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TIME INDEPENDENT MEAN FIELD FOR COLLISIONS

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TIME INDEPENDENT MEAN FIELD FOR COLLISIONS

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The shell model (and its underlying mean field) is probably the most elegant and useful approximation used for both atomic and nuclear physics. The mean field is usually first introduced as time independent, and time dependence is later considered for the description of excitations and collisions. In this lecture, we will use three kinds of shell models, namely i) the traditionnal (**static**) shell model, which may be either spherical or deformed, ii) the **boosted** shell model, which differs from the latter by just boost operations, and iii) a completely new shell model, which accounts for **intermediate** states during transitions.

Even though we are dealing with collisions, we will use only time independent fields and orbitals. Consider a collision A(a,b)B, and the corresponding center-of-mass coordinates R_A, R_a, R_b, R_B . We describe the spectroscopic structures of these nuclei by static shell model wave functions $\chi_A, \chi_a, \chi_b, \chi_B$, respectively, and the initial and final channels by the boosted shell model products

$$\chi = \exp(iKR_a)\chi_a \exp(-iKR_A)\chi_A, \quad \chi' = \exp(iK'R_b)\chi_b \exp(-iK'R_B)\chi_B . \qquad (1)$$

In many practical cases, all these functions $\chi_{a\ldots B}$ reduce to just Slater determinants. We stress the fact that boosting a determinant just generates another determinant. This seriously simplifies practical calculations.

As will be shown, whether the particle number N is small (N=2,3,4...) or large (N ≈ a few hundred), our theory is able to calculate a **microscopic** estimate of the multistep amplitude $\mathcal{T}=\langle\chi'|V'GV|\chi\rangle$, where V' and V are the post and prior interactions, then E and H are the collision energy and total Hamiltonian, respectively, and $G=(E+i\epsilon-H)^{-1}$.

It is understood in the following that proper antisymmetry is included, hence χ and χ' are Slater determinants, with the corresponding boosted shell model orbitals χ_i, χ'_j, respectively. In the same way, the trial functions Φ,Φ', which we will introduce for the variational estimate of $\mathcal{T}$, are determinants, with orbitals φ_i, φ'_j. We will find that these φ,φ'

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make a new model, which we name the transition shell model.

The details of the formalism have been published elsewhere[1]. The essential ingredients of the theory are the variational functional

$$F(\Phi,\Phi') = \frac{\langle\chi'|V'|\Phi\rangle\ \langle\Phi'|V|\chi\rangle}{\langle\Phi'|(E+i\epsilon-H)|\Phi\rangle}, \qquad (2)$$

whose stationnary value with respect to Φ,Φ' provides $\mathcal{T}$, and the corresponding generalized Hartree-Fock equations

$$(\eta_i - h)|\varphi_i\rangle = (\omega+QS)|\chi_i\rangle,\ \langle\chi'_j|(\omega'+S'Q') = \langle\varphi'_j|(\eta_j - h), \qquad (3)$$

where $\eta_i, h, \omega, \omega', Q, Q', S, S'$ are, respectively, a single particle self energy, a self-consistent Hamiltonian, two self-consistent channel energies, two particle-hole projectors and two self-consistent channel average fields.

The reason why the variation of F, Eq.(2), leads to driven Hartree-Fock equations, Eqs.(3), is that the denominator of F has the same structure as the Rayleigh-Ritz functional. Hence the variation of Slater determinants in the denominator just generates Hartree-Fock terms. Driving terms come from the numerator. It will be noticed that it is the numerator of F which depends on the channels, and that both initial and final channels are treated on the same footing. There are two trial functions, Φ and Φ', in order to accomodate this duality. The presence of channel orbitals χ_i, χ'_j in the driving terms is transparent in Eqs.(3).

For all usual values of N the numerical solution of Eqs.(3) is no more difficult than the solution of traditional Hartree-Fock equations. But this solution is not very easy to obtain, either, for we have to face the usual non linearities of Hartree-Fock fields, and furthermore the functional F shows saddle points rather than maxima or minima.

A significant amount of experience has been obtained, however, including a surprisingly good approximation to Faddeev-like equations[2-3] for N=3 and N=4. We show on Fig.1, taken from ref.[3], a comparison between an exact four-body amplitude and its mean field approximation.

We also report here a useful manipulation of Eqs.(3) in order to obtain convergence of the usual iterative algorithm for self consistency.

