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QUANTUM COLLISIONAL EVOLUTION OF A ONE-DIMENSIONAL FERMI-GAS: NUMERICAL SOLUTION

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ABSTRACT

We present a numerical solution to the problem of the quantum collisional evolution of a one-dimensional Fermi gas. The equation governing this dynamics is nonMarkovian non linear and can be solved exactly in this case. We observe two distinct time scales associated with the relaxation process, one connected with the establishment of correlations in the system and which is very short as compared to the second one, related to the evolution of the one body density, once correlations are established.

I. INTRODUCTION

The exact microscopic description of the time evolution of the one body density associated with a many fermion system can be formally given in terms of ingredients of two distinct types: the usual time dependent Hartree-Fock contribution plus additional contributions which arise from the dynamical evolution of quantum correlations in the entire system, and which are essentially related to changes of the coherence properties of the one body density[1]. In fact, it can be shown quite generally[2] that the effective dynamics of any subsystem of a given quantum system (and the nuclear one body density can be regarded as a particular case, i.e., a subsystem of an A-body quantum system, the nucleus) is non-Hamiltonian and closely related in form to equations of the transport type. The physical origin of nonunitarity contributions lies in the complicated dynamical evolution of quantum correlations in the entire system and their consequence is the change in the coherence properties of the given subsystem[2]. The particular case of the exact evolution of the nuclear one body density displays the same feature and in this case the nonunitarity dynamics corresponds directly to the dynamics of occupation numbers[1] which as it is well known, controls the coherence of the one body density. The equations governing the time evolution of the one body density (single particle states and occupation numbers) is very complicated. It is nonlinear and nonMarkovian. Although they do not, in principle, entail irreversible behavior, they can be cast in forms which are

immediately suggestive of irreversible limits or approximations. Equations for the time evolution of occupation numbers, in particular, have been given in the literature, which make use of statistical hypothesis and Markovian approximations[3]. Under these assumptions, the time evolution of the one body density is given in terms of Master type (or Fokker-Planck) equations, which lead the system necessarily to a static equilibrium distribution. We emphasize that the exact macroscopic dynamics of the one body density does not involve in principle any element of irreversibility so that recurrence phenomena cannot be excluded a priori. Therefore the question remains open whether some given system relaxes to an equilibrium distribution or not. The answer to this question would involve solving a nonlinear, nonMarkovian equation. This is obviously hopeless if one considers a finite three dimensional many body system as one has, e.g., in nuclear physics. In this case the equations which describe the time evolution of the one body density, even in the absence of initial correlations, are not tractable either analytically or numerically. The situation is somewhat simpler in the case of an infinite system with translational invariance. For such a system, the eigenfunctions of the one body density are automatically independent of time and given as plane waves, and the full problem of the one body density is reduced to the dynamics of occupation probabilities.

An even simpler problem, which can be solved numerically in a straightforward way, is the problem of the time evolution of the one body density associated to a one dimensional Fermi gas, the correlation dynamics being treated

up to terms of second order in the two body potential. This is a weak coupling approximation to correlation effects, which retains the nonlinear, nonMarkovian character of the evolution. The special case of a one dimensional Fermi gas has the additional advantage of allowing for the choice of self consistent mean-field bound and stable determinantal states (Hartree-Fock) as initial condition, even for simple purely attractive two body potentials.

The study of this simple problem reveals several nontrivial properties of the solution of the nonlinear non-Markovian dynamical equations: It reveals for instance, the details of the process of how two body correlations are established when one starts with a noncorrelated (except for antisymmetrization) initial state. This process, in the cases examined here, could be associated to a distinct (shorter) characteristic time as compared to the characteristic relaxation time of the one body density. The origin of these distinct time scales can also be traced down to the time scales associated a) with the variation in time of the correlation energy (which occurs very rapidly and then stays practically constant) and b) with the further evolution of the distribution of occupation probabilities after correlations are established in the system.

It certainly involves a drastic extrapolation to extend the qualitative aspects of these results to other situations, e.g., for three dimensional infinite systems. However, it is at least amusing to observe that the discussed features of our results have been introduced as a dynamical

hypothesis by Bogoliubov in the classical treatment of kinetic problems[4]. Bogoliubov argued that the dynamical evolution of an (initially uncorrelated) gas of interacting classical particles proceeded in two distinct stages: the one he called pre-kinetic region which corresponded to a very short time scale when correlations were established in the system, and a second stage called kinetic region and described the time evolution of the syustem towards equilibrium, which was then governed by properties of the one body density itself.

The paper is organized as follows: in section II we give the general equations governing the exact dynamics of the translationally invariant one body density, discuss a working approximation to it and present the model. In section III we define two quantities, the reduced one body entropy and the correlation energy, which are calculated and studied in section IV. We show that the total energy (single particle plus correlation energy) is exactly conserved in our model. In fact, it can be shown quite generally that the total energy will be exactly conserved to all orders in the coupling two body potential in the framework of the formalism of ref.(1)[5]. Section IV contains the results and section V the conclusions.

II. GENERAL EQUATIONS AND MODEL

The exact description of the time evolution of the translationally invariant one body density, following ref.(1) yields for the time evolution of the occupation numbers $p_k(t)$:

$$\dot{p}_k(t) = -\mathrm{Tr}\left\{ c_k c_k^{+} \int_0^t dt' \left[H, G(t,t') Q(t') \left[H, \bar{F}_0(t') \right] \right] \right\} \qquad \text{(II.1)}$$

where c_k^{+} and c_k are fermion operators associated with the plane wave number k. The mathematical structure of eq. (II.1) can be physically understood as follows: at time t', the uncorrelated density $F_0(t')$ suffers the action of the Hamiltonian H, which by means of the two body potential will create a correlated state at time t'. The operator $Q(t')$ (see ref.(1)) filters from this state all the contributions having the form of a one body density written in Fock space. The essentially correlated state $Q(t')[H,F_0(t')]$ is propagated from time t' to time t by the Green's function $G(t,t')$

$$G(t,t') = \mathrm{T} \exp\left\{ -i \int_{t'}^{t} d\tau\, Q(\tau) [H, \cdot] \right\} \qquad \text{(II.2)}$$

