Toward an Improved Multi-step Direct Multi-step Compound Reaction Model

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ABSTRACT

A multi-step direct multi-step compound model free of the criticisms suffered by that of Feshbach, Kerman and Koonin is defined in terms of the statistical hypotheses made about the interaction matrix elements. The model is briefly described and discussed. Also described are our unsuccessful attempts to parametrize the level and transition strength densities needed in pre-equilibrium calculations in terms of their moments.

Abstract

In the last decade, an intense effort has been made to obtain a consistent quantum mechanical description of preequilibrium reactions. This has been motivated in great part by the growing body of experimental cross section data, differential in energy and angle, which has been obtained over the same period. The early pre-equilibrium models (1), using emission rates based on the Weisskopf model, were able to describe the energy spectra observed but were not prepared to deal with their forward peaked angular distributions. More recent versions of one of these , the exciton model, have succeeded in describing well the experimental angular distributions (2,3). The pre-equilibrium and Hauser-Feshbach equlibrium compound emission have also been unified within this model through the inclusion of the effects of angular momentum in the emission rates (3). Despite their successes however, these models remain semiclassical ones based on hypotheses which are intuitively reasonable but difficult to evaluate or improve.

The first major step towards a quantum mechanical model of pre-equilibrium reactions was taken by Agassi, Weidenmuller and Mantzouranis (AWM) (4). Using well defined hypotheses on the statistical nature of the matrix elements coupling configurations, they obtained a unified model of pre-equilibrium and equilibrium reactions. Their hypotheses however yield angular distributions symmetric about 90° and can only describe the multi-step compound part of the reaction.

A quantum mechanical model providing the observed anisotropy was developed shortly thereafter by Tamura and Udagawa (TU) (5,6). Applying statistical hypotheses similar to those of AWM to the states excited in direct reactions, they obtained a good description of the multi-step direct component of the pre-equilibrium reaction.

One of the first works to attempt to unite the direct and compound processes in one formalism was that of Feshbach, Kerman and Koonin (FKK) (7). Although their model has been used successfully to describe a large body of experimental data (8), it has also justly suffered many criticisms. Their model of the multi-step compound component makes use of a "never come back" hypothesis which prohibits the unified description of the pre-equilibrium and equilibrium contributions. The latter must be included by hand. Several authors (9,10) have noted that the multi-step direct component cannot be written in terms of DWBA matrix elements as done by FKK. Feshbach claims to have shown that this can in fact be done (11). The fact that all successful comparisons with experimental data have been made using DWBA matrix elements.

ments certainly provides strong motivation for such an attempt. However, Udagawa, Low and Tamura have pointed out other approximations in the model's multi-step direct component which would still leave its accuracy in doubt (10).

Here, we will draw on the works of the Heidelberg (4,12) and University of Texas (5,6) groups to show how the FKK model can be modified so as to satisfy the criticisms above. We will then discuss our not so successful attempts at parametrizing the level densities and transition strength densities necessary for its use.

We can improve the multi-step direct multi-step compound model of .FKK by modifying the statistical hypotheses on which it is based. We will use hypotheses consistent with those of AWM and of TU. The multi-step direct reaction model of deeply inelastic heavy ion collisions developed by Agassi, Ko and Weidenmuller (12) serves as a useful guide in restating the statistical hypotheses used by TU in terms of the interaction matrix elements. In particular, we note their emphasis of the requirement that all statistical hypotheses be made in terms of reduced matrix elements in order to conserve angular momentum.

As in the FKK model, we divide the space of states to be considered into a part in which all particles are in bound single particle states and another in which one and only one of these particles is in a continuum state. We label these by C (for compound) and D (for direct) respectively. We take as statistical hypotheses on the reduced matrix elements the following:

- For the bound state to bound state interaction, V.V.

- For the continuum to bound state interaction, V.V.

(c, I, (s, e), || V== || c| I(s) (e)) (c, I, (s, e,)), || V == || c, I, (s, e) ()

with all other possible pairs averaging to zero. In summary, we suppose that the average coupling is non-zero only for pairs of interactions that couple the same continuum channels and/or bound states.

