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APPROXIMATION FOR A NON-IDEAL BOSE GAS IN
ONE-DIMENSION

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Exact Solution Versus Gaussian Approximation for a Non-Ideal Bose Gas in One-Dimension

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Abstract

We investigate ground-state and excitation spectrum of a system of non-relativistic bosons in one-dimension interacting through repulsive, two-body contact interactions in a self-consistent Gaussian mean-field approximation which consists in writing the variationally determined density operator as the most general Gaussian functional of the quantized field operators. There are mainly two advantages in working with one-dimension. First, the existence of an exact solution for the ground-state and excitation energies. Second, neither in the perturbative results nor in the Gaussian approximation itself we do not have

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to deal with the three-dimensional pathologies of the contact interaction . So that this scheme provides a clear comparison between these three different results.

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1 Introduction

The main objective of this work is to compare the standard perturbation results with the unperturbative ones obtained with the Gaussian approximation in the case of a system of non-relativistic bosons in one dimension interacting through repulsive, two-body contact interactions. The use of an one-dimensional problem gives the advantage of dealing with a repulsive contact interaction without getting into problem due to divergencies [1, 2]. Also the existence of an exact solution in this case show us clearly when the perturbation theory breaks down and how the upperbound non-perturbative results stands in this region.

The Gaussian mean-field approximation which we will use is based in terms of a time-dependent projection approach developed earlier for the non-relativistic nuclear many-body dynamics by Nemes and de Toledo Piza [3]. This approach allows for the formulation of a mean-field expansion for the dynamics of the two-point correlation function from which one recovers the results of the Gaussian mean-field approximations in lowest order, i.e., this approach permit to include and to evaluate higher dynamical corrections effects to the simplest Gaussian mean-field approximation. Moreover, the expansion is energy-conserving (for closed system) to all orders [4]. This approach was recently applied in the context of the field-theoretical models, namely, to treat an uniform relativistic (1+1)-dimensional self-interacting boson system described by the $\lambda\phi^4$ theory [5], to treat an uniform relativistic (1+1)-dimensional self-interacting fermion system described by the chiral Gross-Neveu model [6], and to treat an uniform (3+1)-dimensional relativistic interacting boson-fermion system described by the Plasma Scalar model [7].

Although we developed a temperature dependent formalism in this paper

we will concentrate on the zero temperature case and calculate in Gaussian mean-field approximation the physical quantities related to the optimized free energy such as ground state energy and sound velocity to compare with perturbative and exact results given in literature [8, 9].

In Section 2, we define the problem and its exact solution. In Section 3, the formulation which we adopt is reviewed and the equilibrium solutions are obtained. Through a truncated version of the Gaussian variational equation we obtain the perturbative results in Section 4. In Section 5 our numerical results are detailed. Section 6 contains our conclusions.

2 The problem and the exact solution

We consider an uniform system of non-relativistic, interacting, spinless bosons in one-dimension described by the Hamiltonian

$$H = - \sum_i \left(\frac{\partial^2}{\partial x_i^2} \right) + 2c \sum_{i,j} \delta(x_i - x_j) , \quad (1)$$

where $2c$ is the amplitude of the delta function. The only dimensionless intensive variable in the theory is

$$\gamma = \frac{c}{\rho} .$$

Lieb and Liniger in Ref. [8] has shown that the exact ground state energy can be obtained by solving an inhomogeneous Fredholm equation of the second kind. So that in the thermodynamic limit ($N, L \rightarrow \infty$ such that $\rho = \text{fixed constant}$) we can write the ground state energy per particle as

$$\frac{E_0}{N} = \frac{1}{\rho} \int_{-K}^K f(k) k^2 dk , \quad (2)$$

where $f(k)$ is the solution of

$$2c \int_{-K}^K \frac{f(p)}{c^2 + (p-k)^2} dp = 2\pi f(k) - 1 \quad (3)$$

with the condition

$$\int_{-K}^K f(k) dk = \rho . \quad (4)$$

For computational purposes we can change variables as follows

$$k = Kx ; \quad c = K\lambda ; \quad f(Kx) = g(x) ,$$

in terms of which the Eqs.(2), (3) and (4) become, respectively,

$$\frac{E_0}{N} = \rho^2 \frac{\lambda^3}{\lambda^3} \int_{-1}^1 g(x) x^2 dx \quad (5)$$

$$1 + 2\lambda \int_{-1}^1 \frac{g(x)}{\lambda^2 + (x-y)^2} dx = 2\pi g(y) \quad (6)$$

$$\gamma \int_{-1}^1 g(x) dx = \lambda . \quad (7)$$

For a fixed λ we can calculate $g(x)$ having $\lambda(\gamma)$ and with it follows $\frac{E_0}{N}(\gamma)$ and $K(\gamma)$ [8]. Once we have the ground state energy it is possible to calculate the chemical potential

$$\mu = \frac{\partial E_0}{\partial N} . \quad (8)$$

From μ we can calculate the sound velocity derived from the macroscopic compressibility

$$v_s = 2 \left(\mu - \frac{1}{2} \gamma \frac{\partial \mu}{\partial \gamma} \right) . \quad (9)$$

Lieb, in another work [9], also has shown that this theory exhibit two types of excitations. The energy of the first type of excitation is given by

$$\epsilon_1(p) = -\mu + q^2 + 2 \int_{-K}^K k J(k) dk , \quad (10)$$

where μ is the chemical potential and

$$p = q + \int_{-K}^K J(k) dk , \quad (11)$$

while $J(k)$ is again a solution of a Fredholm equation

$$2\pi J(k) = 2c \int_{-K}^K \frac{J(r)dr}{c^2 + (k-r)^2} - \pi + 2 \tan^{-1}(q-k) . \quad (12)$$

The energy of the second type of excitation have the same structure and is such that

$$\epsilon_2(p) = \mu - q^2 + 2 \int_{-K}^K kG(k)dk \quad (13)$$

$$p = -q + \int_{-K}^K G(k)dk \quad (14)$$

$$2\pi G(k) = 2c \int_{-K}^K \frac{G(r)dr}{c^2 + (k-r)^2} + \pi - 2 \tan^{-1}(q-k) . \quad (15)$$

To solve these equation we use the same procedure used in the ground state energy. Here q plays the same role as λ in the other case.