Additional correlations can be generated during the propagation. At time t, it suffers again the action of H and finally, the trace with $c_\lambda^{+} c_\lambda$ will give the correlation contributions to the time evolution of the one body density. Although their evaluation is rather involved, it is possible to introduce a working "weak coupling" approximation[1]. This approximation consists in neglecting all additional correlations which would be generated within $G(t,t')$. We assume $G(t,t')$ to propagate the initially produced correlations from time t' to time t by means of the mean field dynamics

$$G(t,t') \longrightarrow g_{MF}(t,t') \qquad \text{(II.3)}$$

or, explicitly,

$$g_{MF}(t,t')\,|k,t\rangle\langle k',t'| = |k,t\rangle\langle k',t| \qquad \text{(II.4)}$$

where the states $|k_i,t\rangle$ are defined in such a way as to include the time dependence associated with the mean field dynamics (see eq. (III.5) below). This is a weak coupling approximation, since it considers correlation contributions which are at most quadratic in the coupling potential. The spirit of the approximation is then to retain just the simplest correlation contributions while preserving the mean field dynamics, i.e.,

$$i\frac{\partial}{\partial t}\,|k,t\rangle = h(t)\,|k,t\rangle \qquad \text{(II.5)}$$

Under these approximations one can cast eq. (II.1) into the form

$$\dot{p}_k(t) = -\sum_{k_1k_2k_3}\int_0^t dt'\ Re\Big[\langle k_2k_3|\tilde{v}|kk_1\rangle_t\langle kk_1|\tilde{v}|k_2k_3\rangle_{t'}\cdot \cdot\left(p_k p_{k_1} q_{k_2} q_{k_3} - p\leftrightarrow q\right)_{t'}\Big] \qquad \text{(II.6)}$$

where $q_i = 1 - p_i$ and $\langle k_1k_2|\tilde{v}|k_3k_4\rangle_t$ are antisymmetrized matrix elements of the two body potential at time t. The states in eq. (II.6) contain the full mean field dynamics. A further simplification can be achieved if one restricts the mean field dynamics to its "one body part" i.e., involving differences of single particle energies

$$i\frac{\partial}{\partial t}\,|k_1,t\rangle\langle k_2,t| = \left[h_{k_1}(t) - h_{k_2}(t)\right]\,|k_1,t\rangle\langle k_2,t| = \left[\epsilon_{k_1}(t) - \epsilon_{k_2}(t)\right]\,|k_1,t\rangle\langle k_2,t| \qquad \text{(II.7)}$$

with

$$\epsilon_{k_1}(t) = \frac{\hbar^2k_1^2}{2m} + \sum_{k_2}\langle k_1k_2|\tilde{v}|k_1k_2\rangle\,p_{k_2}(t) \qquad \text{(II.8)}$$

This simplification amounts to identifying the mean field modes with the single particle states. It ignores, in particular, any collective effect, as might emerge from a random phase approximation.. Such effects can actually be included at some computational cost, but we do not consider them here. The interaction we use is a central, spin independent, Gaussian two body potential, given by the matrix elements

$$\langle k_3\lambda_3\,k_4\lambda_4|\tilde{v}|k_1\lambda_1\,k_2\lambda_2\rangle = \frac{V_0}{L}\,\delta_{\lambda_1\lambda_3}\,\delta_{\lambda_2\lambda_4}\,\delta_{k_1+k_2}\,\delta_{k_3+k_4}\cdot \cdot\exp\left\{-4b^2(k_1-k_3)^2\right\} \qquad \text{(II.9)}$$

Translational invariance guarantees, as usual, that the self consistent one body potential depends only on momentum, It is tempting to simplify the numerical calculation by introducing an effective mass approximation. In our case it has been verified numerically to be a good approximation to the full self consistent solution. Substituting the matrix

elements (II.9) into eq. (II.6) we get a non linear integro-differential equation with memory. This equation can be reduced by an analytic quadrature to an integral non linear equation with memory for the occupation probabilities which we solve by the usual integration methods.

III. THE REDUCED ONE BODY ENTROPY, THE CORRELATION ENERGY AND ENERGY CONSERVATION

The reduced one body entropy

$$S' = \sum_i p_i \ln p_i + \sum_i q_i \ln q_i \qquad \text{(III.1)}$$

is a direct measure of the coherence of the one body density. If one has a pure state, S will be zero and it increases as the incoherence in the density increases.

In order to define the correlation energy, we have to go back to ref.(1). In the derivation of the exact dynamics of the one body density, we start by writting the full many body density as

$$F = F_0 + \bar{F}' \qquad \text{(III.2)}$$

where F_0 is an uncorrelated many body density (see. eq. (3.10), ref.(1)) and F' can be expressed, by means of projection techniques, as a function of F_0 (see eq. (3.16) of ref.(1)). The total energy

$$E = T_r (H F) \qquad \text{(III.3)}$$

is obviously a conserved quantity if we make no approximations. We can use eq. (III.2) in order to write it as a sum of single particle energies plus the correlation energy as

$$E = T_r (H \bar{F}_0(t)) + T_r (H F'(t)) \qquad \text{(III.4a)}$$

$$E_{sp} = T_r (H \bar{F}_0(t)) \qquad \text{(III.4b)}$$

$$E_{corr} = T_r (H F'(t)) \qquad \text{(III.4c)}$$

The correlation energy (III.4c) can be evaluated with the same approximation described in section II. We get, for the specific model we study

$$E_{corr} = -\sum_{k k_1 k_2 k_3} \int_0^t dt' \, Im \Big\{ \langle k_2 k_3 | \tilde{v} | k k_1 \rangle_t \langle k k_1 | \tilde{v} | k_2 k_3 \rangle_{t'} \cdot \times \left(p_k p_{k_1} q_{k_2} q_{k_3} - p \leftrightarrow q \right)_{t'} \Big\} \qquad \text{(III.5)}$$

