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A MULTI-STEP DIRECT MULTI-STEP COMPOUND DESCRIPTION OF FAST PARTICLE INDUCED REACTIONS

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This work was performed under IAEA Research Contract No. 4323/R1/RB

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DESCRIPTION OF RESEARCH, RESULTS OBTAINED AND CONCLUSIONS

Since the last progress report, our research effort has concentrated on the development of computer codes to calculate one and two step continuum DWBA angular distributions and cross sections, on the combinatorial calculation of level and transition strength densities and methods to simplify them and on the development of an exciton-like model from the multi-step direct multi-step compound one. In this project report, each of these will be discussed in turn.

1. One and Two Step DWBA Codes

After the failure of our moment method approximation to the one step DWBA transition strength densities, we retreated to the original collective form factor particle-hole approach of Tamura and Udagawa,[1] modifying our code appropriately. Comparison with the experimental data was somewhat encouraging. At sufficiently high excitation energies, we generally found our calculations to lie slightly below the experimental data, suggesting that the use of the full two-body interaction (and not just the Wigner term) could supply the needed transition strength. However, the deficiencies of a simple particle-hole approach to nuclear excitations-its lack of collectivity and inability to describe the low lying states - led us to pursue another path. We are currently preparing to perform one step calculations along the same lines as those of the Bratislava group,[2] which are based on Soloviev's quasi-particle phonon model of nuclear structure.[3]

To perform two step DWBA calculations, we have adopted the coupled channels code ECIS79 [4] as the cross section module. With a suitable choice of form factors and reduced matrix

elements, one iteration of Raynal's ECIS method yields a one step cross section for the first excited state, a two step cross section for the second excited state and so forth. Although we lost several months before succeeding in entering the form factors and matrix elements in a manner acceptable to the code, this problem has now been solved and a driver code is being developed. The driver will prepare the necessary input to ECIS79 and manipulate its output into the desired one and two-step angular distributions and cross sections.

2. Level and Transition Strength Densities

Although we found the moment method approximation to give a poor description of the energy dependence of particle-hole level densities, its description of the spin dependence is generally quite good. We begin this section by demonstrating how this fact can be used to simplify the combinatorial calculation of level densities.

We recall that the generating function for the density of states

$$Z(\beta,\gamma) = \prod_{i=1}^{N_p} \left(1 + x_p e^{-\beta\varepsilon_i - \gamma m_i}\right) \prod_{j=1}^{N_h} \left(1 + x_h e^{-\beta\varepsilon_j - \gamma m_j}\right)$$

can be expanded in terms of the generating functions of the particle-hole densities

$$Z(\beta,\gamma) = \sum_{p,h} (x_p)^p (x_h)^h Z(ph;\beta\gamma)$$

We can then write the particle-hole state densities and their spin moments as inverse Laplace transforms of derivatives of the generating functions.

$$\omega(p,h,U)\langle M^k\rangle(p,h,U) = \frac{1}{2\pi i}\int d\beta \left(-\frac{\partial}{\partial\gamma}\right)^k Z(ph;\beta\gamma)\Big|_{\gamma=0} e^{\beta U}$$

The derivatives and Laplace transforms are easily performed, yielding combinatorial expressions in terms of the single particle levels rather than the single particle states.

We have

$$\omega(p,h,U) = \sum_{\substack{\{n_\kappa, n_\ell\} \\ \sum_\kappa n_\kappa = p \\ \sum_\ell n_\ell = h}} \delta\left(U - \sum_\kappa n_\kappa \varepsilon_\kappa - \sum_\ell n_\ell \varepsilon_\ell\right) \prod_\kappa \binom{g_\kappa}{n_\kappa} \prod_\ell \binom{g_\ell}{n_\ell}$$

and

$$\omega(p,h,U)\langle m^2\rangle(p,h,U) = \sum_{\substack{\{n_\kappa, n_\ell\} \\ \sum_\kappa n_\kappa = p \\ \sum_\ell n_\ell = h}} \delta\left(U - \sum_\kappa n_\kappa \varepsilon_\kappa - \sum_\ell n_\ell \varepsilon_\ell\right) \prod_\kappa \binom{g_\kappa}{n_\kappa} \prod_\ell \binom{g_\ell}{n_\ell}$$

$$\times \left\{ \sum_\kappa \frac{n_\kappa (g_\kappa - n_\kappa)}{(g_\kappa - 1)} \langle m^2\rangle_\kappa + \sum_\ell \frac{n_\ell (g_\ell - n_\ell)}{(g_\ell - 1)} \langle m^2\rangle_\ell \right\}$$

where n_κ and n_ℓ are the occupation numbers of the single particle/hole levels, g_κ and g_ℓ are their multiplicities and $\langle m^2\rangle_\kappa$, $\langle m^2\rangle_\ell$ are their average squared spin projections.