3 Gaussian approximation

In second quantization, rewriting the Hamiltonian (1), in momentum representation with periodic boundary conditions in volume V , follows

$$H = \sum_{\vec{k}} k^2 a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{c}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} a_{\vec{k}_1 + \vec{q}}^\dagger a_{\vec{k}_2 - \vec{q}}^\dagger a_{\vec{k}_2} a_{\vec{k}_1} , \quad (16)$$

where k^2 is the free particle kinetic energy, and the contact repulsive ($c > 0$) interaction potential between a pair of particles is $2c \delta(\vec{x} - \vec{x}')$. The $a_{\vec{k}}^\dagger$ and $a_{\vec{k}}$ are boson creation and annihilation operators, which satisfy the standard boson commutation relations at equal times.

3.1 Projection technique and approximation scheme

In this section we introduce the time-dependent projection technique [3] which will permit to obtain closed approximations to the dynamics of a system. It has been developed earlier in the context of nonrelativistic nuclear

many-body dynamics and was recently applied in the quantum-field theoretical context [5, 6, 7]. It allows for the formulation of a mean-field expansion for the dynamics of the two-point correlation function from which one recovers the results of the Gaussian mean-field approximations in lowest order. If carried to higher orders it allows for the inclusion and evaluation of higher dynamical correlation corrections to the simplest mean-field approximation.

We will describe the quantum state of the system in Heisenberg picture in terms of a many-body density operator \mathcal{F} , a time independent, non-negative, Hermitian operator with unit trace. \mathcal{F} may in general involve statistical mixtures, in particular in the boson number operator, in the spirit of a grand canonical description. Our implementation of the Gaussian approximation will consist in decomposing the full density \mathcal{F} as

$$\mathcal{F} = \mathcal{F}_0(t) + \mathcal{F}'(t) , \quad (17)$$

where $\mathcal{F}_0(t)$ is a Gaussian ansatz which achieves a Hartree-Fock factorization of traces involving more than two field operators. The Gaussian density $\mathcal{F}_0(t)$ is chosen as having the form of an exponential of a bilinear, Hermitian expression in the fields normalized to unit trace [10, 11]. In the momentum basis, it reads

$$\mathcal{F}_0 = \frac{\exp \left[\sum_{(\vec{k}_1, \vec{k}_2)} A_{\vec{k}_1, \vec{k}_2} a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger + B_{\vec{k}_1, \vec{k}_2} a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger + C_{\vec{k}_1, \vec{k}_2} a_{\vec{k}_1} a_{\vec{k}_2} \right]}{\text{Tr} \left\{ \exp \left[\sum_{(\vec{k}_1, \vec{k}_2)} A_{\vec{k}_1, \vec{k}_2} a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger + B_{\vec{k}_1, \vec{k}_2} a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger + C_{\vec{k}_1, \vec{k}_2} a_{\vec{k}_1} a_{\vec{k}_2} \right] \right\}} . \quad (18)$$

The parameters in Eq.(18) are fixed by requiring that mean values in \mathcal{F}_0 of expressions that are bilinear in the fields reproduce the corresponding \mathcal{F} averages [see Eqs.(21) and (22) below]. \mathcal{F}_0 is a time-dependent object, which acquires a particularly simple form when expressed in terms of the Bogolyubov quasi-boson operators

$$\eta_{\vec{k}} = x_{\vec{k}}^* b_{\vec{k}} + y_{\vec{k}}^* b_{-\vec{k}}^\dagger$$

$$\eta_{\vec{k}}^\dagger = x_{\vec{k}} b_{\vec{k}}^\dagger + y_{\vec{k}} b_{-\vec{k}}$$

where

$$b_{\vec{k}} = a_{\vec{k}} - \Gamma_{\vec{k}}$$

$$\Gamma_{\vec{k}} = \langle a_{\vec{k}} \rangle$$

We have used the isotropy of the uniform system to make the c -number transformation parameters x_k , y_k and Γ_k dependent only on the magnitude of \vec{k} . In order for this transformation to be canonical we have still to impose on the x_k and y_k the usual normalization condition

$$|x_k|^2 - |y_k|^2 = 1 \quad (19)$$

In terms of the Bogolyubov quasi-boson operators, the Gaussian truncated density operator is now written explicitly as

$$\mathcal{F}_0 = \prod_{\vec{k}} \frac{1}{1 + \nu_k} \left(\frac{\nu_k}{1 + \nu_k} \right)^{\eta_{\vec{k}}^\dagger \eta_{\vec{k}}} \quad (20)$$

Straightforward calculation shows that

$$Tr(\eta_{\vec{k}}^\dagger \eta_{\vec{k}'} \mathcal{F}_0) = \nu_k \delta(\vec{k} - \vec{k}') \quad (21)$$

so that the ν_k are positive quantities corresponding to mean occupation numbers of the η -bosons. One also finds that

$$Tr[(x_k^* a_{\vec{k}} + y_k^* a_{-\vec{k}}^\dagger)^n \mathcal{F}_0] = Tr[(\eta_{\vec{k}} + A_k)^n \mathcal{F}_0] = A_k^n \quad (22)$$

with $A_k = x_k^* \Gamma_k + y_k^* \Gamma_k^*$ so that non vanishing values of the Γ_k correspond to coherent condensates of unshifted transformed bosons. We again invoke the uniformity of the system to impose

$$\Gamma_k = \delta_{k,0} \Gamma_0 \quad (23)$$

in the calculations to follow.

The "remainder" density $\mathcal{F}'(t)$, defined by Eq.(17), is a traceless, pure correlation density. As already remarked, a crucial point to observe is that $\mathcal{F}_0(t)$ can be written as a time-dependent projection of \mathcal{F} , i.e.,

$$\mathcal{F}_0(t) = \mathcal{P}(t) \mathcal{F} \quad \text{with} \quad \mathcal{P}(t) \mathcal{P}(t) = \mathcal{P}(t) \quad (24)$$

In order to completely define this projector we require further that it satisfies

$$i\dot{\mathcal{F}}_0(t) = [\mathcal{P}(t), \mathcal{L}] \mathcal{F} = [\mathcal{F}_0(t), H] + \mathcal{P}(t) [H, \mathcal{F}] \quad (25)$$

where \mathcal{L} is the Liouvillian defined as

$$\mathcal{L} \cdot = [H, \cdot] \quad (26)$$

H being the Hamiltonian of the field. Eq.(25) is just the Heisenberg picture counterpart of the condition $\dot{\mathcal{P}}(t) \mathcal{F} = 0$ which has been used to define $\mathcal{P}(t)$ in the Schrödinger picture [4]. It is possible to show that conditions (24) and (25) make $\mathcal{P}(t)$ unique and to obtain an explicit form for this object in terms of the quasi-boson operators and of the natural orbital occupations [3, 4, 5, 7].

