FINITE SIZE CORRECTIONS TO THE EQUATION OF STATE

FOR

NUCLEAR MATTER

NEAR THE

PHASE TRANSITION HADRON GAS TO QUARK GLUON PLASMA

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ABSTRACT

It is widely accepted that the finite size of the hadrons must be taken into account in a thermodynamic description of the hadron gas near the phase transition to quark gluon plasma. Existing thermodynamic models introducing a correction due to the finite size of the particles are reviewed and discussed. A new model to describe dense nuclear matter is developed. The model takes into account the different quantum statistical distributions of the hadrons. The grand canonical pressure partition function is used to obtain the thermodynamic limit. The grand canonical partition function is restricted so that only those states where the extended particles fit into the volume of the system, are counted. The configuration space is reduced accordingly. The hadrons are described as MIT bags. The size of the particles depends on the pressure in the system. The pressure in the system compresses the hadrons which leads to an increase of the mass of the hadrons according to the MIT bag equation. The size of the particles is determined by the minimum of the grand canonical potential. A consistent thermodynamic theory is obtained. The equation of state for hadronic matter is discussed for the special cases, zero temperature and zero chemical potential, before the general case of finite temperature and finite chemical potential is used to construct a first order phase transition from hadron gas to quark gluon plasma. At high densities the influence of the description of the hadrons as MIT bags becomes significant. It is found that the phase transition is strongly dependent on the value chosen for the bag constant and the application of α_s corrections. Therefore a reliable value of the bag constant and a generally accepted theory for α_s corrections are essential to obtain a good thermodynamic description of the phase transition from hadron gas to quark gluon plasma.

NOTATIONS

Abbreviations used throughout this thesis:

In equations:

$$\beta = \frac{1}{T} \qquad \lambda = e^{\frac{\mu}{T}} = e^{\beta\mu} \qquad \xi = \beta P$$

If there is a double sign ± or ∓ the upper sign refers to Fermi-Dirac statistics and the lower sign to Bose-Einstein statistics.

The size of the particles (hadrons) is described by the small letters "r" and "v". This notation is different form the definitions used in the bag models where capital letters are assigned. The change is necessary because in the thermodynamic description "V" is the size of the whole system.

In the text:

QGP = Quark gluon plasma	HG = Hadron gas
EOS = Equation of state	QCD = Quantum chromodynamics

"ε-correction" is used as a abbreviation for the proper volume correction used in [34-37] (see also note at end of Ch.(2.3)).

When talking about the pressure ensemble the grand canonical pressure ensemble is meant throughout.

Thermodynamic mean values are in general not specially marked.

The units are chosen so that: $\hbar = c = k = 1$.

Useful constants to convert the units are:

$\hbar c$ = 197.33 MeV fm

$c = 2.997\ 10^{23}$ fm/s

$\hbar = 6.58\ 10^{-22}$ MeV s

$k_B = 8.617\ 10^{-11}$ MeV/K

$\nu_0 = 0.16$ 1/fm^3

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1. INTRODUCTION

Collision experiments in nuclear physics are done at increasing energies and with heavier projectile nuclei [1-6]. During the collision an area with a high density, compared to normal nuclear density, is created. In this dense region (called a "fireball"), particles and antiparticles are created in pair production processes from part of the kinetic energy brought into the system. A new state of matter, "quark gluon plasma" (QGP), is expected to form if the energy density is high enough. The new phase is a prediction of quantum chromodynamics (QCD). In normal nuclear matter, quarks and gluons are confined inside the hadrons. In the QGP the hadrons dissolve. The movement of the quarks is no longer restricted to the inside of the hadrons.

It is also expected to find the QGP in the center of cold neutron stars [7-9]. For the description of such stellar objects it is essential to know the equation of state of nuclear matter for high densities and the conditions which lead to the phase transition. The observed mass and radius of neutron stars cannot be explained by an ideal gas model. Taking into account the finite size of the particles [10] or repulsion between them [9,11] leads to an improved description.

Another application of the EOS for dense hadronic matter is in the evolution of the early universe [12-14]. The early universe was very hot and dense. Initially it was a QGP. During the expansion the temperature dropped. A phase transition to dense hadronic matter occured. The transition time and the further evolution of the universe are strongly dependent on the equation of state of nuclear matter.

Thermodynamics is a well established theory dealing with many-particle systems [15-20]. Instead of an equation of motion for every particle we have an equation of state (EOS) which describes the behaviour of the whole system. The features of the components (for example: mass, volume, charge, magnetic moment, interactions) are still important, but not the path and momentum of every single particle. A good thermodynamic description is obtained if the system has so many possible states that one configuration exists which has a very high probability compared to all other possible configurations. In addition the system must be in local thermal, chemical and mechanical equilibrium which means that it is possible to define a local temperature T and a chemical potential μ.

The main subject of this work is the EOS of dense hadronic matter and the influence of the volume of the constituents (hadrons) on the EOS. The finite size of the hadrons is expected to be of major importance at high densities [21-24].

An illustration of the thermodynamic picture used is shown in fig.(1.1).

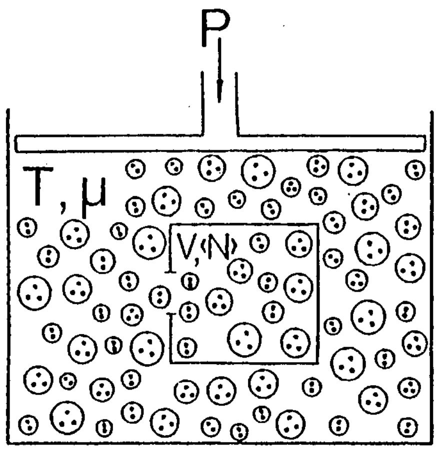

Fig. 1.1: Thermodynamic picture of dense hadronic matter used

The system is imbedded in a temperature and particle bath which has the pressure P. The particles of the "gas", i.e. the hadrons, are MIT bags with a volume v. The hadrons can be baryons and mesons as well as their antiparticles. A grand canonical description is chosen to allow for particle creation and annihilation.

I will start with the ideal gas description to introduce the thermodynamic notation used throughout the thesis. This is followed by a review of the most important volume corrections found in the literature. Most of these models are restricted to special conditions like a single-component system or a gas obeying Boltzmann statistics. The "excluded volume correction" is applicable to nuclear matter. The problem of the maximum number of finite size particles in a given volume does not occur because a special boundary condition ("unusual boundary condition") is introduced. In the new model this problem is solved without the unusual boundary condition. The new model is applicable to multi-component systems and accounts for the different quantum statistical distributions of the components. The grand canonical pressure partition function is used to obtain all thermodynamic quantities in the thermodynamic limit.

The special cases of a hadron gas at T=0 and μ=0 are discussed before the most general problem of a gas at finite T and μ is tackled. With the general EOS of hadronic matter a first order phase transition HG-QGP is constructed. The dependence of the phase transition on the mass of the strange quark, the bag constant and on first order α_s corrections is discussed. The main results are highlighted in the conclusions and suggestions for further improvements are made.

2 LITERATURE REVIEW

2.1 The ideal gas

An ideal gas is a gas of pointlike non-interacting particles. Under these conditions the quantum mechanical problem to determine the energy levels E_n of the gas simplifies to determine the energy levels ε_j of a single particle. All possible sums of energies of the various particles lead to the energy levels E_n of the gas. For comparison, I will review the derivation of the grand potential for fermions and bosons starting from the grand canonical partition function Z of a gas consisting of one kind of particle.

$$Z = \sum_{N=0}^{\infty} \lambda^N Z_N \qquad (2.1)$$

where $\lambda = e^{\mu/T}$ is the fugacity and Z_N is the N-particle partition function, or the canonical partition function.

$$Z_N = \sum_{\{n_j\}} e^{-\beta E\{n_j\}} \cdot \delta_{N, \sum_{j=1}^{\infty} n_j} \qquad (2.2)$$

with $\beta = \frac{1}{T}$.

The Kronecker-delta, $\delta_{i,j}$, restricts the sum over all configurations $\{n_j\}$ so that only configurations with N particles are counted

$$N = \sum_{j=1}^{\infty} n_j \quad . \qquad (2.3)$$

A configuration is described by the number of particles in each energy level, e.g. {0, 1, 0, 1, 0 ... 0} describes a configuration with two particles, one in the second excited state, $n_2=1$, with the energy ε_2 and one in the fourth excited state, $n_4=1$, with the energy ε_4. All other n_j are unoccupied.

The energy of one configuration is:

$$E_{\{n_j\}} = \sum_{j=1}^{\infty} n_j \varepsilon_j \quad . \qquad (2.4)$$

Inserting eq.(2.4) in eq.(2.2), then eq.(2.2) in eq.(2.1) and using eq.(2.3) to substitute the particle number N in eq.(2.1), one gets, after rearranging the terms,

$$Z = \sum_{N=0}^{\infty} \sum_{\{n_j\}} e^{-\beta \sum_{j=1}^{\infty} n_j (\varepsilon_j - \mu)} \cdot \delta_{N, \sum_{j=1}^{\infty} n_j} . \qquad (2.5)$$

Because the sum over $\{n_j\}$ is independent of the particle number N, the Kronecker-delta yields

$$Z = \sum_{\{n_j\}} e^{-\beta \sum_{j=1}^{\infty} n_j (\varepsilon_j - \mu)} . \qquad (2.6)$$

Writing out the sums gives

$$Z = \sum_{n_1=0}^{\kappa} e^{-\beta n_1(\varepsilon_1-\mu)} \cdot \sum_{n_2=0}^{\kappa} e^{-\beta n_2(\varepsilon_2-\mu)} \ldots\ldots \sum_{n_j=0}^{\kappa} e^{-\beta n_j(\varepsilon_j-\mu)} \ldots\ldots$$

$$= \prod_j \left[\sum_{n_j=0}^{\kappa} e^{-\beta n_j(\varepsilon_j-\mu)} \right] \qquad (2.7)$$

For Fermi particles $\kappa=1$ because only one particle is allowed in each energy level (if the energy levels are not degenerate). This leads to

$$Z_{Fermi} = \prod_j \left[\sum_{n_j=0}^{1} e^{-\beta n_j(\varepsilon_j-\mu)} \right]$$

$$= \prod_j \left[1 + e^{-\beta(\varepsilon_j-\mu)} \right] = e^{\sum_{j=1}^{\infty} \ln \left[1 + e^{-\beta(\varepsilon_j-\mu)} \right]} . \qquad (2.8a)$$

For Bose particles there is no restriction as to the number of particles per energy level. Therefore $\kappa \to \infty$ and the sum in the brackets in eq.(2.7) is a geometric progression (provided $\mu \leq 0$).

$$Z_{Bose} = \prod_j \left[\sum_{n_j=0}^{\infty} e^{-\beta n_j(\varepsilon_j-\mu)} \right]$$

$$= \prod_j \left[1 - e^{-\beta(\varepsilon_j - \mu)} \right]^{-1} = e^{-\sum_{j=1}^{\infty} \ln\left[1 - e^{-\beta(\varepsilon_j-\mu)} \right]} \quad . \tag{2.8b}$$

In order to relate the independent sums eq.(2.8) to classical energies E, the sum over all possible states becomes an integral over all phase space.

$$\sum_j \longrightarrow V g \int \frac{d^3p}{(2\pi)^3} \tag{2.9}$$

where g is the degeneracy factor. The grand canonical partition function reads:

$$Z(V,T,\mu)_{Fermi} = e^{V g \int \frac{d^3p}{(2\pi)^3} \ln\left[1 + e^{-\beta(E-\mu)} \right]} \tag{2.10a}$$

$$Z(V,T,\mu)_{Bose} = e^{-V g \int \frac{d^3p}{(2\pi)^3} \ln\left[1 - e^{-\beta(E-\mu)} \right]} \quad . \tag{2.10b}$$

If the gas consists of different kinds of particles, the partition function Z of the whole system is the product of the partition functions Z_k for each component.

$$Z(V,T,\mu) = \prod_k Z_k\,(V,T,\mu)$$

$$= \prod_k e^{\pm V g_k \int \frac{d^3p_k}{(2\pi)^3} \ln\left[1 \pm e^{-\beta(E_k-\mu_k)} \right]}$$

$$= e^{V \sum_k \pm g_k \int \frac{d^3p_k}{(2\pi)^3} \ln\left[1 \pm e^{-\beta(E_k-\mu_k)} \right]} \tag{2.11}$$

where the upper sign refers to fermions and the lower sign to bosons.

The grand canonical potential Ω is defined as

$$\Omega(V,T,\mu) \equiv - T \ln Z(V,T,\mu) \quad . \tag{2.12}$$

For the ideal gas, Ω is

$$\Omega(V,T,\mu) = V\ T \sum_k \mp g_k \int \frac{d^3p_k}{(2\pi)^3} \ln \left[1 \pm e^{-\beta(E_k-\mu_k)} \right] \quad . \tag{2.13}$$

The pressure P, number of particles N, entropy S and the energy E of the gas can be obtained from Ω by partial derivatives (strictly the mean values).

$$P = -\left.\frac{\partial\Omega}{\partial V}\right|_{T,\mu} \quad N = -\left.\frac{\partial\Omega}{\partial\mu}\right|_{V,T} \quad E = \left.\frac{\partial\beta\Omega}{\partial\beta}\right|_{V,\mu} \quad S = -\left.\frac{\partial\Omega}{\partial T}\right|_{V,\mu} \tag{2.14}$$

To arrive at a description which is independent of surface effects one calculates these physical properties in the so-called thermodynamic limit, viz. $N\to\infty$, $V\to\infty$ while the particle density $n = N/V$ stays finite at a pre-assigned value. In this limit the extensive properties of the system are directly proportional to the size of the system V, while the intensive properties become independent thereof. In the grand canonical description it is sufficient to find the pressure P in the thermodynamic limit which can be obtained by

$$P = \lim_{\substack{V\to\infty \\ n = \text{const}}} \left(-\frac{\Omega}{V}\right) = \lim_{\substack{V\to\infty \\ n = \text{const}}} \frac{T \ln Z}{V} \quad . \tag{2.15}$$

All the other intensive properties are obtained by the partial derivatives of $P = -\Omega/V$ in the thermodynamic limit. The particle density n, the energy density ε and the entropy density s are

$$n = \left.\frac{\partial P}{\partial\mu}\right|_{V,T} = \lambda \left.\frac{\partial\lambda P}{\partial\lambda}\right|_{V,T} \qquad \varepsilon = -\left.\frac{\partial\beta P}{\partial\beta}\right|_{V,\mu} \qquad s = \left.\frac{\partial P}{\partial T}\right|_{V,\mu} \ . \tag{2.16}$$

Taking the thermodynamic limit for the ideal gas is trivial because the volume dependence cancels if we insert Z from eq.(2.11) in eq.(2.15). This is not generally true as will become evident in the following chapters.

2.2 The "excluded volume" correction

The so-called "excluded volume" correction is often used in the literature [21,24,25] because the resulting equations are easy to implement. The basic assumption, called the "unusual boundary condition", is that the available volume Δ (the volume which is accessible to the particles with size v) is kept constant

$$\Delta = V - \sum_k N_k v_k = V(1 - \sum_k n_k v_k) \tag{2.17a}$$

or
$$V = \Delta + \sum_k N_k v_k = \Delta(1 + \sum_k \frac{N_k}{\Delta} v_k) \quad . \tag{2.17b}$$

In this formulation all derivatives of Δ vanish and the volume V is never entirely filled with particles because the total volume V changes if more particles are added to the system. For the available volume Δ everything is calculated as an ideal gas and the volume occupied by the particles is added to obtain the volume V of the system. The grand canonical potential Ω_{ex} with the excluded volume correction is the same as the potential Ω_{id} of the ideal gas, eq.(2.13) where V is substituted by Δ

$$\Omega(\Delta,T,\mu)_{ex} = \Delta\ T \sum_k \mp g_k \int \frac{d^3p_k}{(2\pi)^3} \ln\left[1 \pm e^{-\beta(E_k-\mu_k)}\right] \quad . \tag{2.18}$$

Taking the derivatives with respect to ß and μ_k we obtain

$$E = - \frac{\partial\Omega_{ex}}{\partial\beta}\bigg|_{\Delta,\mu} = \frac{\Delta}{V} E_{id} = \Delta\cdot\varepsilon_{id} \tag{2.19}$$

$$N_k = - \frac{\partial\Omega_{ex}}{\partial\mu_k}\bigg|_{\Delta,T} = \frac{\Delta}{V} N_{k,id} = \Delta\cdot n_{k,id} \quad . \tag{2.20}$$

Inserting the last equation (2.20) in eq.(2.17b) we can rewrite the unusual boundary condition, eq.(2.17b), as

$$V = \Delta(1 + \sum_k n_{k,id} v_k) \quad . \tag{2.21}$$

The pressure in the thermodynamic limit is then obtained by $\Delta\to\infty$ using the unusual boundary condition eq.(2.21)

$$P = \lim_{\substack{\Delta \to \infty \\ n = \text{const}}} -\frac{\Omega_{ex}}{V} = \lim_{\substack{\Delta \to \infty \\ n = \text{const}}} \frac{\Delta}{V} P_{id} = \lim_{\substack{\Delta \to \infty \\ n = \text{const}}} \frac{P_{id}}{1 + \sum_k n_{k,id} v_k}$$

$$= \frac{P_{id}}{1 + \sum_k n_{k,id} v_k} . \tag{2.22}$$

The unusual boundary condition, eq.(2.21), used to calculate the energy and particle density leads to very similar equations for these quantities.

$$\varepsilon = \frac{E}{V} = \frac{\varepsilon_{id}}{1 + \sum_k n_{k,id} v_k} \tag{2.23}$$

$$n_k = \frac{N_k}{V} = \frac{n_{k,id}}{1 + \sum_k n_{k,id} v_k} \tag{2.24}$$

Note that the corrections to the ideal gas equation of state in eqs.(2.22-2.24) are the same. If we take ratios of these quantities, the correction cancels and we get the same results as in the case of the ideal gas, i.e. P/ε , $\varepsilon/n = E/N$ and also n_i/n_k are not changed in this model.

