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NUCLEAR STRUCTURE CALCULATION INCLUDING MODIFIED CONTINUUM STATES **)

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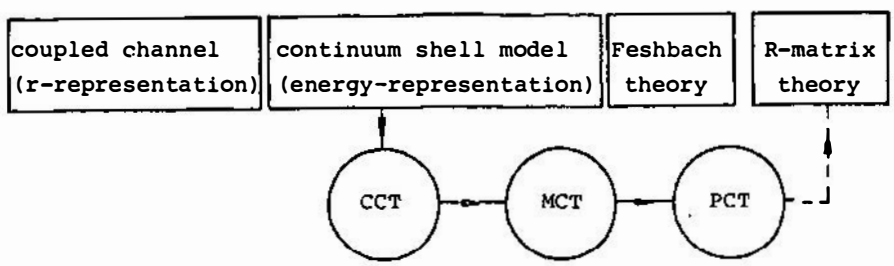
1. INTRODUCTION

Whereas the structure calculations usually solve the Schrödinger equation with a given model Hamiltonian using effective interactions in a given limited model space "exactly", this is not the case for most nuclear reaction calculations. The very successful DWBA, in form of one or two step calculations, treats the problem in a perturbative manner without verification of the convergence properties.

For the description of resonances, however, it is desireable to solve the Schrödinger equation up to all orders in a space consisting of bound and unbound states. Some of such nuclear structure theories in the continuum are given in the following scheme:



In contrast to the DWBA, where just the on-shell T-matrix is obtained, these theories also yield the off-shell matrix elements, which is equivalent to the knowledge of the scattering wave function in the interior region. This is important for the calculation of photonuclear reactions. One obvious question is: What is the price we have to pay for the "exact" solution of the Schrödinger equation? We therefore ask for the numerical feasibility and the physical limitations (configuration, inter-

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action) of the models.

The "coupled channel" approach uses the deformed collective model or simple folding procedures to generate the relevant potentials. As it is formulated in coordinate space, the Pauli Principle is usually neglected. Bound state orbits below the Fermi surface can lead to spurious resonances[1]. A microscopic formulation including antisymmetrization leads to a numerically unpractical integrodifferential equation[2].

The fully antisymmetrized shell model with one particle in the continuum can be applied numerically only in a very limited configuration space[3]. There exist, however, some approximation schemes which reduce the numerical effort substantially[4]. As I will discuss later, these methods are more suitable to describe photonuclear reactions than elastic or inelastic processes.

The "Feshbach Theory" in the usual form[5] (projection on open and closed channels) makes the shell model practical if only one channel is open. The numerical effort, however, increases with increasing energy.

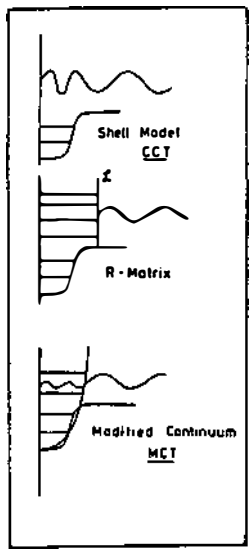
Finally, the R-matrix theory appears on first sight as numerically relatively easy to apply. Although it is in principle exact, in practice difficulties occur with the convergence, and the results may depend strongly on the choice of the channel radii[6].

It is the purpose of this talk to present a formalism which unifies the numerical features of the R-matrix and the physical picture of the shell model. As it treats the bound states and the scattering states in the same basis we calculated both for the $^{12}C + n$ system as a test case. It is found that the results resemble the experimental data quite well, including for the first time the negative parity resonances.

It is well known that single particle resonances cause major numerical difficulties for shell model calculations in the continuum. In the conventional approach[7] the continuum is discretized by a mesh suitable for numerical integration. As the continuum is rapidly varying around the single particle resonances, this procedure (CCT = conventional continuum treatment) demands a narrow discretization in this region. Also, the continuum-continuum coupling is quite large at the resonances.

In the R-Matrix approach there exists no true continuum-

continuum coupling, as the corresponding functions do not extend to the interaction region. The single particle resonances are accounted for by the basis set describing the interior part. In this approach the bound-continuum coupling is done by the surface L-operator[8], which guaranties that the total wave function is smooth at the surface. It is, however, sometimes difficult to establish convergence independent from the channel radius. This stems from the fact that quite a number of basis states in the inner region are necessary to allow the matching at the boundary. As on the other hand the actual continuum (scattering on a hard sphere) is trivial, the calculation of the R-matrix represents numerically no serious problem if convergence is reached.



In the approach presented here (MCT = modified continuum treatment) the wave function in the interaction region is expanded by a finite number of harmonic oscillator functions. The outer region is represented by modified scattering functions which are defined by the demand to be orthogonal to the harmonic oscillator functions. This procedure dampens the scattering functions in the interior region and removes all the single particle resonances from the continuum. The bound-continuum coupling is done by a non-local one-body interaction operator $\tilde{V}$, which describes the decay of the harmonic oscillator states into the continuum[9]. In contrast to the R-matrix theory, the two sets of states are now overlapping in r-space, which gives rise to a continuum-continuum coupling and a bound-continuum coupling via the residual two-body interaction as well. In view of the smallness of the coupling within the modified continuum, one is inclined to treat it in a perturbative manner (PCT = perturbative continuum treatment). By this procedure we shift

just as much from the continuum into the space of harmonic oscillator functions so that the solution of the Schrödinger equation becomes easy in both spaces. The essential demand of the R-matrix theory, that the interior region has to be represented by a complete set of functions, is not given in our approach. The remaining part is contained in the modified continuum.