We note that in a spherical basis, where

$$g_i = 2j_i + 1 \qquad \text{and} \qquad \langle m^2\rangle_i = \frac{j_i(j_i+1)}{3}$$

this method leads to a sizeable reduction in computation time. In an axially symmetric basis, with

$$g_i = 2 \qquad \text{and} \qquad \langle m^2\rangle_i = m_i^2$$

the reduction is much less significant.

We have obtained a similar combinatorial expression for the fourth moment, $\langle m^4\rangle(p,h,U)$, which allows us to calculate the kurtosis,

$$K(p,h,U) = \frac{\langle m^4\rangle}{\langle m^2\rangle^2} - 3$$

With these three quantities, we reconstruct the density of states

as

$$\omega(p,h,U,M) = \frac{\omega(p,h,U)}{\sqrt{2\pi\sigma^2(p,h,U)}}\left(1 + \frac{K(p,h,U)}{4!}\cdot H_4\left(\frac{M}{\sqrt{2\sigma^2(p,h,U)}}\right)\right)\exp\left[\frac{-M^2}{2\sigma^2(p,h,U)}\right]$$

where we have identified the spin cutoff factor, $\sigma^2(p,h,U)$, as

$$\sigma^2(p,h,U) = \langle m^2\rangle(p,h,U)$$

The level density is then determined in the usual manner.

We have found the method to yield excellent results. In Figure 1, we compare the combinatorial level density to the reconstruction in an extreme case of large kurtosis.

