Particle-Hole State Density Calculations with Non-Equidistant Spacing Model: II. Pairing and Exact Treatment

Ahmed Abdul-Razzaq Selman[(1)*], Mahdi Hadi Jasim[(2)], and Shafik Shaker Shafik[(2)#]**

(1) IT Unit, College of Science, University of Baghdad
(2)Department of Physics, College of Science, University of Baghdad,

(*) ahmed@aaselman.com, correspondence author
(**) mhjasim@uobnpg.com
(#) ssalmola@uobnpg.com

Abstract

In an earlier paper, the basic analytical formula for particle-hole nuclear state densities was derived for non-Equidistant Spacing Model (non-ESM) approach. In this paper, an extension of the former equation was made to include pairing. Also a suggestion was made to derive the exact formula for the particle-hole state densities that depends exactly on Fermi energy and nuclear binding energies. The results indicated that the effects of pairing reduce the state density values, with similar dependence in the ESM system but with less strength. The results of the suggested exact formula indicated some modification from earlier non-ESM approximate treatment, on the cost of more calculation time.

Key words
Level Density, Single-Particle Level ensity, Statistical Compound Nucleus Reactions.

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حسابات كثافة الحالة لجسيمة-فجوة حسب نموذج التباعد غير المتساوي: ب. تأثير الإزدواج والمعالجة الدقيقة

أحمد عبد الرزاق سلمان(١)، مهدي هادي جاسم(٢) و شفيق شاكر شفيق(٢)

(١) وحدة تكنولوجيا المعلومات، كلية العلوم – جامعة بغداد و (٢) قسم الفيزياء، كلية العلوم – جامعة بغداد

الخلاصة

في بحث سابق، أُشتقتْ المعادلة التحليلية الأساسية المتعلقة بحساب كثافة الحالات النووية الخاصة بنظام جسيمة-فجوة استنادا على نموذج التباعد الحقيقي الغير متساوي (non-ESM). وفي هذا البحث جرت محاولة لتطوير المعالجة السابقة وذلك لكي تشمل تصحيح طاقة الأزدواج. في البحث الحالي أيضا تم اقتراح طريقة خاصة باشتقاق المعادلة الدقيقة لكثافة الحالات النووية والتي تأخذ بنظر الاعتبار الاعتماد المضبوط على طاقة فيرمي وطاقات الربط النووية. بينت النتائج أن إضافة تأثير الازدواج يقلل من كثافة الحالات المحسوبة وبتصرف مماثل لنموذج التباعد المتساوي (ESM)، ولكن بشدة أقل. أشارت هذه النتائج إلى زيادة الدقة عن المعالجة السابقة، ولكن على حساب الوقت المستغرق لإجراء الحسابات.

Introduction

Various nuclear reactions are classified and interpreted according to the reaction entrance and exit energy channels. The exciton model [1] illustrates the nuclear reaction mechanism

at intermediate energies, where continuum emission is observed. This fraction of nuclear emission has very important applications in nuclear reactors and it is described by the Preequilibrium Emission (PE). In the exciton model, the intermediate stages are treated semi-classically to explain the PE and predict the reaction spectra and cross-sections. A quantity needed for this model calculations is the particle-hole state density, $\omega(n,E)$. This quantity describes the population of the single-particle states per energy interval, thus provides a proper description of the nuclear states that contribute in PE process. Intermediate stages of nuclear reactions have also received a special interest since understanding these stages will reveal important information about the mechanism at which PE occurs. Theoretical interpretation of this emission is required to describe the structure of excited stages. The relation between state and well-known level density $\rho(E)$ is [2],

$$\rho(E)=\sum_{n}\omega(n,E) \qquad (1),$$

It should be mentioned that the level density of the excited nucleus is the quantity that can be experimentally measured [3], although with difficulty. This quantity is determined either from analyzing neutron resonance spectra [4], or from γ-ray strength measurements [5].

A proper literature and theoretical review about the derivation method was given earlier in Part I of this paper [6], thus the theoretical modification described below aims to extend the earlier work.

In this work, we first extend the former treatment to include modified pairing, and compare with modified Williams' formula. Also, the present results are compared with the exact quantum mechanical calculations for selected examples. Finally, a complete derivation of the state density formula that specifies the exact dependence of the state density on binding and Fermi energies is given.