2. ENERGY REPRESENTATION

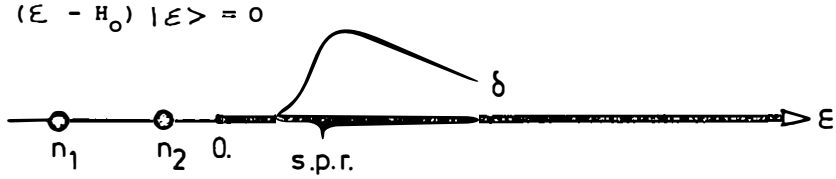
Many nuclear reaction calculations employ the coordinate representation, whereas the shell model is formulated in energy space. In case part of this basis becomes continuous, singularity problems arise which do not occur in bound state calculations. To demonstrate this, we consider a simple single particle state.

The Schrödinger equation with a Saxon-Woods potential has a discrete and a continuous spectrum, which may contain single particle resonances (s.p.r.).

Single Particle Spectrum

$$(\varepsilon_n - H_o)\,|n\rangle = 0$$

$$(\varepsilon - H_o)\,|\varepsilon\rangle = 0$$



The solution of any modified single particle Schrödinger equation (with an additional potential V) can be expanded in this basis.

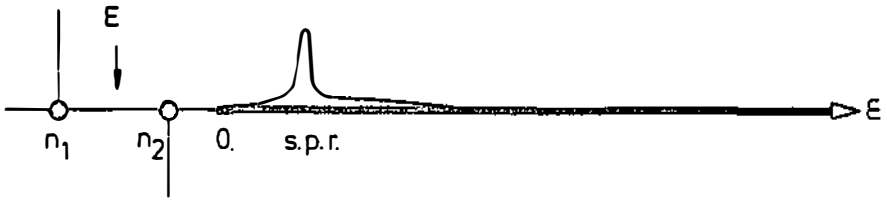
$$(E - H_o - V)\,|\psi^E\rangle = 0 \quad ; \quad |\psi^E\rangle = \sum_n a_n |n\rangle + \int d\varepsilon\, a(\varepsilon)\,|\varepsilon\rangle \qquad (1)$$

The amplitudes a_n and $a(\varepsilon)$ can be viewed as a modified Fourier transform. If the wave function $|\psi^E\rangle$ is bound in coordinate

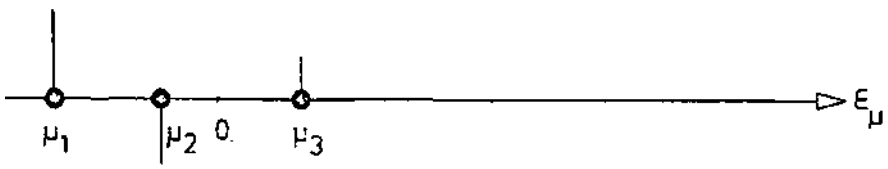
space, the function $a(\varepsilon)$ is regular and in most cases it will be peaked around the s.p.r.

Bound State

$$\langle \varepsilon | \psi^E \rangle = a(\varepsilon)$$
$$\langle n | \psi^E \rangle = a_n$$



HO-Approximation



Taking a harmonic oscillator basis, as many structure calculations do, the s.p.r. is replaced by a bound state.

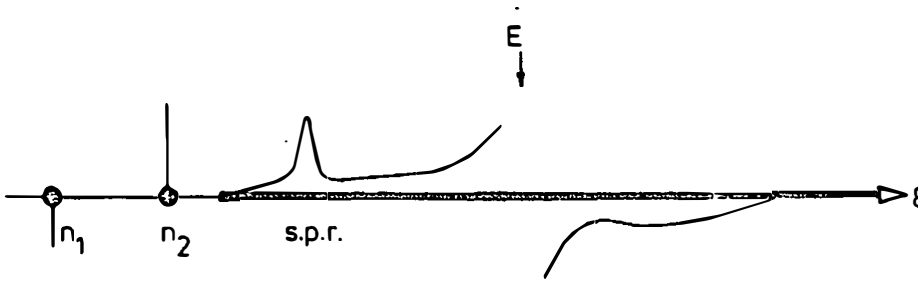
If $|\psi^E\rangle$ is a scattering state, the function $a(\varepsilon)$ will have singularities on the energy shell. The unperturbed (or "ingoing") part of the wave function $|\psi_0\rangle$ is a delta function in the energy representation, whereas the scattered (or "outgoing") part $|\psi_1\rangle$ has a pole singularity.

$$\begin{aligned} \langle \varepsilon | \psi_0^E \rangle &= \delta(E - \varepsilon) \\ \langle \varepsilon | \psi_1^E \rangle &= b(\varepsilon)/(E - \varepsilon) \end{aligned} \qquad (2)$$

$$|\psi^E\rangle = |\psi_0^E\rangle + |\psi_1^E\rangle = |\varepsilon = E\rangle + \sum_n a_n |n\rangle + \int d\varepsilon \frac{b(\varepsilon)}{E - \varepsilon} |\varepsilon\rangle$$

The amplitudes may have the form as given in the following figure.

