formula is a good approximation for the nuclear reactions induced by a nucleon.

1. INTRODUCTION

The state density plays an important role in nuclear reaction theory. It is a significant physical parameter [1] in studying static nuclear properties, such as kinetic energy and ground state energy. In recent years, the average state densities of nuclear excited states have been widely used in many aspects of nuclear reaction theory. Many processes, such as the precompound reactions [2-4], the study of the spreading width of giant resonances [5] and the calculation of the shell model optical potentials [6] demand more accurate knowledge of state densities. Therefore, it is more significant to study state densities in a microscopic approach.

In 1936, Bethe put forward the problem of state densities [7,8]. Since then, most authors have based their studies of state densities on the statistical model [9-17]. They either simply paid no attention to, or just approximately considered, the effect of the Pauli exclusion principle in deriving

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the formula. But as we know, the Pauli principle plays a major role in state densities, especially in the case of high particle-hole number and low excitation energy. The case mentioned above just corresponds to the pre-equilibrium nuclear reaction at excitation energies of few tens of MeV.

In 1983, G. Ghosh et al. [18] obtained a formula for the mean value of the state densities of $g_{1p\text{-}1}h$ and $g_{2p\text{-}2}h$ by applying the semi-classical Thomas-Fermi approximation to the three-dimensional harmonic oscillator model. Their results were consistent with the accurate results of quantum mechanics. Later, in their work Blin et al. [19,20] tried to extend the formula to the case of m particles and n holes. However, they did not take the Pauli exclusion principle into account.

In this paper, starting from the definition of state densities, we turn the restricted summation of the average state densities of m particles and n holes into a summation of a series of non-restricted polynomials. Different from the earlier researchers, we obtained an accurate formula of state densities for multi-particle and multi-hole nuclear systems with the introduction of the Pauli exclusion principle. Being model independent, our formula can in principle be used to calculate the average state densities of nuclear systems consisting of m particles and n holes in any type of single-particle potential well. As a result, our formula is of universal significance. In Section 3, utilizing our formula and the semi-classical Thomas-Fermi approximation, we have calculated the state densities of $g_{1p\text{-}g10p}$, $g_{1h\text{-}g2}h$ and g_{1p1h}--$g_{6p6}h$ for three-dimensional linear oscillators. We have also compared our results with the single-particle state densities from the equi-interval model. We have found that the equi-interval single-particle model is a reasonable approximation in its application to the exciton model.

2. FORMULA FOR CALCULATING THE STATE DENSITIES OF MULTI-PARTICLE AND MULTI-HOLE SYSTEM

The state density of a Fermi system consisting of m particles and n holes is defined as

$$g_{mpnh}(E) = \sum_{\substack{p_1<p_2<\cdots<p_m \\ h_1<h_2<\cdots<h_n}} \delta\left(E - \sum_{i=p_1}^{p_m} \varepsilon_p - \sum_{h=h_1}^{h_n} \varepsilon_h\right), \tag{2.1}$$

where ϵ_p and ϵh are energies of the single-particle and single-hole, respectively. Here the Fermi surface is set as the starting point of energy. $p_1p_2 \ldots p_m$ denote the particle states and $h_1h_2 \ldots h_n$ the hole states. The summations are performed with the restrictions $p_1 < p_2 < \cdots\cdots p_m$ and $h_1 < h_2 < \cdots\cdots < h_n$. The restricted summations are required by the Pauli exclusion principle and the delta function is introduced to ensure energy conservation. By setting $m = 0$ and $n = 0$, we can get the state densities g_{mpoh} and g_{opnh} for systems consisting only of particles and holes, respectively. Eq.(2.1) can be rewritten as