The existence of the projector $\mathcal{P}(t)$ allows one to obtain an equation relating the correlation part $\mathcal{F}'(t)$ to the Gaussian part $\mathcal{F}_0(t)$ of the full density. This can be immediately obtained from Eqs.(17), (24) and (25) and reads

$$(i\partial_t + \mathcal{P}(t)\mathcal{L}) \mathcal{F}'(t) = (\mathcal{I} - \mathcal{P}(t)) \mathcal{L} \mathcal{F}_0(t) \quad (27)$$

This equation has the formal solution

$$\mathcal{F}'(t) = \mathcal{G}(t, 0) \mathcal{F}'(0) - i \int_0^t dt' \mathcal{G}(t, t') (\mathcal{I} - \mathcal{P}(t')) \mathcal{L} \mathcal{F}_0(t') \quad (28)$$

where the first term accounts for initial correlations possibly contained in \mathcal{F} . The object $\mathcal{G}(t, t')$ is the time-ordered Green's function

$$\mathcal{G}(t, t') = T \left(\exp \left[i \int_{t'}^t d\tau \mathcal{P}(\tau) \mathcal{L} \right] \right) \quad (29)$$

We see thus that $\mathcal{F}'(t)$, and therefore also \mathcal{F} [see Eq.(17)], can be formally expressed in terms of $\mathcal{F}_0(t')$ (for $t' \leq t$) and of initial correlations $\mathcal{F}'(0)$. This allows us to express also the dynamics of the system as functionals of $\mathcal{F}_0(t')$ and of the initial correlations. Since, on the other hand, the reduced density $\mathcal{F}_0(t')$ is expressed in terms of the one-boson densities alone, we see that the resulting equations are essentially closed equations. Note, however, that the complicated time dependence of the field operators is explicitly probed through the memory effects present in the expression (28) for $\mathcal{F}'(t)$. Approximations are therefore needed for the actual evaluation of this object. A systematic expansion scheme for the memory effects has been discussed in Refs. [3, 4, 5, 7]. The lowest order correlation corrections to the pure mean field approximation, in which \mathcal{F}' is simply ignored, correspond to replacing the full Heisenberg time-evolution of operators occurring in the collision integrals by a mean-field evolution governed by

$$H_0 = \mathcal{P}^\dagger(t)H .$$

Consistently with this approximation, \mathcal{L} is replaced in (25) and (26) by $\mathcal{L}_0 \cdot = [H_0, \cdot]$. In this way correlation effects are treated to second order in H in the resulting collision integrals.

An important feature of this scheme (which holds also for higher orders of the expansion [4]) is that the mean energy is conserved, namely

$$\frac{\partial}{\partial t} \langle H \rangle = 0$$

where

$$\langle H \rangle = Tr H \mathcal{F}_0(t) + Tr H \mathcal{F}'(t) .$$

In the following sections we apply the general expressions obtained in above to treat a uniform boson system described by the Hamiltonian given in Eq.(16). We will consider only the lowest (mean-field) approximation, corresponding to $\mathcal{F}'(t) = 0$. Collisional correlations will be treated elsewhere.

3.2 Temperature time-dependent Gaussian treatment

First, it is important to note that the truncated density \mathcal{F}_0 in general breaks the global gauge symmetry of H , which is responsible for the conservation of

the number of a -bosons. It is possible to verify that assumption calculating the dispersion

$$\langle N^2 \rangle - \langle N \rangle^2 = Tr[\mathcal{F}_0 \sum_{\vec{k}, \vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} a_{\vec{k}'}^\dagger a_{\vec{k}}] - \{Tr[\mathcal{F}_0 \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}}]\}^2 .$$

Calculating the traces above we have

$$\begin{aligned} \langle N^2 \rangle - \langle N \rangle^2 &= 2|\Gamma_0|^2[|x_0|^2\nu_0 + |y_0|^2(1 + \nu_0)] - 2\Gamma_0^{*2}x_0y_0^*(1 + 2\nu_0) - \\ &\quad - 2\Gamma_0^2y_0x_0^*(1 + 2\nu_0) + |\Gamma_0|^2 + \sum_{\vec{k}}\{|x_k|^2\nu_k + (1 + \nu_k)|y_k|^2\} + \\ &\quad + \sum_{\vec{k}}\{(|x_k|^2\nu_k + (1 + \nu_k)|y_k|^2)^2 + |x_k|^2|y_k|^2(1 + 2\nu_k)^2\} . \end{aligned}$$

Furthermore, mean values of many-boson operators taken with respect to \mathcal{F}_0 will contain no irreducible many-body parts, so that the replacement of \mathcal{F} by \mathcal{F}_0 amounts to a mean field approximation. The states described by \mathcal{F}_0 have therefore to be interpreted as "intrinsic" mean field states.

In order to develop a finite temperature treatment within this framework, we look for variational extrema of an approximation Ω to the grand potential written in terms of the truncated density operator \mathcal{F}_0 as

$$\Omega = Tr[\mathcal{F}_0(H - \mu N + KT \ln \mathcal{F}_0)] \quad (30)$$

with

$$N = \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} ,$$

where K is the Boltzmann constant and the Lagrange multipliers μ and T will play the role of chemical potential and temperature respectively. The replacement of the full density operator \mathcal{F} by \mathcal{F}_0 implies not only truncation of correlation energies but also replacement of the full entropy by the mean field entropy $S_0 = -KTr[\mathcal{F}_0 \ln \mathcal{F}_0]$. Variations will be taken with respect to the parameters which determine the truncated density \mathcal{F}_0 , and the value of μ is fixed by choosing the particle density of the system. A detailed

justification of this general procedure has been given by Balian and Vénéroni [11], who have shown that it corresponds to the optimal determination (in the variational sense) of the grand partition function (hence of the grand potential) for the problem when one restricts oneself to trial density operators of the form given in Eq.(20). We have to emphasize that the use of this functional Ω does not assure that we will have the best variational results for other observables. See discussion in Secs. 5 and 6.