Let us now briefly discuss the pre-equilibrium model which we obtain using these hypotheses. We start with the Born expansion of the Lippmann-Schwinger equation for the Green's functions.

$$\begin{pmatrix}
G_{cc}^{\pm} & G_{cs}^{\pm} \\
G_{oc}^{\pm} & G_{os}^{\pm}
\end{pmatrix} = \begin{pmatrix}
G_{cc}^{\pm} & O \\
C & G_{os}^{\pm}
\end{pmatrix} + \begin{pmatrix}
G_{cc}^{\pm} & O \\
C & G_{cs}^{\pm}
\end{pmatrix} \begin{pmatrix}
V_{cc} & V_{co} \\
V_{dc} & V_{do}
\end{pmatrix} \begin{pmatrix}
G_{cc}^{\pm} & O \\
V_{dc} & V_{co}
\end{pmatrix} \begin{pmatrix}
G_{cc}^{\pm} & O \\
V_{dc} & V_{co}
\end{pmatrix} \begin{pmatrix}
G_{cc}^{\pm} & O \\
C & G_{cs}^{\pm}
\end{pmatrix} \begin{pmatrix}
V_{cc} & V_{co} \\
C & G_{cs}^{\pm}
\end{pmatrix} \begin{pmatrix}
G_{cc}^{\pm} & O \\
V_{dc} & V_{ds}
\end{pmatrix} \begin{pmatrix}
G_{cc}^{\pm} & O \\
C & G_{cs}^{\pm}
\end{pmatrix}$$

Since the terms in the expansion which couple continuum to bound states involve an odd\number of like interactions, they will be zero on the average\.

We obtain equations for the average continuum and bound state components of the Green's function by keeping the lowest order terms in the asymptotic expansion of their average as described in the work of the Heidelberg group. We will use their notation of a bar joining two matrix elements to denote the average.

For the average continuum state Green's function, we obtain

where the optical potential, given by

depends again on the average Green's functions. This optical potential is nonlocal and generally quite complicated, depending on the energy, excitation energy, angular momenta and configuration. To our knowledge, only its ground state elements have been studied (13).

We obtain a similar Lippmann-Schwinger equation for the average continuum wavefunction

which we can write in differential form as

where \mathcal{E}_{\bullet} is the channel excitation energy and $V_{e \, b}$ is the initial distorting potential which we take to be real.

The average bound state Green's function is determined by the equation

where the shift factor and escape width are determined by

while the spreading width is given by

To calculate average cross sections, we first express them in terms of the Born series expansion of the transition matrix.

Beside the average shape elastic cross section, we find in general contributions from multi-step direct and multi-step compound processes.

The average shape elastic cross section is determined by the average transition matrix.

The multi-step direct contribution can be written as

The first term in this expansion is the one-step DNBA while the second is the two-step process (neglecting any nonorthogonality terms) so that the two together reproduce the model of TU. There are, of course, higher order terms that could be included although care should be taken with nonorthogonaltity terms that also might be necessary.

In the multi-step compound contribution to the cross section, the formation of the compound nucleus and the posterior particle emission are described by the factors

while the transitions between classes of states in the compound nucleus are determined by the matrix $\widetilde{\mathcal{N}}$ where

Here, the external mixing matrix is given by

We note that the multi-step compound component depends on the continuum-continuum interaction which modifies the formation/emission factors, the external transition matrix and the escape widths. It is easily seen however that these modifications do not effect the symmetry about 90° of the compound angular distribution. This symmetry is a result of the statistical hypothesis on the continuum to bound state interaction which requires that partial waves differing in total angular momentum or parity contribute incoherently to the cross section.

In the limit in which the continuum to continuum interaction goes to zero, the multi-step compound component almost reduces to the ANM expression for the cross section. The only difference is the elastic enhancement factor which is missing here. This reflects a deficiency in our statistical hypotheses which do not yet contain all of the symmetry to be expected. We are studying the extension of the statistical hypotheses necessary to include this symmetry, although we expect the resulting modifications to have little effect at the energies at which pre-equilibrium reactions are important.

The statistical hypotheses we have given thus define a preequilibrium model which yields cross sections having a multi-step direct component equal to that of TU and a unified multi-step compound component similar to the one obtained by AWM. The model also specifies the average optical potentials, Green's functions and wave functions requiring only the average interaction matrix elements as input parameters.

We admit that the model is exceedingly complex, even more so than the original multi-step model of PRK. Given present computational possibilities, it will be necessary to approximate it in some manner before it can be usefully applied. As it stands however, it could prove useful as a context within which we can better understand and evaluate the approximations and models which we use.