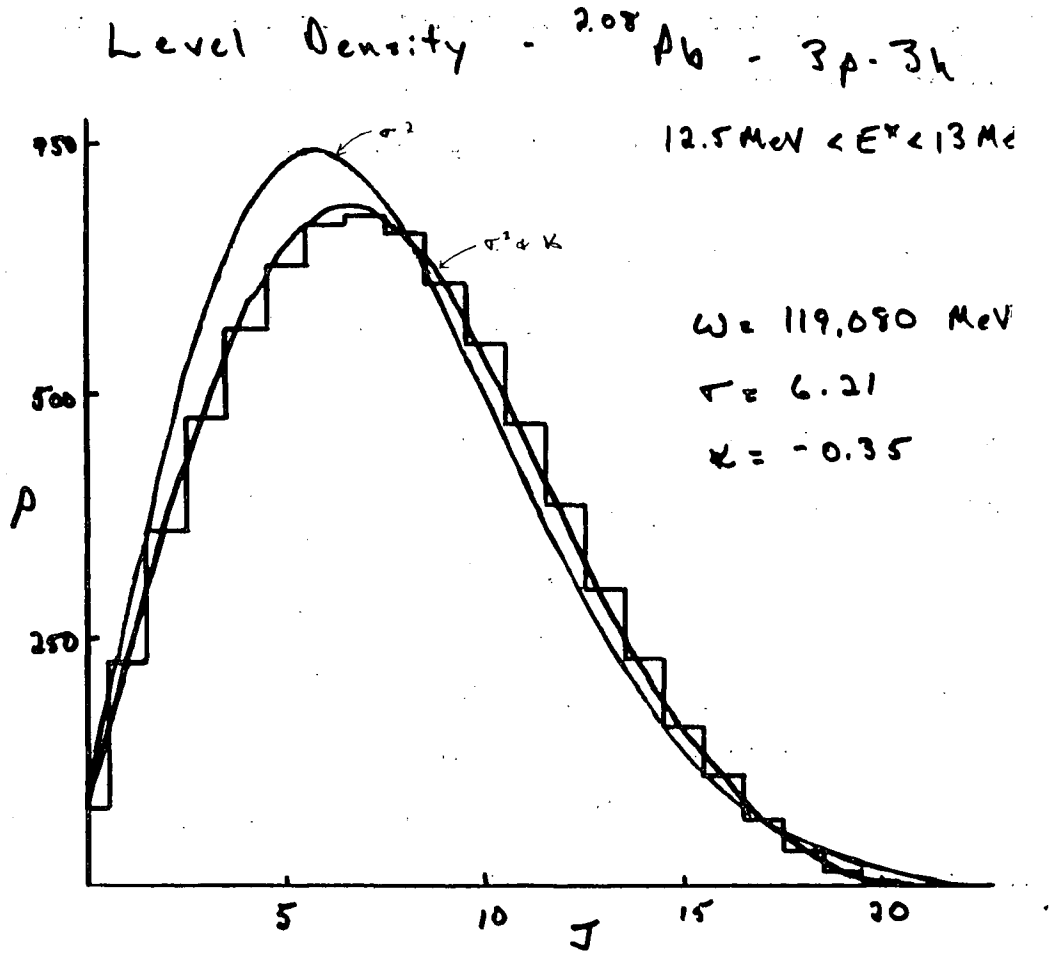

Fig. 1. Spin dependence of the level density as a) calculated combinatorially, b) reconstructed in terms of the spin cutoff parameter and the kurtosis and c) reconstructed in terms of the spin cutoff parameter alone

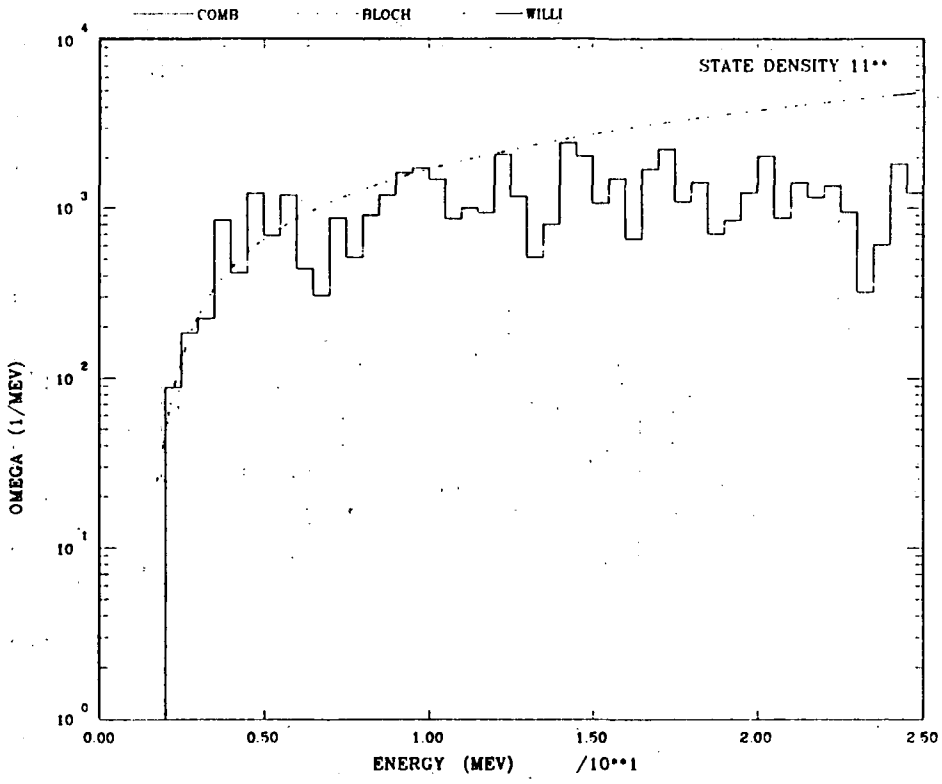

Fig. 2a. The one particle-one hole density of states as obtained combinatorially and as obtained using the Bloch and Williams expressions with adjusted single particle/hole parameters.

For comparison, we also show the reconstructed density obtained when the kurtosis in neglected. Values of the kurtosis as large as that shown are typical near threshold or for low exciton number configurations, as can be seen in Figures 2c and 3c.

We have also used the moment method described here to include spin in the density of states expressions of Bloch [5] and Williams. [6] Using single particle parameters obtained from fits to the single particle spectra used in the combinatorial calculations, we found it possible to obtain a fairly good approximation to the combinatorial results, as can be seen in Figures 2 and 3. However, the Bloch and Williams densities continue to predict poorly the threshold of higher exciton number configurations (see Fig. 3).