Scattering State

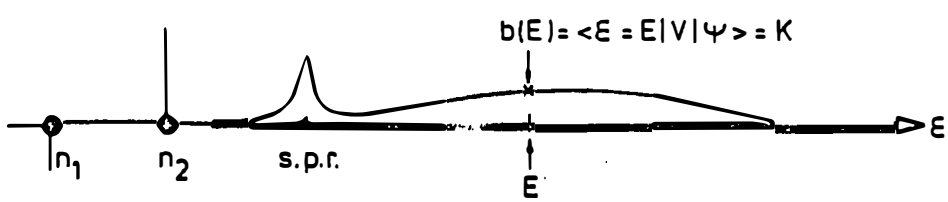


As the potential V is generally in nuclear physics of short range, the state $V|\psi^E\rangle$ is bound in coordinate space and its representation in energy space is regular.

$$V|\psi\rangle = (E - H_o)|\psi\rangle$$
$$\langle\varepsilon|V|\psi\rangle = (E - \varepsilon)\, a(\varepsilon) = b(\varepsilon) \qquad (3)$$

These are half off-shell elements of the transition or reaction operator, depending on the boundary condition. To keep the main part of the calculation real, the principal value integral and hence the reaction operator is used in this study. The on-shell element b(E) constitutes then the K-matrix used for the calculation of the cross section.

Off-Shell Reaction Operator



3. CONVENTIONAL CONTINUUM TREATMENT (CCT)

The Schrödinger equation for the scattering state can be cast into the Lippmann-Schwinger equation for $V|\psi^E\rangle$

$$(1 - V G_o) V|\psi^E\rangle = V|\psi_o^E\rangle \qquad (4)$$

with $(E - H_o)G_o = 1$

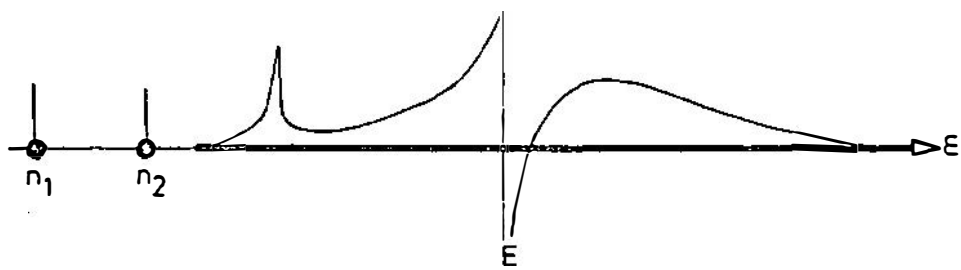
$(E - H_o)|\psi_o\rangle = 0$

In the energy representation, with the discrete part omitted, this becomes:

$$\int d\varepsilon \langle\varepsilon'|1 - \underbrace{V G_o|\varepsilon\rangle}_{I(\varepsilon)} \langle\varepsilon|V|\psi\rangle = \langle\varepsilon'|V|\varepsilon = E\rangle \qquad (5)$$

Because of the propagator $G_o = (E - H_o)^{-1}$ the integrand has a pole:

The Integrand $I(\varepsilon)$



For the numerical solution of this integral equation an integration method for singular integrands is sought. C. Bloch has described a procedure which is based on subtracting the pole term from the integrand[3,7]. The remaining smooth function can be integrated numerically with the use of meshpoints (ε_i) and corresponding integration weight (α_i) for regular integrals. After interpolating the residue, the pole term can be calculated analytically and modified integration weights for

singular integrals are obtained:

$$\int_{\varepsilon_a}^{\varepsilon_b} \frac{f(\varepsilon)}{E^{\pm}_{\circ} - \varepsilon}\, d\varepsilon = \sum_i \frac{\gamma^{\pm\circ}(E)}{E - \varepsilon_i} f(\varepsilon_i) \qquad (6)$$

with

$$\gamma^{\pm}_{\circ}(E) = \alpha_i - (E-\varepsilon_i) g_i(E) \left\{ \sum_j \frac{\alpha_j}{E-\varepsilon_j} + \ln \frac{\varepsilon_b - E}{E-\varepsilon_a} (\pm i\pi) \right\}$$

and Lagrange interpolation weights $g_i(E)$.

As the ratio $\gamma_i(E)/(E-\varepsilon_i)$ stays finite, no matter where E stands with respect to the meshpoint ε_i,

$$\lim_{E \to \varepsilon_i} \left(\frac{\gamma^{\pm\circ}(E)}{E-\varepsilon_i}\right) = \sum_{l \neq i} \frac{\alpha_l - \alpha_i}{\varepsilon_l - \varepsilon_i} - \ln \frac{\varepsilon_b - E}{E-\varepsilon_a} (\mp i\pi) \qquad (7)$$

the integration formula can be applied, even if the pole coincides with one of the meshpoints. With these weights the Lippmann-Schwinger equation becomes a linear system of equations, which can be solved by matrix inversion.

$$\langle \varepsilon_i | V | \psi^E \rangle = \sum_j \frac{E-\varepsilon_i}{\gamma_i(E)} \left[\frac{E-\varepsilon_m}{\gamma_m(E)} \delta_{m,n} - \langle \varepsilon_m | V | \varepsilon_n \rangle \right]^{-1}_{i,j} \langle \varepsilon_j | V | \varepsilon = E \rangle \qquad (8)$$

In this method, which shall be called "conventional continuum treatment", a large number of meshpoints, particularly around the single particle resonance (cf. figures), are required. If we have 40 meshpoints in the single particle basis and allow only 10 configurations, the matrices to be inverted are already 400 x 400. This is the limit where a large number of matrices can be inverted.

