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Particle-Hole State Densitiy with Energy Constraints and Exact Pauli Exclusion Effect

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A formula is derived for the density of particle-hole states in the equidistant spacing model. The formula gives full consideration to the effect of the Pauli exclusion principle. The pairing effect and two energy constrains are considered. The formula is easy to use and can be easily extended to the case where protons and neutrons are distinguished. The calculations indicate that the Pauli effect and the pairing effect play an important role in particle-hole state density.

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1. INTRODUCTION

Particle-hole state density plays an important role in the study of precompound reactions [1-3]. Although the well-known Ericson formula [4] has the simple form, it ignores entirely the effect of the Pauli exclusion principle. The effect was only given rough consideration by means of the Pauli correction term in Williams's formula [5]. In a recent paper [6], Baguer et al. proposed a recursive approach that would give full consideration to the Pauli exclusion effect for the exciton state density. The calculation of the coefficients $\Lambda_{ph}(j)$ (see (21) in Ref. [6]) is so difficult that its results cannot be easily generalized to the case where protons and neutrons are distinguished. Besides, the results obtained by Baguer et al. did not take into account the effect of the finite well depth. Zhang et al. proposed a new approach for calculating particle-hole state density by group theoretical method [7]. This method has the clear advantage of being model independent, and can be extended to arbitrary multifermion systems. In their paper, the Pauli exclusion effect was taken into full account, and the results in the equidistant spacing model were obtained. We will derive an analytical formula of particle-hole state density in order to verify the results in Ref. [7], after considering the pairing effect and the finite well depth. While he considered the density of states with all particles bound and the

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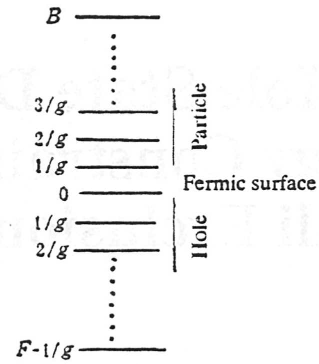

Fig.1
Sequences of energy levels for the single particle and the single hole.

finite well depth [8], Obložinský only gave rough consideration to the Pauli exclusion effect.

The purpose of this paper is to derive a formula of the exciton state density with the constraining conditions as well as the exact Pauli exclusion effect. The formula is easy to use and can be extended easily to the case in which protons and neutrons can be distinguished. Under certain conditions, our result leads to the same results obtained by others with regard to state density expressions. We have calculated the state density for small exciton number, and obtained exact numerical values of the Pauli correction. The results are discussed and compared with those of other authors. These results show that the Pauli exclusion effect and the pairing effect play an important role in particle-hole state density.

2. FORMULATION OF EXCITON STATE DENSITY WITH THE EXACT PAULI EXCLUSION EFFECT

For the sake of simplicity, we assume equidistant single particle level spectrum. The one-particle density of states is g. The excitation energy E is distributed among p particles and h holes. The nucleon binding energy is B and the Fermi energy is F. Thus single particle excitations are expressed by a series of energies $1/g$, $2/g$, ..., B, and possible hole excitations are 0, $1/g$, ... $(F - 1/g)$. The first hole state is taken at the fermi energy (Fig.1). As has been shown by Obložinský [8], we can write the particle-hole state density with energy constraints $\omega(p, h, E)$ in the form

$$\omega(p,h,E) = \sum_{\lambda=0}^{p} \sum_{j=0}^{h} (-1)^{\lambda+j} \binom{p}{\lambda} \binom{h}{j} \cdot \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \mathrm{d}\beta \frac{\exp[\beta(E - \alpha_{ph} - \lambda B - jF)]}{\prod_{k_1=1}^{p} (1 - e^{-\beta k_1/g}) \prod_{k_2=1}^{h} (1 - e^{-\beta k_2/g})}, \tag{1}$$

where

$$\alpha_{ph} = \frac{1}{2g} [p(p+1) + h(h-1)]. \tag{2}$$

The particle-hole state density without energy constraint is [6]

$$\omega(p,h,E) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} d\beta \frac{\exp[\beta(E-\alpha_{ph})]}{\prod_{k_1=1}^{p}(1-e^{-\beta k_1/g})\prod_{k_2=1}^{h}(1-e^{-\beta k_2/g})}. \tag{3}$$