2.3 Volume correction in the bootstrap model

A very interesting way of showing the existence of a phase transition between HG to QGP is done by using the statistical bootstrap model. Because I do not explicitly use this model, I only give a brief overview with the basic assumptions, results and remarks relevant to my work. The details can be found in refs. [26-32].

The basic assumption is that the complicated and as yet unknown interaction (potential) between the particles is represented by the mass spectrum $\tau(m^2,b)$, which describes the number of hadrons of baryon number b in a mass interval dm^2. Our current knowledge of this mass spectrum is restricted to a few known hadrons and their resonances. If the mass spectrum is known, the grand microcanonical level density in the Boltzmann limit is given by an invariant phase space integral.

$$\sigma(p,V,b) = \sum_{N=1}^{\infty} \frac{1}{N!} \delta^4\left(p - \sum_{i=1}^{N} p_i\right) \sum_{\{b_i\}} \delta_K\left(b - \sum_{i=1}^{N} b_i\right) \prod_{i=1}^{N} \frac{2\Delta_\kappa p_i^\kappa}{(2\pi)^3} \tau(p_i^2, b_i) d^4 p_i \tag{2.25}$$

where the particles can move in the "available volume" Δ^κ

$$\Delta^\kappa = V^\kappa - \sum_{i=1}^{N} v_i^\kappa \quad . \tag{2.26}$$

This volume Δ is kept fixed. This is nothing more than the "unusual boundary condition" as presented in Ch.(2.2) written in a Lorentz invariant form. The grand partition function can be obtained from the level density by

$$Z(\beta,V,\lambda) = \sum_{b=-\infty}^{\infty} \lambda^b \int e^{-\beta p} \sigma(p,V,b) \; d^4 p \; . \tag{2.27}$$

with $\lambda = \exp(\mu/T)$ in the rest frame.

The "bootstrap postulate" is now used in order to obtain a self-consistent mass spectrum τ. When a system of many clusters is compressed until the volume is completey occupied by clusters, or when clusters are added to a system of a fixed size until the volume is completely filled, it is in itself an "elementary cluster". This leads to

$$\sigma(p,V,b)\Big|_{V=v_i} = H \; \tau(p^2,b) \tag{2.28}$$

where H is the "bootstrap constant". It also leads to the "bootstrap equation"

$$H\tau(p^2,b) = Hg_b \; \delta_0(p^2 - m_b^2) + \sum_{N=2}^{\infty} \frac{1}{N!} \int \delta^4(p - \sum_{i=1}^{N} p_i) \sum_{\{b_i\}}^{\infty} \delta_K(b - \sum_{i=1}^{N} b_i)$$

$$\cdot \prod_{i=1}^{N} H\tau(p_i^2, b_i) \; d^4 p_i . \tag{2.29}$$

m_b and g_b are the mass and multiplicity of the lowest one-particle contribution to the mass spectrum. Solving eq.(2.29) and interpreting the clusters as Quark-Gluon bags with

$$v_i = \frac{m}{4B} \tag{2.30}$$

leads to:

$$P = \frac{P_{pt}}{1+\frac{\varepsilon_{pt}}{4B}} \quad ; \quad \varepsilon = \frac{\varepsilon_{pt}}{1+\frac{\varepsilon_{pt}}{4B}} \quad ; \quad \nu = \frac{\nu_{pt}}{1+\frac{\varepsilon_{pt}}{4B}} \tag{2.31}$$

for pressure, energy and baryon density. P_{pt} , ε_{pt} , ν_{pt} are given by

$$P_{pt} = - \frac{2T}{(2\pi)^3 H} \frac{\partial}{\partial \beta} \phi(\beta,\lambda)$$

$$\varepsilon_{pt} = \frac{2}{(2\pi)^3 H} \frac{\partial^2}{\partial \beta^2} \phi(\beta,\lambda)$$

$$\nu_{pt} = - \frac{2}{(2\pi)^3 H} \lambda \frac{\partial}{\partial \lambda} \frac{\partial}{\partial \beta} \phi(\beta,\lambda) \tag{2.32}$$

The function $\phi(\beta,\lambda)$ is defined as:

$$\phi(\beta,\lambda) := \int e^{-\beta_\mu p^\mu} \sum_{b=-\infty}^{\infty} \lambda^b H\tau(p_i^2,b_i)\, d^4p \tag{2.33}$$

and has to satisfy the implicit equation

$$\varphi(\beta,\lambda) = 2\,\phi(\beta,\lambda) - e^{\phi(\beta,\lambda)} + 1 \tag{2.34}$$

where $\varphi(\beta,\lambda)$ is defined as

$$\varphi(\beta,\lambda) = \int e^{-\beta_\mu p^\mu} \sum_{b=-\infty}^{\infty} \lambda^b H g_b \delta_0(p^2 - m_b^2) d^4p = 2\,\pi HT \sum_{b=-\infty}^{\infty} \lambda^b g_b m_b K_1\left(\frac{m_b}{T}\right) \quad . \tag{2.35}$$

Solving eq.(2.34) leads to a singular behaviour of φ along a curve in the T-μ plane. It is interpreted as the phase boundary of HG to QGP because on the critical line:

$$\varepsilon \to 4B \quad ; \quad P \to 0 \quad ; \quad \Delta \to 0 \tag{2.36}$$

i.e. the hadronic matter has formed one big cluster with the energy density 4B.

Because the "volume correction" due to the finite size of the particles is done in the same way as in the "excluded volume correction" Ch.(2.2), it is not surprising that again $^P/_\varepsilon$, $^\varepsilon/_\nu$, $^{n_i}/_{n_k}$ are the same as for an ideal gas.

The bootstrap model is formulated in the Boltzmann limit. To generalise it to Fermi-Dirac and Bose-Einstein statistics is, in principle, possible but difficult and tedious.

Equations (2.31) where P_{pt}, ε_{pt}, ν_{pt} is replaced by the expressions for an ideal gas as described in Ch.(2.1) have been used in [33-37]. I will do the same later, but only in order to compare the result and methods in the mentioned articles. Because there is no motivation to use eqs.(2.31) in a different context other than the statistical bootstrap, I am very sceptical about doing so.

2.4 Cluster Expansions

The method of the cluster expansion was developed by Mayer and his collaborators [38-40] (1937) and extended by Kahn and Uhlenbeck [41] and later by Lee and Yang [42-52] (1959). Again, I will briefly outline the method in order to properly discuss volume corrections to the EOS. I will restrict myself to the grand canonical description of a classical, single component gas obeying Boltzmann statistics. The extension to the quantum mechanical system is already too complicated to show but is well described in the literature mentioned above (see also [17,18,53]).

Under the assumption that the potential energy is given by a two-particle interaction u_{ij}, the Hamiltonian of a classical system is

$$H = \sum_i \left(\frac{1}{2m} p_i^2\right) + \sum_{i<j} u_{ij} \quad (i,j = 1,2, \ldots ,N) \quad . \tag{2.37}$$

Inserting this Hamiltonian into the definition of the grand canonical partition function in the Boltzmann limit leads to

$$Z(V,T,\mu) = \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} \frac{1}{(2\pi)^{3N}} \int e^{-\beta H} d^{3N}p \, d^{3N}r$$

$$= \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} \frac{1}{(2\pi)^{3N}} \int \exp\left\{-\beta \sum_i \left(\frac{1}{2m} p_i^2\right) - \beta \sum_{i<j} u_{ij}\right\} d^{3N}p \, d^{3N}r \quad . \tag{2.38}$$

For central forces between the particles, the potential u_{ij} only depends on the relative distance r_{ij} between them.

Standard choices for the potential u(r) are:

1. The hard core potential:

$$u(r) = +\infty \quad \text{for} \quad r \le r_0$$

$$u(r) = 0 \quad \text{for} \quad r > r_0 \qquad r_0 = \text{particle diameter} \tag{2.39}$$

2. The semi-empirical (6,12)-Lennard-Jones potential [54]

$$u(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{2.40}$$

where ε and σ are free parameters. This function has a minimum at

$$r_{min} = 2^{1/6}\sigma \quad \text{and} \quad u(r_{min}) = -\varepsilon \tag{2.41}$$

where ε is interpreted as binding energy and r_{min} as the particle diameter.

In the simplifying case of central forces the integration over the momenta of the particles in eq.(2.38) can be carried out and leads to

$$Z(V,T,\mu) = \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} \left(\frac{mT}{2\pi}\right)^{\frac{3}{2}N} \int e^{-\beta \sum\limits_{i<j} u_{ij}} d^{3N}r \quad . \tag{2.42}$$

The main problem above is to solve the "configuration integrals" C_N defined as

$$C_N(V,T) \equiv \int e^{-\beta \sum\limits_{i<j} u_{ij}} d^{3N}r = \int \prod_{i<j} (e^{-\beta u_{ij}}) \, d^{3N}r \quad . \tag{2.43}$$

For non-interacting particles $C_N = \int d^{3N}r = V^N$. In order to solve C_N for interacting particles the idea of the cluster expansion is to substitute u_{ij} by f_{ij} which is defined as

$$f_{ij} \equiv e^{-\beta u_{ij}} - 1 \quad . \tag{2.44}$$

The function f_{ij} is zero in the absence of interactions and equal to minus one for an infinitely strong repulsion. Inserting f_{ij} and rearranging the terms in eq.(2.43) yields

$$C_N(V,T) = \int \prod_{i<j} (1 + f_{ij})\, d^3r_1 \dots d^3r_N$$

$$= \int [1 + \Sigma f_{ij} + \Sigma f_{ij} f_{kl} + \dots]\, d^3r_1 \dots d^3r_N \quad . \qquad (2.45)$$

The integrals are interpreted as ℓ particle clusters. The integral $\int f_{ij}\, d^3r_i\, d^3r_j$, for example, is a two-particle cluster (ℓ=2) and $\int f_{ij} f_{jk}\, d^3r_i\, d^3r_j\, d^3r_k$ a three-particle cluster (ℓ=3) with an interaction between particle i and j and between j and k but not between i and k. $\int f_{ij} f_{ik} f_{jk}\, d^3r_i\, d^3r_j\, d^3r_k$ is another three-particle cluster (ℓ=3) but here there is an interaction between particle i and k.

Rearranging the terms in eq.(2.45) according to the number of particles connected by an interaction i.e. according to ℓ and inserting this into eq.(2.43) finally leads to the cluster expansion of the grand canonical partition function

$$Z(V,T,\mu) = \prod_{\ell=1} e^{b_\ell \lambda^\ell}\, V \left(\frac{mT}{2\pi}\right)^{3/2} \qquad (2.46)$$

with the "cluster integrals" b_ℓ defined by

$$b_\ell(V,T) = \frac{1}{\ell! V} \left(\frac{mT}{2\pi}\right)^{\frac{3}{2}(\ell-1)} \cdot \text{(sum over all possible } \ell \text{ clusters)}. \qquad (2.47)$$

For dilute systems it is assumed to be sufficient to take only the first terms of the cluster expansion, i.e. to neglect the interaction between many particles and to avoid the complicated multi-dimensional integrals.

The cluster integrals b_ℓ can be related to the virial expansion of the equation of state [55]

$$P = \frac{N \cdot T}{V} \left[1 + \frac{N}{V} B(T) + \left(\frac{N}{V}\right)^2 C(T) + \dots \right] \qquad (2.48)$$

where B(T), C(T), ... are called second, third, ... virial coefficient. The second and third virial coefficients, for example, are

$$B(T) = - b_2$$

$$C(T) = 4\, b_2^2 - 2\, b_3 \quad . \tag{2.49}$$

Moreover it is possible, with further assumptions, to obtain a Van der Waal's type equation of state [56-58]

$$(P + a\,\frac{N^2}{V^2})\ (V - bN) = N\ T \tag{2.50}$$

which is a frequently used interpolation formula to describe a two-phase system. The parameters a and b have to be fitted to experimental data. A simple equation of state can be obtained if the temperature dependence of a and b is neglected. The interpretation of b as four times the particle volume can be used as an estimate of the order of b, but not to determine its actual value (see note in Landau and Lifschitz, Statistical Physics, Pergamon Press, 3rd Edition, Part 1, Page 234).

3 THE MODEL

3.1 Motivation

Having reviewed the most common volume corrections found in the literature (Ch.(2)) their application to dense hadronic matter is discussed.

The van der Waals equation of state (eq.(2.50)) derives its utility from fits to experimental measurements. It is already constructed to describe a phase transition. With only two free parameters it describes two phases of a system of one species. However, the quantitative results of the van der Waals equation are generally not very satisfactory and all attempts to improve the equation were finally unsuccessful, mainly because they lacked a theoretical foundation (A. Münster [16] page 492 and references therein). For the purpose of describing dense nuclear matter the van der Waals equation of state cannot be applied because there is no reliable measurement of the equation of state to fit the free parameters, neither do we expect a gas of one species only. The expected density is too high to talk about a dilute system. The expansion in virial coefficients and the cluster expansion are not valid for dense systems. One of the main problems in these theories is to find the proper interaction energy U_{ij} between two particles and the non-additive multi-particle interaction energy i.e. $U_{ijk} \neq U_{ij} + U_{ik} + U_{jk}$. The extension to systems containing different particle species is complicated because each particle species will have a different size. It is necessary to distinguish between the interactions of the same type of particle and all possible mixed combinations. Until now no attempt has been made to tackle this problem because there are still other reasons to question the results even if it were possible to calculate a sufficient number of terms of the expansions. When calculating the grand canonical partition function eq.(2.38) the sum over the particle number is not restricted. For finite size particles the sum should, however, have an upper limit so that states where the volume is overfilled with particles are not counted. In the extended volume correction and in the application of the bootstrap model to hadronic matter such a restriction is avoided by using the unusual boundary condition eq.(2.2) and by changing the limiting procedure to obtain the thermodynamic limit (eq.(2.22)). The unusual boundary condition together with this limiting procedure is essential for the bootstrap model to find a singularity which is interpreted as a phase transition QGP-HG [32]. To improve the model it seems necessary to give up the unusual boundary condition because there is no reason why reality should obey the unusual boundary condition and use the usual limiting procedure for the thermodynamic limit (eq.(2.15)).

In this thesis I will develop a more involved model than the simple excluded volume approximation and will show that it is possible to take the usual thermodynamic limit, even with a restriction to the sum over the particle number. The general problem remains i.e. the difficulty of handling the restriction over the particle number N in the upper limit of the sum, which results from the dependence of the total volume in the upper limit. With no restriction the sum can be written as a geometric series and the thermodynamic potential Ω can be split into a product of the volume and a function independent of the volume $\Omega = V \cdot f(T,\mu)$. With the restriction, the volume cannot be separated and taking the thermodynamic limit (eq.(2.15)) is no longer trivial.

3.2 The pressure ensemble

Before applying the concept of the pressure ensemble to extended particles, I will outline the general concept.

Starting from the microcanonical partition function $Z(V,E,N)$ other partition functions are subsequently obtained by Laplace transformations. Each Laplace transformation replaces an extensive variable by its conjugated intensive variable ($E \to T$; $N \to \mu$; $V \to P$). The different possible combinations were formally introduced by Guggenheim [59] in 1939.

Any partition function depending on P is referred to as a pressure ensemble. In this work I will use the grand canonical pressure partition function $\pi(P,T,\mu)$ where all extensive variables are replaced by intensive variables. Prigogine [60] found that this partition function has a singularity. The corresponding thermodynamic potential $\Omega(P,T,\mu)$ is 0. This reflects the fact that the actual physical size of the system is not specified by the parameters. These conditions are illustrated in fig.(3.1).