4. MODIFIED CONTINUUM TREATMENT (MCT)

In order to reduce the dimension of the matrices, the harmonic oscillator approximation for $V|\psi^E>$ can be used (cf. next figure)

$$V|\psi^E> = \sum_\mu a_\mu |\mu> \tag{9}$$

In this basis the Lippmann-Schwinger equation is cast in the form:

$$\sum_\mu \left[\delta_{\mu\mu'} - <\mu'|VG_0|\mu> \right] \overbrace{<\mu|V|\psi^E>}^{a_\mu} = <\mu'|V|\varepsilon=E> \tag{10}$$

J. Birkholz[9] has shown that the results for the photonuclear reaction are stable with only a few basis states $|\mu>$ (~4). For the elastic and inelastic scattering, however, we need the on-shell K-matrix, whereas the solution of eq.(10) yields the reaction operator in the HO-basis. As the expansion

$$K = <\varepsilon=E|V|\psi> \cong \sum_\mu f_\mu(\varepsilon) <\mu|V|\psi> \tag{11}$$

is only slowly converging, the eq.(10) has yet to be solved with a large number of basis states. In order to avoid this expansion the Lippmann-Schwinger equation can be solved in a basis consisting of HO-function and a modified continuum. The notion of this "modified continuum treatment" can be seen from the following figure. Here some interaction matrix elements, which enter into the integrand, are plotted.

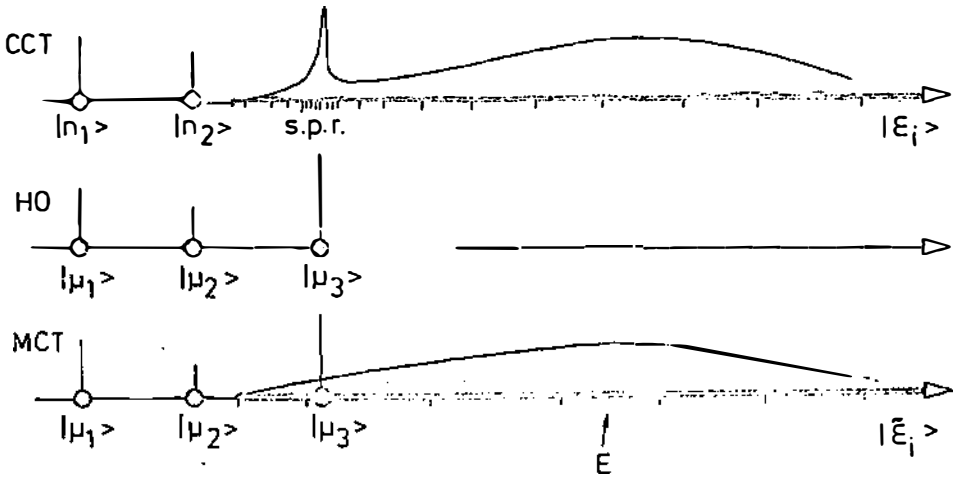
The modified continuum states $|\tilde{\varepsilon}>$ shall be chosen that they are orthogonal to the HO-states. In generalization of the procedure given by W.L. Wang and C.M. Shakin[10] they can be obtained from the original continuum states $|\varepsilon>$ by:

$$|\tilde{\varepsilon}> = |\varepsilon> - g^+(\varepsilon) \sum_{i,j} |\mu_i> \left[<\mu_i|g^+|\mu_j> \right]^{-1}_{ij} <\mu_j|\varepsilon> \tag{12}$$

with

$$g^+ = \sum_n \frac{|n><n|}{\varepsilon - \varepsilon_n} + \int d\varepsilon' \frac{|\varepsilon'><\varepsilon'|}{\varepsilon^+ - \varepsilon'}$$

The Modified Continuum



The main advantage of the new continuum states is that they show no resonance behaviour any more, and the single particle resonance is now replaced by the bound state (here $|\mu_3>$). This allows a discretization of the integral with only a few strongly weighted meshpoints. Thus the dimension of the matrices to be inverted will be drastically reduced.

In this new orthonormal set of states $\{|\mu>\ |\tilde{\varepsilon}>\}$ the single particle Hamiltonian is not diagonal any more: The bound "s.p.r." couples to the modified continuum and decays:

$$<\mu|h_0|\tilde{\varepsilon}> = \sum_{\mu_i} \left[<\mu''|q^+|\mu'>\right]^{-1}_{\mu\mu_i} <\mu_i|\varepsilon> \qquad (13)$$

This one-body "residual interaction" $\tilde{v}$ has been neglected in earlier work[11]. In order to solve the Lippmann-Schwinger equation in the new basis we have to replace $|\varepsilon_i>$ by $|\tilde{\varepsilon}_i>$ in eq.(8). In addition, the (unwritten) bound state configurations have to be extended by the single particle resonance. If we then add the one-body interaction to V, the solution of

this equation (MCT) should give the same results as the CCT. As the number of meshpoints can now be drastically reduced, this method is most favourable from the numerical point of view. In contrast to the HO (Birkholz)method the on-shell K-matrix is obtained directly.

5. PERTURBATIVE CONTINUUM TREATMENT (PCT)

As the continuum-continuum coupling is much reduced in the modified continuum, it might be a reasonable approximation to neglect it. Using the projection operator technique the solution of the Lippmann-Schwinger equation then reads

$$\langle \tilde{\varepsilon} \mid V \mid \psi^E \rangle = \langle \tilde{\varepsilon} \mid VQ \; (E - H_{QQ} - W_{QQ})^{-1} \; QV \mid \tilde{\varepsilon} \rangle \tag{14}$$

with $W_{QQ} = V_{QP} \; (E - PH_oP) \; V_{PQ}$

and $Q = \sum_{\mu} |\mu\rangle\langle\mu| \qquad P = \int d\varepsilon \; |\varepsilon\rangle\langle\varepsilon|$

For the numerical solution of this equation it is advisable to diagonalize the energy dependent matrix $H_{QQ} - W_{QQ}$ (E):

$$\varepsilon_\mu \delta_{\mu\mu'} - \langle\mu|V|\mu'\rangle + \sum_i \langle\mu|V|\tilde{\varepsilon}_i\rangle \frac{\psi_i(E)}{E-\varepsilon_i} \langle\tilde{\varepsilon}_i|V|\mu'\rangle \tag{15}$$

Using the eigenstates $|\omega\rangle$ with energies E_ω the on-shell reaction operator reads simply

$$K = \sum_\omega \langle \tilde{\varepsilon} = E|V|\omega\rangle \frac{1}{E-E_\omega(E)} \langle\omega \mid V \mid \tilde{\varepsilon} = E\rangle \tag{16}$$

Hence, in this approximation no matrix inversion is necessary. It is important to note that the above formula holds only if the continuum functions are orthogonal to the bound state wave functions.