In this simple case it is easy to see that energy will be conserved. The time derivative of the single particle energy is given by

$$\frac{d}{dt} T_r (H \bar{F}_0) = \sum_k h_k \frac{d}{dt} p_k \qquad \text{(III.6)}$$

where h_k is defined in eq. (II.7). Using eq. (3.16) of ref. (1), neglecting initial correlations and working within the approximation described in section II we can write

$$F'(t) = -i \int_0^t dt' \, g_{MF}(t,t') \, Q(t') [H, \bar{F}_0(t')] \qquad \text{(III.7)}$$

The time derivative of the correlation energy can then be written as

$$\frac{d}{dt} Tr(H\bar{F}') = -i\, Tr\left(H g_{MF}(t,t)\, Q(t)\, [H, F_0]\right)$$
$$- i\, Tr\left(\int_0^t dt'\, H \frac{\partial}{\partial t} g_{MF}\, Q(t')\, [H, F_0]\right) \qquad \text{(III.8)}$$

The first term on the r.h.s. can easily be shown to be zero. It can be written as

$$-i\, Tr\left(H Q(t) [H, \bar{F}_0(t)]\right) = i\, Tr\left(h_{MF} [h_{MF}, F_0]\right) = 0 \qquad \text{(III.9)}$$

The second term on the r.h.s. can be written as

$$- Tr\left(\int_0^t H\, [h_{MF}(t), g_{MF}(t,t')\, Q(t')\, [H, \bar{F}_0(t')]]\right) \qquad \text{(III.10)}$$

given that

$$i \frac{\partial}{\partial t} g_{MF}(t,t') = [h_{MF}(t), g_{MF}(t,t')] \qquad \text{(III.11)}$$

Therefore

$$- Tr\left(\int_0^t dt'\, H\, [h_{MF}, g_{MF}(t,t')\, Q(t')\, [H, \bar{F}_0(t')]]\right) =$$

$$= Tr\left(h_{MF}(t) \int_0^t dt'\, [H, g_{MF}(t,t') Q(t')\, [H, \bar{F}_0(t')]]\right) =$$

$$= - \sum_k h_k(t) \frac{d}{dt} p_k \qquad \text{(III.12)}$$

which completes the proof that energy is conserved in the model presented here. It is possible to show that energy conservation holds in a more general context within the formalism of ref.(1)[5], as already pointed out in the introduction.

IV. RESULTS AND DISCUSSION

In this section we exhibit the most instructive results which illustrate clearly the presence of two distinct time scales in the evolution of the occupation probabilities. In fig. 1 we plot the time evolution of occupation probabilities having as initial condition the self consistent excited determinantal state (full line) as well as a determinantal state (dashed lines). For the excited determinantal state as initial condition we observe that for times of order τ_{corr} (marked in the figure) there is a rapid change in the occupation probabilities for states lying below and above the Fermi sea, which stay practically constant afterwards. This characteristic time is associated with the establishment of correlations in the system as can be seen from fig. 2 where the correlation energy is plotted against time. Here we see very clearly that the correlation energy in both cases (the excited determinantal state and the determinantal state) exhibit the same short time scale, associated with the establishment of correlations in the system. As for the determinantal initial state we observe from fig. 1 that at time 0.1 MeV^{-1} it has practically attained its

equilibrium distribution, whereas the excited state has not yet filled in the hole due to the excitation. The equilibration process for this case proceeds after τ_{corr} in a slower time scale which can be most clearly seen in fig. 3 where the one body entropy is plotted against time, again for both cases. We see immediately that the fast process of establishment of correlations manifests itself clearly in the entropy. For the case of the determinantal state the entropy attains equilibrium after τ_{corr}, but the excited state has not yet relaxed after τ_{corr}. Therefore the entropy continues to change in a slower time scale until it saturates. The behavior of all quantities exhibited depend very much on initial conditions and also on the coupling potential.

It is very simple to estimate τ_{corr}. It can be associated to the off-the-energy shell character of correlation process, which is in turn linked to the range of the two body potential. In fact, the energy mismatch involved in the correlated state can be estimated as

$$\Delta E \sim \frac{\hbar^2}{m} k_F \, \Delta k$$

with $\Delta k \sim \frac{1}{b}$ (b being the typical range of the two body potential) so that

$$\tau_{corr} \simeq \frac{\hbar}{\Delta E} = \frac{m b}{\hbar k_F} \qquad \text{(IV.1)}$$

This linear dependence with the potential range has been verified in the calculations. It is also easy to show

that for short times[2]

$$n_k \simeq n_k(0) + \frac{t^2}{\tau_{corr}^2} \qquad \text{(IV.2)}$$

where

$$\tau_{corr} = \frac{2}{A\hbar^2} \sum_{\substack{i,j \in A \\ k,\ell > A}} |\langle k\ell|\bar{v}|ij\rangle|^2 \qquad \text{(IV.3)}$$

which yields the same result as (IV.1), when estimated in a simplified way. This short time behavior should be valid for all occupation probabilities. This can be easily checked in Figs. 4, 5, 6 and 7. In these figures we plot a logarithmic scale the time evolution of the occupation probabilities for the two cases studied. In figs. 4 and 5 we display the variation with time of the various occupied and unoccupied states for the determinantal state as initial condition. We observe immediately that all occupations exhibit the same behavior for short times. After that each occupation probability evolves differently. This is an effect of the nonlinearity in the problem, and, in fact the system exhibits many different time scales. We observe that states which are symmetric around the Fermi sea tend to oscillate out of phase. This might be the reason why there is no contribution to the entropy for times later than τ_{corr}. The same thing happens in the case of the excited determinantal state as we see in figs. 6 and 7 except that the states near the Fermi sea (as states 5 and 7 in fig. 6 and 4 and 6 in fig. 7) do not seem to exhibit an oscilatory behavior. This conspiracy of nonlinear effects, we believe, might be

responsible for the second time scale in the entropy as seen in fig. 3.