By comparing Eq. (1) with Eq. (3), it can be seen that the term for $\lambda = 0$ and $j = 0$ in (1) (corresponding to $B \to \infty$ and $F \to \infty$) is just the right-hand side of Eq. (3). The other terms give the correction arising form the energy constraints B and F. α_{ph} is called Fermi energy, which is the minimum energy of the p particles and h holes due to the Pauli blocking. It represents partial effect of the Pauli exclusion principle. Another effect comes from the products in the denominator. Approximating the products results in Williams's formula [5,8] with the Pauli correction. In order to take into full account the effect of Pauli exclusion principle, we must treat the products in the denominator of Eq. (3) strictly. The same is true for Eq. (1). Let us first evaluate the integral in Eq. (1). Define

$$F(m,n,t) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\exp(tz)dz}{\prod_{k_1=1}^{m}(1-e^{-k_1 z/g})\prod_{k_2=1}^{n}(1-e^{-k_2 z/g})}, \tag{4}$$

where both m and n are integers. Let

$$S(k,z) = \frac{kz/g}{1-\exp\left(\frac{-kz}{g}\right)}, \tag{5}$$

$$Q(m,z) = \prod_{k_1=1}^{m} S(k_1,z), \tag{6}$$

$$f(m,n,z) = Q(m,z)Q(n,z), \tag{7}$$

Then

$$F(m,n,t) = \frac{g^{m+n}}{m!n!}\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} dz \frac{f(m,n,z)\exp(tz)}{z^{m+n}}. \tag{8}$$

We expand $S(k, z)$ at $z = 0$

$$S(k,z) = \sum_{n=0}^{\infty} b_n \left(-\frac{kz}{g}\right)^n \frac{1}{n!}, \tag{9}$$

where b_n is Bernouli number, the values of which can be found in any mathematical tables. In addition,

$$b_0 = 1,\ b_1 = -\frac{1}{2},\ b_{2k+1} = 0\ (k \geq 1).$$

Eqs. (6) and (7) show that $Q(m, z)$ and $f(m, n, z)$ can be written in the classical form (the coefficient of the zero power of z equal to 1) as

$$Q(m,z) = \sum_{\mu=0}^{\infty} C(m,\mu)z^{\mu}, \tag{10}$$

$$f(m,n,z) = \sum_{\lambda=0}^{\infty} B(m,n,\lambda) z^{\lambda}. \tag{11}$$

Hence, the integrand in Eq. (8) has a pole of the order of $m + n$ at the origin. We obtain

$$F(m,n,t) = \frac{g^{m+n}}{m!n!} \frac{1}{2\pi i} \oint \frac{f(m,n,z) e^{tz}}{z^{m+n}} \theta(t) dz, \tag{12}$$

because if $t < 0$, the contour must be closed in the right half-plane, without containing the pole. Here, $\theta(t)$ is step function. Substituting (11) into (12) and using the residue theorem, we have

$$\begin{aligned} F(m,n,t) &= \frac{g^{m+n}}{m!n!} \sum_{\lambda=0}^{\infty} B(m,n,\lambda) \frac{1}{2\pi i} \oint \frac{e^{tz}}{z^{m+n-\lambda}} dz \theta(t) \\ &= \frac{g^{m+n}}{m!n!} \sum_{\lambda=0}^{m+n-1} B(m,n,\lambda) \frac{t^{m+n-1-\lambda}}{(m+n-1-\lambda)!} \theta(t). \end{aligned} \tag{13}$$

Now let us find the explicit expression of the coefficient $B(m, n, \lambda)$. We have the following formula for the derivative:

$$(u_1 u_2 \cdot \cdots \cdot u_m)^{(n)} = \sum_{\substack{0 \leq i_1 \leq n \\ 0 \leq i_2 \leq n \\ \vdots \\ 0 \leq i_m \leq n \\ (i_1 + i_2 + \cdots + i_m = n)}} \frac{n!}{i_1! i_2! \cdots i_m!} u_1^{(i_1)} u_2^{(i_2)} \cdot \cdots \cdot u_m^{(i_m)}, \tag{14}$$

where (n) and (i) denote the nth and ith derivatives. From Eqs. (11), (7) and (14), we obtain

$$\begin{aligned} B(m,n,\lambda) &= \frac{1}{\lambda!} f^{(\lambda)}(m,n,z)\big|_{z=0} \\ &= \frac{1}{\lambda!} (Q(m,z)Q(n,z))^{(\lambda)}\big|_{z=0} \\ &= \sum_{\substack{0 \leq \lambda_1 \leq \lambda \\ 0 \leq \lambda_2 \leq \lambda \\ (\lambda_1 + \lambda_2 = \lambda)}} \frac{Q(m,z)^{(\lambda_1)} Q(n,z)^{(\lambda_2)}}{\lambda_1! \lambda_2} \Big|_{z=0}, \end{aligned} \tag{15}$$