An important simplification occurs in the case of stationary problems. In this case x_k, y_k and Γ_0 can be taken to be real and we can use a simple parametric representation that automatically satisfies the canonicity condition. It reads

$$x_k = \cosh \sigma_k, \quad y_k = \sinh \sigma_k. \quad (31)$$

It is then straightforward to evaluate the traces involved in Ω to obtain

$$\begin{aligned} \Omega = & \sum_{\vec{k}} \left(e(k) - \mu + \frac{4c\Gamma_0^2}{V} \right) \left[\frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] - \mu\Gamma_0^2 + \frac{c\Gamma_0^4}{V} \\ & - \frac{c\Gamma_0^2}{V} \sum_{\vec{k}} (1 + 2\nu_k) \sinh 2\sigma_k + \frac{2c}{V} \left\{ \sum_{\vec{k}} \left[\frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] \right\}^2 \\ & + \frac{c}{4V} \left\{ \sum_{\vec{k}} (1 + 2\nu_k) \sinh 2\sigma_k \right\}^2 \\ & - KT \sum_{\vec{k}} [(1 + \nu_k) \ln(1 + \nu_k) - \nu_k \ln \nu_k]. \end{aligned} \quad (32)$$

In a similar way the number constraint $Tr[\mathcal{F}_0 N] = \langle N \rangle$ evaluates to

$$\langle N \rangle = \Gamma_0^2 + \sum_{\vec{k}} \left[\frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right]. \quad (33)$$

3.3 Equilibrium solutions

Equations determining the form of the truncated density \mathcal{F}_0 appropriate for thermal equilibrium are in general derived by requiring that Ω , Eq.(32), is

stationary under arbitrary variations of Γ_0, σ_k and ν_k . Variation with respect to Γ_0 gives the gap equation

$$\Gamma_0 \left\{ \frac{4c}{V} \Gamma_0^2 - 2\mu - 4cA + 8cB \right\} = 0, \quad (34)$$

where the quantities A, B and C , in the thermodynamic limit as $\sum_k \rightarrow \frac{L}{2\pi} \int_{-\infty}^{+\infty} dk$, are given by

$$\begin{aligned} A &= \frac{1}{4\pi} \int_{-\infty}^{\infty} \sinh 2\sigma_k k^2 dk \\ B &= \frac{1}{4\pi} \int_{-\infty}^{\infty} [\cosh 2\sigma_k - 1] k^2 dk \\ C &= \frac{1}{4\pi} \int_{-\infty}^{\infty} e(k) [\cosh 2\sigma_k - 1] k^2 dk. \end{aligned}$$

The gap equation, Eq.(34), besides the trivial solution $\Gamma_0 = 0$ (non-condensed phase), may also admit a solution with a non-vanishing value of Γ_0 (condensed phase) obtained by requiring that the expression in curly brackets vanishes. This condensed phase solution involves the number constraint, Eq.(33), in addition to the values of ν_k and σ_k , which are determined by the remaining variational conditions on Ω . In order to simplify the algebraic work involved in the study of this class of solutions, it is sometimes convenient to use the gap equation, Eq.(34), to eliminate Γ_0 from Ω , which then becomes

$$\Omega = F - \mu \langle N \rangle.$$

This identifies the free energy F as

$$\begin{aligned} F = & CV - \lambda \rho (A - B)V + \frac{\lambda}{2} (\rho^2 + A^2 - B^2)V + \lambda ABV \\ & - KT \sum_{\vec{k}} [(1 + \nu_k) \ln(1 + \nu_k) - \nu_k \ln \nu_k]. \end{aligned} \quad (35)$$

For condensed phase, the chemical potential follows from Eqs.(33) and (34)

$$\mu = 2c(\rho - A + B) . \quad (36)$$

Extremizing F by setting derivatives with respect to σ_k and ν_k equal to zero one gets

$$\tanh 2\sigma_k = \frac{2c[\rho - B - A]}{e(k) + 2c[\rho - B + A]} \quad (37)$$

and

$$\nu_k = \frac{1}{\{exp[\sqrt{\Delta}/KT] - 1\}} \quad (38)$$

where

$$e_g(k) = \sqrt{\Delta} = \sqrt{e(k)^2 + 4ce(k)[\rho - B + A] + 16c^2[\rho - B]A} . \quad (39)$$

corresponds to the excitation spectrum in our approximation. This result can be confirmed through an RPA calculation Ref. [12]. Particularly in this paper we are interested on properties for $T = 0$ so that A and B can be found from gap equation (37), for a given ρ , solving the system

$$\begin{cases} A = \frac{1}{4\pi} \int_{-\infty}^{\infty} \frac{2c[\rho - B - A]}{\sqrt{\Delta}} dk \\ B = \frac{1}{4\pi} \int_{-\infty}^{\infty} \left\{ \frac{e(k) + 2c[\rho - B + A]}{\sqrt{\Delta}} - 1 \right\} dk \end{cases} . \quad (40)$$

The ground state energy is then given by

$$\frac{F(T=0)}{N} = \frac{E}{N} = \frac{C}{\rho} - 2c\rho^2(A - B) + c\rho(\rho^2 + A^2 - B^2) + 2c\rho AB . \quad (41)$$

For the trivial solution $\Gamma_0 = 0$ (non-condensed phase), we obtain the gap equation below

$$\tanh 2\sigma_k = \frac{-2cA}{e(k) - \mu + 2cB} . \quad (42)$$

The only possible solution is $A = 0$ following that $\sigma_k = 0$. Therefore, from Eq.(33), we have the solution

$$\rho = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dk}{\exp[(k^2 - \mu + 4c\rho)/KT] - 1}$$

That is the standard Hartree-Fock result which corresponds to a shift in the chemical potential when compared with the ideal Bose gas [13]. In this phase, we show in Ref. [12] that when $T \rightarrow 0$ we have $\mu \rightarrow 4c\rho$.