$$g_{mpnh}(E) = \sum_{\substack{\mu_1<\mu_2<\cdots<\mu_m \\ \nu_1<\nu_2<\cdots<\nu_n}} \langle \mu_1\mu_2\cdots\mu_m, \nu_1\nu_2\cdots\nu_n | \delta\left(E - \sum_{\mu=\mu_1}^{\mu_m} H_\mu - \sum_{\nu=\nu_1}^{\nu_n} H_\nu\right) \cdot | \mu_1\mu_2\cdots\mu_m, \nu_1\nu_2\cdots\nu_n \rangle. \tag{2.2}$$

where summation indexes p_i and h_i are replaced by μ_i and ν_i and the summation is now over all particle and hole states. H_i and ϵ_i are the Hamiltonian and the corresponding eigenvalues of the single-particle and single-hole states. By means of the Laplace transformation a convenient expression of Eq.(2.2) can be obtained,

$$G_{mpnh}(E) = \int_0^\infty dE e^{-\beta E} g_{mpnh}(E) = z_p(\beta, m) z_h(\beta, n), \tag{2.3}$$

The result is factorized into two parts, a particle component and a hole component

$$z_p(\beta, m) = \sum_{\mu_1<\mu_2<\cdots<\mu_m} \langle \mu_1\mu_2\cdots\mu_m | e^{-\beta \sum_\mu H_\mu} | \mu_1\mu_2\cdots\mu_m \rangle , \tag{2.4a}$$

$$z_h(\beta, n) = \sum_{\nu_1<\nu_2<\cdots<\nu_n} \langle \nu_1\nu_2\cdots\nu_n | e^{-\beta \sum_\nu H_\nu} | \nu_1\nu_2\cdots\nu_n \rangle . \tag{2.4b}$$

In order to transform Eq.(2.4) into a trace form, we define

$$f^{(l)}(\mu) \equiv \langle \mu | e^{-l\beta H_\mu} | \mu \rangle , \tag{2.5}$$

indicating that there are l particles in the μ-th state.

In the following discussion, as an example we only consider the particle case, while the treatment of holes can be carried out in a similar way. We consider the case with $m = 2$. From Eq.(2.4), we have

$$\sum_{\mu_1<\mu_2} f(\mu_1)f(\mu_2) = (2!)^{-1} \Big\{ \sum_{\mu_1,\mu_2} f(\mu_1)f(\mu_2) - \sum_{\mu_1} f^2(\mu_1) \Big\} . \tag{2.6a}$$

In Eq.(2.6a), the first term on the right-hand side is obtained without taking the Pauli exclusion principle into account. If the Pauli principle is considered, the correction term for a given state having two particles must be subtracted. Thus the case of $\mu_1 > \mu_2$ is included and the equation must be divided by the identity factor 2!.

Analogously, in the case of $m = 3$ and $m = 4$, we have

$$\begin{aligned} \sum_{\mu_1<\mu_2<\mu_3} f(\mu_1)f(\mu_2)f(\mu_3) = (3!)^{-1} \Big\{ & \sum_{\mu_1,\mu_2,\mu_3} f(\mu_1)f(\mu_2)f(\mu_3) \\ & - 3 \sum_{\mu_1\mu_2} f^2(\mu_1)f(\mu_2) + 2 \sum_{\mu_1} f^3(\mu_1) \Big\} \end{aligned} \tag{2.6b}$$

$$\begin{aligned} \sum_{\mu_1<\mu_2<\mu_3<\mu_4} f(\mu_1)f(\mu_2)f(\mu_3)f(\mu_4) = (4!)^{-1} \Big\{ & \sum_{\mu_1,\mu_2,\mu_3,\mu_4} f(\mu_1)f(\mu_2)f(\mu_3)f(\mu_4) \\ & - 6 \sum_{\mu_1,\mu_2,\mu_3} f^2(\mu_1)f(\mu_2)f(\mu_3) + 3 \sum_{\mu_1,\mu_2} f^2(\mu_1)f^2(\mu_2) \\ & + 8 \sum_{\mu_1,\mu_2} f^3(\mu_1)f(\mu_2) - 6 \sum_{\mu_1} f^4(\mu_1) \Big\} . \end{aligned} \tag{2.6c}$$