According to Eq. (10), we have

$$\begin{aligned} Q(m,z)^{(\lambda_1)}\big|_{z=0} &= C(m,\lambda_1)\lambda_1!, \\ Q(n,z)^{(\lambda_2)}\big|_{z=0} &= C(n,\lambda_2)\lambda_2!, \end{aligned} \tag{16}$$

A combination of Eqs. (15) and (16) yields

$$B(m,n,\lambda) = \sum_{\lambda_1=0}^{\lambda} C(m,\lambda_1) C(n,\lambda-\lambda_1), \tag{17}$$

Using Eqs. (14), (16) and (6), we obtain

$$C(m,\lambda_1) = \frac{1}{\lambda_1!} Q(m,z)^{(\lambda_1)}|_{z=0}$$

$$= \frac{1}{\lambda_1!} \sum_{\substack{0\leq i_1\leq\lambda_1 \\ 0\leq i_2\leq\lambda_1 \\ \vdots \\ 0\leq i_m\leq\lambda_1 \\ (i_1+i_2+\cdots+i_m=\lambda_1)}} \frac{\lambda_1! S(1,z)^{(i_1)} S(2,z)^{(i_2)}\cdot\cdots\cdots S(m,z)^{(i_m)}}{i_1! i_2! \cdot\cdots\cdots i_m!}\Big|_{z=0}$$

$$\equiv \sum_{\substack{0\leq i_k\leq\lambda_1 \\ \left(\sum_{k=1}^{m} i_k=\lambda_1\right)}} \prod_{k=1}^{m} \frac{S(k,z)^{(i_k)}}{i_k!}\Big|_{z=0}. \tag{18}$$

From Eq. (9), we have

$$S(k,z)^{(i_k)}|_{z=0} = b_{i_k}\left(\frac{-k}{g}\right)^{i_k}, \tag{19}$$

Substituting this into Eq. (18), we have

$$C(m,\lambda_1) = \sum_{\substack{0\leq i_k\leq\lambda_1 \\ \left(\sum_{k=1}^{m} i_k=\lambda_1\right)}} \prod_{k=1}^{m} \frac{1}{i_k!} b_{i_k}\left(-\frac{k}{g}\right)^{i_k}$$

$$= \sum_{i_m=0}^{\lambda_1} \frac{1}{i_m!} b_{i_m}\left(-\frac{m}{g}\right)^{i_m} \cdot \sum_{\substack{0\leq i_k\leq(\lambda_1-i_m) \\ \left(\sum_{k=1}^{m-1} i_k=\lambda_1-i_m\right)}} \prod_{k=1}^{m-1} \cdot \frac{b_{i_k}\left(-\frac{k}{g}\right)^{i_k}}{i_k!}, \tag{18'}$$

which yields the following recursive relation of coefficient C:

$$C(m,\lambda_1) = \sum_{i_m=0}^{\lambda_1} \frac{1}{i_m!} b_{i_m}\left(-\frac{m}{g}\right)^{i_m} C(m-1,\lambda_1-i_m). \tag{20}$$

Due to $Q(m = 0, z) = 1$ when $m = 0$, from Eq. (10), we have

$$C(0,\lambda) = \begin{cases} 1, & \text{when } \lambda = 0, \\ 0, & \text{when } \lambda \neq 0. \end{cases} \tag{21}$$

Substituting Eq. (13) into Eq. (1), we find immediately the final result in the following form

$$\omega(p,h,E) = \frac{g^N}{p!h!} \sum_{i=0}^{p} \sum_{j=0}^{h} (-1)^{i+j} \binom{p}{i}\binom{h}{j} \sum_{\lambda=0}^{N-1} (E-\alpha_{ph}-iB-jF)^{N-1-\lambda}$$

$$\cdot\, \theta(E-\alpha_{ph}-iB-jF) B(p,h,\lambda) \frac{1}{(N-1-\lambda)!}, \tag{22}$$

where $N = p + h$ (the number of excitons),

$$B(p,h,\lambda) = \sum_{\lambda_1=0}^{\lambda} C(p,\lambda_1)C(h,\lambda-\lambda_1), \tag{23}$$

$$C(m,\lambda) = \sum_{i=0}^{\lambda} \frac{1}{i!} b_i \left(-\frac{m}{g}\right)^i C(m-1,\lambda-i). \tag{24}$$

It is easy to calculate coefficient C according to the recursive relation (24) because Bernouli number b_i is provided in mathematical handbooks.