We note that the perturbative continuum treatment, particularly eq.(16), is formally somewhat similar to the R-matrix approach. Mahaux and Weidenmüller[12] already remarked that the more bound states exist in the continuum, the more the K-matrix parameters resemble the R-matrix parameters, if no single particle resonances occur and the continuum-continuum coupling is small. All these conditions which are not satisfied in the conventional continuum shell model, are fulfilled in our approach. This procedure is therefore a connection of the numerical simple R-matrix method with the more physical shell model basis, without using a channel radius.

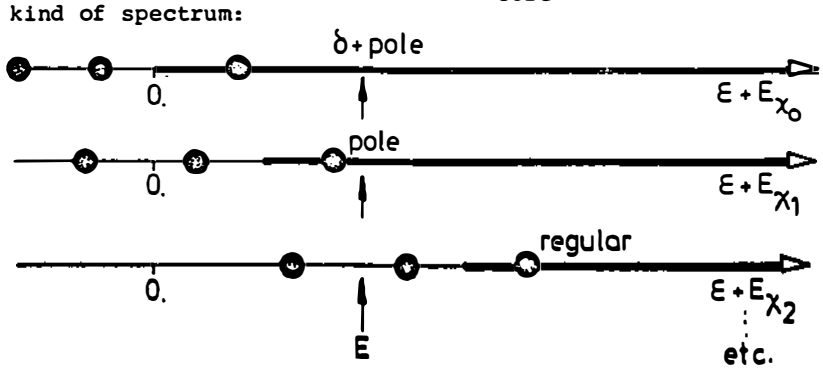
6. RESULTS FOR NEUTRON SCATTERING BY ^{12}C

To test the different methods, the ^{12}C + n - system has been chosen because of the existence of several structure calculations in the continuum for this system using different theories. In the collective model employed, the particle-core-basis is used: i.e. in addition to the single particle states, the core states $|\chi>$ are used to form the basis $\{|\mu\chi>, |\tilde{\varepsilon}\chi>\}$.

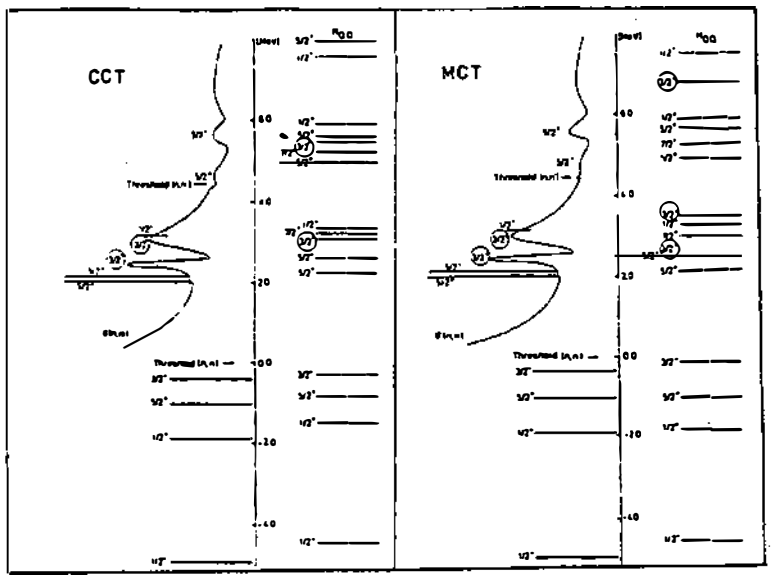
$$(H_o + H_{core})\,|\tilde{\varepsilon}\chi> = (\varepsilon + E_\chi)\,|\tilde{\varepsilon}\chi>$$

$$|\psi> = \sum_{\mu\chi} a_{\mu\chi}\,|\mu\chi> + \sum_{\chi}\int d\varepsilon\; a_\chi(\varepsilon)\,|\tilde{\varepsilon}\chi> \qquad (17)$$

The unperturbed Hamiltonian ($H_o + H_{core}$) has the following kind of spectrum:

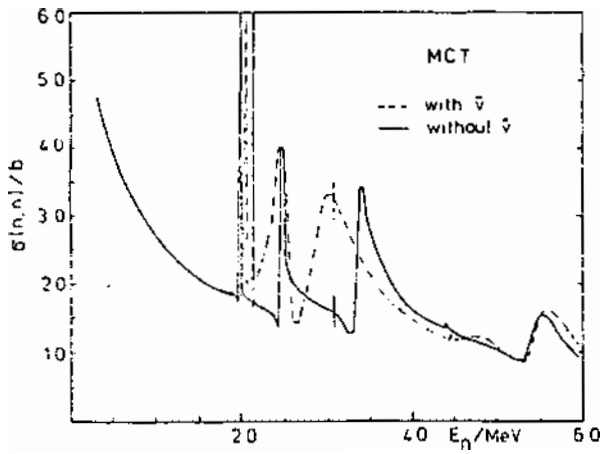


For the interaction V we took a quadrupole-quadrupole and octupole-octupole particle-core interaction[13]. As the wave function shall have only an incoming wave in the elastic channel χ_o, the function $a_{\chi_o}(\varepsilon)$ has a δ- and pole-singularity, whereas $a_{\chi_1}(\varepsilon)$ has only a pole. The function $a_{\chi_2}(\varepsilon)$ is regular because χ_2 represents a closed channel and the corresponding wave function in coordinate space is bound.