Noting that each summation on the right-hand side of Eq.(2.6) is independent and non-restricted, Eq.(2.6) can be rewritten in the trace form. To get the independent reduced summation

form for arbitrary m particles, we introduce the representation for $(l+1)$ particles occupying the same state:

$$A_m^{(l)}(\beta) = m! \sum_{\mu_1<\mu_2<\cdots<\mu_m} f(\mu_1)f(\mu_2)\cdots f^{(l+1)}(\mu_i)\cdots f(\mu_m)$$
$$= m! \sum_{\mu_1<\mu_2<\cdots<\mu_m} \langle \mu_1\cdots\mu_m | e^{-\beta\sum_\mu H_\mu} e^{-\beta l l H_{\mu_i}} | \mu_1\cdots\mu_m\rangle, \tag{2.7}$$

The relationship between $A_m^{(l)}(\beta)$ and $z_p(\beta,m)$ is $z_p(\beta,m) = (m!)^{-1}A_m^{(0)}$, while

$$A_m^{(0)}(\beta) = (m!) \sum_{\mu_1<\cdots<\mu_m} \langle \mu_1\cdots\mu_m | e^{-\beta\sum_\mu H_\mu} | \mu_1\cdots\mu_m\rangle$$
$$- (m!) \sum_{\mu_1<\cdots<\mu_m} f(\mu_1)f(\mu_2)\cdots f(\mu_m), \tag{2.8}$$

rewriting Eq.(2.6) by means of Eq.(2.8), one finds,

$$\begin{aligned} A_2^{(0)}(\beta) &= A_1^{(0)}A_1^{(0)} - A_1^{(1)} \\ A_3^{(0)}(\beta) &= A_1^{(0)}A_1^{(0)}A_1^{(0)} - 3A_1^{(1)}A_1^{(0)} + 2A_1^{(2)} \\ A_4^{(0)}(\beta) &= A_1^{(0)}A_1^{(0)}A_1^{(0)}A_1^{(0)} - 6A_1^{(1)}A_1^{(0)}A_1^{(0)} + 3A_1^{(1)}A_1^{(1)} \\ &\quad + 8A_1^{(2)}A_1^{(0)} - 6A_1^{(3)}. \end{aligned} \tag{2.9}$$

In this way, we can get the expressions for $m = 5, 6, \ldots$ Finally, we find out their regularity and come to the following recurrence formula

$$\begin{cases} A_m^{(0)}(\beta) = \sum_{i=0}^{m-1} (-1)^i \dfrac{(m-1)!}{(m-i-1)!} A_1^{(i)}(\beta)A_{m-i-1}^{(0)}(\beta), \\ A_0^{(0)}(\beta) \equiv 1, \end{cases} \tag{2.10a}$$

In a similar way, for a system with n holes we get

$$\begin{aligned} B_n^{(0)}(\beta) &= \sum_{j=0}^{n-1} (-1)^j \frac{(n-1)!}{(n-j-1)!} B_1^{(j)}(\beta)B_{n-j-1}^{(0)}(\beta), \\ B_0^{(0)}(\beta) &\equiv 1, \end{aligned} \tag{2.10b}$$

With the help of the inverse Laplace transformation, from Eqs.(2.10) we can get the expression of the state density $g_{mpnh}(E)$.

As a general formula of the state density for a multiparticle and multi-hole system, Eqs.(2.10) are model independent and valid for any single-particle Hamiltonian, hence possessing a universal significance. Furthermore, from another point of view, utilizing the method for evaluating coefficients [21] by means of the field diagrams, we can obtain the same result. All terms but the first one on the right-hand side of Eqs.(2.10) reflect the effect of the Pauli exclusion principle and are known as the Pauli exclusion correction terms.