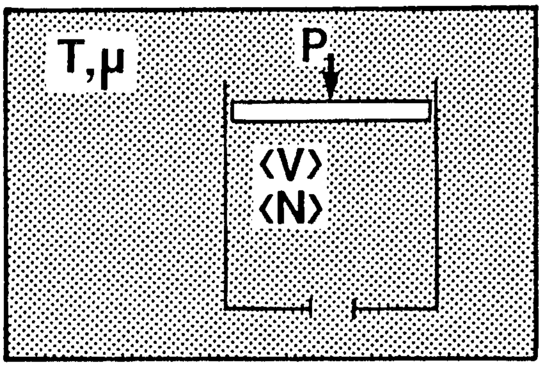

Fig. 3.1: Illustration of the grand canonical pressure ensemble.

The system is immersed in a "temperature", "particle" and "pressure" bath. The piston can be in any position. A closer examination of the singularity of the grand canonical pressure partition function shows that the singularity is a representation of the thermodynamic limit. This is easy to show:

The grand canonical pressure partition function can conveniently be obtained from the grand canonical partition function $Z(V,T,\mu)$ by

$$\pi(P,T,\mu) = \int_0^\infty e^{-\frac{PV}{T}} Z(V,T,\mu)\, dV \quad . \tag{3.1}$$

This can be written as

$$\pi(P,T,\mu) = \int_0^\infty e^{-\frac{V}{T}\left(P - \frac{T \ln Z}{V}\right)} dV \quad . \tag{3.2}$$

Looking at π as a function of the pressure P, π has a pole for

$$P = \frac{T \ln Z}{V} \quad . \tag{3.3}$$

The right hand side is equal to the pressure P in the thermodynamic limit only

$$P = \lim_{\substack{V \to \infty \\ n = \text{const}}} \left(-\frac{\Omega}{V} \right) = \lim_{\substack{V \to \infty \\ n = \text{const}}} \frac{T \ln Z}{V} \quad . \tag{3.4}$$

Consequently the pole of the grand canonical pressure partition function represents the pressure in the thermodynamic limit. In my applications there will always be only one pole of first order. The grand canonical pressure partition function can therefore be used as a mathematical tool to find the pressure in the thermodynamic limit, when it is too difficult to obtain the pressure directly from $Z(V,T,\mu)$ by the limiting procedure in eq.(3.4).

Before going on I have to mention some difficulties arising from the definition of the grand canonical pressure partition function eq.(3.1). The same definition is used by A. Münster ([16] page 177) and Hagedorn [32,61]. A partition function should be dimensionless. Obviously eq.(3.1) leads to a partition function with the unit of a volume and is strictly speaking, not a partition function. A possible constant factor (normalisation factor) in the definition of the grand canonical pressure partition function is of no relevance for the following calculations since I am not interested in obtaining the grand canonical pressure potential (Massieu-Planck function). The grand canonical pressure partition function will only be used as a mathematical tool to identify the thermodynamic limit. In any case, the physical interpretation of the transformation $V\to P$ or $V\to P/T$ within the concept of the generalized ensembles is distinguished from all other transformations because the volume does not represent an eigenvalue of a quantum mechanical operator. Other definitions and a more general discussion can be found in [62,63]. Even if the definition of the grand canonical pressure partition function can be done more consistently with the general concept of thermodynamic ensembles, it is more convenient to use the definition eq.(3.1).

Introducing the short notation

$$\xi = \frac{P}{T} = \beta P \tag{3.5}$$

the mean values of E,N,V are "in principle" defined by

$$E(P,T,\mu) = -\frac{\int_0^\infty e^{-\xi V} E(V,T,\mu)\, Z(V,T,\mu)\, dV}{\int_0^\infty e^{-\xi V} Z(V,T,\mu)\, dV} = -\frac{\left.\frac{\partial\pi}{\partial\beta}\right|_{\xi,\mu}}{\pi}$$

$$N(P,T,\mu) = \frac{\int_0^\infty e^{-\xi V} N(V,T,\mu)\, Z(V,T,\mu)\, dV}{\int_0^\infty e^{-\xi V} Z(V,T,\mu)\, dV} = \frac{\left.\frac{\partial\pi}{\partial\mu}\right|_{P,T}}{\pi}$$

$$V(P,T,\mu) = - \frac{\int_0^\infty e^{-\xi V} \quad V \quad Z(V,T,\mu)\ dV}{\int_0^\infty e^{-\xi V}\ Z(V,T,\mu)\ dV} = - \frac{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}}{\pi} \tag{3.6}$$

with the grand canonical mean values $E(V,T,\mu)$ and $N(V,T,\mu)$ as already defined in eq.(2.4).

"In principle" because in the thermodynamic limit π has a pole and only the energy density $\varepsilon=E/V$ and the particle density $n=N/V$ are determined

$$\varepsilon(P,T,\mu) = \frac{E}{V} = \frac{\left.\frac{\partial\pi}{\partial\beta}\right|_{\xi,\mu}}{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}} \tag{3.7a}$$

$$n(P,T,\mu) = \frac{N}{V} = - \frac{\left.\frac{\partial\pi}{\partial\mu}\right|_{P,T}}{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}} = - \frac{\lambda \left.\frac{\partial\pi}{\partial\lambda}\right|_{P,T}}{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}} \quad . \tag{3.7b}$$

Singular expressions still left in nominator and denominator always cancel. With the two eqs.(3.7) and the pressure in the thermodynamic limit (the pressure to the singularity of the grand canonical pressure partion function π) the EOS is completely determined. The entropy density s can be obtained using the first law of thermodynamics

$$E = -PV + TS + \sum_i \mu_i N_i \qquad \varepsilon = -P + Ts + \sum_i \mu_i n_i \tag{3.8}$$

$$\longrightarrow \quad s = \frac{\varepsilon + P - \sum_i \mu_i n_i}{T} \quad . \tag{3.9}$$

This is easier than to calculate

$$s(P,T,\mu) = \frac{S}{V} = - \frac{\left.\frac{\partial\pi}{\partial T}\right|_{\xi,\mu}}{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}} \quad . \tag{3.10}$$

Both are, of course, identical and lead to the same result.

It is interesting to see that the grand canonical pressure partition function leads to the EOS in the thermodynamic limit, i.e. in an infinite system, without considering a finite size subsystem (sample) first. In all other ensembles the size of the system is given by at least one extensive parameter and only after taking the thermodynamic limit are, all effects connected with the finite size are eliminated.

3.3 Volume correction using the pressure ensemble

In this chapter I will develop an improved model for a proper volume correction due to the finite size of the particle. In contrast to the other models (Ch.(2)) the restriction in the summation over the particle number for the grand canonical partition function is taken into account. This prevents the counting of unphysical states where the total volume is filled with more particles than will fit into it (i.e. these states do not exist). With the help of the pressure ensemble, the usual thermodynamic limit (eq(2.15)) is obtained. There is no restriction to small temperatures because Fermi-Dirac and Bose-Einstein statistics are used, respectively. Application and comparison to the previously introduced models are covered in the next chapters.

As for the ideal gas description (Ch.(2.1)) I will start with the grand canonical partition function Z for one species (eq.(2.1)). For extended particles of volume v, Z changes to

$$Z = \sum_{N=0}^{\infty} \lambda^N Z_N \, \theta(V-kNv) \qquad (3.11)$$

where $\lambda = e^{\mu/T} = e^{\beta\mu}$ is again the fugacity and Z_N the N-particle partition function (canonical partition function). The θ-function restricts the sum over the particle number N. There is no contribution to the sum when

$$N > \frac{V}{k\,v} \quad . \qquad (3.12)$$

The factor k is introduced to assist taking into account the fact that for hard spherical particles one is unable to fill the volume to more than the closest packing (k=1.35). If it is possible to deform the particles the volume can be filled up completely (k=1).

The canonical partition function remains the same for the ideal gas (eq.(2.2))

$$Z_N = \sum_{\{n_j\}} e^{-\beta E\{n_j\}} \cdot \delta_{N,\sum_{j=1}^{\infty} n_j} \tag{3.13}$$

and again the Kronecker-delta, $\delta_{i,j}$, restricts the sum over all configurations $\{n_j\}$ so that only configurations with N particles are counted.

The total particle number N is again given by

$$N = \sum_{j=1}^{\infty} n_j \tag{3.14}$$

and the energy of one configuration is

$$E_{\{n_j\}} = \sum_{j=1}^{\infty} n_j \, \varepsilon_j \quad . \tag{3.15}$$

Inserting eq.(3.15) and eq.(3.14) into eq.(3.13) and the result into eq.(3.11) leads to

$$Z = \sum_{N=0}^{\infty} \sum_{\{n_j\}} e^{-\beta \sum_{j=1}^{\infty} n_j (\varepsilon_j - \mu)} \cdot \delta_{N,\sum_{j=1}^{\infty} n_j} \cdot \theta(V-kNv) \quad . \tag{3.16}$$

At this stage, without volume corrections, the argument under the sum over N is independent of the particle number and the Kronecker-delta breaks down the sum over the particle number. For extended particles the particle number remains in the θ-function. In principle it is possible to replace the particle number N by the sum over all occupation numbers n_j, eq.(3.14), but then the argument of the θ-function becomes more complicated. To proceed in a similar way as for pointlike particles I use the integral representation of $\delta_{i,j}$

$$\delta_{N,\sum_{j=1}^{\infty} n_j} = \frac{1}{2\pi} \int_0^{2\pi} e^{i(\sum_{j=0}^{\infty} n_j - N)\alpha} \, d\alpha \quad . \tag{3.17}$$

. . . .

Proof:

$$N = \sum_{j=1}^{\infty} n_j \longrightarrow \frac{1}{2\pi}\int_0^{2\pi} e^0 \, d\alpha = 1$$

$$N \neq \sum_{j=1}^{\infty} n_j \longrightarrow \frac{1}{2\pi}\int_0^{2\pi} \cos\left[\left(\sum_{j=1}^{\infty} n_j - N\right)\alpha\right] + i \sin\left[\left(\sum_{j=1}^{\infty} n_j - N\right)\alpha\right] = 0$$

. . . .

so that eq.(3.17) reads

$$Z = \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} \sum_{\{n_j\}} e^{-\beta \sum_{j=1}^{\infty} n_j \left(\varepsilon_j - \mu - \frac{i\alpha}{\beta}\right)} \cdot e^{-iN\alpha} \, \theta(V-kNv) \, d\alpha \qquad (3.18)$$

Now I write out the sum over j and split up the sum over the configurations $\{n_j\}$ as it was done for the ideal gas (eq.(2.7))

$$Z = \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha}$$

$$\sum_{n_1=0}^{\kappa} e^{-\beta n_1 \left(\varepsilon_1 - \mu - \frac{i\alpha}{\beta}\right)} \cdot \sum_{n_2=0}^{\kappa} e^{-\beta n_2 \left(\varepsilon_2 - \mu - \frac{i\alpha}{\beta}\right)} \; \ldots\ldots \; \theta(V-kNv) \, d\alpha$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \prod_j \left(\sum_{n_j=0}^{\kappa} e^{-\beta n_j \left(\varepsilon_j - \mu - \frac{i\alpha}{\beta}\right)} \right) \theta(V-kNv) \, d\alpha \qquad (3.19)$$

where I have used κ to distinguish between particles obeying Fermi-Dirac and Bose-Einstein statistics

$\kappa = 1$ Fermions

$\kappa \to \infty$ Bosons.

Performing the sum in brackets in the case of Fermions yields

$$Z_{Fermi} = \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \prod_j \left[\sum_{n_j=0}^{1} e^{-\beta\, n_j\, (\varepsilon_j-\mu-\frac{i\alpha}{\beta})} \right] \theta(V-kNv)\, d\alpha$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \prod_j \left[1 + e^{-\beta\, n_j\, (\varepsilon_j-\mu-\frac{i\alpha}{\beta})} \right] \theta(V-kNv)\, d\alpha$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha}\, e^{\sum_{j=1}^{\infty} \ln(1 + e^{-\beta(\varepsilon_j-\mu-\frac{i\alpha}{\beta})})} \theta(V-kNv)\, d\alpha \qquad (3.20)$$

For Bosons the summation in brackets is a geometric progression

$$Z_{Bose} = \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \prod_j \left[\sum_{n_j=0}^{\infty} e^{-\beta\, n_j\, (\varepsilon_j-\mu-\frac{i\alpha}{\beta})} \right] \theta(V-kNv)\, d\alpha$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \prod_j \left[1 - e^{-\beta\, n_j\, (\varepsilon_j-\mu-\frac{i\alpha}{\beta})} \right]^{-1} \theta(V-kNv)\, d\alpha$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha}\, e^{-\sum_{j=1}^{\infty} \ln(1 - e^{-\beta(\varepsilon_j-\mu-\frac{i\alpha}{\beta})})} \theta(V-kNv)\, d\alpha \qquad (3.21)$$

If we go over to the classical energy E, I will use the same assumption as in the excluded volume correction, the bootstrap model [26-32] and several other models [21-25,64-69] : replace the sum over all possible states by an integral over all phase space but change the volume into the available volume Δ = V-kNv.

$$\sum_j \longrightarrow (V-kNv)\; g \int \frac{d^3p}{(2\pi)^3} \quad . \qquad (3.22)$$

This accounts for the fact that the finite particle volume reduces the number of available states. Using eq.(3.22) yields

$$Z(V,T,\mu) = \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha \pm (V-kNv)\, g\int \frac{d^3p}{(2\pi)^3} \ln(1\pm e^{-\beta(\varepsilon_j-\mu-\frac{i\alpha}{\beta})})}\, \theta(V-kNv)\, d\alpha \tag{3.23}$$

where the upper sign applies to fermions and the lower sign to bosons.

The easiest way to find the thermodynamic limit is to insert Z into eq.(3.1) to obtain the grand canonical pressure partition function

$$\pi(P,T,\mu) = \int_0^{\infty} e^{-\beta PV}\, Z(V,T,\mu)\, dV$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \int_0^{\infty} e^{-\beta PV}\, e^{(V-kNv)\, F(T,\mu,i\alpha)}\, \theta(V-kNv)\, dV\, d\alpha \tag{3.24}$$

with the abbreviation

$$F(T,\mu,i\alpha) = \pm g \int \ln(1 \pm e^{-\beta(E-\mu-\frac{i\alpha}{\beta})})\, \frac{d^3p}{(2\pi)^3} \quad . \tag{3.25}$$

The θ-function can be used as a restriction on the limits of the integration if the volume v is substituted by

$$V = x + kNv \qquad x = V - kNv \qquad dx = dV \tag{3.26}$$

The boundaries of the integration change to

$$V = 0 \longrightarrow x = -kNv \longrightarrow 0$$
$$V = \infty \longrightarrow x = \infty$$

because $\theta(V-kNv) = \theta(x)$ only allows positive x-values.

$$\pi(P,T,\mu) = \frac{1}{2\pi}\int_0^{2\pi} \sum_{N=0}^{\infty} e^{-iN\alpha} \int_0^{\infty} e^{-\beta P(x+kNv)}\, e^{x\, F(T,\mu,i\alpha)}\, dx\, d\alpha$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \left[\int_0^{\infty} e^{-x(\beta P - F(\mu,T,i\alpha))} \, dx \right] \cdot \left[\sum_{N=0}^{\infty} \left[e^{-(\beta Pkv+i\alpha)} \right]^N \right] d\alpha \qquad (3.27)$$

The integration over x is an analytic integral (provided $\beta P > F(\mu,T,i\alpha)$) and the sum over n is a geometric progession

$$\pi(P,T,\mu) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{\beta P - F(\mu,T,i\alpha)} \, \frac{1}{1 - e^{-i\alpha} \, e^{-\beta Pkv}} \, d\alpha \quad . \qquad (3.28)$$

With the help of the complex variable

$$z = e^{i\alpha} \qquad dz = iz \, d\alpha \qquad d\alpha = \frac{1}{iz} \, dz \qquad (3.29)$$

the integral over α is transformed into a complex path integration over a closed loop in the complex plane.

$$\pi(P,T,\mu) = \frac{1}{2\pi i} \oint_{|z|=1} \frac{1}{\beta P - F(\mu,T,z)} \, \frac{1}{z - e^{-\beta Pkv}} \, dz \quad . \qquad (3.30)$$

Because there is only one pole of first order at $z_0 = e^{-\beta Pkv}$ inside the integration circle the residuum theorem leads to

$$\pi(P,T,\mu) = \frac{1}{\beta P - F(\mu,T,z=z_0)} = \frac{1}{\beta P - \left[\pm g \int \ln(1 \pm e^{\beta(E-\mu+Pkv)} \frac{d^3p}{(2\pi)^3}) \right]} \quad . \qquad (3.31)$$

To find the pressure in the thermodynamic limit one has to look for the pole of the grand pressure partition function π (see Ch.(3.2)), which is obviously where the denominator has a root. This leads to an implicit equation for the pressure which has to be solved numerically.

$$P = \pm g \, T \int \ln \left(1 \pm e^{-\beta(E-\mu+Pkv)} \right) \frac{d^3p}{(2\pi)^3} \quad . \qquad (3.32)$$

Note that for $v \to 0$ eq.(3.32) is not implicit any more and the expression for the pressure P for pointlike noninteracting particles is reobtained as expected. In the Boltzmann-limit where $1 \gg e^{-\beta(E-\mu-Pkv)}$ the logarithmic function can be expanded leading to

$$P_{Boltz} = T\, e^{\beta(\mu - Pkv)} \int e^{-\beta E} \frac{d^3p}{(2\pi)^3} \tag{3.33}$$

This result was already obtained by R. Hagedorn [61].