For this we notice that, formally, the variation of F leads to an equation $|\Phi\rangle=(E+i\epsilon-H)^{-1}V|\chi\rangle$. In order to generate the proper on-shell limit, we first select ImE finite rather than infinitesimal. As wave packets, χ and χ' are square integrable and thus the condition "ImE finite" leads to square integrability of Φ and Φ'. If now H splits into a channel Hamiltonian H_0 and a prior interaction V, the auxilliary problem where $H=H_0+\lambda V$, $\lambda \to \infty$, provides the trivial limit solution $|\Phi\rangle \to -|\chi\rangle$ for Eqs.(3). It is then easy to reduce λ to 1 and obtain a smooth extrapolation to the physical solution. Simultaneously, we reduce ImE back to ϵ.

We find the following result, which is of some practical importance: even though the exact on-shell scattered waves are not square integrable, **the mean field approximations Φ, Φ' are still square integrable when ImE vanishes.** This violation of boundary conditions must not be too surprising on second thoughts: in order to approximate a scalar product $[\langle\chi'|V'] [GV|\chi\rangle]$ by another scalar product $[\langle\chi'|V'] |\Phi\rangle$, nothing forces Φ to show the same boundary conditions as $GV|\chi\rangle$. In other words, just one scalar product does not define a whole vector.

Among several few-body collisions, we have programmed Eqs.(3) for an elastic p-t scattering, governed by a Gaussian two-body local force

$$v_{ij} = -V_0 \exp\left(-(r_i-r_j)^2/\mu^2\right), \; V_0 = 50 \text{ MeV}, \; \mu = 2 \text{ fm}. \qquad (4)$$

The target is described by boosted, spherical shells,

$$\chi_{2,3,4}(r_{2,3,4}) = \pi^{-3/4} \beta^{-3/2} \exp\left(-r^2_{2,3,4}/2\beta^2 + i r_{2,3,4} K/3\right), \; \beta = 2 \text{ fm}, \qquad (5)$$

with a similar formula for the final orbitals $\chi'_{2,3,4}$ boosted by $-K'/3$. For the sake of simplicity, we freeze the orbitals in the direction perpendicular to the reaction plane defined by the two vectors K,K'.

We have solved Eqs.(3) on an 11x11 mesh in the reaction plane, for many energies and angles. The momentum density plots for variational orbitals shown on Fig.2 are taken from the whole atlas we have generated. In all cases, the self consistent φ,φ' show very smooth shapes. A zoology of such "transition orbitals" is still an open problem, but it can be seen already at this stage that these shapes make smoothly deformed shells, without major singularities so far.

From the form of the functional, Eq.(2), it is seen that the amplitude $\mathfrak{C}$ is the product of two widths, divided by an energy denominator. An interpretation of Φ,Φ' as intermediate states is thus in order. Their smoothness indicates that there is a whole extension of the shell model concept: it not just a convenient picture of bound states, but also of transition steps in a collision.

We have tested the quality of the mean field approximation in the case of several soluble models, for N=2 for instance, where the comparison with the exact multistep amplitude is trivially available. Our experience contains the case of long range forces (Coulomb) and the case of trial functions with much fewer parameters than the full flexibility of orbitals φ,φ'. It turns out that F provides excellent approximations in general.

The interested reader may look into ref.[4] for a case with N=5, a semi-quantitative calculation of elastic π-α scattering. There an exact solution is not available for comparison with the variational estimate, but the outlook of the variational estimate is definitely sound enough. This is very encouraging for calculations for higher values of N.

In conclusion, the same methods which have been so successful in the history of the static shell model for the diagonalization of H are available for the inversion of E-H. In particular, a suitable inhomogeneous term can be added to Hartree-Fock equations, in a self consistent way, in order to microscopically define a collision term without ad hoc parameters. This extended Hartree-Fock theory provides a parameter free calculation (no ad hoc optical potentials for instance) of collision amplitudes.

References:

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2) Y.Abe and B.G.Giraud, Nucl. Phys. A 440, 311 (1985)
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Figure Captions:

Fig.1: Exact versus mean field amplitudes for a soluble N=4 model.

Fig.2: Momentum density plot of variational orbitals for an elastic p-t collision at 90°. Left plots for projectile, right plots for target.