Bearing in mind the character (21) of coefficient C, from Eq. (23), we have

$$B(p,0,\lambda) = C(p,\lambda),$$
$$B(0,h,\lambda) = C(h,\lambda).$$

Hence, a pure particle (hole) state density can be obtained from Eq. (22):

$$\begin{aligned}\omega(p,0,E) &= \frac{g^p}{p!}\sum_{i=0}^{p}(-1)^i\binom{p}{i}\sum_{\lambda=0}^{p-1}(E-\alpha_{p0}-iB)^{p-1-\lambda} \\ &\cdot \theta(E-\alpha_{p0}-iB)\frac{C(p,\lambda)}{(p-1-\lambda)!}, \\ \omega(0,h,E) &= \frac{g^h}{h!}\sum_{j=0}^{h}(-1)^j\binom{h}{j}\sum_{\lambda=0}^{h-1}(E-\alpha_{0h}-jF)^{h-1-\lambda} \\ &\cdot \theta(E-\alpha_{0h}-jF)\frac{C(h,\lambda)}{(h-1-\lambda)!}.\end{aligned} \tag{25}$$

If we keep only the term corresponding to $i = 0$, $j = 0$ in Eq. (22), Eq. (22) can be reduced to the state density expression without the energy constraints derived by Baguer et al. [6].

$$\omega(p,h,E) = \frac{g^N}{p!h!}\sum_{\lambda=0}^{N-1}(E-\alpha_{ph})^{N-1-\lambda}\theta(E-\alpha_{ph})\frac{B(p,h,\lambda)}{(N-1-\lambda)!}. \tag{26}$$

where $B(p, h, \lambda)$ is equivalent to $G_{ph}(\lambda)$ in Ref. [16]. The other terms corresponding to $i = 0$, $j = 0$ give the correction of the state density caused by the energy constraints. Obložinský's result [8] is

$$\begin{aligned}\omega(p,h,E) &= \frac{g^N}{p!h!(N-1)!}\sum_{i=0}^{p}\sum_{j=0}^{h}(-1)^{i+j} \\ &\cdot \binom{p}{i}\binom{h}{j}\theta(E-\alpha_{ph}-iB-jF)\end{aligned} \tag{27}$$

where

$$\cdot (E - A_{ph} - iB - jF)^{N-1},$$

$$A_{ph} = \frac{1}{4}\frac{p^2+p}{g} + \frac{1}{4}\frac{h^2-3h}{g}$$

Expanding the factor $(E - A_{ph} - iB - jF)^{N-1}$ in Eq. (27) by the binomial theorem,

$$(E - A_{ph} - iB - jF)^{N-1} = \left[(E - \alpha_{ph} - iB - jF) + \left(\frac{p^2+p}{4g} + \frac{h^2+h}{4g} \right) \right]^{N-1}$$

$$= \sum_{\lambda=0}^{N-1} \binom{N-1}{\lambda} (E - \alpha_{ph} - iB - jF)^{N-1-\lambda} \left(\frac{p^2+p}{4g} + \frac{h^2+h}{4g} \right)^{\lambda},$$

Eq. (27) can be rewritten as

$$\omega(p,h,E) = \frac{g^N}{p!h!} \sum_{i=0}^{p} \sum_{j=0}^{h} (-1)^{i+j} \binom{p}{i} \binom{h}{j} \sum_{\lambda=0}^{N-1} (E - \alpha_{ph} - iB - iF)^{N-1-\lambda}$$

$$\cdot\, \theta(E - \alpha_{ph} - iB - jF) \left[\frac{1}{\lambda!} \left(\frac{p^2+p}{4g} + \frac{h^2+h}{4g} \right)^{\lambda} \right] \frac{1}{(N-1-\lambda)!}. \tag{28}$$

A comparison between Eq. (28) and Eq. (22) shows that Obložinský's result is an approximate one in which the exact coefficient is replaced by the following factor:

$$B(p,h,\lambda) = \frac{1}{\lambda!} \left(\frac{p^2+p}{4g} + \frac{h^2+h}{4g} \right)^{\lambda}, \tag{29}$$

This approximation suggests that the Pauli exclusion effect is taken into account approximately. The result (22) can be easily extended to the case in which protons and neutrons are distinguishable because the coefficient $B(p,\ h,\ \lambda)$ can be calculated systematically by the aid of Eqs. (23) and (24).