Doing the same steps as before for i different particles yields to

$$P = T \sum_{j=1}^{i} \pm g_j \int \ln \left(1 \pm e^{-\beta(E_j - \mu_j + Pkv_j)} \right) \frac{d^3p_j}{(2\pi)^3} . \tag{3.34}$$

It is interesting to look at the term Pkv_j in the exponent which acts like an additional potential. Through the pressure P it depends on all particles in the system. Because of v_j it is more "difficult" to add a big particle to the system, therefore small particles will be "preferred". In contrast to a description without volume correction and in contrast to the volume corrections discussed earlier (Ch.(2.2) and Ch.(2.3)), particles in a multi component system are not only suppressed by their mass but also by their volume. The ratio between two species in a system of different components will deviate from the ratio obtained from an ideal gas description for the same temperature and the same chemical potential. This is not unexpected. The pressure ensemble description seems more plausible.

The dependence of the additional term on the pressure is more difficult to understand. P is determined by the implicit equation (3.34). If P is changed, at least one of the other parameters μ_i, T, m_i, v_i has to change in order for the system to remain within the thermodynamic limit. The pressure in the exponent prevents the system from filling up completely with particles. It becomes more and more difficult to add the same type of particles if the pressure increases. In this model the additional term Pkv_j in eq.(3.34) acts as an "interaction" between the different particles.

Once the pressure P in the thermodynamic limit is known by solving the implicit equation (3.34) on a computer, energy density and particle density can by calculated from the grand canonical pressure partition function eq.(3.31) using equation (3.7a) und (3.7b). It turns out that the statement by Hagedorn [61] that the grand canonical pressure partition function nearly always has the form

$$\pi(P,T,\mu) = \frac{1}{\xi - F(\mu,T,\xi)} \qquad \text{with } \xi = P/T \tag{3.35}$$

is also true for the application of the pressure ensemble done here. For a pressure partition function of this type the energy density and the particle density can be written as

$$\varepsilon(P,T,\mu) = \frac{\left.\frac{\partial\pi}{\partial\beta}\right|_{\xi,\mu}}{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}} = - \frac{\left.\frac{\partial F}{\partial\beta}\right|_{\xi,\mu}}{1 - \left.\frac{\partial F}{\partial\xi}\right|_{\mu,T}}$$

$$n(P,T,\mu) = - \frac{\lambda\left.\frac{\partial\pi}{\partial\lambda}\right|_{P,T}}{\left.\frac{\partial\pi}{\partial\xi}\right|_{\mu,T}} = \frac{\lambda\left.\frac{\partial F}{\partial\lambda}\right|_{P,T}}{1 - \left.\frac{\partial F}{\partial\xi}\right|_{\mu,T}} \quad . \tag{3.36}$$

Doing all the partial derivations of $F(P,T,\mu)$ (see eq.(3.25)) leads to

$$\varepsilon(P,T,\mu) = \frac{\frac{g}{2\pi^2}\int_0^\infty \frac{E\, p^2\, dp}{1 \pm e^{\beta(E-\mu+Pkv)}}}{1 + kv\frac{g}{2\pi^2}\int_0^\infty \frac{p^2\, dp}{1 \pm e^{\beta(E-\mu+Pkv)}}}$$

$$n(P,T,\mu) = \frac{\frac{g}{2\pi^2}\int_0^\infty \frac{p^2\, dp}{1 \pm e^{\beta(E-\mu+Pkv)}}}{1 + kv\frac{g}{2\pi^2}\int_0^\infty \frac{p^2\, dp}{1 \pm e^{\beta(E-\mu+Pkv)}}} \tag{3.37}$$

where the integration over the spherical angles of the momentum have been carried out. For a gas of i different types of particles the energy density and the particle density of species j are given by

$$\varepsilon_j = \frac{\frac{g_j}{2\pi^2}\int_0^\infty \frac{E_j\, p_j^2\, dp_j}{1 \pm e^{\beta(E_j-\mu_j+Pkv_j)}}}{1 + k\sum_i v_i \frac{g_i}{2\pi^2}\int_0^\infty \frac{p_i^2\, dp_i}{1 \pm e^{\beta(E_i-\mu_i+Pkv_i)}}}$$

$$n_j = \frac{\frac{g_j}{2\pi^2}\int_0^\infty \frac{p_j^2\, dp_j}{1 \pm e^{\beta(E_j-\mu_j+Pkv_j)}}}{1 + k\sum_i v_i \frac{g_i}{2\pi^2}\int_0^\infty \frac{p_i^2\, dp_i}{1 \pm e^{\beta(E_i-\mu_i+Pkv_i)}}} \quad . \tag{3.38}$$

The contribution of one component to the total energy density and total particle density is dependent on all other types of particles in the system due to the sum in the denominator and the pressure in the exponent of the distribution function .

In the next chapter I will consider the special case $T=0$ in more detail. In this case analytical solutions for the integrals in eq.(3.34) and eq.(3.38) can be obtained.

4 RESULTS AND DISCUSSION

4.1 The equation of state at zero temperature

A gas at zero temperature consists of fermions only. All states up to the fermi level E_f are occupied by particles. For ideal particles (v=0, no interaction) the fermi level is at $E_{f,id} = \mu$. In the model using the pressure ensemble I have obtained an additional factor in the exponent of the distribution function (eq.(3.31)). For T=0 only particles with an energy lower than the fermi energy E_f occur. In other words, the energy for which the exponent of the distribution function vanishes is

$$E_{f,i} = \mu_i - Pkv_i \quad . \tag{4.1}$$

Fig.(4.1) illustrates the fact that the volume correction reduces the number of occupied states compared to the number of occupied states without correction ($E_f = \mu$).

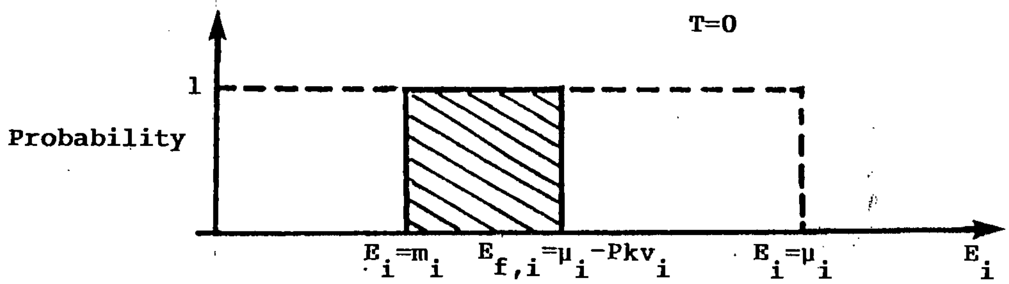

Figure 4.1: Filled energy level for T=0

The finite volume of the particles acts like a repelling force. It increases with the particle size and with the total number of states in the whole system, because P is an increasing nonlinear function of the number of states in the system.

Replacing the integrals over the distribution function with integrals limited by the Fermi energy leads to analytic integrals. The implicit equation for the pressure in the thermodynamic limit (eq.(3.34)) and the explicit equations for the energy density and particle density of the component j (eq.(3.36)) simplify:

$$P^0 = \sum_{j=1}^{i} \frac{m_j^4 g_j}{48 \pi^2} \left(x_j (x_j^2-1)^{\frac{1}{2}} (2x_j^2-5) + 3 \ln \left[x_j + (x_j^2-1)^{\frac{1}{2}} \right] \right)$$

$$\varepsilon^{0} = \frac{\frac{m_j^4 g_j}{16\pi^2}\left(2x_j(x_j^2-1)^{\frac{1}{2}} - \ln\left[x_j+(x_j^2-1)^{\frac{1}{2}}\right]\right)}{1 + k\sum_i v_i \frac{m_i^3 g_i}{6\pi^2}(x_i^2-1)^{3/2}}$$

$$n^{0} = \frac{\frac{m_j^3 g_j}{6\pi^2}(x_j^2-1)^{3/2}}{1 + k\sum_i v_i \frac{m_i^3 g_i}{6\pi^2}(x_i^2-1)^{3/2}}$$

$$\text{with} \quad x_j = \frac{\mu_j - Pkv_j}{m_j}\,. \qquad (4.2)$$

The superscript ⁰ refers to the zero temperature case. The equation for the pressure is still implicit and again has to be solved numerically before calculating the energy and particle densities. For $v_1=v_2=\ldots=v_i=0$ the equations (4.2) reduce to the expressions for pointlike particles, as expected:

$$P^{0}_{j,id} = \frac{m_j^4 g_j}{48\pi^2}\left(x_j(x_j^2-1)^{\frac{1}{2}}(2x_j^2-5) + 3\ln\left[x_j+(x_j^2-1)^{\frac{1}{2}}\right]\right)$$

$$\varepsilon^{0}_{j,id} = \frac{m_j^4 g_j}{16\pi^2}\left(2x_j(x_j^2-1)^{\frac{1}{2}} - \ln\left[x_j+(x_j^2-1)^{\frac{1}{2}}\right]\right)$$

$$n^{0}_{j,id} = \frac{m_j^3 g_j}{6\pi^2}(x_j^2-1)^{3/2}$$

$$\text{with} \quad x_j = \frac{\mu_j}{m_j} \qquad (4.3)$$

where P is now an explicit equation and ε and n are independent of the pressure P. For m=0 or μ>>m the equations change to

$$P^{0,0} = \sum_{j=1}^{i} \frac{g_j}{24\pi^2}x_j^4 \quad ; \quad P^{0,0}_{j,id} = \frac{g_j}{24\pi^2}\mu_j^4$$

$$n_j^{0,0} = \frac{\frac{g_j}{6\pi^2} x_j^3}{1 + k \sum_i v_i \frac{g_i}{6\pi^2} x_i^3} \quad ; \quad n_{j,id}^{0,0} = \frac{g_j}{6\pi^2} \mu_j^4$$

$$\varepsilon_j^{0,0} = \frac{\frac{g_j}{8\pi^2} x_j^4}{1 + k \sum_i v_i \frac{g_i}{6\pi^2} x_i^3} \quad ; \quad \varepsilon_{j,id}^{0,0} = \frac{g_j}{8\pi^2} \mu_j^4$$

with $x_j = \mu_j - P^{0,0} k v_j$. (4.4)

The second ^{0} in the superscript refers to m=0.

Before I consider some applications I want to point out an interesting difference between an ideal gas description and the model developed here with the pressure ensemble. In the ideal gas approximation as well as in the approach using the excluded volume correction (Ch.(2.2)) a particle of mass m_j is found in the system when the chemical potential μ_j of the particle exceeds its mass m_j, i.e. a heavy particle can always be found if the chemical potential is high enough and

$$\mu_j > m_j \qquad \text{(ideal gas, excluded volume correction).} \qquad (4.5)$$

With finite size particles in the pressure ensemble the Fermi level E_f is a function of the pressure in the system (eq.(4.1)). If an increase of the chemical potential μ_j leads to a stronger increase of the pressure i.e.

$$\frac{P(\mu_j)}{\mu_j} < \frac{P(\mu_j+\Delta\mu_j)}{\mu_j+\Delta\mu_j} \quad \text{for all } \mu_j \qquad (4.6)$$

or in other words: if the curvature of the pressure P as a function of μ_j is greater than 1, i.e. if

$$\frac{\partial^2 P}{\partial \mu_j^2} > 1 \quad \text{for all } \mu_j \qquad (4.7)$$

then the condition

$$m_j < \mu_j - Pkv_j \qquad (4.8)$$

to find particles of mass m_j and volume v_j will only be satisfied up to a certain value of the pressure P. Certain particles may not appear at all. An illustration of this behaviour is nuclear matter at zero temperature, as described in the next chapter.

4.2 Nuclear Matter of "hard" particles at zero temperature

As a first example I will calculate the EOS of nuclear matter as an ideal gas ($v_1=v_2=\ldots=v_i=0$) and compare to the EOS with the volume correction in the context of the pressure ensemble, the excluded volume correction (Ch.(2.2)) and the correction used in [34-37] (see also end of Ch.(2.3)) which will be referred to as "ε-correction", because of the appearence of the energy density in the correction. For the calculation I will use the following values for nucleon and delta:

$$m_N = 939 \text{ MeV} \qquad v_N = 2.16 \text{ fm}^3 \longrightarrow \qquad r_N = 0.80 \text{ fm}$$

$$m_\Delta = 1232 \text{ MeV} \qquad v_\Delta = 2.83 \text{ fm}^3 \longrightarrow \qquad r_\Delta = 0.88 \text{ fm}$$

where m_N (m_Δ) is the average mass of proton and neutron ($\Delta^-,\Delta^0,\Delta^+,\Delta^{++}$) [78]. The size of the spherical particles N and Δ was obtained from a MIT-bag description (see Ch.(3.3.1)) for a bag constant of $B^{1/4}$= 170 MeV. To get an idea of where to expect a phase transition to the QGP the EOS for massless quarks is also shown (see Ch.(4.4.1)). In order to compare the phases I will use the quark chemical potential μ_q. The chemical potential of the nucleon and the delta can be obtained from

$$\mu_q = 1/3\ \mu_N = 1/3\ \mu_\Delta \qquad (4.9)$$

because a nucleon can be converted into a delta and vice versa and because at the phase boundary nucleon and delta dissolve into three quarks each.

Fig.(4.2) shows the pressure as a function of μ_q. For the pressure ensemble two curves are shown. For k=1 the entire volume can be filled with particles. For k=1.35 the volume can only by filled up to the densest packing of hard spheres.

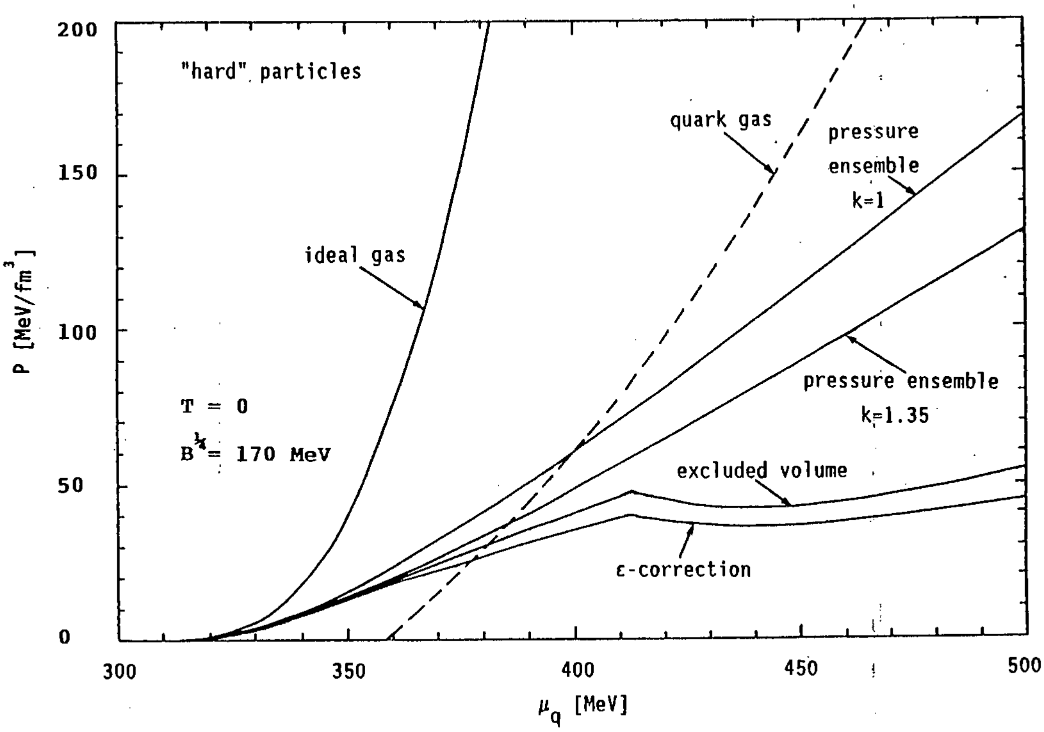

Figure 4.2: Pressure as a function of μ_q for different models

If the transition HG to QGP is of first order, the phase transition occurs at the chemical potential where the curve for the quark gas crosses the model curve for our volume corrected HG. At the first glance one might be surprised to find a kink in some of the curves at $\mu_q = 1/3\ m_\Delta$ i.e. $\mu_\Delta = m_\Delta$. This kink is readily explained. From this point Δ-particles can be formed. For T=0 the degeneracy of the system changes discontinuously. For higher temperatures the kink smoothes out. The only curves without a kink for T=0 are the curves calculated with the use of the pressure ensemble. The curve marked "ideal gas" also has a kink at $\mu_q = 1/3\ m_\Delta$ but far outside the chosen range of the ordinate. In the pressure ensemble description, the condition (eq.(4.8)) to find a Δ-particle of mass m_Δ and volume v_Δ is never fulfilled. The pressure at $\mu_q > 1/3\ m_\Delta$ is already so high that particles bigger and heavier than the nucleon cannot be found in the system, even at very high chemical potentials because P is an always strongly increasing function of μ. It is interesting to note that $P \sim \mu^4$ for large μ, with a proportionality factor different from the one of an ideal gas. Really unexpected is that the pressure within the "excluded volume correction" and the "ε-correction" show a temporary decrease of the pressure after the deltas appear. This is an artefact of these models and is mainly due to the fact that the composition is unchanged from that of an ideal gas description.