V. CONCLUSION

The numerical solution to the quantum collisional dynamics of a one dimensional interacting Fermi Gas presented in this work reveals several nontrivial properties of a non linear nonMarkovian process. We studied, in particular, the details of the process of establishment of correlations in an initially uncorrelated system. There is a short time scale associated with this process which depends essentially on the range of the two body potential. We learn also that the short times behavior of the system is mainly governed by the single particle energies. These contribute to the dynamics as phases (see eq. (II.6)) and vary very rapidly in time while the occupation probabilities have a definite sign. A Markovian approximation to the occupation probabilities turns out to be a good approximation in this case. Nonlinear effects become important after τ_{corr}. Up to the times for which we integrated the differential equations, relaxation occurs for the two cases examined. We believe that there will be no physical recurrence in the calculated quantities due to the continuum of phases. It is tempting but dangerous to extrapolate this conclusion to finite nuclei. The lesson to be learned is that it is very important to treat the single particle energies correctly. We should also like to remark that eq. (II.6) was solved self consistently with the single

particle energies. However, it was checked numerically that the effective mass approximation is very good.

We do not believe the results would change qualitatively if we extend the calculation to two or three dimensions.

It is interesting to speculate whether the correlation energy liberated in a nucleus-nucleus collision could have any measurable effect. Depending on the initial conditions of the problem it could for instance lead to the formation of a hot spot or thermalize. While this work was being written, a recent work along these lines came to our attention[6].

REFERENCES

(1) M.C. Nemes and A.F.R. de Toledo Piza, Phys. Rev. C27, 862 (1983).

(2) M.C. Nemes and A.F.R. de Toledo Piza, to be published.

(3) G. Wolschin, Lecture Notes in Physics 171, 142.

(4) N.N. Bogoliubov, Studies in Statistical Mechanics, de Boer and Uhlenbeck, eds., N.H. 1962.

(5) H. Feldmeier and M.C. Nemes, to be published.

(6) M. Tohyama, Preprint Giessen (1985).

FIGURE CAPTIONS

Fig. 1 - Time evolution of occupation probabilities for two initial conditions: the self consistent Hartree-Fock ground state (dashed line) and a particle-hole excitation based on it (full line).

Fig. 2 - Correlation energy as a function of time for the same two cases as in fig. 1.

Fig. 3 - Entropy as a function of time for the same two cases as in fig. 1.

Fig. 4 - Variation with time of the occupied states indicated in the figure.

Fig. 5 - Variation with time of the unoccupied states indicated in the figure.

Fig. 6 - Variation with time of the occupied states indicated in the figure.

Fig. 7 - Variation with time of the unoccupied states indicated in the figure.

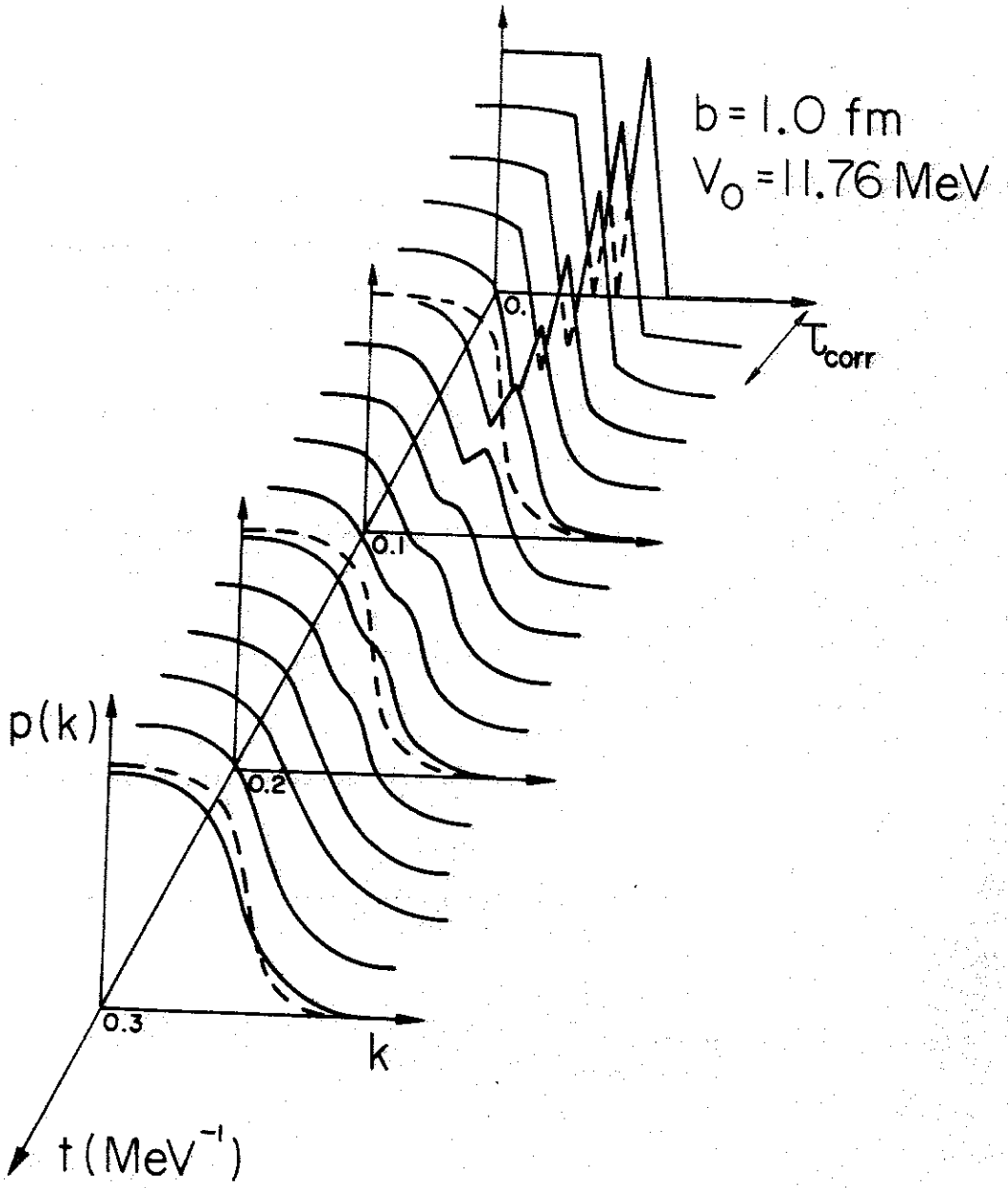

b = 1.0 fm
V_0 = 11.76 MeV
τ_{corr}
0.
0.1
0.2
0.3
p(k)
k
t (MeV^{-1})