3. FORMULATION OF EXCITON STATE DENSITY WITH THE PAIRING CORRECTIONS

The pairing effect also plays an important role in particle-hole state density. As has been pointed out by Kalbach [9], we can obtain an expression of the particle-hole state density with pairing corrections simply by replacing the Pauli energy α_{ph} with $E_{\rm thresh}$. $E_{\rm thresh}$ [9,10] can be taken as

$$E_{\rm thresh} = g\,\frac{(\Delta_0^2 - \Delta^2)}{4} + p_m \left[\left(\frac{p_m}{g} \right)^2 + \Delta^2 \right]^{\frac{1}{2}}, \tag{30}$$

where

$$p_m = \max(p,h), \quad \Delta_0 = 2\left(\frac{c}{g} \right)^{\frac{1}{2}}$$

Δ_0 is the condensation energy, and c is the constant obtained by fitting experimental level density data. Pairing gap Δ can be taken as

$$\frac{\Delta}{\Delta_0} = \begin{cases} 0.996 - 1.76 \left(\dfrac{N}{N_c} \right)^{1.6} \left(\dfrac{E}{c} \right)^{-0.68}, & E > E_{\rm phase} \\ 0, & E < E_{\rm phase} \end{cases} \tag{31}$$

where E_{phase} is the energy of the pairing phase transition given by

$$E_{phase} = \begin{cases} c[0.716 + 2.44\left(\frac{N}{N_c}\right)^{2.17}], & \frac{N}{N_c} > 0.446, \\ 0 & \text{Otherwise} \end{cases} \quad (32)$$

and $N_c = 0.792g\Delta_0$ is the critical number of excitons.

The replacement of α_{ph} in Eq. (22) by E_{thresh} yields the following formula of exciton state density

$$\omega(p,h,\lambda) = \frac{g^N}{p!h!}\sum_{i=0}^{p}\sum_{j=0}^{h}(-1)^{i+j}\binom{p}{i}\binom{h}{j}$$
$$\cdot\sum_{\lambda=0}^{N-1}(E - E_{thresh} - iB - jF)^{N-1-\lambda}\theta(E - E_{thresh} - iB - jF)B(p,h,\lambda)\frac{1}{(N-1-\lambda)!}. \quad (33)$$

in which the pairing corrections as well as the energy constraints are involved and the effect of the Pauli exclusion principle is taken into full account.

4. RESULTS AND DISCUSSION

In order to emphasize the study of the Pauli exclusion effect, we ignore the pairing effect and eliminate the energy constraints on particles and holes for the time being. We set the Fermi level at halfway between the last-filled and first-vacant single particle level. In doing so, α_{ph} in Eq. (26) need be changed to the following form

$$\alpha_{ph} = \frac{1}{2g}(p^2 + h^2),$$

Then, from Eq. (26) we can obtain the maximum zero point of the state density and the Pauli correction $A(p, h)$ with exact Pauli exclusion effect. In this case, Kalbach's Pauli correction $A_K(p, h)$ is equal to Williams's

$$A_K(p,h) = \frac{1}{4}(p^2 - p) + \frac{1}{4}(h^2 - h). \quad (34)$$

A comparison between $A(p, h)$ and $A_K(p, h)$ is shown in Table 1. Roughly $A(p, h)$ is twice as large as $A_K(p, h)$. Considering the approximation for Exciton model's trace employed in Ref. [7], we obtain for the Pauli correction [6,7] the same results as in Ref. [7]. This situation suggests that the Pauli exclusion principle plays an important role in particle-hole state density.