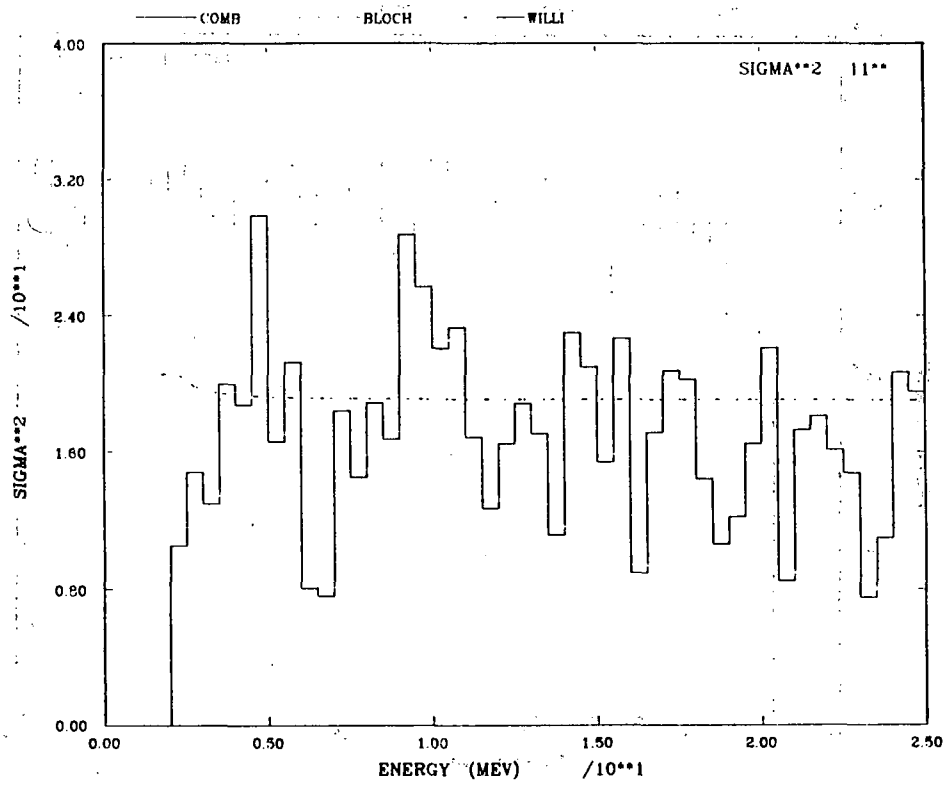

Fig. 2b. The spin cutoff parameters corresponding to the one-particle one-hole densities of Fig. 2a.

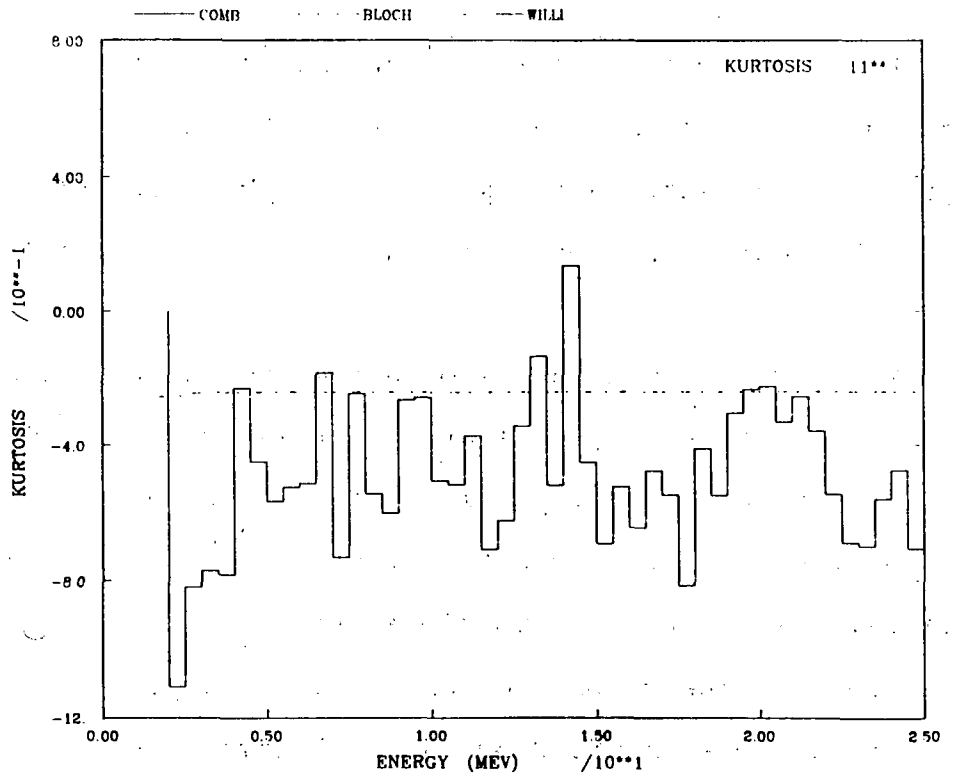

Fig. 2c. The spin kurtoses corresponding to the one-particle one-hole densities of Fig. 2a.