Fig 1

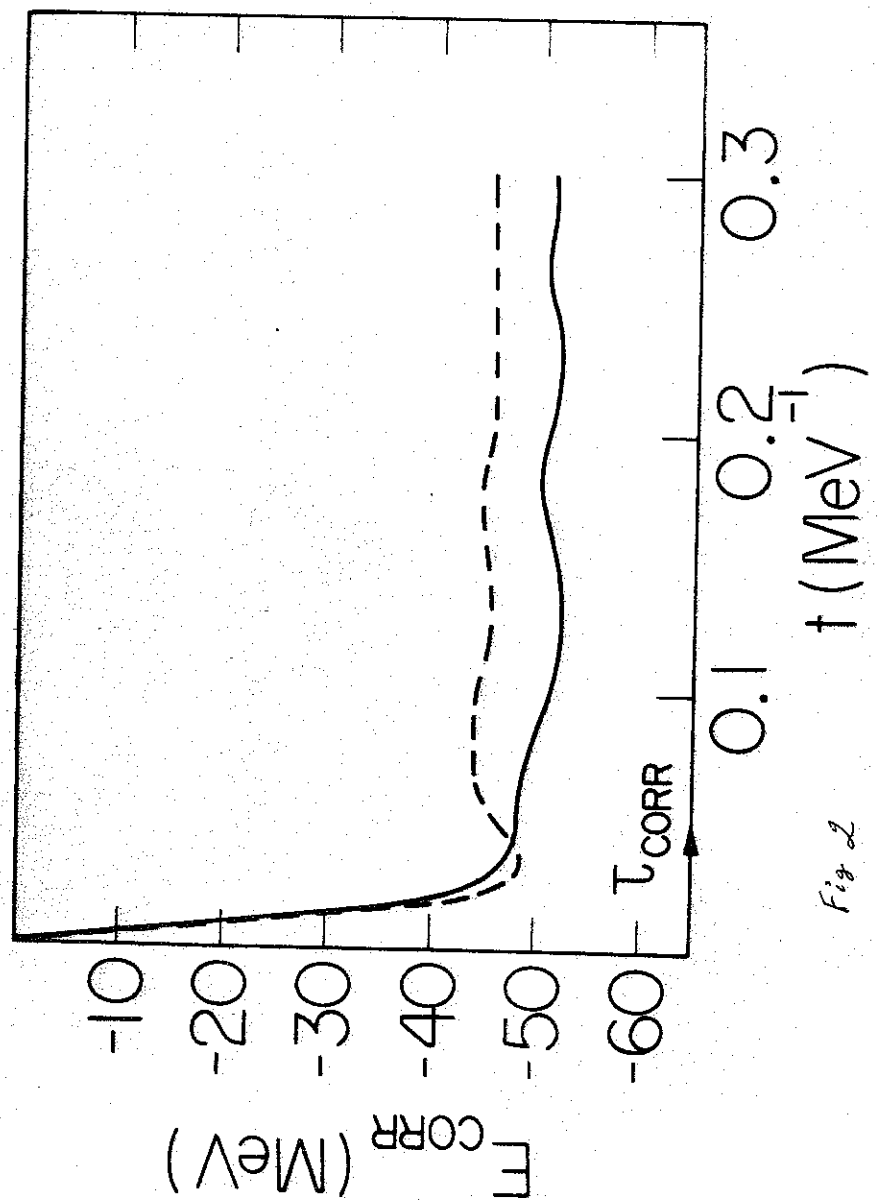

E_{CORR} (MeV)
-10
-20
-30
-40
-50
-60
τ_{CORR}
0.1
0.2
0.3
t (MeV^{-1})