3. STATE DENSITIES OF THE THREE-DIMENSIONAL HARMONIC OSCILLATORS IN THE SEMI-CLASSICAL APPROXIMATION

Consider the Hamiltonian of the three-dimensional harmonic oscillator

$$\hat{H}_i = \frac{\hat{P}_i^2}{2m} + \frac{1}{2} m_0 \omega_0^2 \hat{r}_i^2, \tag{3.1}$$

where m_0 is the nucleon mass and ω_0 the harmonic oscillator parameter. In the semiclassical approximation, in the lowest order with respect to $\vec{\hbar}$, the operator $\hat{H}_i$ can be replaced by its classical counterpart and the tracing process can be replaced by the integration over the phase space, namely,

$$\hat{H}_i \longrightarrow H_i; \quad \mathrm{Tr}_i \longrightarrow \frac{d}{(2\pi\hbar)^3} \int d^3 r_i d^3 p_i \tag{3.2}$$

where d denotes the spin degeneracy of Fermions and is equal to 2. In the present work, the non-spin degree of freedom is not taken into account.

From Eqs.(2.10), the state density of m particles can be reduced into a sum of the products of a series of single states. And in the oscillator model, $A_1^{(l)}(\beta)$ and $B_1^{(l)}(\beta)$ can be written as

$$A_1^{(l)}(\beta) = \frac{d}{(\hbar\omega_0)^3} \left\{ \frac{\varepsilon_F^2}{2(l+1)\beta} + \frac{\varepsilon_F}{(l+1)^2\beta^2} + \frac{1}{(l+1)^3\beta^3} \right\}, \tag{3.3a}$$

$$\beta_1^{(l)}(\beta) = \frac{d}{(\hbar\omega_0)^3} \left\{ \frac{\varepsilon_F^2}{2(l+1)\beta} - \frac{\varepsilon_F}{(l+1)^2\beta^2} + \frac{1}{(l+1)^3\beta^3} - \frac{e^{-(l+1)\beta\varepsilon_F}}{(l+1)^3\beta^3} \right\}. \tag{3.3b}$$

The inverse Laplace transformation of $e^{-\mu\beta\varepsilon_F}\beta^{-\nu}(\nu = 1, 2..., \mu = 0, \pm1, \pm2 ...)$ can be easily performed. As both μ and ν are constants, the inverse Laplace transformation yields $(E - \mu\epsilon_F)^{\nu-1}/(\nu - 1)!\theta(E - \mu\epsilon_F)$. In Ref. [18], the average state densities for excitation energies of $g_{1p\text{-}1}h$ and $g_{2p\text{-}2}h$ are calculated and the results are in good agreement with those of quantum mechanics. This shows that the semiclassical approximate method and quantum mechanics give the same results. In Ref. [19], the state density of $g_{3p\text{-}3}h$ was correctly calculated. Table 1 gives the Pauli correction factors for various cases, and comparisons of the calculations with the results from the equi-interval model [22] are also presented.

As is known, owing to some physical reasons, if there is no restriction on the energy and well-depth of particles and holes [23,24], the state densities must be positive and monotonous functions of energy E. Therefore there exists a point $B = g_0 E_0$ (here $g_0 = 3A/\epsilon_F$ is the state density of the single particle in the region near the Fermi surface, E_0 is the excitation energy), at which $g(B) = 0$. If the energy is lower than E_0, the state densities will be located in the non-physical region. If the energy is higher than E_0, the state densities will always be positive. B is called the Pauli exclusion factor.