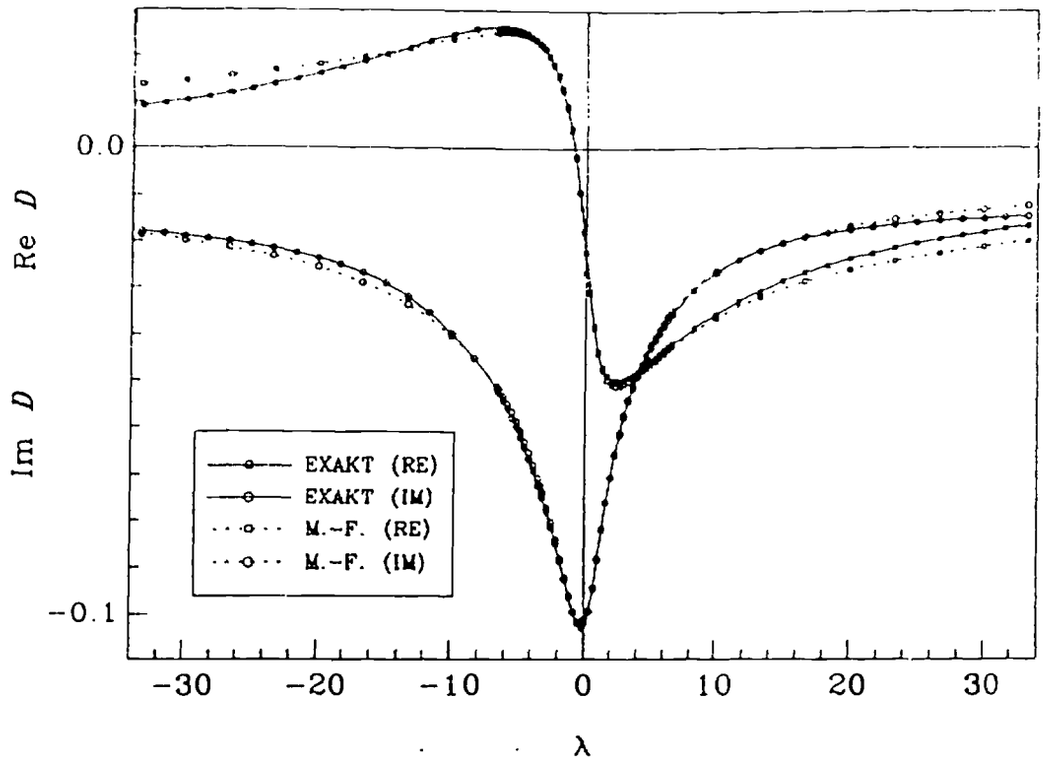


Abbildung 4.4: Die Diagonalamplitude D für die exakte und die Mean-Field-Rechnung bei $K = 1$ und $\epsilon = 8$.