Preparatory studies to the development of a code to calculate the transition strength densities discussed in the last progress report revealed the need for a slight reformulation of the model in order to extract mean field contributions contained in the densities. This was performed by redefining the creation/annihilation operators as

$$a_\nu^\dagger \Rightarrow a_\nu^\dagger \qquad a_\nu \Rightarrow a_\nu \qquad \text{for particle states}$$

and

$$a_\nu^\dagger \Rightarrow b_\nu \qquad a_\nu \Rightarrow b_\nu^\dagger \qquad \text{for hole states}$$

The unnormalized single particle density operator could then be rewritten as

$$\begin{aligned}
Z(\rho_1, n_1, \beta, \chi; \rho n \rho' \nu') = {} & \prod_{\tau} (1 + x_{\rho\tau} x'_{\rho'\tau}) \prod_{\omega} (1 + x_{n\omega} x'_{n'\omega}) \\
& * \Bigg\{ \tfrac{1}{2} \sum_{\substack{\mu\nu\sigma\tau\rho \\ \rho\neq n}} |V_{\mu\nu\rho\tau}|^2 \frac{x_{\rho\mu}}{1 + x_{\rho\mu} x'_{\rho\mu}} \cdot \frac{x_{\rho\nu}}{1 + x_{\rho\nu} x'_{\rho\nu}} \cdot \frac{x_{\rho\tau}}{1 + x_{\rho\tau} x'_{\rho\tau}} \cdot \frac{x_{n\rho}}{1 + x_{n\rho} x'_{n\rho}} \\
& + \tfrac{1}{2} \sum_{\substack{\mu\nu\rho\tau \\ \nu\neq\rho\neq\tau\neq n}} |V_{\mu\nu\rho\tau}|^2 \frac{x_{\rho\mu}}{1 + x_{\rho\mu} x'_{\rho\mu}} \cdot \frac{x'_{\rho\nu}}{1 + x_{\mu\nu} x'_{\mu\nu}} \cdot \frac{x_{n\tau}}{1 + x_{n\tau} x'_{n\tau}} \cdot \frac{x_{n\rho}}{1 + x_{n\rho} x'_{n\rho}} \\
& + \sum_{\substack{\mu\sigma\tau\rho \\ \rho\neq n}} |V_{\mu\sigma\rho\tau}|^2 \frac{x_{\rho\mu}}{1 + x_{\rho\mu} x'_{\rho\mu}} \cdot \frac{x_{\rho\tau} x'_{\rho\tau}}{1 + x_{\rho\tau} x'_{\rho\tau}} \cdot \frac{x_{n\rho}}{1 + x_{n\rho} x'_{n\rho}} \\
& + \sum_{\substack{\mu\rho \\ \rho\neq\tau\neq n}} |V_{\mu\tau\rho\tau}|^2 \frac{x_{\rho\mu}}{1 + x_{\rho\mu} x'_{\rho\mu}} \cdot \frac{x_{n\tau} x'_{n\tau}}{1 + x_{n\tau} x'_{n\tau}} \cdot \frac{x_{n\rho}}{1 + x_{n\rho} x'_{n\rho}} \Bigg\}
\end{aligned}$$

where the last term is different from that given in the last progress report. The transition state density obtained after Laplace transforming and restricting to the energy conserving transitions is identical to that given previously. In this case,