II. State Density for non-ESM System With Modified Williams' Formula

The uncorrected state density formula obtained in Part I [6] is given by,

$$\omega(p,h,E)=\frac{g_o^n}{2^n\pi^{n/2}\,p!h!}\,\widehat{\Xi}\,\frac{E^{N-1}}{F^{N-n}(N-1)!} \qquad (2),$$

where the special mathematical multiplication operator $\widehat{\Xi}$ is defined by,

$$\widehat{\Xi}\equiv\sum_{\substack{a_1,a_2,..a_p,\\ b_1,b_2,..b_h=0}}^{\infty}\prod_{j=1}^{p}C_{a_j}^{p}\prod_{\lambda=1}^{h}C_{b_\lambda}^{h} \qquad (3),$$

and C^p and C^h are coefficients of integrating the special functions $P(k)$ and $H(k)$ –see Part I [6]. These functions represent part of the state density integration. Modification of equation (3) to include Pauli effect was written as,

$$\omega^{non-ESM}(p,h,E)=\frac{g_o^n}{2^n\pi^{n/2}\,p!h!}\,\widehat{\Xi}\,\frac{\left(E-A(p,h)\right)^{N-1}}{F^{N-n}(N-1)!} \qquad (4),$$

where $\omega^{non-ESM}(p,h,E)$ is the state density, E is the excitation energy, g_o is the s.p.l.d. for ground state, $A_{p,h}$ is Pauli blocking energy for system configuring of p particles and h holes, n is the exciton number ($n=p+h$), F is Fermi energy of the target nucleus

Modified Williams' formula takes particle pairing into consideration. Pairing can add considerable amount of correction to the state density calculation [7,8]. This effect is included in such a way that the excitation energy is corrected by more subtracting the amount of energy $P(\Delta)$ which accounts for paring as a function of the energy gap, Δ.

The treatment was well described by Harangozo et al. and Avrigeanu et al. [9,10] in practical calculation and here only the basic formulae are listed. The state density with modified Pauli blocking is (modified Williams' formula) [10],

$$\omega^{\mathrm{mW}}(n,E,P)=\frac{g^{n}\left(E-P(\Delta)-B_{p,h}\right)^{n-1}}{p!h!\,(n-1)!}$$
$$\times\quad \Theta(E-P(\Delta)-B_{p,h}) \qquad (5),$$

where

$$P(\Delta)=g\frac{\left(\Delta_o^2-\Delta^2\right)}{4} \qquad (6),$$

is the pairing energy. B is the binding energy of the emitted nucleon, $B_{p,h}$ is a modified Pauli energy given as,

$$B_{p,h}=A_{p,h}\sqrt{1+\left(\frac{2g\Delta}{n}\right)^2} \qquad (7),$$

Δ and Δ are energy gaps of the nuclear levels for the ground and excited states, The relation between Δ and Δ_o is,

$$\left.\begin{aligned}\frac{\Delta}{\Delta_o}&=0.996-1.76\left(\frac{n}{n_c}\right)^{1.60}\times\\ &\left(\frac{E}{C_e}\right)^{-0.68} \quad if\ \ E\ge E_{phase}\\ \frac{\Delta}{\Delta_o}&=0 \quad if\ \ E<E_{phase}\end{aligned}\right\} \qquad (8),$$

C_e is the condensation energy, and E_{phase} is pairing energy due to phase transition, it is defined as [7],

$$\left.\begin{aligned}E_{phase}&=\\ C_e&\left[0.716+2.44\left(\frac{n}{n_c}\right)^{2.17}\right] \text{ if } \frac{n}{n_c}\ge 0.446\\ E_{phase}&=\ 0 \qquad \text{otherwise}\end{aligned}\right\} \qquad (9),$$

C_e is given by,

$$C_e=g\frac{\Delta_o^2}{4} \qquad (10),$$

n_c in eq.(9 and 10) is the critical exciton number given as $n_c=0.792\ g\Delta_o$. For full discussions about this treatment, see Refs.[9,10] for both ESM and non-ESM approaches.