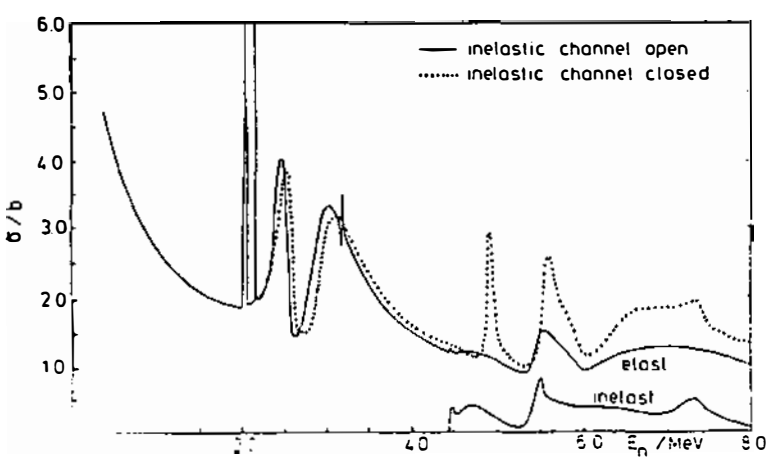
The results of the full continuum calculation are summarized in the figure above, where H_{QQ} stands for the diagonalization in the bound state space. As we treated the $d_{3/2}$ -single particle resonance as bound state in the MCT calculation, a few points were enough in discretizing the continuum. In the CCT many more mesh points are necessary, so that for each channel spin and energy the matrix to be inverted was about 400 x 400. The computer time was therefore about 100 times longer; although the results for the cross sections were practically the

same. This was, however, only checked at some energy points, whereas the full CCT-curve given in the figure was calculated with less (not quite sufficient) mesh points. In the bound state calculation there is one $3/2^+$ -state less as compared to MCT. The additional $3/2^+$ -resonance in the full continuum calculation stems from the single particle resonance in the continuum.



In the next figure the effect of the one-body operator $\tilde{v}$ is studied. This coupling contributes most of the width to the resonances which have large components of the single particle resonance. From this figure it is obvious that $\tilde{v}$ cannot be neglected as has been done before[11].

We have also found that the interesting behaviour at the inelastic threshold is sensitive to the position of the $5/2^+$ -resonance around 4.8 MeV. This resonance is suppressed very much due



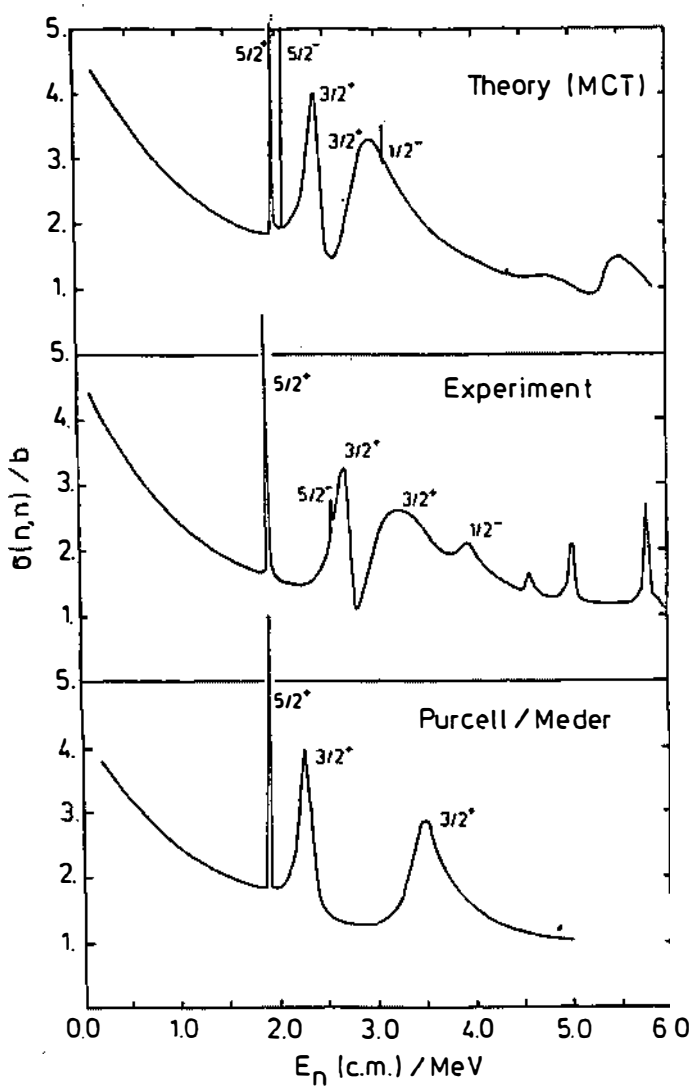
to the strong coupling to the inelastic channel. If we remove the inelastic channel from the continuous part of the basis, this resonance as well as others appear much more pronounced than before. This is demonstrated in the preceding figure.