We have calculated particle-hole state density from Eq. (22) and compared our results with Obložinský's. For the convenience of comparison, we have taken the same values of parameters as Ref. [9], i.e., $g = 8\ \text{MeV}^{-1}$, $B = 8$ MeV and $F = 32$ MeV. The calculated results are shown in Figs. 2 and 3. As is seen, for small exciton number, such as $2p0h$, $0p2h$ and $1p1h$, our results agree with Obložinský's values. This suggests that the Pauli exclusion effect is not important for small exciton number, and that an approximate method is accurate enough. The deviation between two results

Table 1
A comparisons of Pauli corrections.

p	h	$A(p,h)$	$A_K(p,h)$	p	h	$A(p,h)$	$A_K(p,h)$
1	1	0.000	0.000	4	3	10.701	4.500
2	1	1.207	0.500	4	4	14.109	6.000
2	2	2.581	1.000	5	1	11.053	5.000
3	1	3.436	1.500	5	2	12.702	5.500
3	2	4.916	2.000	5	3	15.146	6.500
3	3	7.298	3.000	5	4	18.554	8.000
4	1	6.720	3.000	5	5	22.989	10.000
4	2	8.289	3.500				

occurs with increasing exciton number. For $2p1h$ and $1p2h$, the relative deviations are about 1%. They are too small to appear in Fig.2. When $N = 5$, such as $2p3h$ and $3p2h$, the maximum relative deviation between them is about 30%. This shows that for large exciton number the Pauli exclusion effect is very important. In this situation we must give it full consideration because an approximate result is not accurate enough.

Due to the constraints B and F on particles and holes, the state density for a particular number of particles and holes is no longer a monotonous function of the excitation energy. It can be seen from the calculated results (Fig.3) that for small E our results are smaller than Obložinský's but for large E ours are larger, i.e., each solid line and the corresponding dashed line intersect. This is caused by the factor$(-1)^{1+j}$ and the summation with respect to i and j in Eq. (22). The major reason may be explained with complex effects of the constraints. Further calculations show that as B and F increase, the point of intersection is displaced in the right direction. In the limit case of $F \to \infty$ and $B \to \infty$, they do not intersect, and each solid line is below the corresponding dashed line. Apparently, increasing the Pauli correction is equivalent to decreasing the excitation energy.

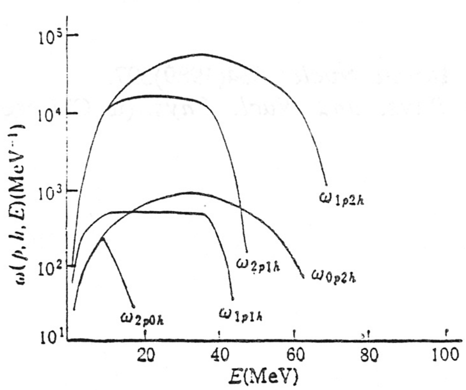

Fig.2
Density of particle-hole states
versus excitation energy.

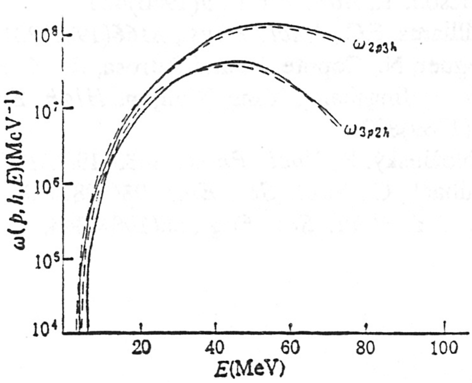

Fig.3
Density of particle-hole states
versus excitation energy.
___ present results;
----- P. Obložinský.

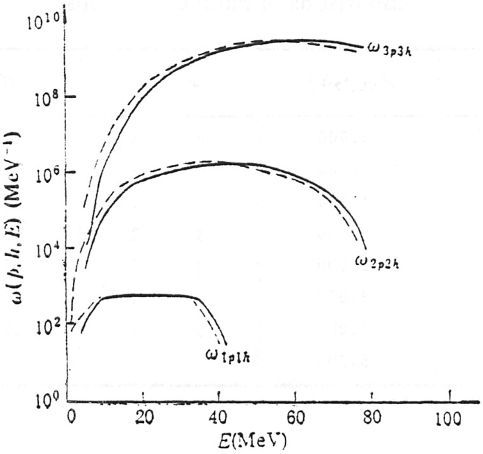

Fig.4
Density of particle-hole states versus excitation energy.
___ with pairing corrections;
----- without pairing corrections.

Fig.4 shows the calculated results with the pairing effect obtained by Eq. (33), with $\Delta_0 = 1$ MeV, $g = 8$ MeV^{-1}, $B = 8$ MeV and $F = 32$ MeV. When they are compared with the results without the pairing effect, the pairing effect enhances the values of the state density for large E and reduces it for small E. To sum up, the pairing effect plays an important role in exciton state density.

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