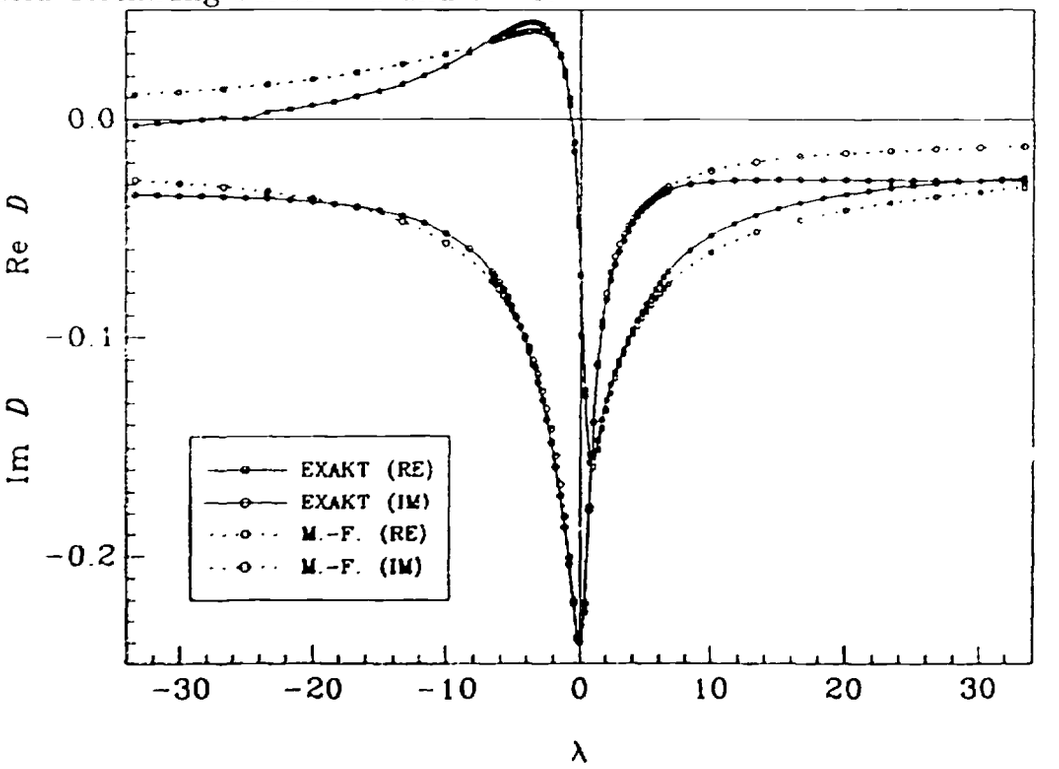
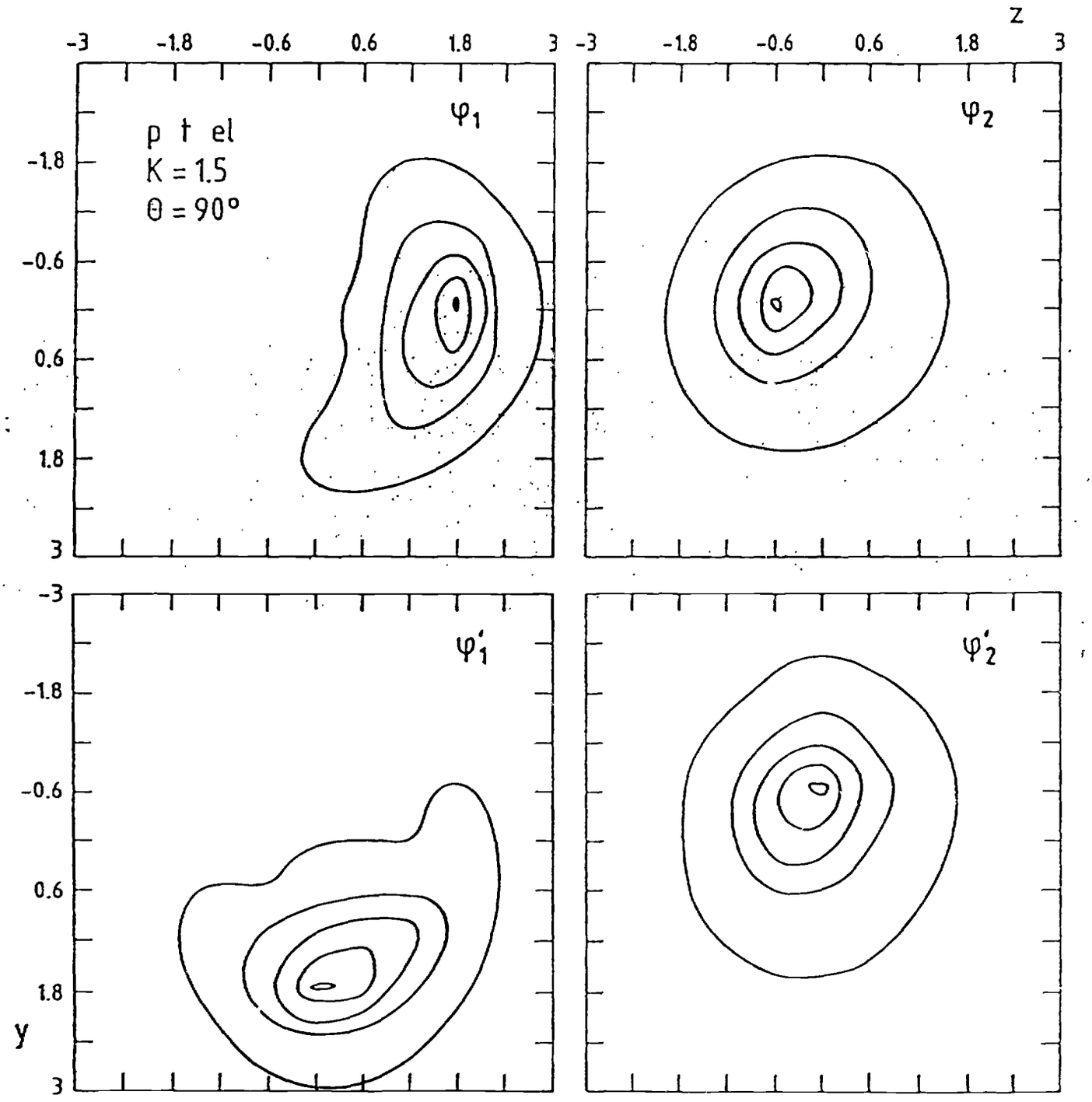


Abbildung 4.5: Die Diagonalamplitude D für die exakte und Mean-Field-Rechnung bei $K = 1$ und $\epsilon = 2$.


p t el
K = 1.5
θ = 90°
φ1
φ2
φ'1
φ'2
z
y
-3
-1.8
-0.6
0.6
1.8
3