ALTERNATIVE APPROACH TO THE R-MATRIX DESCRIPTION OF THE SHELL MODEL CONTINUUM

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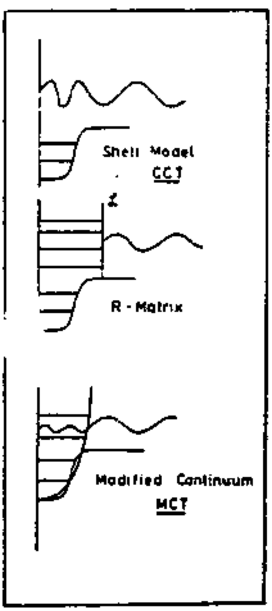
Introduction

It is well known that single particle resonances cause major numerical difficulties for shell model calculations in the continuum[1]). In the conventional approach[2]) 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 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[4]), 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 the continuum is no serious problem, the R-matrix is relativly easy to calculate numerically 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[3]). 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.

Formalism

In order to keep the main part of the calculation real we used the Hermitian reaction operator K, which can be calculated by[3])

$$G_o^o K = (G_o^{o^{-1}} - V)^{-1} V$$

Here G_o^o is the principle value free propagator

$$G_o^o = \sum_i |i\rangle \frac{\gamma_i(E)}{E - E_i} \langle i|$$

The states $|i\rangle$ are either the bound or discretized unbound (many-body) states, and the $\gamma i(E)$ are the integration weights for singular integrands. The K-matrix can now be evaluated by matrix inversion

$$\langle i|K|j\rangle = \sum_l \frac{E - E_i}{\gamma_i(E)} \left[\frac{E - E_m}{\gamma_m(E)} \delta_{m,n} - \langle m|V|n\rangle \right]^{-1}_{i,l} \langle l|V|j\rangle$$

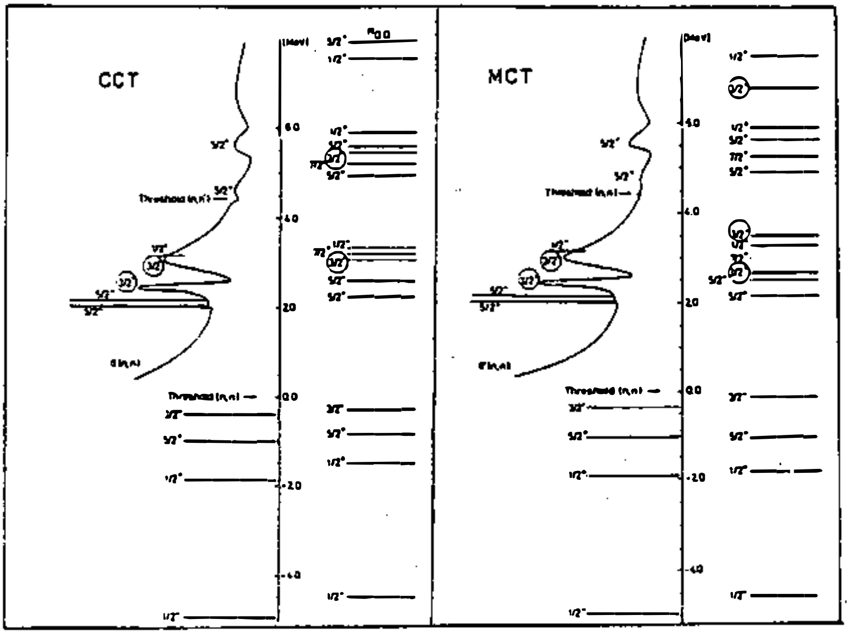
As the modified continuum behaves smooth, only a few mesh points are necessary in the discretization. In case we neglect the coupling within the modified continuum (PCT), the K-matrix reads simply[3]):

$$\langle i|K|j\rangle = \sum_\omega \langle i|V|\omega\rangle \frac{1}{E - E_\omega} \langle \omega|V|j\rangle$$