Fig.(4.3) illustrates the strong increase of deltas in the system once the chemical potential is high enough.

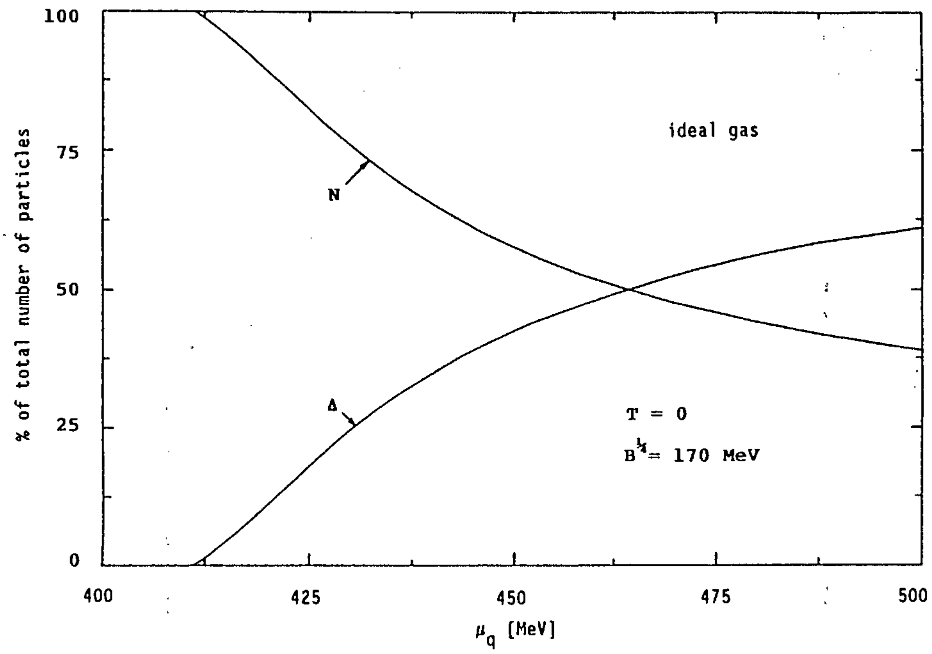

Figure 4.3: Change of composition with μ_q for an ideal gas

Because of the bigger volume of the deltas compared to the nucleons, the rise in the amount of the deltas leads in the case of the "excluded volume correction", to an increase of the volume correction which over-compensates the increase of P_{id} with μ (eq.(2.22)). Hence the pressure drops. In the case of the "ε-correction" the increase of the slope of ε_{id} caused by the increasing fraction of Δ-particles causes the same effect. This effect is also found if the particles are assumed to be smaller i.e. larger bag constants. This was confirmed up to $B^{1/4}$= 250 MeV where the particles already seem unrealistically small. (see Ch.(4.3.1)).

Before going on it is useful to look at the amount of space not filled up with particles (Fig.(4.4)). The crosses indicate the position of the first order phase transition to the QGP as constructed in fig.(4.2). The dashed line shows where spherical particles will start to overlap (densest packing). In general the figure shows why the volume correction is expected to have a dominant influence on the EOS for nuclear matter near the phase transition. In all cases shown, more than half of the volume is filled up with particles when the phase transition sets in. The increase of the free space in the case of the "ε-correction" cannot be motivated.

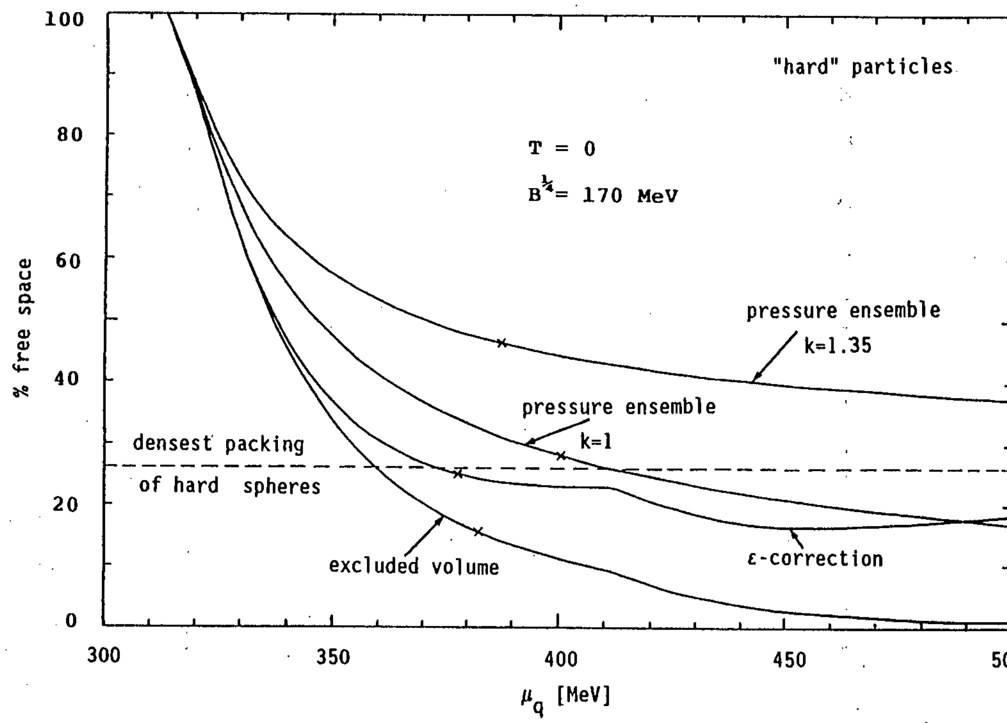

Figure 4.4: Space not taken up by the particles as a function of μ_q

Fig.(4.5) shows the baryon density (for this example equal to the total amount of particle because at T=0 there are neither antibaryons nor mesons in the system) in units of normal nuclear baryon density ν_0.

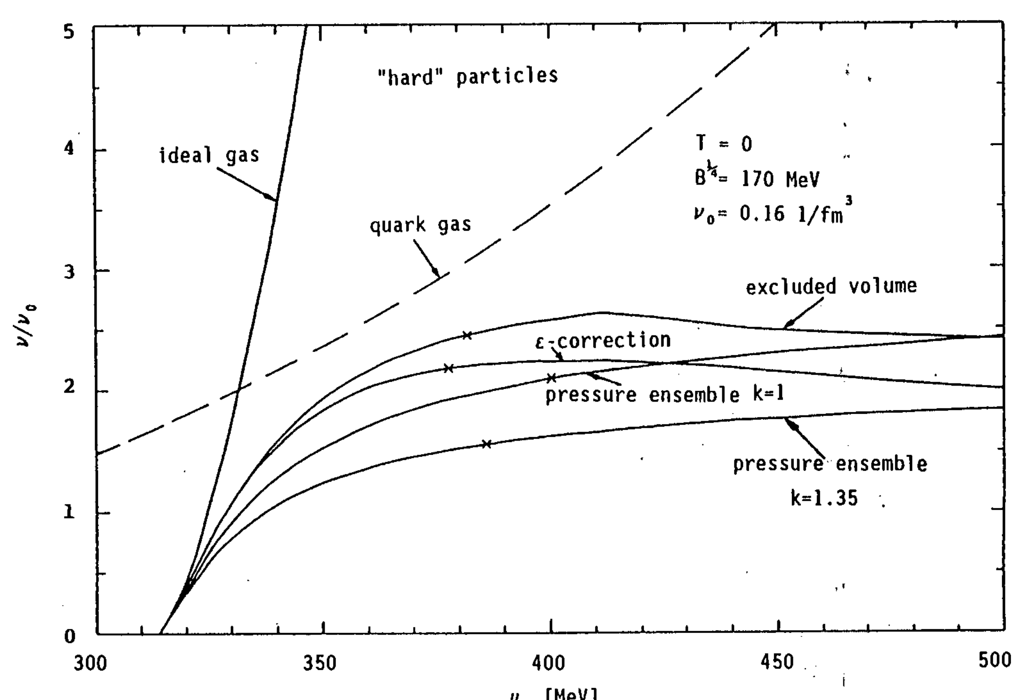

Figure 4.5: Baryon density as a function of μ_q for various models

All curves with a proper volume correction seem to approach a limiting density. For k=1 this limit is the density where the space is filled up completely with particles and for k=1.35 the limit is the density of densest packing. For the "excluded volume correction" first the limit for nucleons is approached and after the kink when the deltas start to dominate, the limiting density for the deltas is approached. Because the density before the kink is already higher than the limiting density for a system containing only deltas, the density starts to drop at $\mu_q = 1/3\ m_\Delta$ where the first deltas appear. Careful examination shows that this effect does not disappear for smaller particles. The reason is that for smaller particles the volume correction is also smaller and it is easier to fill up the space again. For our example with $B^{1/4} = 170$ MeV the problems connected with the kink seem unimportant because the phase transition to the QGP has already occurred. For smaller particles and a larger bag constant however, the phase transition immediately moves to higher chemical potentials while the position of the kink is unchanged. There will be even more kinks because other particles and resonances occur at higher μ_q.

I would now like to move to a more realistic model. A model for nuclear matter using hard particles will always lead to a phase transition close to the point where the volume starts to be filled up completely. For a reasonable size of the nucleon [70] this leads to a density at the phase transition of $1\text{-}2\nu_0$ for T=0. Because there is still no experimental evidence for a phase transition it is believed that the density for a phase transition at T=0 will be higher. To have higher densities for the phase transition is definitely one of the reasons why the bag constant is often chosen to be rather high ($B^{1/4}$ above 200 MeV) [33-37]. A high bag constant also leads to a high critical temperature (phase transition temperature for $\mu_q=0$ as seen later in Ch.(4.4.5)). The strongest argument against the description as "hard" particles is the sound velocity

$$v_s^2 \equiv \left.\frac{\partial P}{\partial \varepsilon}\right|_S \quad . \tag{4.9a}$$

Fig.(4.6) shows P as a function of ε at zero temperature.

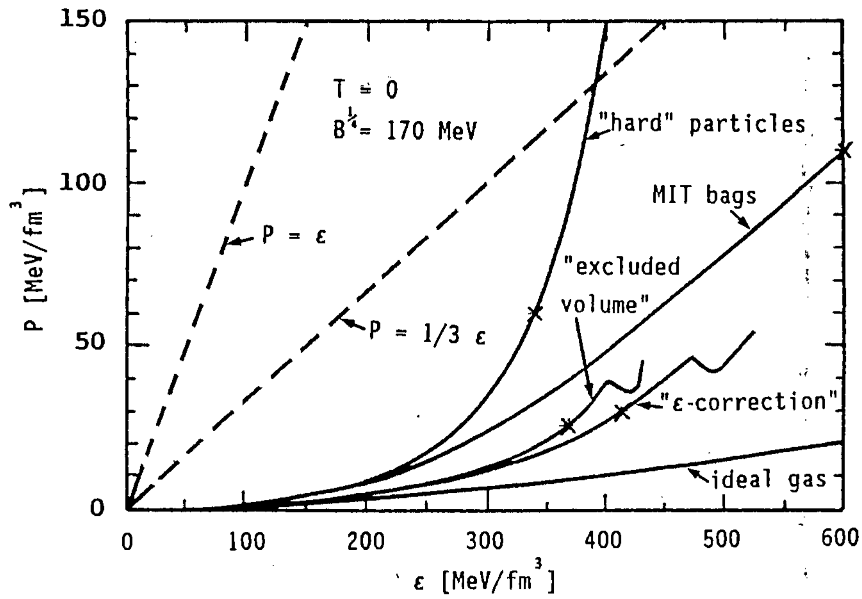

Figure 4.6: P as function of ε at T=0 (slope is the sound velocity)

The slope of P(ε) is the square of the sound velocity because the entropy S is zero for T=0. The two straight lines are P=1/3 ε and P=ε; the slope are the square of the sound velocity of a relativistic gas and the square of the velocity of light, respectively. In all the models shown the sound velocity can exeed the sound velocity of a relativistic gas. For my choice of the bag constant ($B^{1/4}$= 170 MeV) the sound velocity at the phase transition is almost as high as the velocity of light if hard particles are described by the pressure ensemble. With the "excluded volume correction" and the "ε-correction" the sound velocity is still below the relativistic limit at the phase transition. Note that if the bag constant is increased, the phase transition occurs at higher values of ε where the sound velocity becomes unphysical. As before the kinks are caused by the appearance of Δ-particles. A better approach would be to give up the concept of hard particles for nuclear matter. It makes more sense if the particles themselves feel the pressure in the system and reduce their size if the pressure increases. Instead of using a "soft potential" or describing the nuclear matter as a compressible liquid [71,72] I will obtain an EOS for "soft" particles using the MIT-bag model. The sound velocity of such a description (see Ch.(4.3)) never reaches the relativistic limit, as shown in fig.(4.6).

Before I calculate the EOS for "soft" MIT-bag particles I will review the MIT-bag model in the next chapter.

4.3 Nuclear matter of MIT bags

4.3.1 The MIT bag model

The MIT-bag model was developed at the Massachusetts Institute of Technology (MIT) [73-75] in order to describe the hadron mass spectrum on the basis of QCD (quark and gluon fields). The fields are localized to a certain area in space, the bag, which is interpeted as a hadron. It is assumed that the region opened up in the vacuum to contain the fields has a constant positive energy density called B, the bag constant. B is also interpreted as the pressure that the vacuum exerts on the bag. It is assumed that the bag is spherical and that the flux of the quark fields through the surface of the bag vanishes, i.e. the number of quarks and antiquarks inside the bag are conserved. The following ansatz for the particle mass is used

$$m(v) = E_V + E_0 + E_Q + E_M + E_E \qquad (4.10)$$

with

E_V = Volume term of the zero point energy
E_0 = Zero point energy from the fluctuations of the fields
E_Q = Rest and kinetic energy of the quarks in the bag
E_M = Colour magnetic interaction energy
E_E = Colour electric interaction energy .

Other bag models [76,77] will not be discussed here.

Eq.(4.10) contains several free parameters in the different energy terms. For the explicit expressions of the complicated terms in eq.(4.10) see ref [74,75]. The free parameters B, E_0, α_c, m_s (m_q is assumed to be 0) were fitted by applying the mass formula (4.10) to the mass of N, Δ, ω and Ω so that the experimental values [78] of the mass belong to the minimum of eq.(4.10). Examples for the volume dependence are given in fig.(4.7b) and fig.(4.7d). The reason for fitting the particle masses to the minimum of eq.(4.10) with respect to v or r is that at this point the pressure inside the bag balances the vacuum pressure B. The presence of only one isolated hadron has been assumed. If other particles are around there should be an additional pressure. Assuming that the MIT bag equation is still valid, the volume of the particles decreases due to the additional pressure, as expected. At the same time the mass (total energy) of the hadrons increases because more energy is needed to confine the quark fields to a smaller volume.