In the present paper, pairing modifications are added by inspection to formula (2), as done by Harangozo et al. [9]. This will result in the following -corrected- formula,

$$\omega^{non-ESM}(p,h,E)=$$
$$\frac{g_o^n}{2^n\pi^{n/2}\,p!h!}\widehat{\Xi}\frac{\left(E-P(\Delta)-B_{p,h}\right)^{N-1}}{F^{N-n}(N-1)!}$$
$$\times\Theta(E-P(\Delta)-B_{p,h}) \qquad (11),$$

which takes pairing effect into account. $\Theta(x\text{-}x_o)$ is the Heaviside step function. The results of comparing state density values from this formula and eq.(5) are shown in Figs.(1-3). The comparisons of these figures were made using data found from the code PLD [10].

In Fig.(1) it is seen that the state density calculated from eq.(11) in the (1,1) configuration is always less than that found from eq.(5), and in the case of F=38 MeV, three terms gave the only adequate results. However, as the exciton configuration develops the behavior of the state density in the case of F=38 MeV becomes much consistent with the reasonable behavior of state density, as seen from Figs.(2 and 3) for (2,1) and (3,2) exciton configurations. As a matter of fact, at these configurations even the number of summation terms tend to improve the state density behavior much more than in the previous results listed so far in the present paper. Figs.(2-*a*) and (3-*a*) clearly show that increasing the number of terms only slightly changes the calculated state densities. The state density ratio in these figures crosses the line corresponding to unity at energies 70 MeV in the case (2,1) and 77 MeV in (3,2). These correspond to the energy value ~ 2F. On the other hand, the maxima in both cases occurred at

energies ~ 40 MeV. These results indicate that as the excitation energies approach ~*F*, a maximum value occurs which means that states will gather mostly near such energy, *i.e*., more important distribution probabilities will occur. Also, at excitation energies ~2*F*, the state densities found from both improved Williams formula and the formula for non-ESM are almost being equal in magnitude, and above such energy the ratio decreases in favor of Williams'.

III. Comparisons with Exact Calculations

In Fig.(4) we plot the results of the present treatment against the exact quantum-mechanical results for 1*p*-1*h* in the case of ^{56}Fe and 2*p*-1*h* for ^{54}Mn as reported by Herman and Reffo [11], where the exact results illustrated there are for state density calculation with pairing, compared to our results with no interaction assumed (thin lines) and with pairing (heavy lines). The calculations of Ref.[11] were described without using the approximations based on saddle-point and ESM, thus provide well-referenced data for comparison with the present results. The specifications of including pairing effect are -taken from Table (1) of Ref.[11], units of MeV- for ^{56}Fe: Δ_o=1.49, S=0.53, C_e=2.22 and for ^{54}Mn: Δ_o=2.6, S=-0.45, C_e=1.55.

Comparison among these figures shows that our results are still higher ~20% than the exact results made for the same system specifications, where even in the range below 40 MeV of excitation energy the match was not achieved. This indicates that the results obtained by correcting the analytical expression by inspection may give good (but not exact) results of the state density calculations. This also strongly suggests that one should try to apply the general formula eq.(11) if more accurate results required.

IV. Exact Inclusion of Fermi and Binding Energies

When the limits of B and F are very large, the effect of the Heaviside step function will be neglected because the integrals in this case will extend from zero to infinity without any restrictions. The results discussed so far were obtained from adding some corrections to eq.(2) by inspection, that is to add these corrections to the energy term. There should be, however, a certain (and more accurate) change in the indices of summations used in the development of eqs.(2 and 11). This comes from the fact that the basic derivation of the original formula, eq.(2), was based on specified method that takes into account these indices. Below this is made as a suggestion for the present development of the state density calculation using the non-ESM approach. The exact inclusion of the effects of Fermi and binding energies is determined as in Ref.[6], which takes into account the reasonable limitations that u not to exceed F (in the case of holes) and B(in the case of particles). Then, using this exact definition, the functions $P(k)$ and $H(k)$ can be found equal to -compare to eqs.(16 and 17) of [2],

$$P(k) = g_o \sum_{m=0}^{\infty} \frac{C_m^p}{F^m (ik)^{m+1}} \times \left(1 - \exp(-ikB) \sum_{s=0}^{m} \frac{(ikB)^s}{s!} \right) \qquad (12),$$