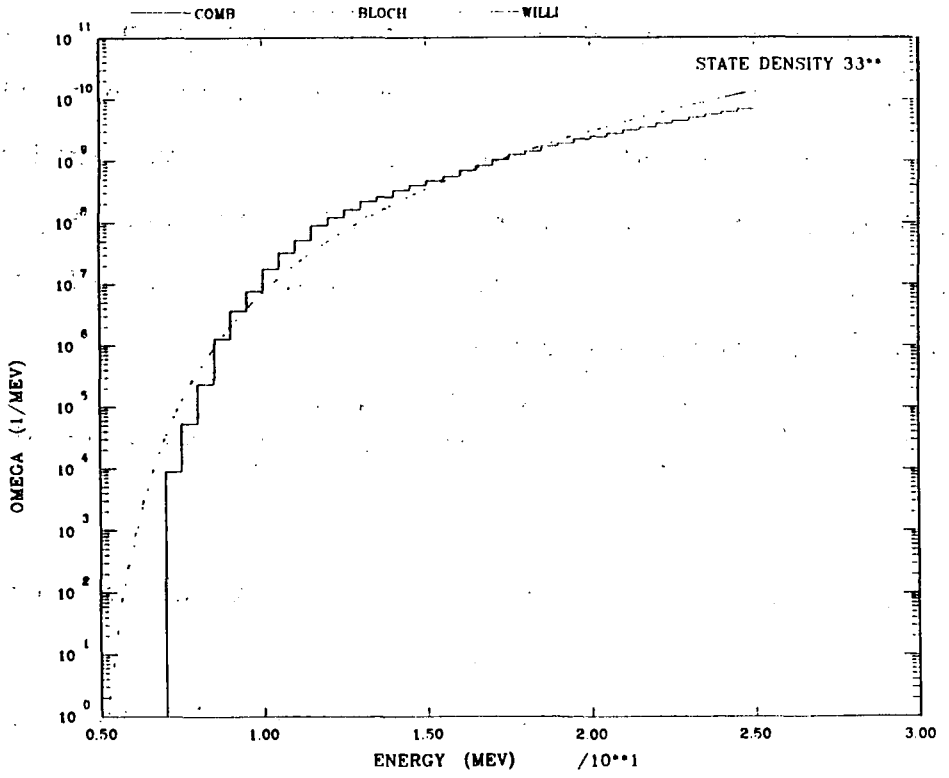

Fig. 3a. The three-particle three-hole density of states as obtained combinatorially and as obtained using the Bloch and Williams expressions with adjusted single particle/hole parameters.

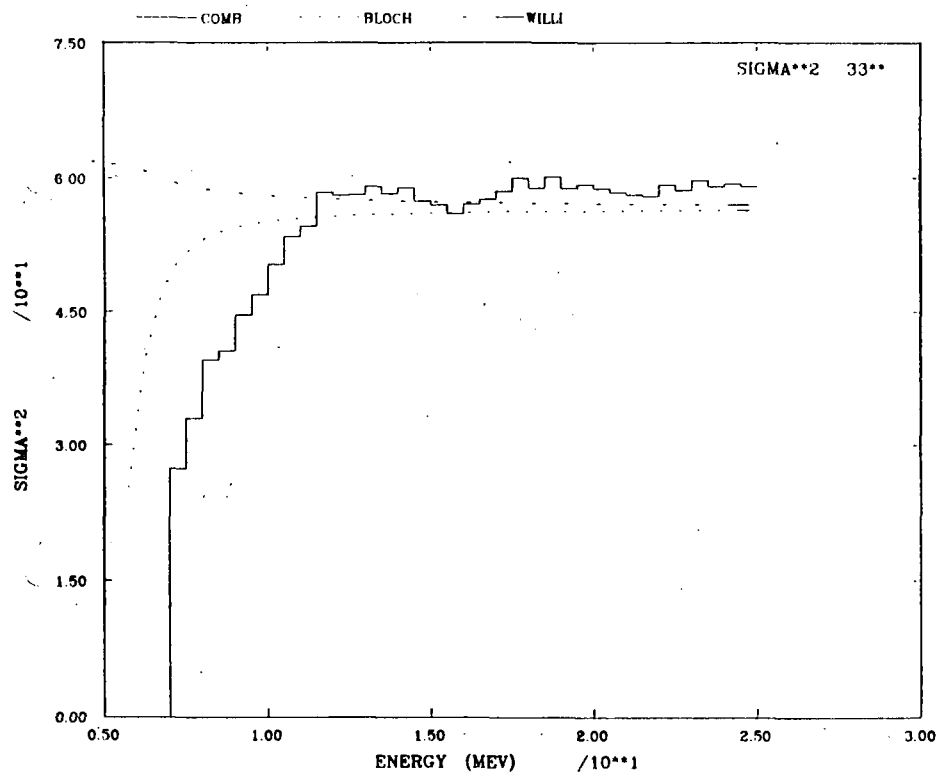

Fig. 3b. The spin cutoff parameters corresponding to the three-particle theree-hole densities of Fig. 3a.