In a thermodynamic theory of "soft" particles it should be possible to use the MIT bag equation to describe the mass of the particles (hadrons) as a function of their volume. The volume varies according to the ambient conditions. Following up this idea leads to several problems. The bag constant obtained from the MIT bag model (eq.(4.10)) is $B^{\frac{1}{4}} \approx 145$ MeV if massless light quarks are assumed. If one wants to use a thermodynamic theory to predict the phase transition from hadronic matter to the quark gluon plasma (QGP) at T=0, $B^{\frac{1}{4}}$ must exceed 148.5 MeV unless α_s corrections are applied. For smaller values of B the pressure of the quark phase is always larger than the pressure of a nucleon gas at $\mu_q = 1/3\ m_N$ [21]. This means that the system will be in the quark phase before nucleons can exist, independent of the particular model for the hadron phase. This is in contradiction to reality. A bag constant of $B^{\frac{1}{4}} =$ 148.5 MeV leads to a phase transition at densities far below nuclear density. The existence of nuclei at T=0 implies that the phase transition should occur at densities above ν_0. Therefore even higher bag constants are required. The size of the particles obtained from the MIT-bag model is another reason to prefer a higher bag constant. A radius of ≈1 fm for the nucleon seems very high because scattering experiments indicate a smaller radius of ≈0.85 fm [70]. Another weak point especially for the application to the thermodynamic description of the phase transition HG to QGP is that the pion mass obtained is nearly twice as the experimental value of m_π=139 MeV. As the lightest meson it will be the dominant particle at high temperature and low chemical potential. Therefore an incorrect pion mass will cause a huge error. To obtain the right mass in the MIT bag model is difficult because the low mass requires that energy terms differing by a factor of ten in the MIT bag eq.(4.10) have to cancel each other. In this case the result is not trustworthy because the single energy terms are already only estimates. Also the mass of the strange quark of about 300 MeV as calculated from the bag model is believed to be rather high. Strange quark masses between 150-200 MeV are used more often [79,80]. In an attempt to improve the situation I tried to fit the free parameters through a least squares fit to all light hadrons by minimizing the relative difference between theoretical and experimental mass to fit all masses to a similar relative error i.e. to the minimum of

$$\chi^2 = \sum_i \left[\frac{m_{theo,i} - m_{exp,i}}{m_{exp,i}} \right]^2 . \qquad (4.11)$$

The results are discouraging. Although the fit improves in general with respect to equation (4.11) the abovementioned problems still occur. Furthermore the mass obtained for the well known nucleon deviates considerably from the experimental value even though the nucleon is expected to be well described by the bag model. This problem remains even if the fit is restricted to the relatively stable particles and if a weight factor is introduced depending on the instability (width) of the particles.

There is no doubt that it is possible to improve on some of the points mentioned above when modifying (playing around with) the MIT bag equation and introducing some new phenomenological constants [81]. Even then there is a limit in having more parameters as they will be correlated. It is difficult to compare the fits because of the unequal amount of degrees of freedom and the different conditions chosen (e.g. fitting the stable particles only or including or excluding the pion into the fit, introducing weight factors for unstable particles). Even though I obtained a better fit (see appendix D) no physical reason could be found why this special type of bag equation should lead to a better fit than any that were tried. For the thermodynamic model it should suffice to use the "basic" form of the MIT bag equation:

$$m_i(v_i) = \frac{c_i}{r_i} + Bv_i \qquad \text{with} \quad v_i = \frac{4}{3}\pi r_i^3 \tag{4.12}$$

to be able to see the effect if the hadrons are not hard any more.
The form of eq.(4.12) with c_i as a constant is the same as eq.(4.10) for all hadrons not containing strange quarks. If strange quarks are present and the $1/r_i$ dependence is taken out of the energy term, c_i is still a function of r_i. Neglecting this dependence leads to bigger particles. Taking c_i as a constant is regarded as a satisfactory fit here. With c_i as a constant eq.(4.12) has a minimum at

$$m_{i,min} = 4Bv_{i,min} = \frac{4}{3}\left[4\pi c_i^3 B\right]^{1/4} . \tag{4.13}$$

Because I want the hadrons to have their experimental measured mass at the minimum because I want to use B as an external parameter, the constants c_i and $v_{i,min}$ are calculated from eq.(4.13).

$$c_i = \left[\frac{(3/4\ m_i)^4}{4\pi B}\right]^{1/3} \qquad v_{i,min} = \frac{m_{i,min}}{4\ B} . \tag{4.14}$$

Eq.(4.12) together with the value of c_i obtained from eq.(4.14) is used as the equation for $m_i(v_i)$ for the "soft" particles throughout the rest of this thesis. Fig.(4.7a) and fig.(4.7c) give an overview about the particle size at the minimum of eq.(4.14) as a function of the minimum mass for different bag constants B. Fig.(4.7b) and fig.(4.7d) show how eq.(4.12) depends on the choice of the bag constant and the mass of the minimum.

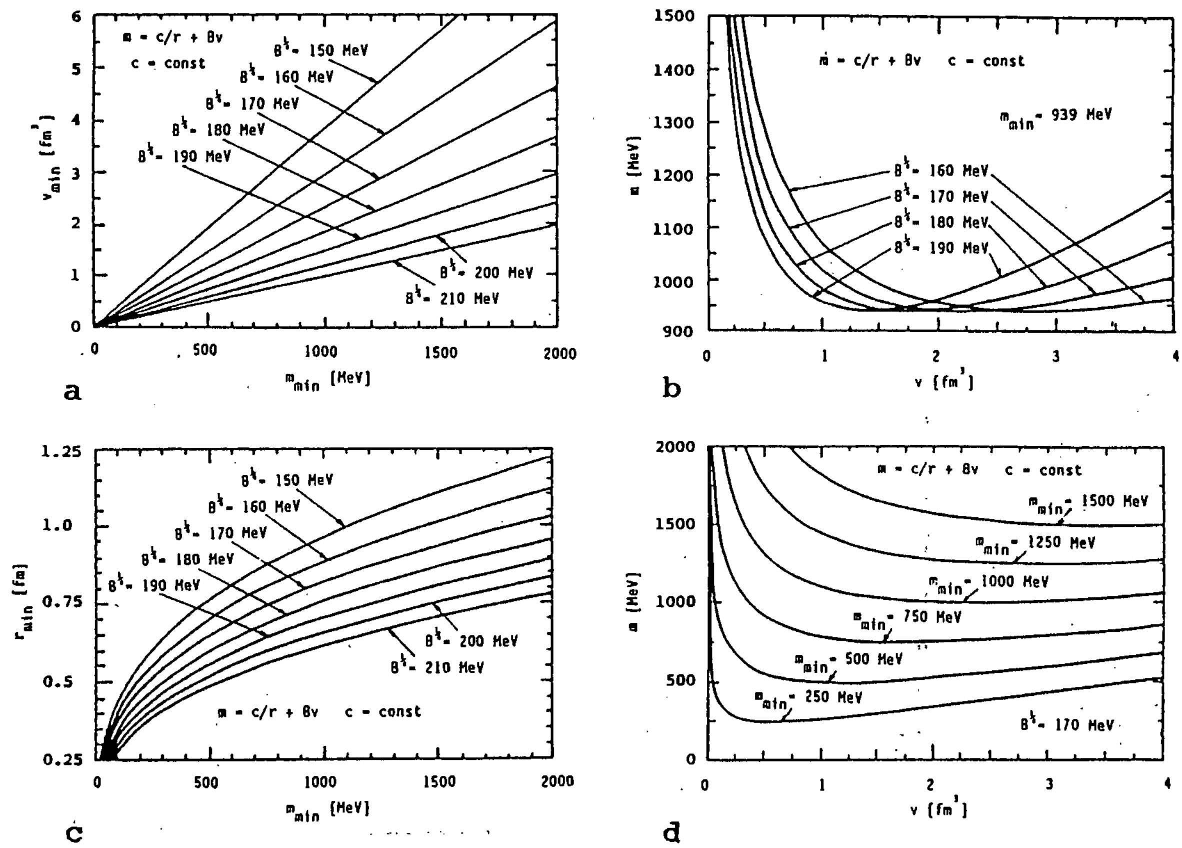

Figure 4.7: Illustration of the behaviour of eq.(4.12)

4.3.2 Nuclear matter of MIT bags at zero temperature

In the last chapter the MIT bag model for hadrons was reviewed. In this chapter I will show that the basic form of the MIT bag equation

$$m_i(v_i) = \frac{c_i}{r_i} + Bv_i \quad \text{for spherical particles with } r_i = \left(\frac{3v_i}{4\pi}\right)^{1/3} \qquad (4.15)$$

is already sufficient to obtain an EOS for particles which are "soft" in the sense that the spherical particles will change their volume and mass according to eq.(4.15). Compared to the EOS obtained from the "hard" particle model (Ch.(4.2)) a completely different behaviour at high densities is obtained.

For soft particles the volume and mass are not constants so the question of how to determine one of them, arises. The other variable is then given by the MIT bag eq.(4.15). Here the particle volume will be regarded as the new independent parameter. The value of this new independent parameter will be such that the system is in the state where the thermodynamic potential has a minimum with respect to the new variable [82]. Using the grand canonical potential $\Omega(V,T,\mu,v)$ the system should choose the value of v such that

$$\left.\frac{\partial\Omega(V,T,\mu,v)}{\partial v}\right|_{V,T,\mu} = 0 \quad \text{and} \quad \left.\frac{\partial^2\Omega(V,T,\mu,v)}{\partial v^2}\right|_{V,T,\mu} > 0 \quad . \qquad (4.16)$$

This condition depends on the size V of the system. In the thermodynamic limit $\Omega = -PV$. Inserting this into eq.(4.16) leads to

$$\left.\frac{\partial P(T,\mu,v)}{\partial v}\right|_{T,\mu} = 0 \quad \text{and} \quad \left.\frac{\partial^2 P(T,\mu,v)}{\partial v^2}\right|_{T,\mu} < 0 \qquad (4.17)$$

i.e. in the thermodynamic limit the system chooses the state with the maximum pressure. To see whether a maximum exists at all fig.(4.8) shows the pressure obtained from the pressure ensemble description (eq.(4.2)) using eq.(4.15) for the particle mass as a function of the particle volume.

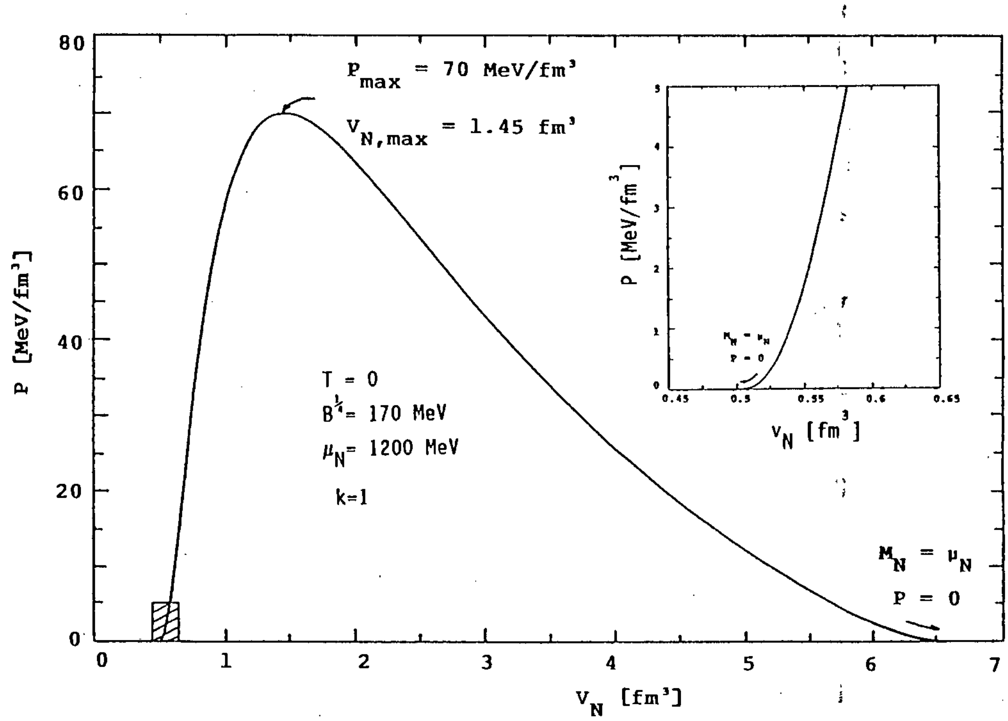

Figure 4.8: Pressure as a function of the particle volume

As already discussed in Ch.(4.2) only nucleons are present at T=0 and the pressure P is only a function of one particle volume, v_N. The constant c_N in eq.(4.15) is determined by eq.(4.14) with $m_{N,min}$= 939 MeV and $B^{1/4}$= 170 MeV. In fig.(4.8) μ was chosen as μ_q= 1/3 μ_N= 1200 MeV. In this example P develops a maximum at P_{max}= 70 MeV/fm^3, $v_{N,max}$= 1.45 fm^3 ($m_{N,max}$= 962 MeV). The maximum appears because for both big and small particle volumes the mass of the particles increases according to the MIT bag eq.(4.15) until the chemical potential reaches μ_N= m_N= $3\mu_q$ and no state to be occupied exists (P=0). The value for v or m at the maximum of P is different from the value obtained from the minimum of the MIT bag equation. A look back at fig.(4.1) helps to explain the reason. The system chooses the state with the maximum number of states. For T=0 all possible states are between $m_N(v_N)$ and the Fermi level $E_{f,N}$= μ_N - Pkv_N. If the particle volume v_N is reduced to below $v_{N,min}$ (the volume corresponding to the minimum mass of the MIT bag equation) the Fermi level rises and more states are possible because the pressure is not increasing as fast as v_N is reduced. Close to the minimum of the MIT bag equation a change in v_N leads to a very small increase in m_N so that the lower boundary for the number of states is nearly unchanged. The particles shrink until the increase of $m_N(v_N)$ is faster than the increase of the Fermi level $E_{f,N}$= μ_N- Pkv_N. Calculating all physical properties to the maximum pressure for different values of μ_q leads to the EOS of the soft particles in the thermodynamic limit, i.e. the pressure is always calculated by finding the pole of the grand canonical pressure partition function (eq.(3.31)) or the root of the denominator of the grand canonical pressure partition function for given μ and T. Fig.(4.9) shows what happens to our soft nucleons if there is no phase transition HG→QGP. The HG would also exist at very high pressure i.e. large chemical potential. Volume and radius shrink with increasing densities. For an infinite dilution, volume and radius would have their values according to the minimum of the bag equation (eq.(4.14)), i.e. $v_{N,min}$= 2.16 fm^3, $r_{N,min}$= 0.80 fm (for $B^{1/4}$= 170 MeV). In this case the pressure is very small and the EOS turns into the ideal gas EOS, as expected. For normal nuclear matter density ν_0= 0.16 baryons/fm^3, the nucleons are slightly smaller. Only at densities greater than $2\nu_0$ do the particles start to become really compressed. In the limit of infinite density $\nu\to\infty$ or $\nu_0/\nu\to 0$ they are reduced to point particles with an infinite mass. The amount of space still left between the particles, called free space, reaches a finite limit for an infinitely dense system (fig.(4.10)).

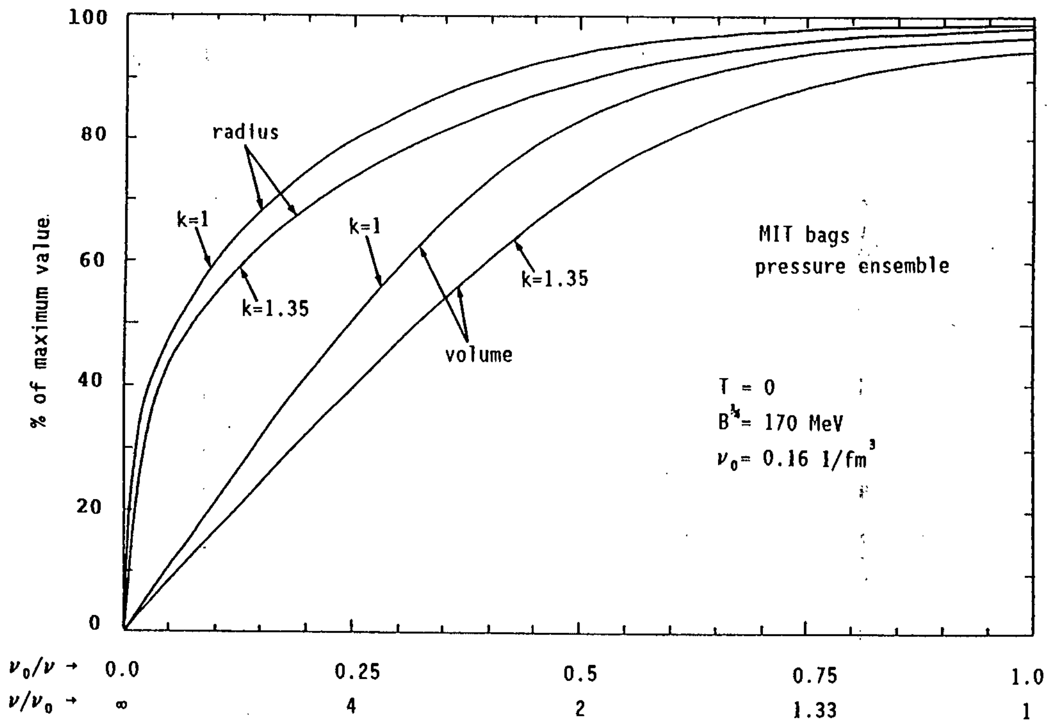

Figure 4.9: Density dependence of the particle volume and radius

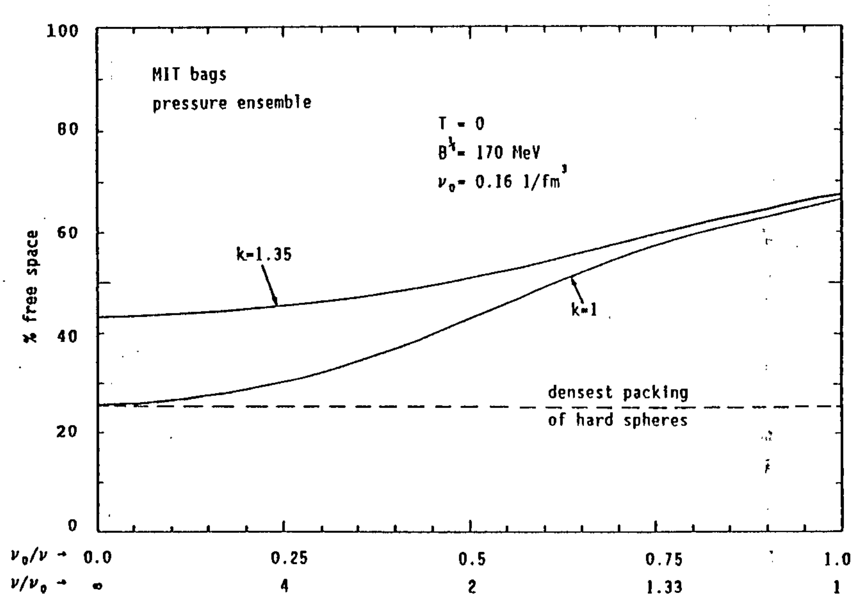

Figure 4.10: Free space as a function of the density

Even if k=1 the system stays away from the densest packing of hard spheres. It seems as if the system itself knows that there is a limit where we have the closest packing. This is not so. It is possible by logical arguments to motivate the final volume left for the infinite dense systems. The system will be in the state with the highest number of possible states per volume with respect to m,v,N. This is only possible because the system with the maximum pressure is considered. With the correction to the phase space (eq.(3.22)) the number of states is proportional to the free space. It is unfavourable for the system to fill the space completely with particles. On the other hand, the number of states is proportional to the number of particles. It is good to have as many small particles as possible (see eq.(3.11)). For small particles, the number of possible states is larger than for big particles due to the restriction in the sum over the particle number. Because the mass of the particles increases if the particles are compressed, the number of states is again reduced by mass suppression. The free space is determined by a balance between mass suppression and "volume suppression". The limit of the densest packing for spherical particles is never reached for a description using the pressure ensemble with k=1.35. There is no reason why this limit should not be reached for very high densities. Therefore I will use k=1 in all further discussions. Fig.(4.11) again shows the free space as a function of the density, but for different values of the bag constant B.