Fig 2

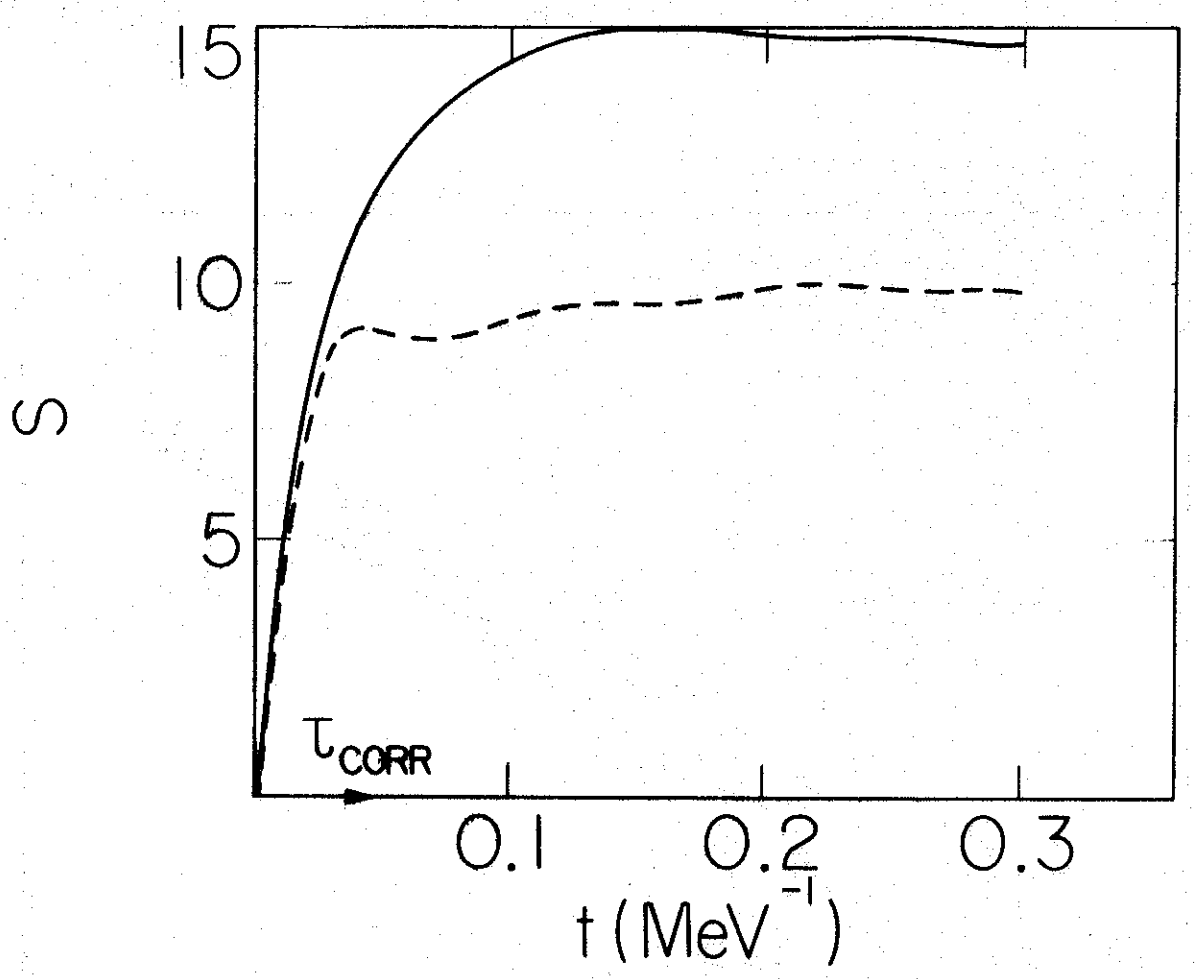

15
10
5
S
τ_{CORR}
0.1
0.2
0.3
t (MeV^{-1})

Fig 3

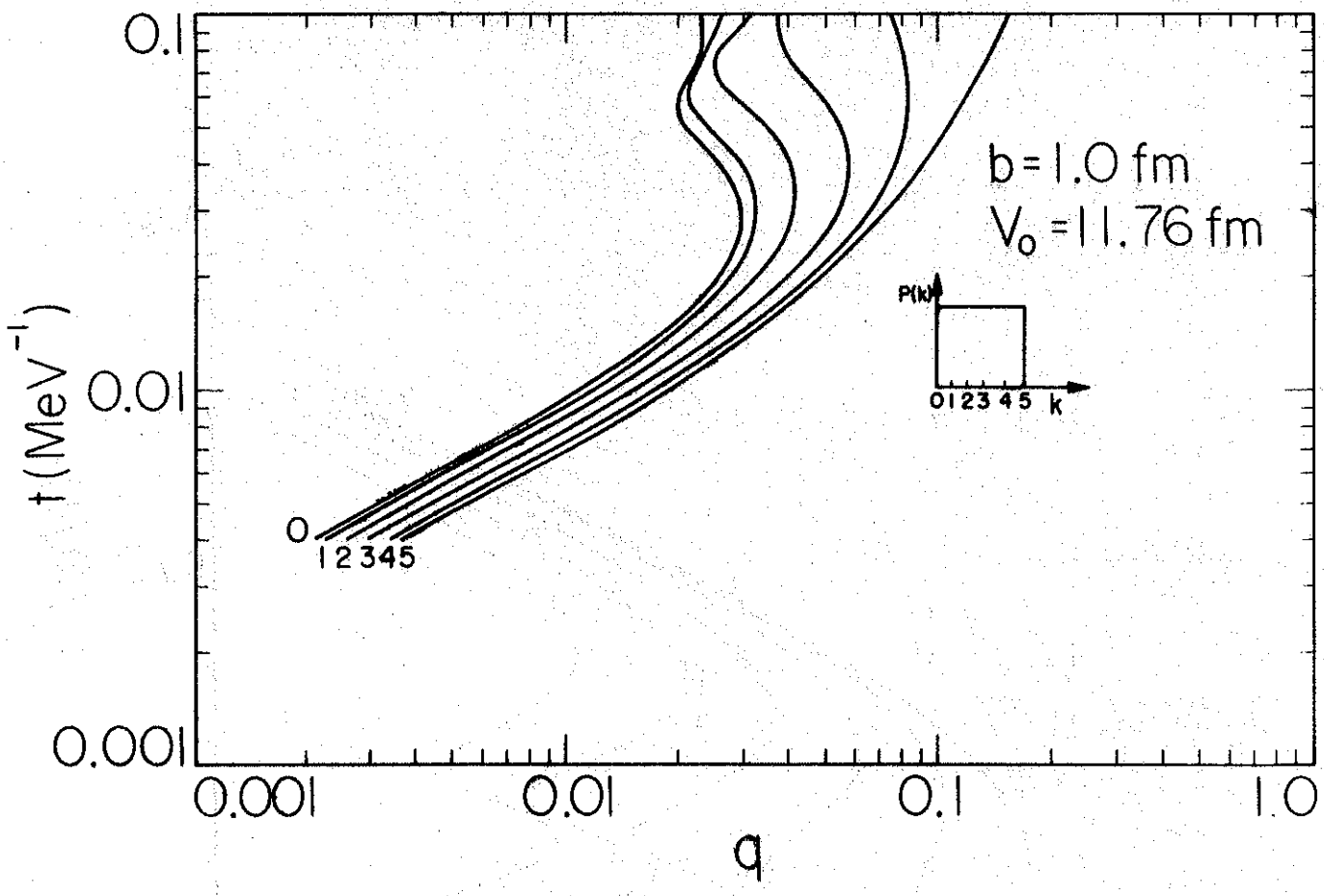
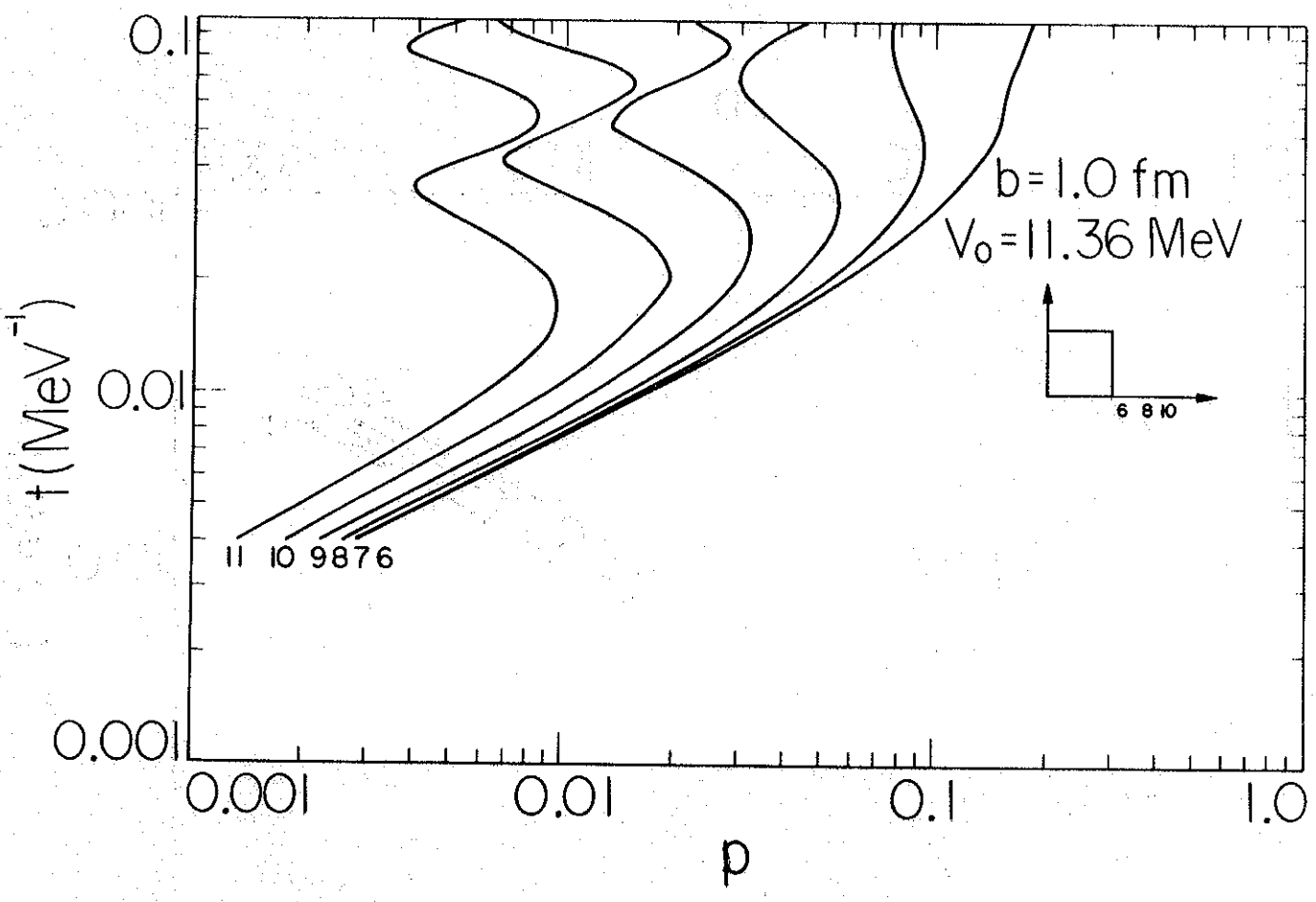