We still have to decide what phase shall we use when $T = 0$. To do so, let us examine the chemical potential μ since from Eq.(36). When $A > 0$ follows from Eq.(36) that $\mu_{\Gamma_0 \neq 0} < 4c\rho = \mu_{\Gamma_0 = 0}$ and it is easy to check that for a given ρ at $T = 0$ there are always A and B that are solutions of the system (40). This does not happen in the case of non-condensed phase at $T = 0$ [1]. Therefore, we conclude that the stable phase at $T = 0$ for any ρ is the one with $\Gamma_0 \neq 0$.

Finally, in this calculation A, B and C are finite meaning that no renormalization is needed. This is a quite different result from the three-dimensional case Ref. [1, 12]

4 Independent η -bosons - Perturbative results

In Ref. [1] it is shown that from a convenient truncation of the Gaussian approximation in the three-dimension problem, it is possible to obtain the usual perturbative results in the parameter γ . Here we will do the something obtaining the results of Ref.[8, 9].

This truncation of the Gaussian approximation consists in neglecting all terms representing interactions between η -bosons. If we discard interaction between η -bosons amounts to dropping all double integrals in Eq.(35). The variational conditions on σ_k and ν_k appear then as

$$\tanh 2\sigma_k = \frac{2c\rho}{k^2 + 2c\rho} \quad (43)$$

and

$$\nu_k = \frac{1}{e^{\frac{1}{RT}} \sqrt{k^4 + 4c\rho k^2} - 1} \quad (44)$$

which gives us the usual phonon excitation spectrum

$$\epsilon(p) = \sqrt{p^4 + 4\gamma p^2} \quad (45)$$

When we using these results for calculating F , replacing the sums by integrals, we obtain

$$F(T=0) = E = c\rho^2 L + \frac{L}{2\pi} \int_{-\infty}^{\infty} \left\{ \sqrt{k^4 + 4c\rho k^2} - (k^2 + 2c\rho) \right\} dk \quad (46)$$

Evaluating the integral and once again stressing that there is no need for regularization here

$$\frac{E}{N} = \rho^2 \gamma \left(1 - \frac{4\sqrt{\gamma}}{3\pi} \right) \quad (47)$$

Using Eq.(8) and Eq.(9) for the chemical potential and the sound velocity we get

$$\mu = 2\gamma \left(1 - \frac{\sqrt{\gamma}}{\pi} \right) \quad (48)$$

$$v_s = 2\rho \left[\left(\gamma - \frac{1}{2\pi} \gamma^{\frac{3}{2}} \right) \right]^{\frac{1}{2}} \quad (49)$$

We can check that the sound velocity obtained from the excitation spectrum Eq.(45) defined by

$$v_s = \lim_{p \rightarrow 0} \frac{\partial \epsilon(p)}{\partial p} \quad (50)$$

gives us $v_s = 2\rho\sqrt{\gamma}$, that is exactly one order lower of the one obtained through the compressibility Eq.(49)

5 Numerical Results

We did all our calculations for a fixed $\rho = 1$. For the exact solution we follow the steps of Ref.[8] solving numerically the Eqs.(5),(6) and (7). For the Gaussian approximation we solve the system of Eqs.(39) and (40), and we calculate the ground state energy given by the Eq.(41). Finally for the perturbative results we use closed expression (46). All this results are shown in Fig.1, where we plot the ground state energy as a function of γ . We clearly see the upperbound Gaussian results and the, as expected, good results for low γ of both perturbative and Gaussian results.

For the exact and Gaussian sound velocity we differentiate numerically the respective ground state curve. For the perturbative solution we have two possibilities one using the compressibility through Eq.(49) or in lower order using the excitation spectrum Eq.(45). We plot the sound velocity as a function of γ in Fig.2. We note that the Gaussian result is also an upperbound and for this range of γ the results obtained from perturbative theory using the compressibility and the exact solution are graphically indistinguishable.

Finally for the excitation spectrum we solve numerically (10), (11) and (12) for the first type of excitations and (13), (14) and (15) for the second type. To calculate the excitation spectrum in the Gaussian approximation using Eq.(39), once we have solved the system (40). For the perturbative theory we use Eq.(45). In Fig.3 and Fig.4 we plot the excitation energy as a function of the momentum for $\gamma = 0.787094$ and $\gamma = 3.07725$ respectively. Neither perturbative nor Gaussian approximation describe the exact second type of excitations and the Gaussian approximation introduces a gap in the excitation energy that gets bigger if we go to the non-perturbative limit.

6 Conclusion

Using a one-dimensional problem help us to understand in a clear way the nature of the Gaussian approximation from the grand-potential functional. We avoid problems related to renormalization [1] and have the exact solution for the ground state energy and excitation spectrum [8, 9].

We were able to see in Fig. 1 that the ground state energy for low values of γ both perturbative and Gaussian (non-perturbative) results are quite good. As γ increases we have a region where the exact solution is in between the

two approximations. For higher values of γ the perturbative results breaks down completely and the Gaussian approximation still gives us an good upperbound result. This shows us that for high values of γ a self-consistent non-perturbative calculation should be used.

For the sound velocity, Fig. 2, we see that both perturbative and Gaussian results are upperbound approximation to the exact result.

From Figs.3 and 4, we see a very interesting feature of the Gaussian approximation, namely, it produces a coherent macroscopic occupation for $k = 0$. This occupation is artificial because as we can see from the exact solution there is no macroscopic occupation for $k = 0$.

Therefore, the results that are related directly from the thermodynamic potential as the ground state energy, the sound velocity obtained through the compressibility are good upperbounds. Yet the gap in the excitation spectrum, that came from the occupations, are very different from the exact solution. So, the fact that using the optimal determination of the grand potential does not assure that we will have the best variational result for the occupations /citeBV.

This confirm that we shall use our Gaussian approximation that introduce quantum correlations at the level of a mean field calculation, through a coherent condensate and pairing introduced in a non-perturbative self-consistent way, as a good upperbound for thermodynamic properties derived directly from the thermodynamic potentials. For better results in other observables we should involve ourselves in a more difficult task of finding the best functional related to this specific observable with the same trial density operator of the form given in Eq.(20).