$$H(k) = g_o \sum_{m=0}^{\infty} \frac{C_m^h}{F^m (ik)^{m+1}} \times \left(1 - \exp(-ikF) \sum_{s=0}^{m} \frac{(ikF)^s}{s!} \right) \qquad (13),$$

which leads to the following,

$$\omega(p,h,E) =$$

$$\frac{g_o^n}{\pi\, p!h!}\sum_{a_1=0}^{\infty}\sum_{a_2=0}^{\infty}\cdots\sum_{a_p=0}^{\infty}\sum_{s_1=0}^{a_1}\sum_{s_2=0}^{a_2}\cdots\sum_{s_p=0}^{a_p}\sum_{b_1=0}^{\infty}\sum_{b_2=0}^{\infty}\cdots\sum_{b_h=0}^{\infty}\sum_{q_1=0}^{b_1}\sum_{q_2=0}^{b_2}\cdots\sum_{q_h=0}^{b_h}\prod_{j=1}^{p}C_{a_j}^{p}\times$$

$$\prod_{\lambda=1}^{h}C_{b_\lambda}^{h}\sum_{\ell=0}^{p}\sum_{r=0}^{h}(-1)^{\ell+r}\binom{p}{\ell}\binom{h}{r}\frac{B^{(s_1+s_2+\ldots+s_p)\ell}\,F^{(q_1+q_2+\ldots+q_h)r-(b_1+b_2+\ldots b_h)-(a_1+a_2+\ldots a_p)}}{\left[\prod_{j=1}^{p}(s_j)!\right]^{\ell}\left[\prod_{\lambda=1}^{h}(q_\lambda)!\right]^{r}}I \qquad (14),$$

where the integral I is defined as,

$$I=\int_0^{\infty}\frac{\exp\left(ik(E-rF-\ell B)\right)}{(ik)^N}dk \qquad (15),$$

and N in this case is,

$$N=n+\sum_{j=1}^{p}(a_j-\ell s_j)+\sum_{\lambda=1}^{h}(b_\lambda-r q_\lambda) \qquad (16).$$

Then, our solution is,

$$\therefore \omega(p,h,E)=\frac{g_o^n}{p!h!}\hat{\Xi}\,B^{\ell\sum_{j=1}^{p}s_j}\,F^{\sum_{\lambda=1}^{h}(r q_\lambda-b_\lambda)-\sum_{j=1}^{p}a_j}\,\frac{(E-rF-\ell B)^{N-1}}{(N-1)!} \qquad (17),$$

and the $\hat{\Xi}$ operator in this case is,

$$\hat{\Xi}=\sum_{a_1=0}^{\infty}\sum_{a_2=0}^{\infty}\cdots\sum_{a_p=0}^{\infty}\sum_{s_1=0}^{a_1}\sum_{s_2=0}^{a_2}\cdots\sum_{s_p=0}^{a_p}\sum_{b_1=0}^{\infty}\sum_{b_2=0}^{\infty}\cdots\sum_{b_h=0}^{\infty}\sum_{q_1=0}^{b_1}\sum_{q_2=0}^{b_2}\cdots\sum_{q_h=0}^{b_h}\times$$

$$\prod_{j=1}^{p}C_{a_j}^{p}\prod_{\lambda=1}^{h}C_{b_\lambda}^{h}\sum_{\ell=0}^{p}\sum_{r=0}^{h}\frac{(-1)^{\ell+r}\binom{p}{\ell}\binom{h}{r}}{\left[\prod_{j=1}^{p}(s_j)!\right]^{\ell}\left[\prod_{\lambda=1}^{h}(q_\lambda)!\right]^{r}} \qquad (18).$$

Eq.(17) represents the exact state density formula for non-ESM dependence on B and F.

The above set of equations, eq.s(17, 18), clearly indicate how complicated formula one will find if the exact dependence was needed. Beside the need for numerical calculations of eq.(17), further inclusion of Pauli blocking and pairing terms should also be made. These tasks are left for further investigation.