3.0 A MOMENT METHOD APPROXIMATION OF LEVEL AND TRANSITION STRENGTH DENSITIES

The most important quantities which enter pre-equlibrium calculations are the average interacti matrix elements and the level densities. An alternative description uses the appropriate product of the two, the density of interaction matrix elements, which we will call the transition strength density.

Combinatorial methods can calculate densities to within the accuracy of the set of single particle states and the residual interaction used. Such calculations become prohibitive for large energies and/or complex configurations however. We have thus studied the possibility of using a simple moment method to reproduce the average trend of combinatorial calculations.

3.1 LEVEL DENSITIES

We will illustrate the moment method calculation of level densities with a simple case involving one type of particle and hole. We will assume that we have N particle states and N hole states and will write their energies as positive ones with respect to the Fermi energy.

We first define an appropriately unnormalized one-body density operator for the system.

$$F_{c}(\beta, x) = \frac{N_{t}}{1} \left(\alpha_{t}^{2} \alpha_{t}^{2} + \alpha_{t}^{2} \alpha_{t}^{2} x_{p} e^{\beta \epsilon_{t}^{2} - x_{m}} \right)$$

$$\times \frac{N_{t}}{1} \left(\alpha_{1}^{2} \alpha_{1} + \alpha_{3}^{2} \alpha_{1}^{2} x_{m}^{2} e^{\beta \epsilon_{1}^{2} - x_{m}} \right)$$

$$1=1$$

We note that when $\beta \to \infty$, for fixed γ , this becomes the density operator for the independent particle ground state. We

obtain the partition function by taking the trace of this operator.

A power expansion in the factors x_n and x_n , a device first used by Bloch (14), then permits us to identify the partition function of each configuration.

The density of states could be obtained by performing the inverse Laplace transform of the partition function.

In terms of a configuration's partition function, we can calculate its moments using

where

It turns out, however, to be easier to calculate the moments for all configurations at the same time using

For example, we have

$$\frac{Z(\beta,\gamma)}{\beta=\gamma=0} = \frac{(1+\chi_{\beta})^{N_{\beta}}(1+\chi_{\gamma})^{N_{\beta}}}{(1+\chi_{\gamma})^{N_{\beta}}(\chi_{\gamma})^{N_{\beta}}(\chi_{\gamma})^{N_{\beta}}(\chi_{\gamma})^{N_{\beta}}(\chi_{\gamma})^{N_{\beta}}}$$

$$= \sum_{\beta,\gamma} (\chi_{\gamma})^{\beta}(\chi_{\gamma})^{\gamma} N_{\beta}$$

$$= \sum_{\beta,\gamma} (\chi_{\gamma})^{\beta}(\chi_{\gamma})^{\gamma} N_{\beta}$$

so that the number of states with p particles and h holes is

Likewise,

so that the centroid in energy of the p particle h hole configuration is

where $\langle \xi \rangle_{i}$ and $\langle \xi \rangle_{i}$ are the average energies of the single particle and single hole states, respectively.

Other low moments of interest are the variance in energy

$$\langle U^2 \rangle_{p_N} - \langle U \rangle_{p_N}^2 = \frac{p(N_1 - p)}{N_0 - 1} \left(\langle \varepsilon^2 \rangle_p - \langle \varepsilon \rangle_p^2 \right) + \frac{h(N_0 - h)}{N_0 - 1} \left(\langle \varepsilon^2 \rangle_n - \langle \varepsilon \rangle_n^2 \right)$$

and the variance of the spin projection, the spin cutoff factor,

The reconstruction of the density is most easily performed in terms of the cumulants rather than the moments. These are defined as

and are simple polynomial functions of the moments.

We calculate the cumulants through sixth order in A and Y and approximate the configuration partition function as

We can then write the density of states as a derivative expansion about a Gaussian,

whore

$$\widetilde{K}_{PN} = \begin{pmatrix} (K'')^{PN} & (K^{02})^{PN} \\ (K^{20})^{PN} & (K'')^{N} \end{pmatrix} = \begin{pmatrix} \langle 0M \rangle^{N} - \langle 0 \rangle^{PN} & \langle 0M \rangle^{N} - \langle 0 \rangle^{N} \langle 0M \rangle^{N} \\ \langle 0M \rangle^{N} - \langle 0 \rangle^{N} \langle 0M \rangle^{N} & \langle 0M \rangle^{N} - \langle 0 \rangle^{N} \langle 0M \rangle^{N} \end{pmatrix}$$

We expand the exponential derivative keeping terms through sixth order. Finally, we obtain the level density using Bethe's difference formula.