From the table we find that when the number of particles or holes is small, the Pauli correction factors are almost the same as the results from the equi-interval method; when the number of particles increases, the Pauli factors become slightly smaller; but when the number of holes increases, the Pauli factors become slightly bigger. All these show that the higher the particle states above the Fermi surface, the denser the state densities, and the lower the hole states below the

TABLE 1. Pauli Correction Factors

N	N Particles			N Holes			N Particles – N Holes		
	Harmonic oscillator		Equi-interval	Harmonic oscillator		Equi-interval	Harmonic oscillator		Equi-interval
	$A=56$	$A=100$		$A=56$	$A=100$		$A=56$	$A=100$	
2	0.50	0.50	0.50	0.50	0.50	0.50	2.37	2.37	2.37
3	2.44	2.45	2.46	2.47	2.46	2.46	7.29	7.29	7.29
4	5.61	5.63	5.66	5.71	5.69	5.66	14.02	14.04	14.04
5	9.80	9.86	9.93	10.08	10.01	9.93	22.85	22.83	22.83
6	14.95	15.07	15.22	15.49	15.38	15.22	33.99	33.97	33.97
7	20.99	21.21	21.52	22.06	21.83	21.52			
8	27.82	28.23	28.86						
9	35.21	35.99	37.26						
10	42.62	44.13	46.68						

Parameter: $\varepsilon_F = 39\text{MeV}$, $g_0 = A/13$.

Fermi surface, the sparser the state densities. If particles and holes exist simultaneously, because of their mutual interference, the Pauli correction factors will be bigger than the sum of the corresponding factors when they exist individually. Compared with the results from the equi-interval method, if the particle number and the hole number are equal, they will coincide with each other fairly well. From Table 1 we can conclude that the bigger the nucleon number A, the closer the results from the oscillator method to those from the equi-interval method.

Fig.1 shows the calculated state densities of particle systems from 1 particle to 10 particles with $\epsilon_F = 40.77$ MeV and $A = 40$. From the figure one finds that for different particle numbers, the state densities always start from zero and go up monotonously. For low energies the state densities change slowly with the increase of the particle number. But at relative higher energies, there exists a saturation tendency. The reason is that the farther the states are away from the Fermi surface, the

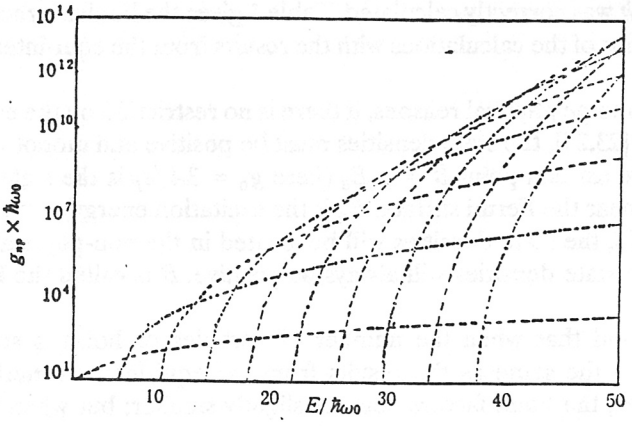

FIG.1 State densities of particle systems. The energy begins with zero. From left to right, the curves correspond to g_1p, g_2p, g_3p, g_4p, g_5p, g_6p, g_7p, g_8p, g_{9p} and $g_{10}p$, respectively.

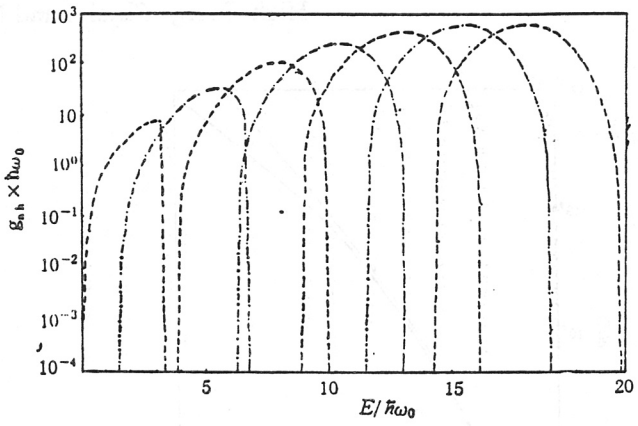

FIG.2 State densities of hole systems. The energy begins with zero. From left to right, the curves are for g_1h, g_2h, g_3h, g_4h, g_5h, g_6h and g_7h, respectively with ϵ_F = 40.77 MeV, A = 40 and n = 1--7.

smaller the state intervals and the more the states in unit energy interval will become. Therefore, the change of state densities becomes smoother.