V. Conclusions

In conclusion, it is seen that pairing correction adds an important modification to state density values in the non-ESM system. Comparisons with the standard treatment showed that the present non-ESM formula for state density calculation corresponds to the best results. The comparison with exact calculations for (1*p*-1*h*) and (2*p*-1*h*) configurations showed that the present results may give better state density values when including pairing effect. A comparison with exact quantum mechanical treatment showed that the present formula still ~ 20% higher, thus a conclusion is made that more corrections are still needed.

The inclusion of exact effects of binding and Fermi energies for particles and

holes, respectively on the state density calculation made it clear that the state density formula will have a highly complicated form. This indicates that the problem of non-ESM can actually be solved to give better description of the system, but on the price of more calculation time and efforts.

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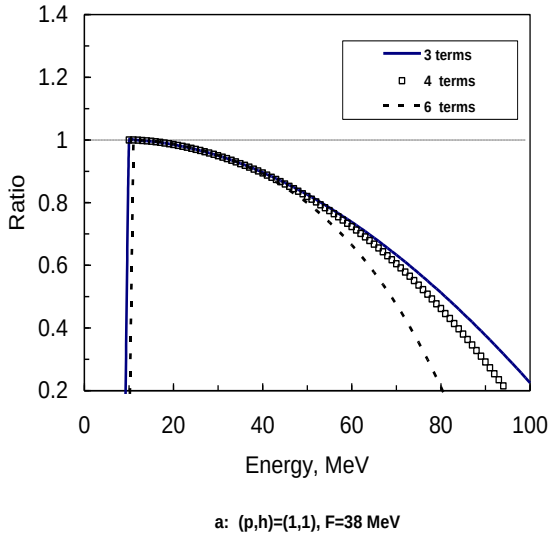


Fig.(1-a)

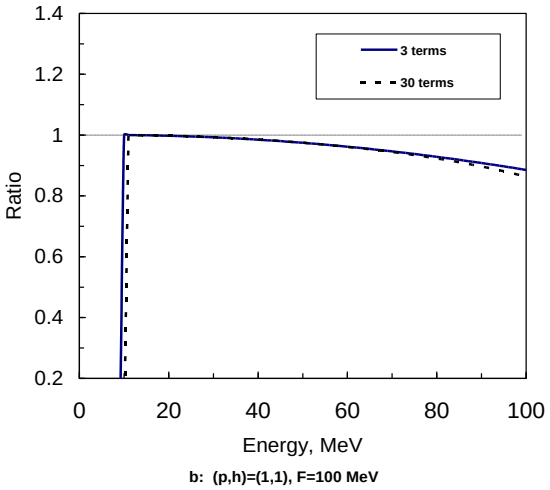
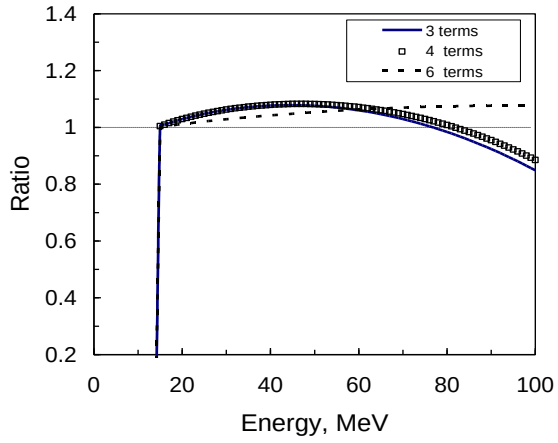


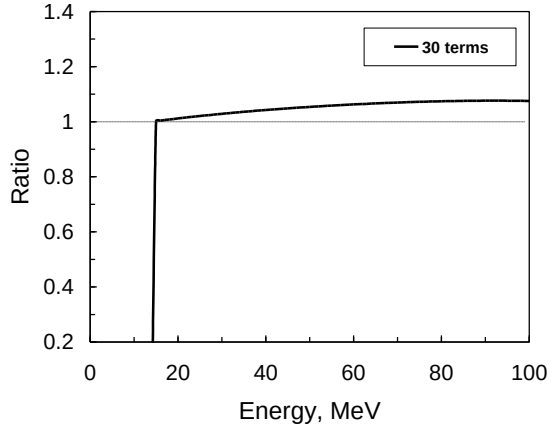
Fig.(1-b)