Finally, we want to compare our results with other calculations and with the experimental data. One of the first continuum calculations for this system is the work of Lovas[5], which is based on the Feshbach formalism. However, due to the separation in open and closed channels, the calculation was restricted to energies below the inelastic threshold. Although the results describe some aspects of the experiment fairly well, they are conflicting with the results of Robson and van Megen[14], who repeated this calculation. Whereas Lovas employed the microscopic intermediate coupling model, Robson and van Megen used this as well as the rotational model. At the same time they compare the Feshbach formalism with the R-matrix approach.

A perfect agreement with the experiment is reached by Reynold et.al.[1] in their coupled channel calculation. One should note, however, that their Hamiltonian is completely parameterized and some parameters used do not agree with the experiment. For example, an unrealistic β_2-value was taken, which also depends on the configuration. It has been criticized[15] that in contrast to all structure calculations, including ours, Reynold et.al. consider the first $5/2^+$ -resonance as a $|1d_{5/2} \times 2^+ : 5/2^+>$ configuration. They obtain this result by artificially lowering the energy of the 2^+-core state for this configuration. We point out that in contrast to the energy representation, the coupled channel formalism completely neglects the Pauli-principle (as long as a integro-differential equation is avoided). This leads, at least virtually, to forbidden configurations (bound states below the Fermi surface) and to unphysical resonances. Such antisymmetrization effects are discussed in the coupled channel calculation of A. Mori and T. Terasawa[16], using a microscopic form factor.

A. Mori also performed R-matrix calculations for the $^{12}C + n$ system[17], where he found strong dependence on the channel

radius. Later R-matrix calculations investigate the convergence properties applying different boundary conditions. R.J. Philpott and J. George[18] use basis functions with homogeneous boundaries, whereas S.S. Ahmed, R.F. Barrett and B.A. Robson[6] employ the so-called natural boundary conditions Both investigations use the same parameters as J.T. Reynold et.al. and they reproduce the coupled-channel results.



The most recent study in this field is the work of J.E. Purcell and M.R. Meder[19]. It is the extension of their bound state calculation using the L-operator i.e. R-matrix formalism. To deal with the continuum, however, they had to require certain changes in the model as compared to the bound state model. Their result is shown in the preceeding figure, where we also plotted our calculated cross section and the experimental data[20]. As for the positive parity resonances it is obvious that their results are similar to ours, although they miss some of the width of the second $3/2^+$-resonance. On the other hand they obtain neither the $5/2^+$ nor the $1/2^-$ - resonance. They claim that the $1/2^-$ - state $|1p_{1/2} x 0_2^+>$ can couple to the continuum only via the monopole interaction. In our model, however, it can decay via the continuum-continuum interaction

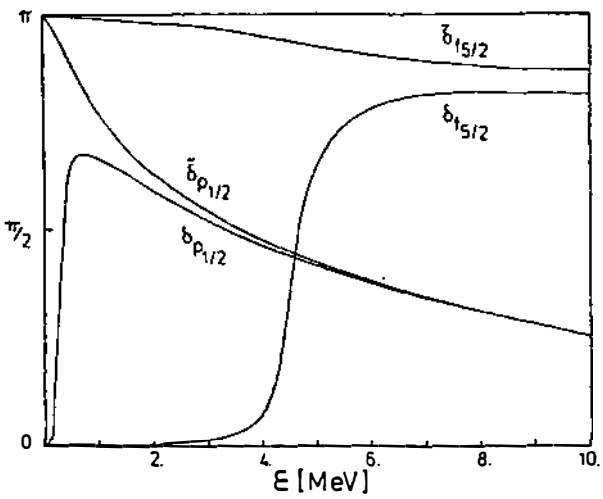
$$|1\, p_{1/2} \times 0_2^+ > \rightarrow |\tilde{\varepsilon} p_{3/2} \times 2^+ > \rightarrow |\tilde{\varepsilon} p_{1/2} \times 0_1^+ >$$

There is no reason why this should not be the case in a R-matrix calculation, provided the basis is large enough. However, as the continuum-continuum coupling is small and the resonance state can only be excited in a two-step process, the calculated width of the resonance is too small.

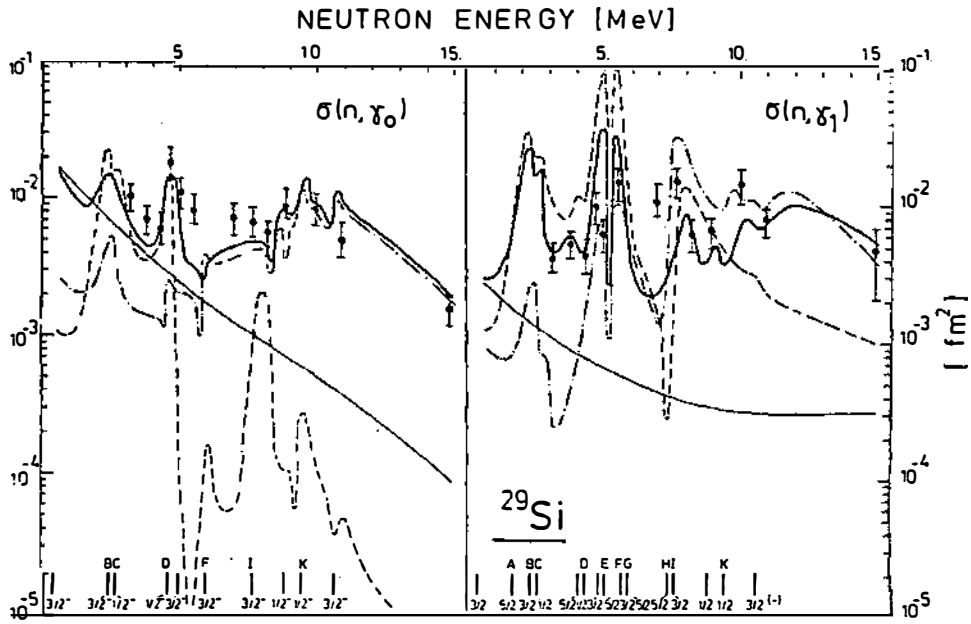
We also calculated the elastic cross section using the perturbative continuum treatment (PCT). As in the PCT the continuum-continuum coupling is neglected, the $1/2^-$ -resonance did not appear in such a calculation. It is, however, interesting to note that aside from this point, the PCT-results do not differ much from the MCT-results, but the computer time was only half as long. It is obvious from the figure that using the MCT-method with relatively little numerical effort (as compared to the CCT), a quite satisfactory agreement between theory and experiment can be achieved.