Fig.2 shows the state densities for hole systems. Due to the Pauli exclusion principle, the Pauli correction factors for the state densities exist not only in the region near the Fermi surface but also at the bottom of the well. So there is another correction factor in this case. The reason is that when the excitation energy increases fr ɔm zero, the holes will fill the states downwards from the Fermi surface, but as the excitation decreases gradually from a large value, the holes will fill the states upwards from the bottom of the well. So no matter in which direction the holes fill the states, they are affected by the Pauli exclusion principle. This is the so-called finite well-depth effect. Furthermore, if the energy levels distribute evenly, then one will find $B_1 = B_2$. But for the harmonic oscillator model, we obtain $B_1 \neq B_2$. This means that the oscillator model can describe the uneven distribution of the energy levels. From the figure we also find that the state densities increase monotonously with the increase of E and then begin to decrease gradually to zero after a maximum

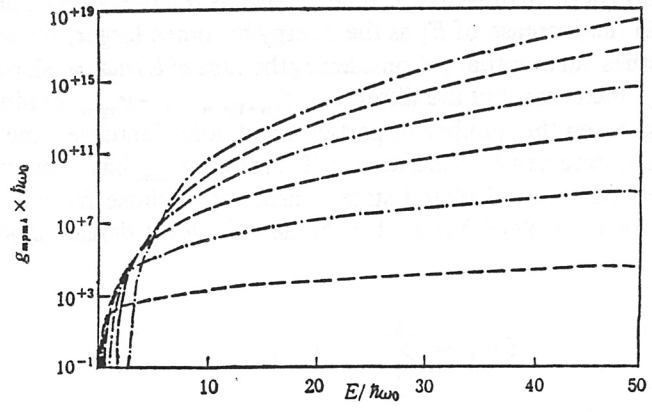

FIG.3 State densities of particle-hole systems. From top to bottom, the curves are for g_{1p1}h, g_{2p2}h, g_{3p3}h, $g_{4p4}h$, $g_{5p5}h$ and g_{6p6h} respectively.

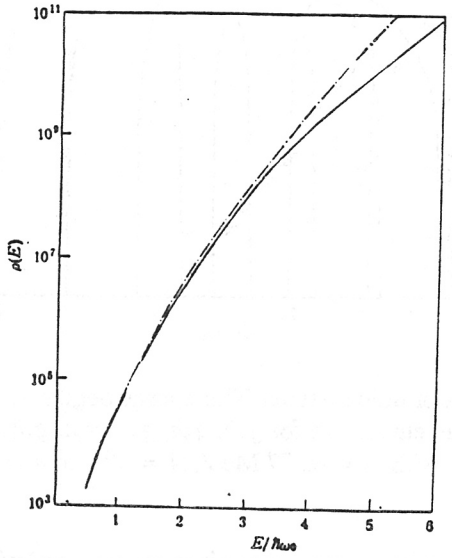

FIG.4 Comparison of state densities from the harmonic oscillator model and the equi-interval model. ----- results of the equi-interval model; ------ result of the harmonic oscillator model.

point. This is quite different from the particle case because there are no restrictions on the particle states in the potential well of single-particle harmonic oscillators as the particles fill the states upwards from the Fermi surface. But the hole states are restricted by the finite well-depth, so when the energy increases to a certain value, all states will be filled up. If the energy continues to increase, due to the Pauli exclusion principle, the states cannot be filled up any more, thus making the corresponding overall state density zero.