0.1
0.01
0.001
t (MeV^{-1})
0.001
0.01
0.1
1.0
q
b = 1.0 fm
V_0 = 11.76 fm
P(k)
0 1 2 3 4 5 k
0
1 2 3 4 5

Fig 4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0.01
0.001
t (MeV⁻¹)
b = 1.0 fm
V₀ = 11.36 MeV
6 8 10
11 10 9 8 7 6
0.001
0.01
0.1
1.0
p

Fig 5

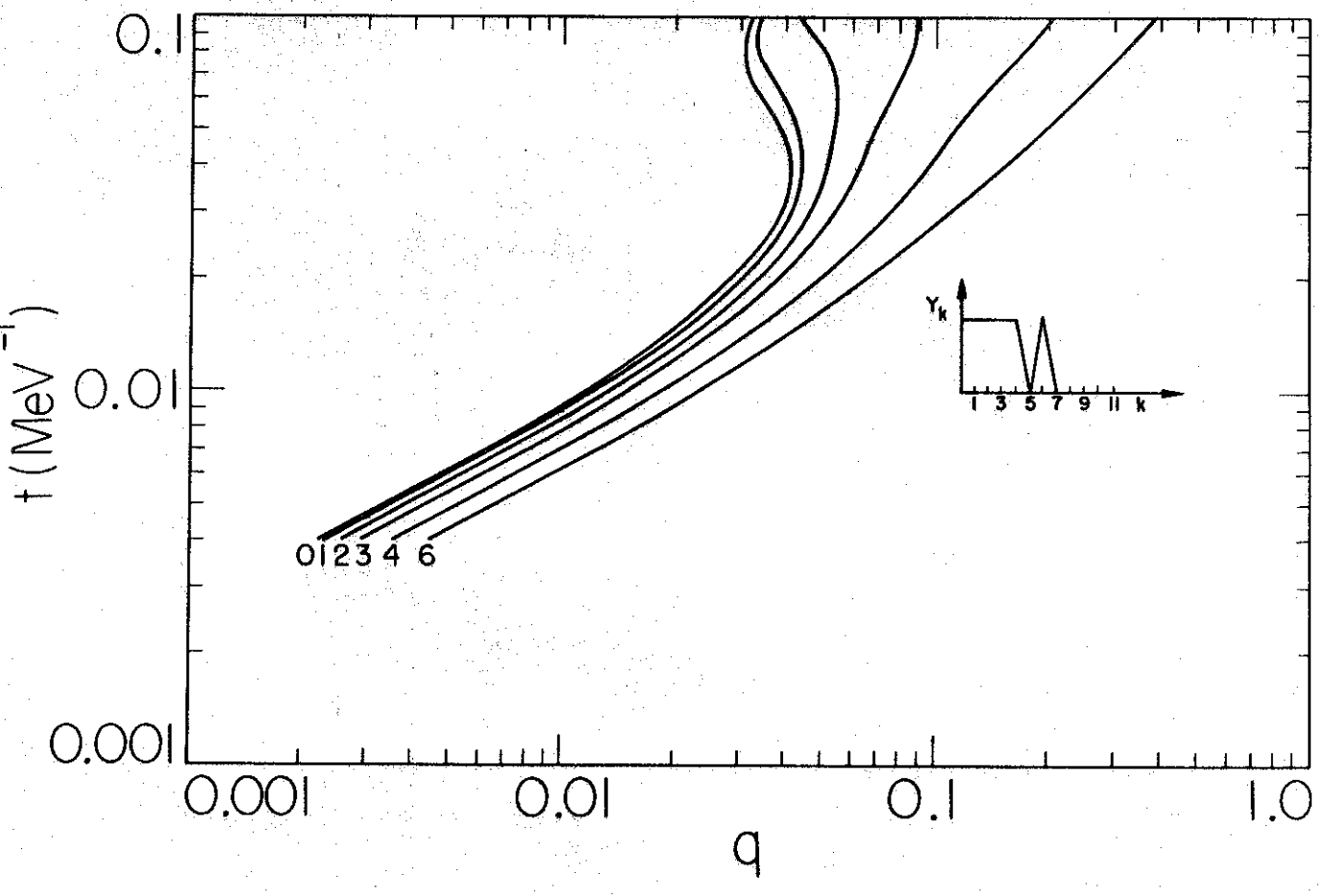
0.1
0.01
0.001
t (MeV⁻¹)
Yk
1 3 5 7 9 11 k
0 1 2 3 4 6
0.001
0.01
0.1
1.0
q