Finally we want to point out that the formalism developed here allows us to go in straightfoward way to $T \neq 0$ still keeping the variational characteristic of having an upperbound result.

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References

- [1] P.R.I. Tommasini and A.F.R. de Toledo Piza, in *Non-Ideal Boson System in the Gaussian Approximation* (to be published in Ann. Phys.); P.R.I. Tommasini, Doctoral thesis, University of São Paulo, Brazil, 1995.
- [2] K. Huang and P.R.I. Tommasini, in Journal of Research of the N.I.S.T. on Bose-Einstein Condensation, August 1996.
- [3] A.F.R. de Toledo Piza, in *Time-Dependent Hartree-Fock and Beyond*, edited by K. Goeke and P.-G. Reinhardt, Lectures Notes in Physics **171** (Springer-Verlag, Berlin, 1982); M.C. Nemes and A.F.R. de Toledo Piza, Phys. Rev. C **27**, 862 (1983); B.V. Carlson, M.C. Nemes and A.F.R. de Toledo Piza, Nucl. Phys. A **457**, 261 (1986).
- [4] P. Buck, H. Feldmeier and M.C. Nemes, Ann. Phys. (N.Y.) **185**, 170 (1988).
- [5] L.C. Yong and A.F.R. de Toledo Piza, Phys. Rev. D **46**, 742 (1992).
- [6] P.L.Natti and A.F.R. de Toledo Piza, Phys. Rev. D **54**, 7867 (1996); P.L.Natti and A.F.R. de Toledo Piza, (to be published in Phys. Rev. D**55** in march/97).
- [7] E.R. Takano Natti and A.F.R. de Toledo Piza, in *Mean-Field and Collisional Dynamics of Interacting Fermion-Boson System in a Soluble Model* (to be published in Physica A**236**, 321, 1997); E.R. Takano Natti, A.F.R. de Toledo Piza and P.L. Natti in *Initial-Condition Problem for a Relativistic Scalar Plasma System* (to be published).
- [8] E. H. Lieb and W. Liniger, Phys. Rev. **130**, 1605, (1963).
- [9] Elliott H. Lieb, Phys. Rev. **130**, 1616, (1963).
- [10] J. Des Cloizeaux, in *The Many Body Physics*, edited by C. de Witt and R. Balian (Gordon and Breach, New York, 1968).
- [11] R. Balian and M. Vénéroni, Ann. Phys (N.Y.) **187**, 29 (1988).
- [12] P.R.I. Tommasini and A.F.R. de Toledo Piza, in *Time-Dependent Gaussian Approximation for a Non-Ideal Bose Gas* (to be published).

7 Figure captions

Fig.1. The ground-state energy as a function of $\gamma = c/\rho$. The full curve 1 gives the exact solution obtained numerically. Curve 2 show the Gaussian approximation also obtained numerically. Curve 3 is the result of perturbation theory.

Fig.2. The sound velocity v_s , as a function of $\gamma = c/\rho$. Curve 1 is the result obtained from perturbative theory using the excitation spectrum. Curve 2 derived from the macroscopic compressibility using the Gaussian approximation. Curves 3 and 4, that is graphically indistinguishable in this region, are the exact result and the perturbation solution obtained through the macroscopic compressibility.

Fig.3 The excitation energy as a function of the momentum for $\gamma = 0.787$. The full curves 1 and 2 corresponds of the two types of excitations (exact result). Curve 3 corresponds to the Gaussian spectrum and curve 4 is the perturbative spectrum.

Fig.4 The excitation energy as a function of the momentum for $\gamma = 3.07$. The full curves 1 and 2 corresponds of the two types of excitations (exact result). Curve 3 corresponds to the Gaussian spectrum and curve 4 is the perturbative spectrum.