In the calculations performed, we have distinguished between protons and neutrons permitting independent particle and hole states for each. As the cumulants of the state densities for noninteracting particles are additive, the generalization to this case is trivial.

We have compared the moment method densities with combinatorial ones obtained using the same sets of single particle states. Although protons and neutrons were distinguished in the calculations, this distinction was not investigated. We have compared densities summed over all configurations with the same number of particles and holes.

In Figures 1 and 2, we show two examples of the relatively good agreement obtained for the density of four particle two hole levels in "1 Zr. Similar results were obtained for other values of the angular momentum. We note however that the oscillations in the combinatorial densities due to shell effects are not reproduced by the moment method results.

We would expect the shell effects to become less important for more complex configurations. Indeed, as we can see in Figure 3, the combinatorial total level density of five particle three hole states in Y1Zr is much smoother than the four particle two hole one. However, we encounter here the principal drawback of the moment method. It can describe the energy dependence of the density only within the first few standard deviations of the centroid. Although the density falls about four orders of magnitude from its centroid value in this range, we can see from the figure that the error is still extremely large. Similar results, using up to 18 moments, have been reported recently by Jacquemin and Rataria (15). We thus cannot hope to solve the problem by simply extending the expansion to include higher moments.

3.2 TRANSITION STRENGTH DENSITIES

We have also applied the moment method to the calculation of the average spectroscopic amplitudes to be used in the DWBA calculation of one-step direct reactions. Following TU we assume a Wigner form for the residual interaction and write its reduced matrix elements as

We use a single form factor f(r), proportional to the radial derivative of the optical potential, for all angular momentum transfers and all excitation energies.

As we will look only at the one-step excitation from the ground state, we write the spectroscopic amplitudes as

To be consistent with the statistical hypotheses discussed earlier, we must have

The total one-step angular distribution will then take the form

$$\frac{d\tau''(E_{x}, \Sigma)dE_{x}}{d\Omega} = \sum_{k} \beta_{k}^{2} \left(\frac{d^{k}}{d\lambda}\right)^{2} \frac{d\tau_{out}(E_{x}, \Sigma)}{d\Omega}$$

As a single application of the residual interaction will only excite one particle one hole states,

the necessary squared spectroscopic amplitudes are simply

In general, to calculate moments of the distribution of spectroscopic amplitudes, we would start with a partition function

where F_c is the one body density operator described earlier and & is the appropriate transition operator. The function & now has two pairs of arguments, referring to the initial and final states respectively. For arbitrary configurations, the

calculation of such a partition function is an extremely difficult problem. Fortunately, it simplifies considerably in the case of interest here. Because we specify the angular momentum transferred and the initial state, the number of arguments reduces to one.

We can then calculate the moments as before.

We have used the moment method to calculate the density of spectroscopic amplitudes in Ni. The same set of single particle states, shown in Figure 4, were used for protons and neutrons. The resulting one particle one hole spectrum and the allowed angular momentum transfers are also shown there. We note that, because of the Wigner form assumed for the residual interaction, only natural parity transitions are possible.

We have used the resulting spectroscopic densities to calculate the energy-angular distributions for 5 Fe at 14.6 and 25.7 MeV. We introduced two free parameters, β_{+}^{3} and β_{-}^{3} , which multiplied the contributions to the angular distribution of even and odd transferred angular momenta, respectively. These were adjusted to obtain the best fit to the data at 25.7 MeV (16). The strength density so obtained (β_{\pm}^{3} times the spectroscopic density) can be seen in Figure 5.

The fit to the 25.7 MeV data can be seen in Figure 6. In Figure 7, we show the results obtained at 14.7 MeV, where the same parameters, β_+^2 and β_-^2 , have been used but an isotropic Hauser-Feshbach component has been added at the higher energy losses. We see that the resulting fits are not at all good. Comparing the results at the two energies however, we find the poorness of fit, at a given excitation energy, to be about the same for the two. A look at the combinatorial spectroscopic distribution suggests that it could better reproduce the experimental cross sections. The moment method has failed here because it cannot reproduce the structure of the combinatorial density but only its global trend.