Fig.(1): The ratio between the results of eq.(11) and Williams' formula with improved pairing effect, eq.(5) for configuration (1,1). The drop at energies less than ~10MeV is due to the effect of the Heaviside function.



a: (p,h)=(2,1), F=38 MeV

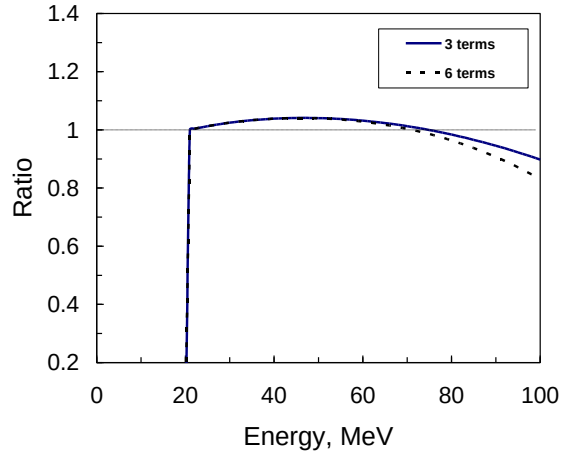
Fig.(2-a)



b: (p,h)=(2,1), F=100 MeV

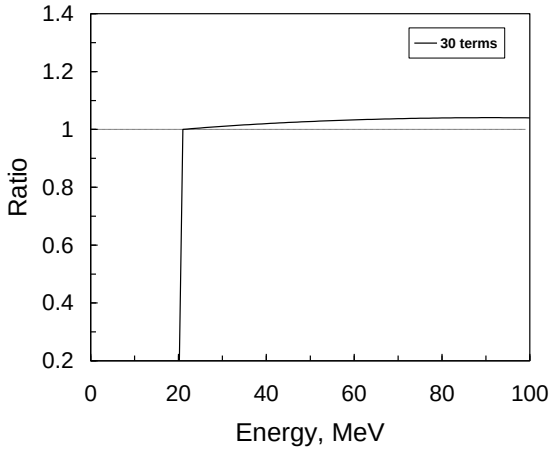
Fig.(2-b)

Fig.(2): The same as Fig.(1) for configuration (2,1).



a: (p,h)=(3,2), F=38 MeV

Fig.(3-a)



b: (p,h)=(3,2), F=100 MeV

Fig.(3-b)

Fig.(3): The same as Fig.(1) for configuration (3,2).

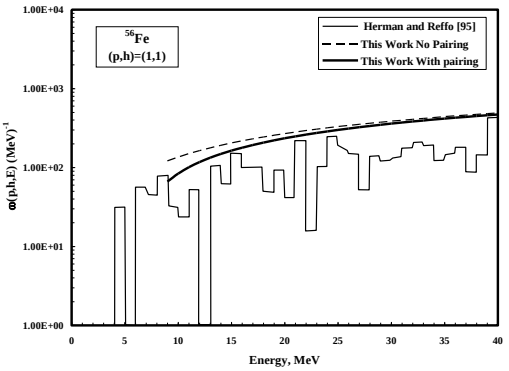


Fig. (4-*a*): State density for 1*p*-1*h* of ^{56}Fe as calculated according to eq.(11) for 50 terms of summation for non-interacting system (thin line) and for a system which includes pairing (thick line), compared with the exact results of Ref.[11] (histogram).

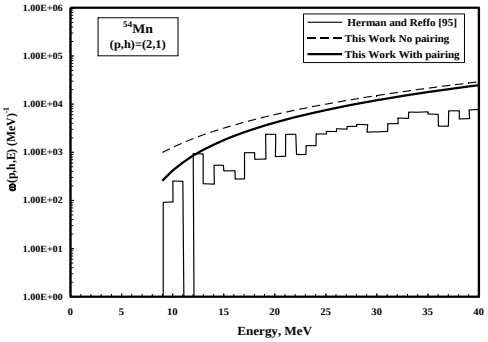


Fig.(4-*b*)

Fig. (4-*b*): The same as Fig.(4-*a*) for 2*p*-1*h* of ^{54}Mn.