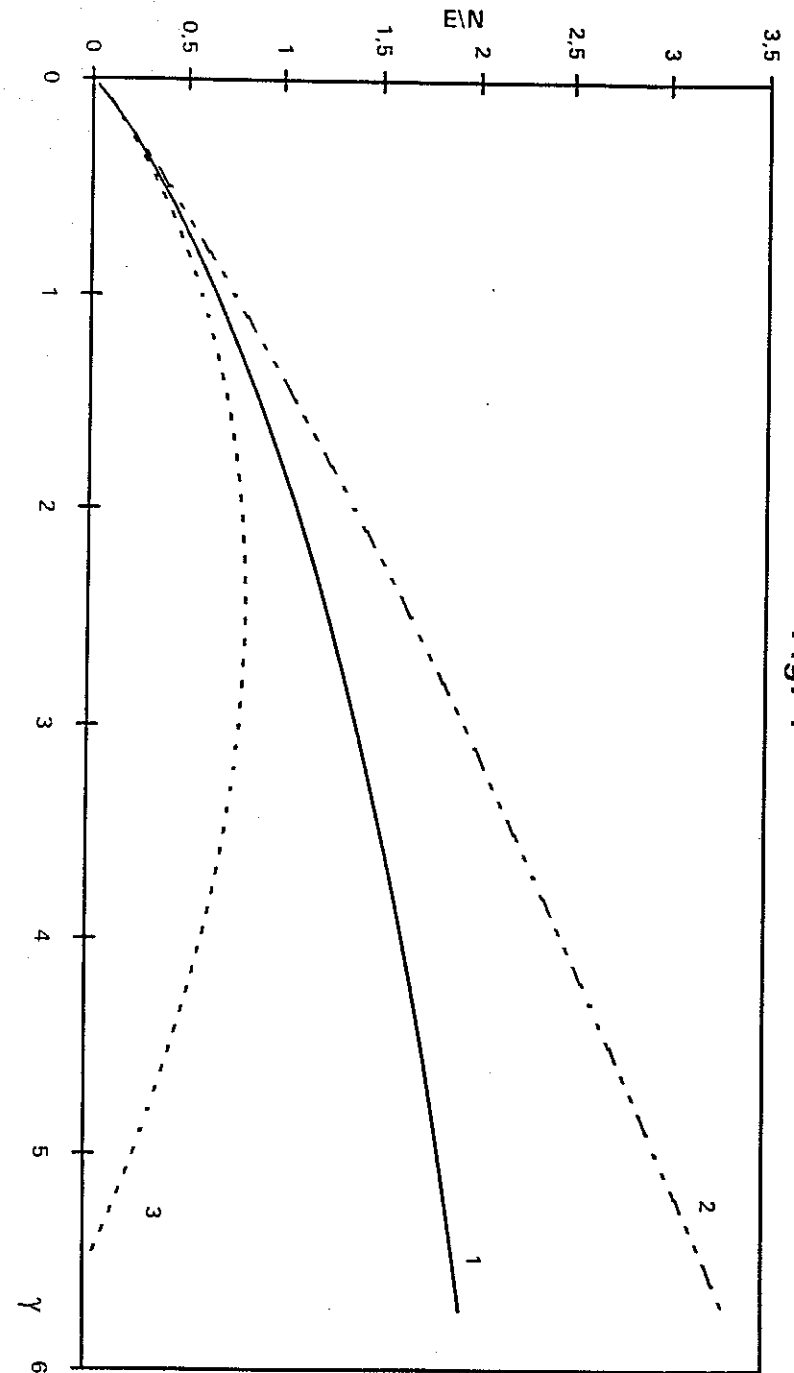


Fig. 1

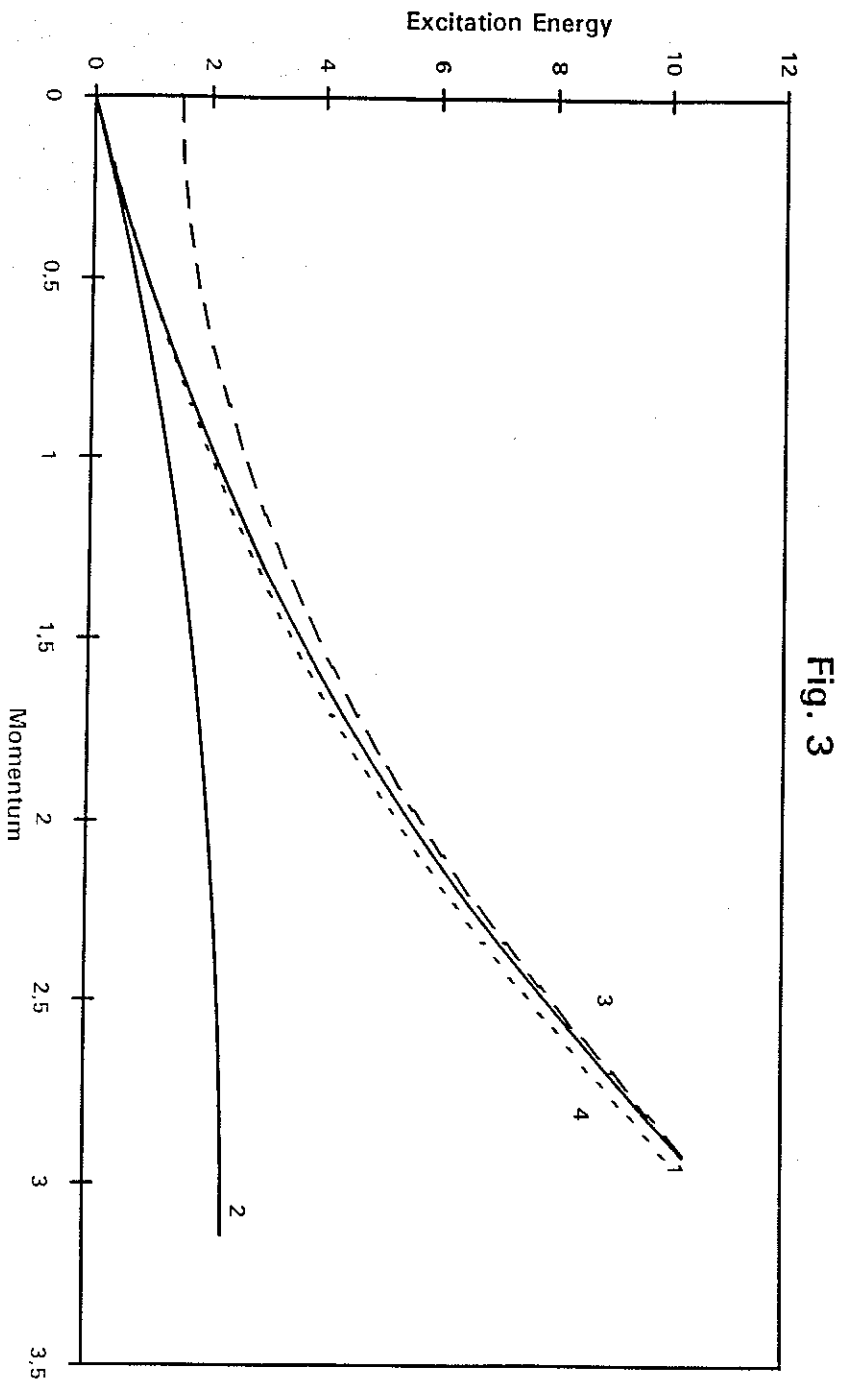


Fig. 3