We thus conclude that the moment method will not provide an immediate solution to the problem of precision in level and transition strength densities. The combinatorial method could provide the necessary precision for simple configurations or at low energy. In some cases, such as that of the one particle one hole transition strength, even more precise methods could be warranted (6,18). Such methods cannot offer a complete solution to the problem however. They are too

time consuming to be practical for the calculation of densities involving complex configurations. We believe that the moment method could still provide a partial solution in these cases (19). It will be necessary though to supplement it with other approximate expressions in order to describe these densities over the entire energy range.

4.0 CONCLUSIONS

We have given statistical hypotheses on the interaction matrix elements which define a multi-step direct multi-step compound pre-equilibrium model. The model specifies the average optical potentials, Green's functions, wave functions and cross sections in terms of the average matrix elements. The resulting cross sections have the multi-step direct component of TU and a multi-step compound component similar to that of AWM. As it stands, the model is too complex to be useful for practical calculations but it can furnish a context within which more approximate models could be understood and evaluated.

The most important quantities which enter pre-equilibrium calculations are the average matrix elements and the level densities or, alternatively, the transition strength densities. We have studied the possibility of using the moment method as a means of efficiently parametrizing these and found it to be generally unsuccessful. The method does not succeed in reproducing the structure observed in densities involving simple configurations and, for more complex ones, can describe the densities only near their energy centroids. We have not completely discarded the method however but continue to look for some combination of methods (combinatorial, moment and others) which could provide a good approximation to the necessary densities.

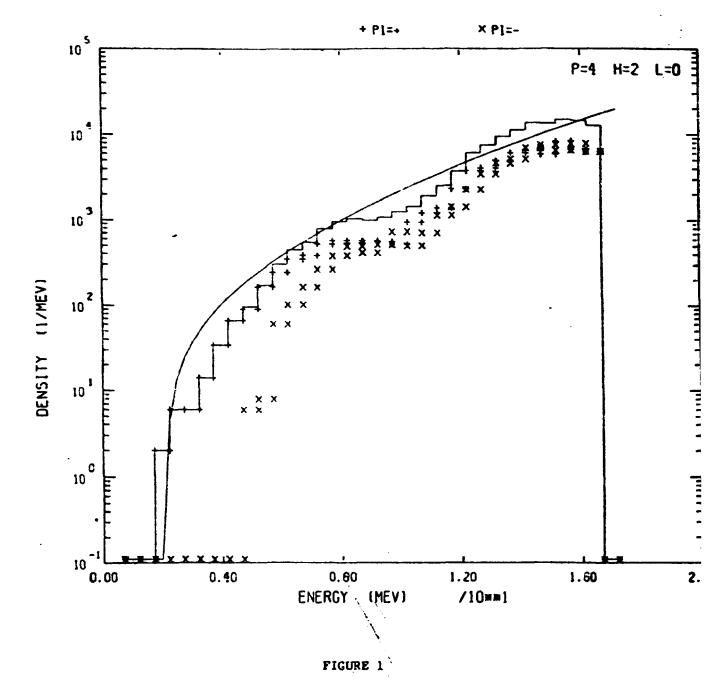
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6.0 FIGURE CAPTIONS

- Fig. 1 Comparison of the density of 4 particle 2 hole levels of spin 0 in Tr calculated using the combinatorial method (histogram) and the moment method (smooth curve).
- Fig. 2 Comparison of the density of 4 particle 2 hole levels of spin 10 in 92 Zr calculated using the combinatorial method (histogram) and the moment method (smooth curve).
- Fig. 3 Comparison of the density of all 5 particle 3 hole levels in ¹²Zr calculated using the combinatorial method (histogram) and the moment method (smooth curve).
- Fig. 4 Neutron (and proton) single particle levels.used for ⁵¹Ni, the resulting 1 particle 1 hole spectrum and possible transferred angular momenta.
- Fig. 5 Transition strength densities obtained for ⁵⁶Fe based on the moment method spectroscopic amplitude distribution of ⁶⁶Ni.
- Fig. 6 Comparison of the calculated one-step DWBA angular distributions to the experimental data at 25.7 MeV (ref. 16).
- Fig. 7 Comparison of the calculated one-step DWBA angular distributions to the experimental data at 14.6 MeV (ref. 17).