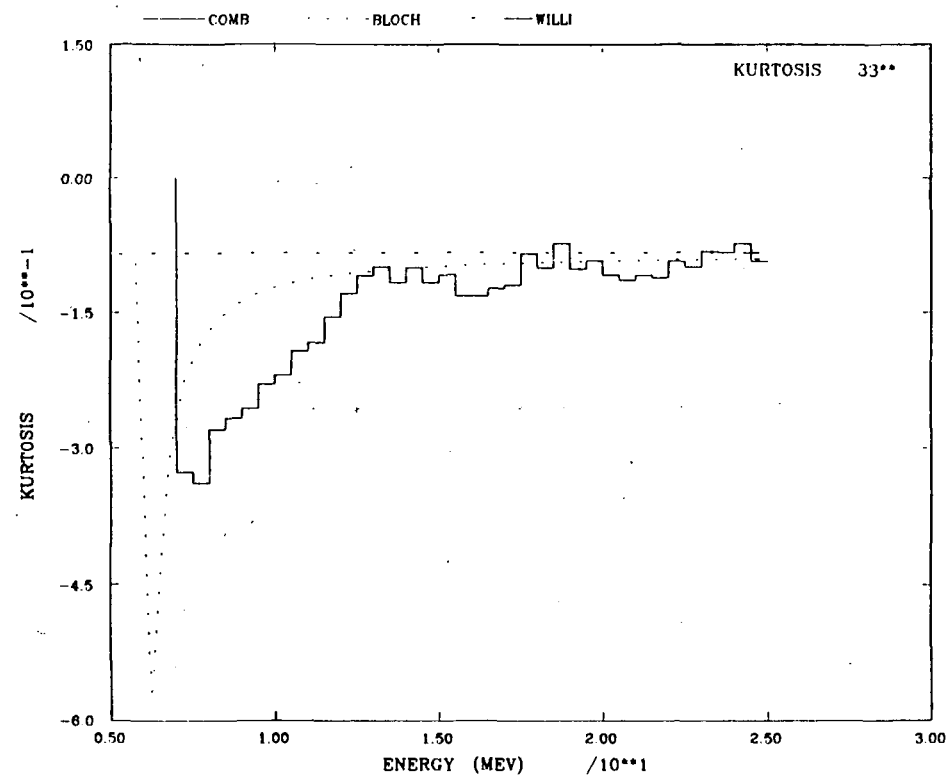

Fig. 3c. The spin kurtoses corresponding to the three-particle three-hole densities of Fig. 3a.

the modified term only contributes to nonconserving transitions. However, modifications do occur in the energy conserving transition rates which leave the exciton number unchanged.

We have developed a code to calculate combinatorially the transition strength densities which increase the number of particles and holes by one each. We have used a neutron/proton formalism rather than an isospin one and have begun by attempting to calculate the transition state density, $\omega_{+}(p,h,U,M)$. The matrix elements of this quantity are

$$\text{"}V_{+\alpha\beta<\delta}\text{"} = \sum_{JM} \langle j_\alpha j_\beta m_\alpha m_\beta | JM \rangle \langle JM j_\delta -m_\delta | j_\gamma m_\gamma \rangle \sqrt{(1+(-1)^J\delta_{\alpha\beta})(1+(-1)^J\delta_{\gamma\delta})} \times \frac{(1+\pi_\alpha\pi_\beta\pi_\gamma\pi_\delta)}{2}$$

which ensure the conservation of angular momentum and parity. Neutron and proton number conservation is taken into account explicitly in the code.

The matrix elements of the transition state density differ from those of a general interaction only in the reduced matrix elements which enter the sum over J. In order to eventually calculate average matrix elements, $\overline{|V|^2}$, it will be necessary to have at hand the density $\omega_\pi(p,h,U,M)$ as the transition strength density which we have defined corresponds to the exciton model quantity $\overline{|V|^2}\,\omega_\pi(p,h,U,M)\,\omega(p,h,U,M)$.

As stated above, we have developed the code necessary to calculate the transition rates, $\lambda_\pi(p,h,U,M)$, and have begun by attempting to calculate the transition state densities, $\omega_\pi(p,h,U,M)$. We have discovered, however, that the computation time necessary is too great to permit any but the simplest calculations. As an example, our calculation of the near energy conserving transitions (1100) $\rightarrow$ (2200), (1111), using an average of ten single particle orbitals for the neutron proton particle/hole levels, requires about 5000 s. on our CYBER 750. We thus need a faster method of counting, the obvious one being the reduction from state to level counting described earlier.

We have performed the algebra necessary to program the reduced level counting calculation. Although much more tedious than the level density example discussed earlier, the calculation is straight forward but for one point. The single complication involves Pauli correction terms which enter as sums over squared matrix elements in which one of the initial single particle states is also a final one.

$$\sum_{m's} |V_{\alpha\beta\alpha\gamma}|^2 \quad , \quad \sum_{m's} m_\alpha^2 |V_{\alpha\beta\alpha\gamma}|^2 \quad , \quad \sum_{m's} m_\alpha m_\beta |V_{\alpha\beta\alpha\gamma}|^2 \quad , \text{ etc.}$$

We have not yet succeeded in analytically reducing these sums to sums over reduced matrix elements. For the calculation of λ_π and ω_π, this difficulty is not important as, in this case, the correction terms do not contribute to the near energy conserving

transition rates. These terms do contribute, however, to the energy conserving transitions in λ_0 and ω_0. Calculation of the latter will thus require further work. At the moment, we are developing the code necessary to calculate the near energy conserving contributions to λ_+ and ω_+.