Fig 6

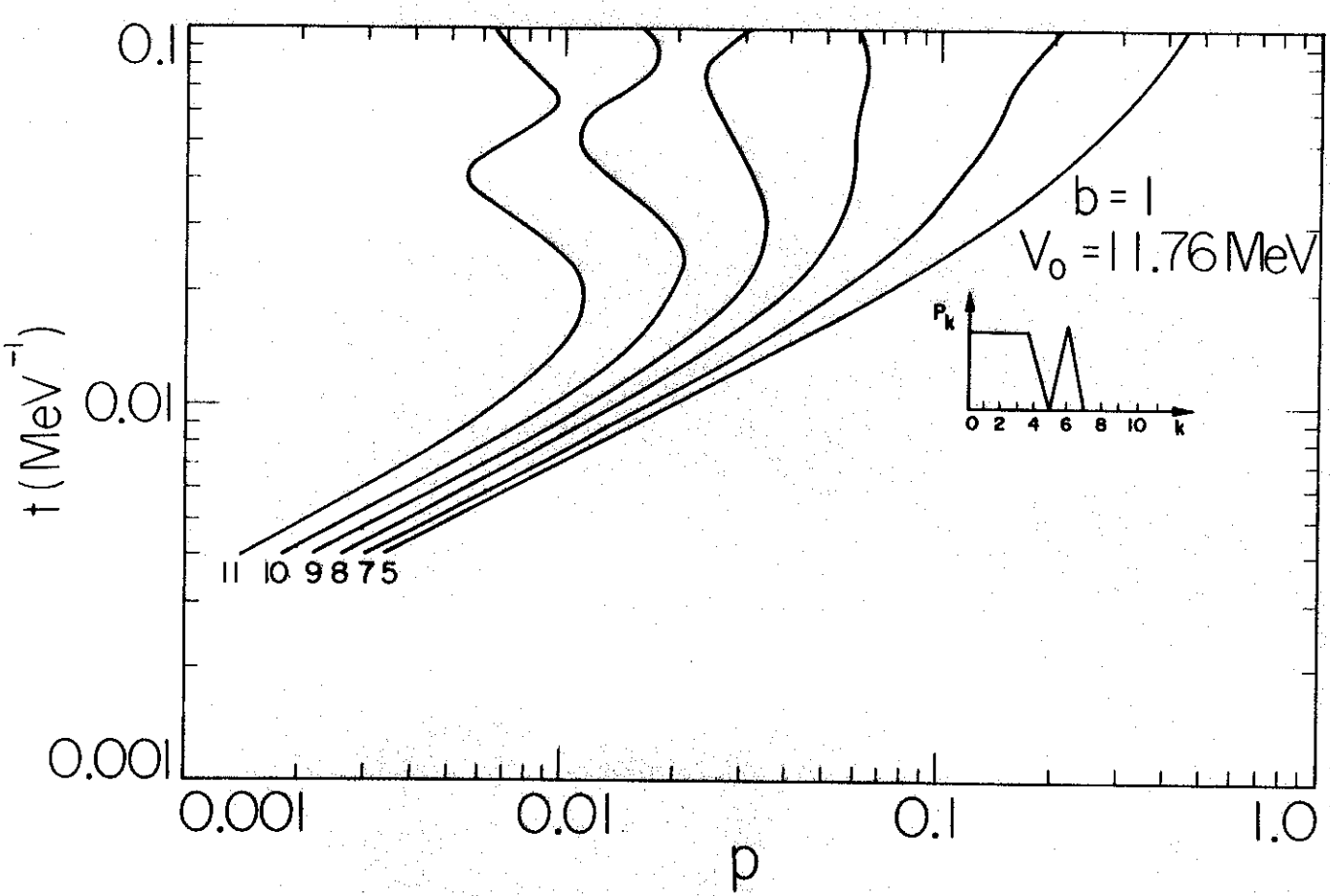
0.1
0.01
0.001
t (MeV⁻¹)
b = 1
V₀ = 11.76 MeV
P_k
0 2 4 6 8 10 k
11 10 9 8 7 5
0.001
0.01
0.1
1.0
p

Fig 7