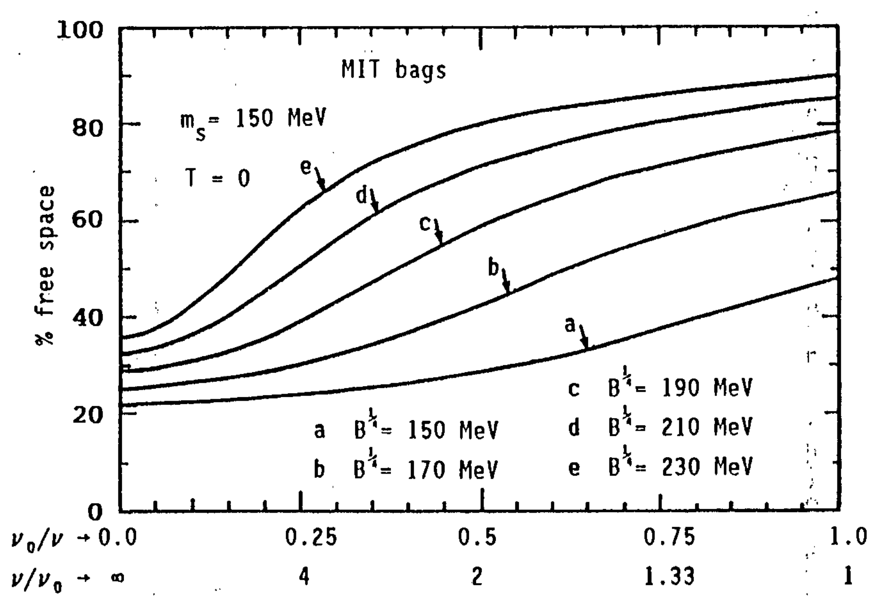

Figure 4.11: Dependence of the free space on the chosen bag constant

For bigger bag constants the particles are smaller and for the same density more space is free. This difference becomes smaller for high densities but does not vanish for infinitely high densities. It cannot be expected that the same limit is reached because the different bag constant changes the dependence of the particle mass from the particle volume m(v) (see fig.(4.7a)).

Fig.(4.12) shows several curves. Marked with (1) is the chemical potential for the nucleon μ_N, with (2) the energy per baryon E/b and with (3) the nucleon mass m_N which changes with the density. The changing mass m_N is the reason why I have to deviate from the usual form when drawing the energy per baryon, i.e. the plot shows the total energy per baryon and not the energy minus the rest mass. The difference between the energy per baryon and the changing rest mass, i.e. the mean kinetic energy of the particles and also the difference between μ_N and m_N is shown in the inset of fig.(4.12).

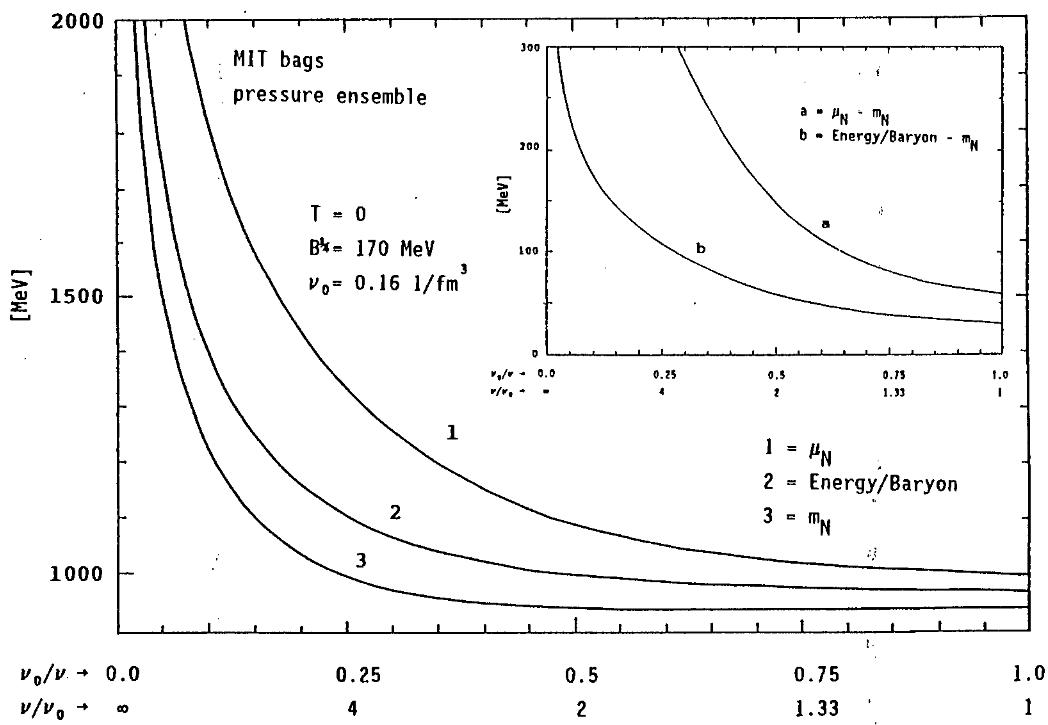

Figure 4.12: Density dependence of μ_q, m_N and E/b and their differences Both differences increase as higher densities are reached. Curve (a) shows that the rest mass can be neglected against the chemical potential. Curve (b) shows that at high densities the kinetic energy increases rapidly. This means that the gas should behave like a relativistic Fermi gas because I have already shown in fig.(4.9) that the volume of the particles, v_N reduces to "pointlike" particles. This is confirmed by the fact that for high densities P/ε approaches the relativistic Fermi gas result, i.e. $P/\varepsilon = 1/3$ (fig.(4.6)). In fig.(4.13) the results for the energy per baryon obtained so far are compared to each other and to the energy per baryon found in the literature.

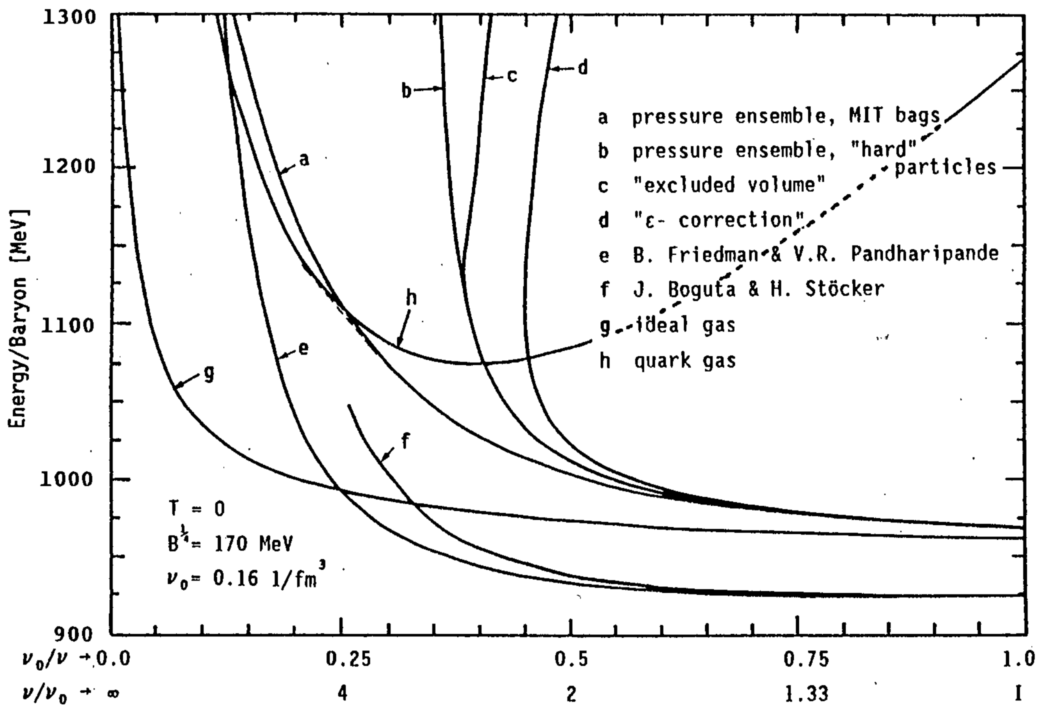

Figure 4.13: Comparison of E/b obtained from different models

The curve marked "e" is taken from [9]. Its calculation is based on a soft-core nucleon potential and a lowest order variational theory. The curve marked "f" is taken from [83] and is their best choice with the parameters m^*/m_N = 0.7 and k = 210 MeV (k = compressibility modulus, m^* = effective mass). The main difference from my calculation is that they have a minimum for the energy per baryon (saturation) at normal nuclear density ν_0 with a binding energy of 16 MeV/baryon. Binding effects were not included in the presented soft particle model with the pressure ensemble because it is not yet known whether there is a binding effect if nuclear matter consists of very many nucleons. The presence of many particles is the basis for the thermodynamic calculation. The expected phase transition to the quark gas for the soft particles would be from ν = 3.5 ν_0 to ν = 4.3 ν_0 if a first order phase transition is assumed. This is indicated in fig.(4.13)

Instead of keeping T constant at T=0 and increasing μ, which immediately leads to applications in the description of complex stellar objects like neutron stars [7,8,10,84], it is also interesting to fix μ at μ=0 and increase the temperature. The results for this case are presented in the following chapter.

4.3.3 Nuclear matter of MIT bags at zero chemical potential

The choice of the baryon chemical potential μ=0 means that the total baryon number $N_{b,total}$ is zero, i.e. the number of baryons N_b is always equal to the number of antibaryons $N_{\bar{b}}$.

$$0 = N_{b,total} = N_b - N_{\bar{b}} \tag{4.18}$$

or
$$0 = \nu = \nu_b - \nu_{\bar{b}} \tag{4.19}$$

where ν_b ($\nu_{\bar{b}}$) is the baryon (antibaryon) density

$$\nu_b = \frac{N_b}{V} \qquad \nu_{\bar{b}} = \frac{N_{\bar{b}}}{V} \quad . \tag{4.20}$$

The interest in the case μ=0 results from some theoretical predictions that for high energy collisions of heavy nuclei the central area will be without any net baryon number and only a hot area in space is left once the nuclei have passed through each other (Bjorken picture [85]).

For finite temperature, mesons like π, K, ρ ... and all hadron resonances will be present. The total number of particles and antiparticles in the system is

$$N_{total} = N_b + N_{\bar{b}} + N_m \tag{4.21}$$

and the density

$$\rho_{total} = \nu_b + \nu_{\bar{b}} + \rho_m \quad . \tag{4.22}$$

Assuming thermal equilibrium between the particles the calculation is now much more involved than in the case of T=0 because all particles in the hadron mass spectrum can be present. Each type of particle will have a different mass m_i and size v_i. Again we will use the basic form of the MIT bag equation (eq.(4.12)) as a relation $m_i(v_i)$. The pressure in the system will be the maximum pressure with respect to all different particle volumes v_i (Appendix C explains the numerical procedure) because the volume of each type of particle is a new independent variable (see Ch.(4.3.2)) i.e. if there are i different types of particles in the system the pressure will be so that

$$\left.\frac{\partial P}{\partial v_j}\right|_{T,v_1,\ldots,v_{j-1},v_{j+1},\ldots,v_i} = 0$$

and
$$\left.\frac{\partial^2 P}{\partial v_j^2}\right|_{T,v_1,\ldots,v_{j-1},v_{j+1},\ldots,v_i} < 0 \qquad (4.23)$$

for each particle species j = 1 ... i. The pressure P is calculated in the thermodynamic limit according to the solution of the implicit equation (3.34). Table (4.1) shows which particles were included in the calculation. Volume and radius belong to the minimum of the basic MIT bag equation (eq.(4.12)) and represent the size of the particles for infinite dilution.

particle name	mass [MeV]	radius [fm]	volume [fm^3]	Quark content q	$\bar{q}$	s	$\bar{s}$	spin	iso-spin	statis-tics	degen-eracy
N	939.0	0.80	2.16	3	0	0	0	1/2	1/2	FD	4
$\bar{N}$	939.0	0.80	2.16	0	3	0	0	1/2	1/2	FD	4
Λ	1115.6	0.85	2.57	2	0	1	0	0	1/2	FD	2
$\bar{\Lambda}$	1115.6	0.85	2.57	0	2	0	1	0	1/2	FD	2
Σ	1194.0	0.87	2.75	2	0	1	0	1	1/2	FD	6
$\bar{\Sigma}$	1194.0	0.87	2.75	0	2	0	1	1	1/2	FD	6
Ξ	1318.0	0.90	3.03	1	0	2	0	1/2	1/2	FD	4
$\bar{\Xi}$	1318.0	0.90	3.03	0	1	0	2	1/2	1/2	FD	4
Δ	1232.0	0.88	2.83	3	0	0	0	3/2	3/2	FD	16
$\bar{\Delta}$	1232.0	0.88	2.83	0	3	0	0	3/2	3/2	FD	16
Σ^*	1385.0	0.91	3.19	2	0	1	0	1	3/2	FD	12
$\bar{\Sigma}^*$	1385.0	0.91	3.19	0	2	0	1	1	3/2	FD	12
π	139.0	0.42	0.32	1	1	0	0	1	0	BE	3
η	547.6	0.67	1.26	1	1	0	0	0	0	BE	1
η′	958.8	0.81	2.21	1	1	0	0	0	0	BE	1
ρ	770.0	0.75	1.77	1	1	0	0	1	1	BE	9
ω	782.6	0.76	1.80	1	1	0	0	0	1	BE	3
K	495.8	0.65	1.14	1	0	0	1	1/2	0	BE	2
$\bar{K}$	495.8	0.65	1.14	0	1	1	0	1/2	0	BE	2
K^*	892.1	0.79	2.05	1	0	0	1	1/2	1	BE	6
$\bar{K}^*$	892.1	0.79	2.05	0	1	1	0	1/2	1	BE	6

q = up or down quark
$\bar{q}$ = anti up or down quark
s = strange quark
$\bar{s}$ = anti strange quark

FD = Fermi-Dirac statistics
BE = Bose-Einstein statistics
Bag constant used to determine r and v
B = 109 MeV/fm^3 or $B^{1/4}$ = 170 MeV

Table 4.1: Hadrons included in the calculations

Fig.(4.14) shows the total particle density ρ_{total} of the soft particles compared to the ideal gas description.