Finally, we confess that we have made no progress in the collaboration with Dr. Reffo of ENEA on the modified exciton model. The responsibility for this is entirely ours, as we have not yet supplied him with the transition state densities necessary for performing calculations within the modified model. However, as we have made progress in the calculation of transition strength densities, we believe that we are now at a point where we can provide the necessary modified densities. After the CRP meeting, this researcher will spend ten days with Dr. Reffo in Bologna with this intention.

3. Development of an Exciton-Like Model

Our attempt to derive an exciton-like model from the multi-step direct multi-step compound one is based on the following objection raised by Blann and Reffo: (7) The distinction between bound compound nucleus states and resonant states is an arbitrary model dependent one. It is lost after introducing the residual interaction. All states then become resonant states.

It thus seemed reasonable to attempt to include the resonant continuum contribution with the bound compound nucleus states to obtain an exciton-like model. An obvious attraction of such a model is that the resonant terms would permit contributions of the form

$$\overline{T^{J\pi}\ T^{J'\pi'}}$$

which could yield angular distributions asymmetric about 90.

However, our simple minded attempt to derive such a model encountered serious difficulties.

The decomposition of the Green's function into a sum of bound state terms, resonant terms and a background,

$$G = \sum_b \frac{|b\rangle\langle b|}{E-\mathcal{E}_b} + \sum_r \frac{|r\rangle\langle\tilde{r}|}{E-\mathcal{E}_r - \frac{\Gamma_r}{2}} + G_B$$

as well as methods for the use of this expansion in calculating matrix elements and perturbation series have been well documented.(8) If we expand the continuum part of the Green's function into a resonant sum and background,

$$G_c = \sum_{r_c} |r_c\rangle D^\circ_{r_c}(E) \langle\tilde{r}_c| + G_{cB}$$

and apply a perturbing potential, U, (small enough to not create new resonances), we can resum to write the perturbed Green's function as

$$G = \sum_{r's'} |r'\rangle D_{r's'}(E) \langle\tilde{s}'| + G_B$$

where

$$G_B = G_{cB} + G_{cB} U G_B$$

$$|s'\rangle = |s_0\rangle + G_{cB} U |s'\rangle$$

$$\langle\tilde{s}'| = |s\rangle^T$$

and

$$D = D_c + D_c \langle\tilde{s}_c|U|s\rangle D$$

As D is complex but symmetric, it can be diagonalized by a complex orthogonal transformation, yielding an expansion similar to the original one for G_c

$$G = \sum_r |r\rangle D_r(E) \langle\tilde{r}| + G_B$$

However, to calculate the average Green's function, we must also calculate the optical potential. Definition of the latter is complicated by terms such as

$$\overline{V G_{cB} V G V |r_0\rangle D^\circ \langle r_0| V}$$

We would like these terms to average to zero but our statistical hypotheses do not require this. If we assume that the above terms are zero, we can define the optical potential in a natural manner,

$$U = \overline{V G_0 V} + \overline{V |r\rangle D_r \langle \tilde{r}| V} + \overline{V |s\rangle D_s \langle s| V}$$

and calculate the average Green's functions as above.

This, however, is not sufficient to eliminate our problems. When we turn to the calculation of cross sections, we now encounter contributions such as

$$\overline{\langle \tilde{\psi}_f^- | V | s\rangle D_s \langle \tilde{s}| V |\psi_i^+\rangle \langle \tilde{\psi}_i^+ | V | r\rangle D_r \langle \tilde{r}| V |\psi_f^-\rangle}$$

which require further statistical hypotheses for their evaluation.

What we have reencountered here are the same old problems which plagued the derivation from more fundamental hypotheses, of the Hauser-Feshbach cross section. One of the advantages of the statistical ensemble of matrix elements is its ability to circumvent these difficulties. That we have reencountered then here suggests that we have not chosen our statistical hypotheses wisely. Although we have not yet succeeded in obtaining statistical hypotheses which are reasonable within this new context, we have not yet abandoned hope of doing so.

Beside the chief investigator, several other members of the Theoretical Nuclear Physics Group at IEAv have taken an active part in this research project. They are T. Frederico, R. Mastroleo, A.C. Merchant and R.A. Rego.

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