Fig.3 shows the calculated state densities of $\epsilon_F = 40.77$ MeV and $A = 40$ with particles and holes existing simultaneously (here $1p1h$ —$6p6h$). When $E/\hbar\omega_0$ is relatively small, at the beginning g_{mpmh} increases rapidly with the increase of E; as the energy becomes larger, the increase rate of g_{mpmh} slows down and smoothes out eventually. Considering the case of $E/\hbar\omega_0 = 50$, with the increase of particles and holes, g_{mpmh} increases, but the difference $g_{(m+1)p(m+1)h} - g_{mpmh}$ gradually decreases. The reason is the following: when the number of particles and holes increases, the average phase space becomes bigger and the state densities are denser. Therefore g_{mpmh} has a saturation tendency.

The comparison between our calculated state densities and those from the equi-interval method is shown in Fig.4 for $\epsilon_F = 59.09$ MeV, $A = 50$ and the level densities of the harmonic oscillators are given by

$$\rho(E) = \sum_{i=1}^{5} g_{ipih}(E). \tag{3.4}$$

Fig.4 indicates that when $E/\hbar\omega_0$ is small, the results of the equi-interval model and the oscillator model are almost the same. As the energy increases, the difference becomes greater with the results of the oscillator model being smaller. This is caused partially by the effect of the finite well-depth on the state densities of holes in the oscillator model and partially by the neglect of the contribution from the states higher than $5p5h$ to the state densities in our summation. Thus, we conclude that the results of the equi-interval method are in good agreement with those of the

conclude that the results of the equi-interval method are in good agreement with those of the oscillator method and that the application of the equi-interval method in the exciton model is reasonable.

In addition, we have calculated the state densities for two cases with and without the Pauli principle effect. The results show that for lower energy and a larger bigger number of particles (or holes), the effect of the Pauli principle is greater. Conversely, the effect of the Pauli principle is smaller. Moreover, the results indicate that the state densities change greatly with the harmonic oscillator parameter ϵ_F.

4. CONCLUSION

We have derived a general formula of the state densities for m-particle and n-hole systems. In the process of derivation, we have fully taken the Pauli exclusion principle into consideration. The formula is model independent. By applying our formula to three-dimensional linear harmonic oscillators, we have obtained various state densities based on a semi-classical approximation. To verify the reasonability of the equi-interval approximation, we have made a comparison between the results of the two methods. It shows that when the energy is not too high, the results from the two methods are almost the same, but when the energy is relatively higher, the results from the oscillator method become smaller. The reasons have been analyzed. When the particle number and the hole number are almost the same, the Pauli correction factors from these two methods are almost identical; but when the particle number increases, the value from the oscillator method becomes smaller and when the hole number increases, the value from the oscillator method becomes bigger. Due to the cancellation of the unequal-interval effects from particles and holes, the results from the harmonic oscillator method tend to be closer to that from the equi-interval method when the nucleon number A is bigger. From $(\varepsilon_F/\hbar\omega_0)^3 = 3A$ and $g_0 = 3A/\epsilon_F$, we find
for particles,

$$\mathrm{Tr}\, e^{-l\beta H_p} = (g_0/l\beta) + \frac{2}{(3A)}(g/l\beta)^2 + \frac{2}{(3A)^2}(g_0/l\beta)^3,$$

and for holes,

$$\mathrm{Tr}\, e^{-l\beta H_p} = (g_0/l\beta) - \frac{2}{(3A)}(g_0/l\beta)^2 + \frac{2}{(3A)^2}(g_0/l\beta)^3(1 - e^{-l\beta\varepsilon_F}),$$

In the case of the equi-interval model [22], we have

$$\mathrm{Tr}\, e^{-l\beta H} = g_0/l\beta.$$

So we can say that the equi-interval model is the large A limit of the harmonic oscillator model. Because $3A$ is a big number, the correction for A is just a small quantity. This can be regarded as the reason for the small differences among Pauli correction factors for various A.

Summing up our analysis, we come to the conclusion that the equi-interval model widely used in the exciton model is a good approximation for the low-energy nuclear reactions induced by nucleons.

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