The states $|\omega\rangle$ and energies E_ω are obtained by diagonalization of the energy-dependent matrix

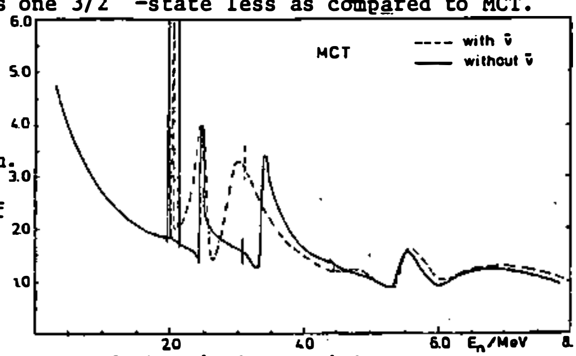
$$E_\alpha \delta_{\alpha,\beta} - \langle \alpha|V|\beta\rangle - \sum_i \langle \alpha|V|i\rangle \frac{\gamma_i(E)}{E - E_i} \langle i|V|\beta\rangle$$

where $|\alpha\rangle$, $|\beta\rangle$ are bound basis states and the states $|i\rangle$ belong to the discretized continuum. These results are formally similar to the R-matrix equations.



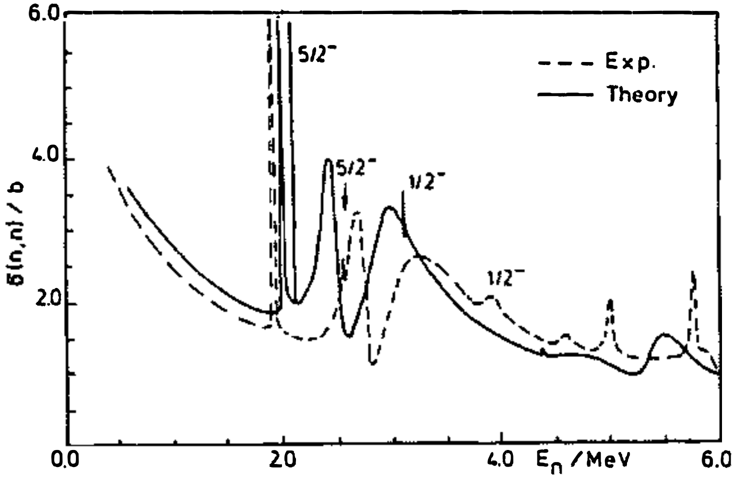
Results

The results of a weak-coupling continuum calculation for the ^{12}C+n -system are given 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.



Finally, the comparison of the calculated curve with experiment is given. The positive parity resonances agree very well in shape, width and position, whereas the width of the negative parity resonances appears somewhat too small. This is an effect of our model space. Within this space the $1/2^-$-resonance $(2p_{1/2} \times 0_1^+)$ can only be excited via the continuum-continuum coupling and therefore cannot appear in the PCT-calculation. Besides this point however, we found only small differences in the PCT-method from the "exact" calculation.

Conclusion

Starting from the conventional shell model continuum we introduced a modified continuum which is free from single particle resonances. This reduces the numerical expenditure drastically. Neglecting then the continuum-continuum coupling leads to the perturbative approach (PCT) which is formally similar to the R-matrix theory. As in this approach, however, no convergence problems exist, we feel that this method is most favourable from the numerical point of view.[5)]

1) J. Raynal, M.A. Melkanow and T. Sawada, Nucl.Phys. A101(1967)369; M. Micklinghoff, B. Castel, Z. Phys. A282(1977)117

2) C. Bloch, XXXVI Intern. School of Physics, E.Fermi Course, Varenna(1966)

3) M. Micklinghoff, submitted to Nucl.Phys.

4) A.M. Lane, D. Robson, Phys.Rev. 151(1966)774

5) This method has recently been applied for the calculation of doorway structures in the radiative neutron capture in Silicon and Sulfur. (M. Micklinghoff, B. Castel to be published).