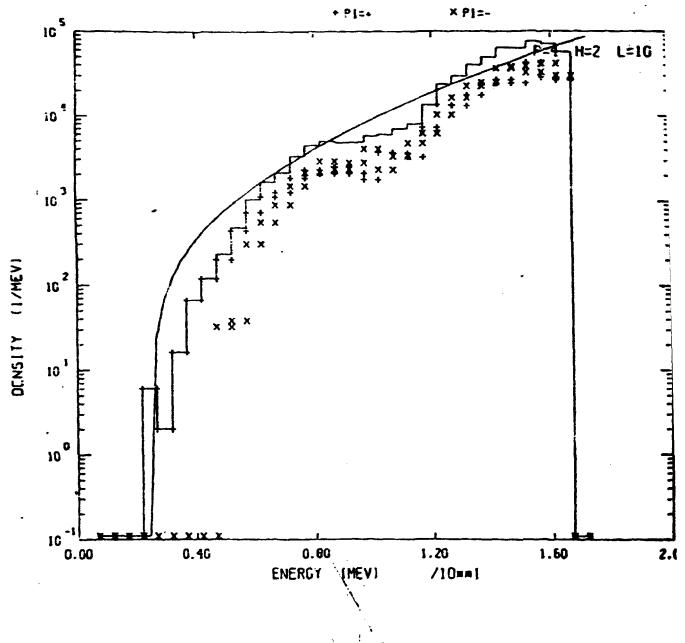


FIGURE 2

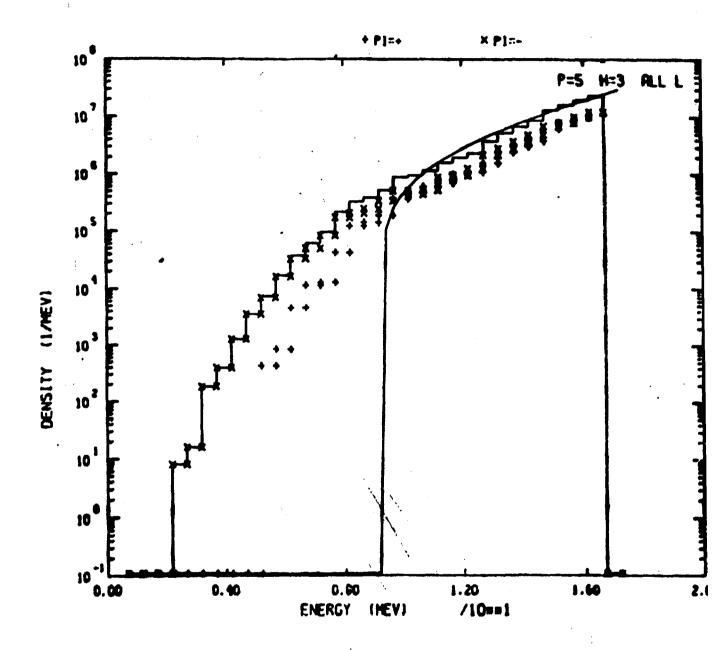


FIGURE 3

Hide /Hole EX

FIGURE 4

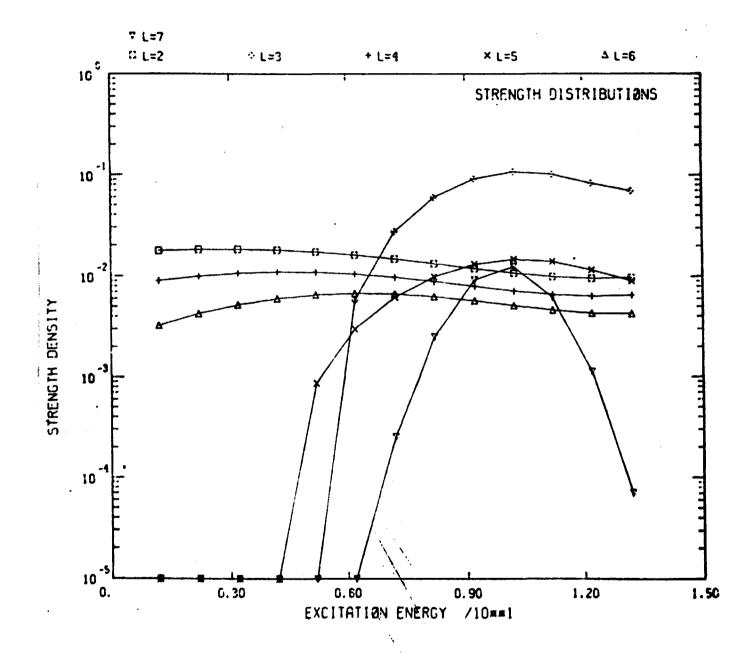


FIGURE 5