7. RESULTS FOR THE NEUTRON CAPTURE BY ^{28}Si

The perturbative continuum treatment is particularly useful for the description of more complex systems. Using this method, doorway structures in the radiative capture of neutrons by ^{28}Si can be successfully explained[21]. The $p_{1/2}$ and $f_{5/2}$ phase shifts δ for the $^{28}Si + n$ system are plotted in the figure, and the existence of single particle resonances is obvious. We therefore removed these resonances from the continuum as described above and included them as bound states in the Q-space. This modifies the phase shifts, which now vary smooth with energy. In the particle core model for this system we also included the giant dipole resonance of the core and an isovector particle-core interaction. The results are summarized in the following figure. At the bottom, the energies of the intermediate states $|\omega>$ are displayed. They are mainly doorway states (i.e. particle coupled to the first excited core state). These states, however, split due to the coupling to more complicated configurations.



The different curves represent the different contributions to the total capture cross section (full line). The thin full line is the direct capture, the dashed line marks the single particle decay of the resonance states, whereas the dot-dashed line represents the collective decay.



8. CONCLUSION

Starting from the continuum version of the shell model we have derived a procedure which simplifies the continuum treatment significantly. The characteristics of this method (no single particle resonance in the continuum, small continuum-continuum coupling, many bound states embedded in the continuum) come close to those of the R-matrix approach which is also manifest in the formalism (e.g. eq.16).

Whereas in the conventional shell model the difficulty lies in the continuum, the problem of the R-matrix theory is the complete description of the interior region. The method proposed here is a compromise, which leads to a formalism which is numerically simple although it uses the usual shell model basis. This basis allows us to take care of the Pauli principle and to treat the bound state and continuum calculation exactly on the same footing.

In the $^{12}C + n$ calculation it was possible to reproduce the positive parity as well as the negative parity resonances. We also demonstrated that in order to get the full width it is not justified to neglect the one-body bound-continuum interaction. The results indicate that the continuum-continuum coupling within the modified continuum can be neglected. The resulting perturbative continuum treatment allows calculations for more complicated systems. By this method, doorway structures in the radiative capture of neutrons by ^{28}Si could be successfully reproduced.

As the proposed formalism employs the usual shell model basis without the need for a channel radius and is nevertheless easy to realize numerically, we think that it is an interesting alternative to the L-operator (i.e. R-matrix) approach.

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DISCUSSION

D.R. Thompson: What happens when you go to energies above the first reaction threshold? Do you see "spurious" resonances due to the omission of reaction channels?

M. Micklinghoff: As we have seen in the comparison of the results including or excluding the inelastic channel, "spurious" resonances can occure easily. The calculated width of a resonance, which couples strongly to open reaction channels not included in the model space, will be far too small.

R.J. Philpott: In your calculations you are using a macroscopic collective model. When you use a microscopic model, it is necessary to antisymmetrize the intrinsic states. It is then convenient to reduce as much as possible the amplitude of the continuum functions within the interior region. This can be accomplished (see Ref. 39 of previous paper) by using a weight function of finite range when projecting out the oscillator functions. By this means, the amplitude in the interior can be made very small with only a few oscillator functions. Channel-channel coupling can now be truly neglected and antisymmetrization can be implemented much more easily.

M. Micklinghoff: The macroscopic model was used to allow the application of the conventional as well as the modified continuum treatment numerically. I think a weight function in the projection procedure demands more oscillator functions

in order to assure completeness. As on the other hand in the approach I am using more continuum functions are needed, the methods are probably equivalent with respect to the numerical expenditure. I also believe that the antisymmetrization in a microscopic model presents no difficulty for the MCT, because there is no overlap of the continuum with the harmonic oscillator space.

H. Horiuchi: I think, in microscopic treatments of composite particle scattering, they adopt various kinds of basis wave functions to describe the behaviour in the interaction region like the translated Gaussian functions in GCM and harmonic oscillator function with different width parameters in RGM. Is there any special reason in choosing the harmonic oscillator basis? I understand in Dr. Philpott's talk he needed the Moshinsky coefficients to handle the recoil problem. How does it look in your case? Especially I am interested in the number of basis functions which concerns the convergence of the calculation.

M. Micklinghoff: There is no need to choose harmonic oscillator functions in my approach. The basis states, however, should be orthogonal to each other (and to the continuum), and should at the same time describe the single particle resonances and the bound single particle states. The number of basis states for the PCT is then the same as needed for bound shell model calculations. For the MCT you have to add about seven continuum states for each channel.

R.J. Philpott: I comment on the question by H. Horiuchi about oscillator functions and the center-of-mass problem.

The model used by Dr. Micklinghoff is essentially a macroscopic one. Recoil effects are presumably treated correctly in the model itself. Once the model has been determined, oscillator functions are introduced into each channel merely as a device to aid the calculations. Thus the center-of-mass coordinate never apprears in the problem and no recoil error is introduced.