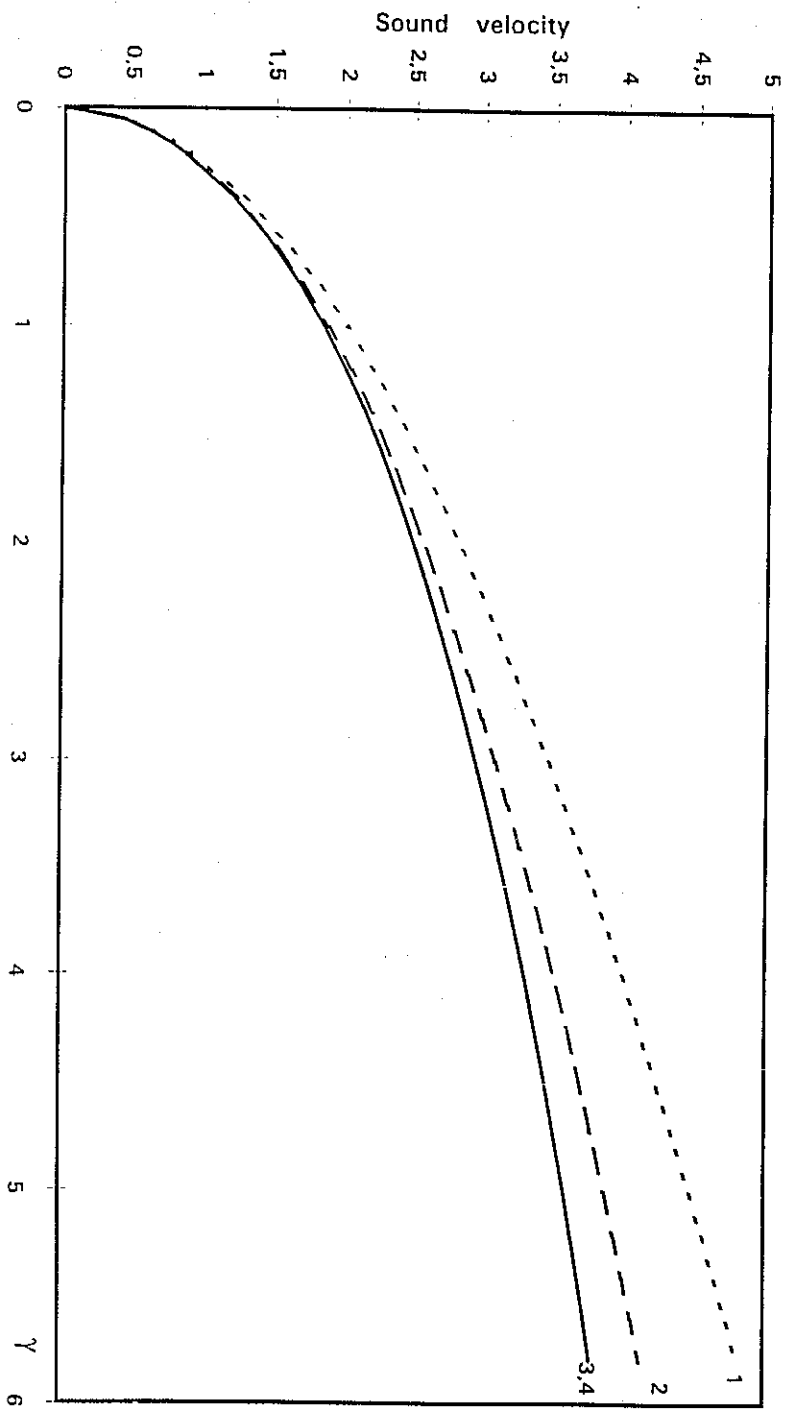


Fig. 2

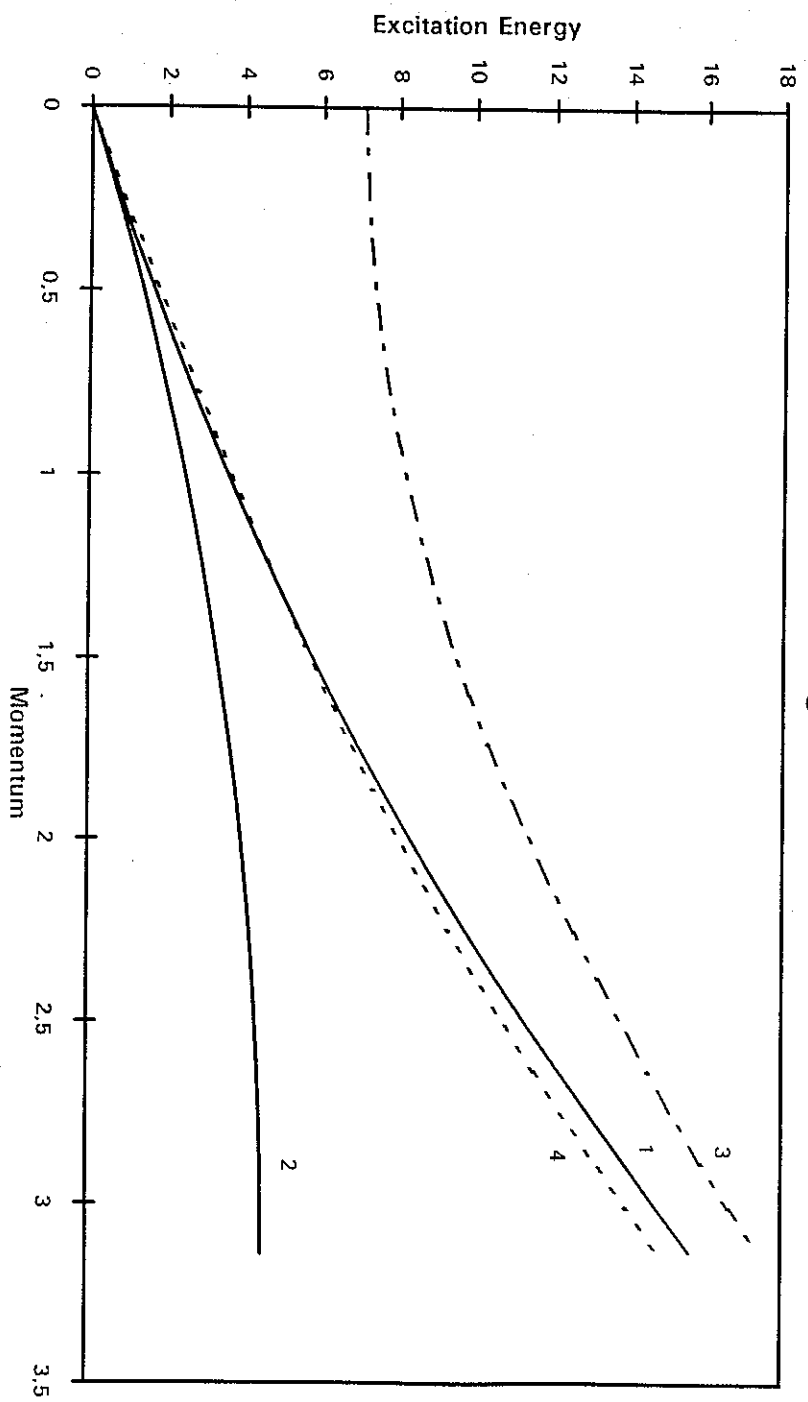


Fig. 4