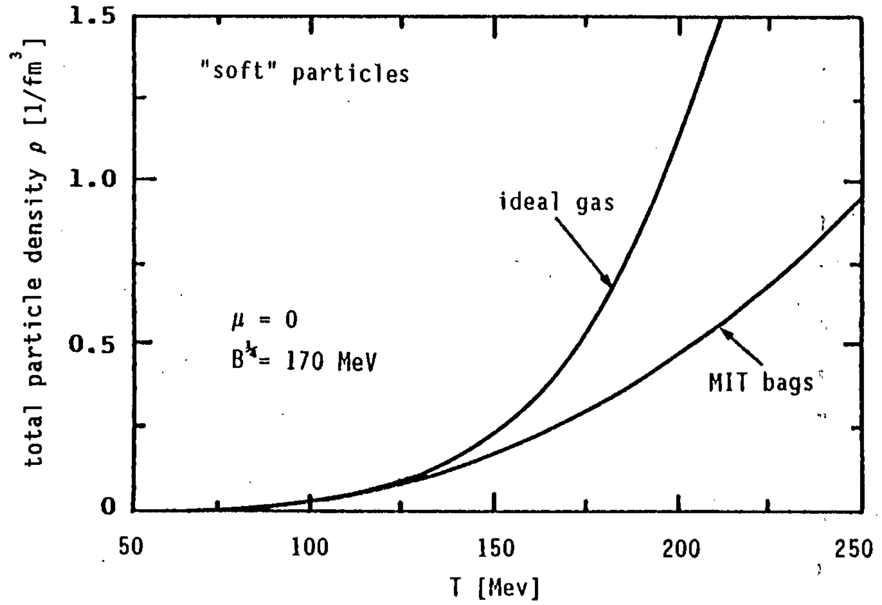

Figure 4.14: Total particle density as a function of the temperature

At low temperatures the system is so dilute that the effects of the particle volumes can be neglected. For higher temperatures the difference becomes significant because the space becomes filled with particles. Fig.(4.15a) shows the free space left. Fig.(4.15b) shows P/ε to see if the gas behaves like a relativistic gas in which case $P/\varepsilon = 1/3$.

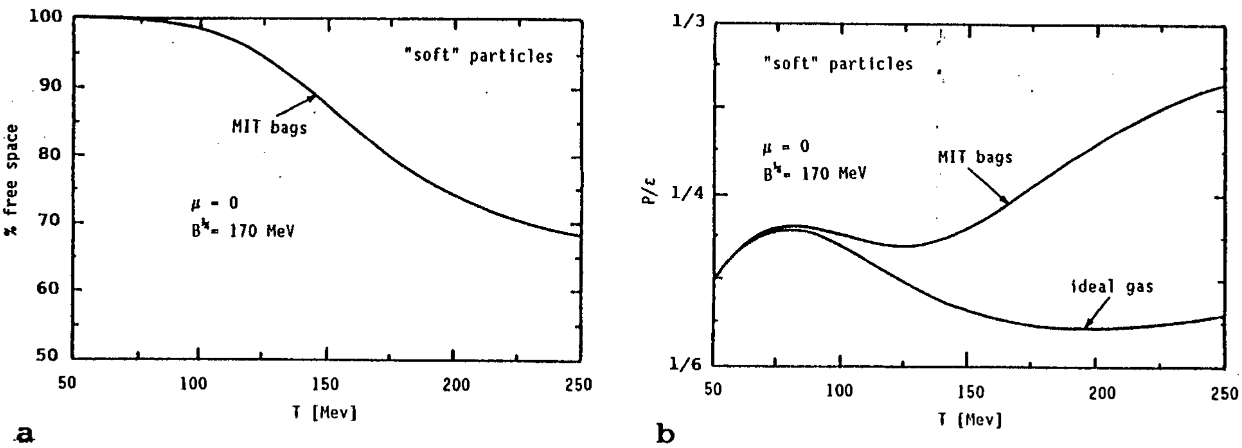

Figure 4.15: Free space and P/ε as a function of the temperature

The bump in the curves originates from a change in composition (see fig.(4.16) below). The soft particle model presented here for the nuclear matter reaches the limit $P/\varepsilon=1/3$ faster than the description of an ideal gas. The reason is that the energy in the system is divided amongst fewer particles. As a consequence, the energy per particle rises. The particles become relativistic because the increase in the rest mass due to the decreased particle volume becomes negligible for higher temperatures. The behaviour found here for varying T at $\mu=0$ resembles the behaviour found for varying μ at T=0 presented in the last chapter. At $T\neq0$ not only the nucleons but all other hadrons in the mass spectrum can occur. The most important particle is the pion as the lightest and smallest hadron. The change of the composition of the system with temperature is shown in fig.(4.16).

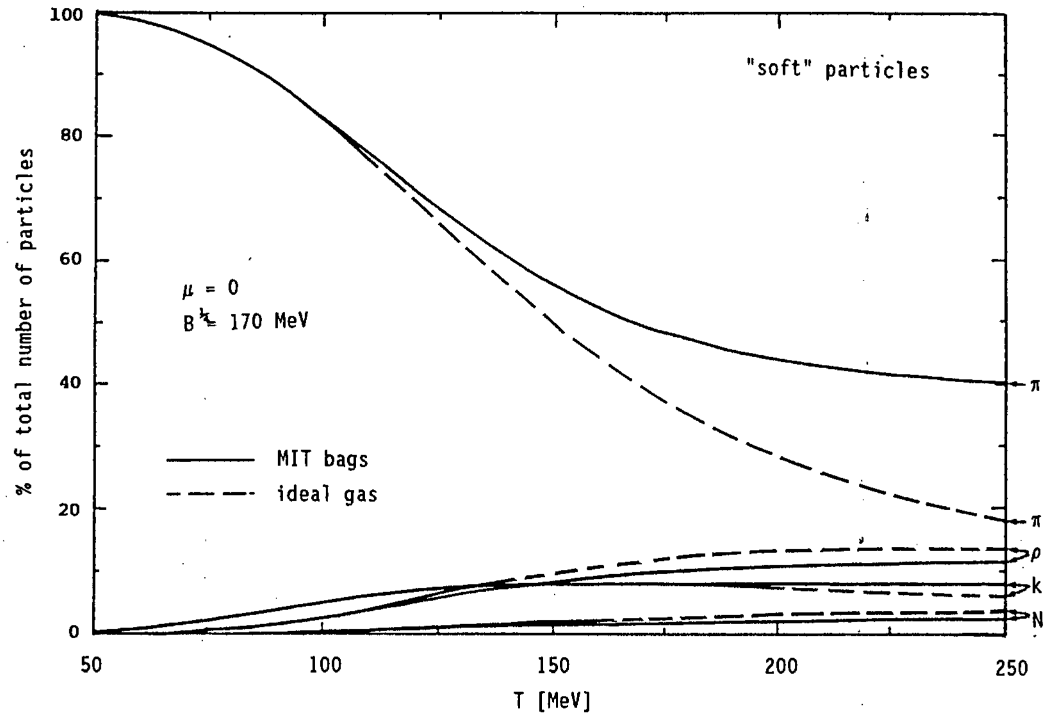

Figure 4.16: Temperature dependence of the particle composition

In an ideal gas the amount of heavy particles with a high g-factor increases markedly with increasing temperature. When the mass of the particle becomes negligible the particle composition is governed by the g-factor, i.e. particles with high g-factors dominate. In the soft particle description the composition is always dominated by the pion because it is the smallest particle. Bigger and heavier particles are suppressed even at high temperatures because the system rejects the particles due to their size. In contrast to the "excluded volume correction", the "ε-correction" or the bootstrap model, the composition differs from the composition obtained from an ideal gas description. All ratios between different types of particles are shifted towards the side of the smaller type of particle! This effect increases with higher temperatures.

Fig.(4.17) shows the pressure in the system. It also shows the pressure of a QGP comprising non-interacting (α_s=0) quarks, antiquarks and gluons at the same temperature for different strange quark masses.

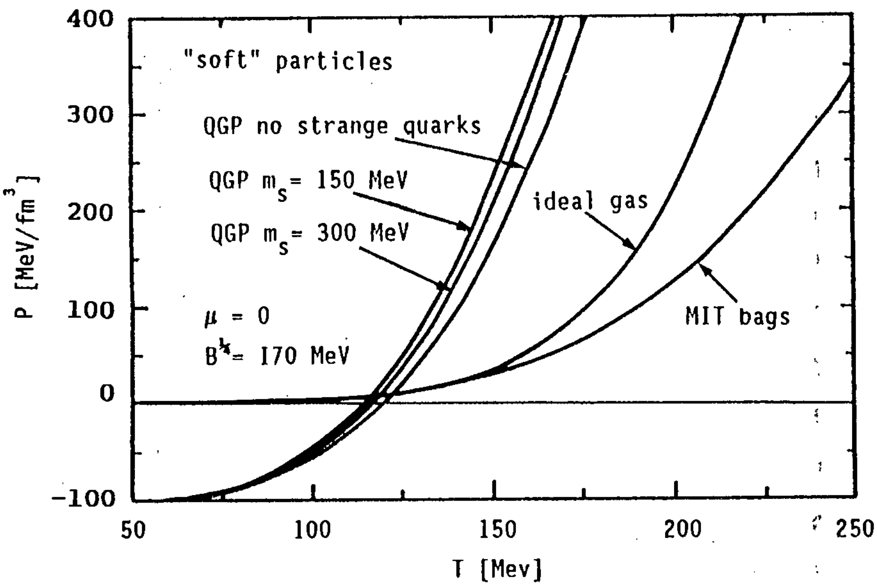

Figure 4.17: Pressure as a function of the temperature

A first order phase transition HG to QGP would be where the pressure curve of the HG crosses the QGP curve. The temperature for the phase transition at μ=0, called critical temperature T_c, is nearly independent of the choice of the strange quark mass. Even if the strange quarks are totally neglected the critical temperature is about $T_c \approx$ 115 MeV. Compared to other calculations and predictions [27,86] this is a very low value. The reason is not the model used here (see the comparison to other models in Ch.(4.4.6)). For this critical temperature the description with the soft particles in the context of the pressure ensemble is very close to the ideal gas description. A "stronger" correction always leads to a lower temperature. The main reason for the low critical temperature is the choice of the bag constant $B^{\frac{1}{4}}$ = 170 MeV. The very strong influence of the bag constant B on the critical temperature due to a shift of the pressure curve describing the QGP is discussed in Ch.(4.4.5).

4.4 The hadron gas of MIT bag at T≠0 and μ≠0 and the phase transition hadron gas to quark gluon plasma

Since the internal structure of hadrons could be explained by the introduction of quarks and gluons the question arose whether there could be a phase in which the quarks and gluons can move freely without being "confined" into particles. QCD calculations indicate that for high densities nuclear matter dissolves and forms a new phase called QGP. Since then several approaches have been made, both theoretical and experimental to find the conditions and indications for this phase transition from nuclear matter to QGP [1-6,79].

In order to calculate the conditions of the phase transition, two different approaches are generally used. The first method is based on the QCD interactions in conjunction with lattice calculations [86,87]. These calculations are still restricted to very small values of the chemical potential μ, i.e. to baryon free systems.

The second approach is based on a thermodynamic description of both phases. The hadron side and the plasma side are calculated independently. A first order phase transition is then constructed based on the assumption that for a given T and μ the system will always be in the state with the lowest value of the thermodynamic potential per volume $\Omega/V = -P$ or in the state with the largest pressure, respectively. The two phases co-exist if:

$$P_{\text{Hadron phase}} = P_{\text{Plasma phase}} \qquad \text{(Mechanical equilibrium)}$$

$$T_{\text{Hadron phase}} = T_{\text{Plasma phase}} \qquad \text{(Thermal equilibrium)}$$

$$\mu_{\text{Hadron phase}} = \mu_{\text{Plasma phase}} \qquad \text{(Chemical equilibrium)}\ . \qquad (4.24)$$

The constructed phase transition is of first order because, with equations (4.24), $\varepsilon_{\text{Hadron phase}}$ is in general different from $\varepsilon_{\text{Plasma phase}}$.

It would be desirable to have one thermodynamic potential describing **both** phases including the phase transition. Unfortunately no such potential has yet been constructed.

In the next chapters I will first present the thermodynamic description of the QGP and then construct the phase transition to the hadron phase as described above. For the hadron phase I use the pressure ensemble description derived in Ch.(3.3). In contrast to the applications already discussed in Ch.(4.3.2) and Ch.(4.3.3), both μ and T will be different from zero.

4.4.1 The equation of state for the quark gluon plasma

The EOS for the QGP used in this thesis is derived from the grand canonical thermodynamical potential Ω_{QGP} [31,34,88,89] for massless quarks

$$\Omega_{QGP} = - PV_{QGP} = \frac{-V}{360\pi^2} \left\{ g_q \left(\left[15\mu_q^4 + 30\mu_q^2 (\pi T)^2 \right] (1 - \frac{2\alpha_s}{\pi}) + 7(\pi T)^4 (1 - \frac{50}{21}\frac{\alpha_s}{\pi}) \right) \right.$$
$$\left. + 4g_g \, (\pi T)^4 (1 - \frac{15}{4}\frac{\alpha_s}{\pi}) \right\} + BV \qquad (4.25)$$

which contains the lowest order of α_s perturbative corrections in the strong coupling constant due to the quantum chromodynamic interactions between quarks and gluons [89]. g_q and g_g are the degeneracy of the quarks and gluons.

Partial derivatives of eq.(4.25) with respect to μ_q , T and ß lead to the quark density ν_q , the entropy density s and the energy density ε

$$\nu_q = \rho_q - \rho_{\bar{q}} = \frac{g_q \mu_q}{18\pi^2} \left[\mu_q^2 + (\pi T)^2 \right] (1 - \frac{2\alpha_s}{\pi}) \qquad (4.26)$$

$$s = \frac{1}{90\pi} \left[g_q \left\{ (15\mu_q^2 \pi T \, (1 - \frac{2\alpha_s}{\pi}) + 7(\pi T)^3 (1 - \frac{50}{21}\frac{\alpha_s}{\pi}) \right\} \right.$$
$$\left. + 4g_g \, (\pi T)^3 (1 - \frac{15}{4}\frac{\alpha_s}{\pi}) \right] \qquad (4.27)$$

$$\varepsilon = \frac{1}{120\pi^2} \left[(15 g_q \mu_q^4 + 30 g_q \mu_q^2 \, (\pi T)^2)(1 - \frac{2\alpha_s}{\pi}) + 7 g_q (\pi T)^4 (1 - \frac{50}{21}\frac{\alpha_s}{\pi}) \right.$$
$$\left. + 4g_g \, (\pi T)^4 (1 - \frac{15}{4}\frac{\alpha_s}{\pi}) \right] + B \quad . \qquad (4.28)$$

Interpreting three quarks (three antiquarks) as a baryon (antibaryon) the baryon density is

$$\nu = \frac{1}{3} \nu_q \quad . \qquad (4.29)$$

Because in this thesis I am only interested in showing the principle behaviour of the EOS and the phase transition on the finite particle size of the hadrons, α_s correction will not be applied. To estimate the influence one example is calculated where α_s is taken as a constant (see Ch.(4.4.7)). Several approaches with running coupling constants have been suggested [34,89,90] differing in dependence of α_s on for example Λ (Λ = QCD scale parameter),T,μ,ν,r and the stage at which they are applied. Running coupling constants will not be used because up to now it has been impossible to decide which is the best approximation to reality. Eqs.(4.25-4.28) are only valid for massless quarks. In the case of $\alpha_s = 0$ heavy quarks (the strange quarks) can be considered when their contribution is calculated according to Ch.(2.1), i.e. they are regarded as an independent ideal gas. This contribution is then added to the expressions in eq.(4.25). An overview dealing with the properties of the QGP is found in [91].

4.4.2 The chemical potential of the different particles

The equations needed to describe the hadron gas have already been derived in Ch.(3.3) (eq.(3.34) and eq.(3.38)). For $T \neq 0$ and $\mu \neq 0$ the additional problem arises how to determine the chemical potential μ_i of each particle species. This problem is generally solved by using the assumption that at the phase boundary the particles dissolve into their quark content. Assigning the light quarks (up and down quarks) the chemical potential μ_q and the heavy strange quarks the chemical potential μ_s, the chemical potential for the particles in the hadron gas are related to the chemical potentials μ_q and μ_s in the plasma phase by, e.g.

$$
\begin{array}{ll}
N \leftrightarrow qqq & \mu_N = 3\mu_q \\
\overline{N} \leftrightarrow \overline{qqq} & \mu_{\overline{N}} = -3\mu_q = -\mu_N \\
\Lambda \leftrightarrow qqs & \mu_\Lambda = 2\mu_q + \mu_s \\
\Omega \leftrightarrow sss & \mu_\Omega = 3\mu_s \\
\pi \leftrightarrow q\overline{q} & \mu_\pi = \mu_q + \mu_{\overline{q}} = 0 \\
K \leftrightarrow q\overline{s} & \mu_K = \mu_q + \mu_{\overline{s}} \\
\overline{K} \leftrightarrow \overline{qs} & \mu_{\overline{K}} = \mu_{\overline{q}} + \mu_{\overline{s}} \\
\vdots & \vdots
\end{array}
\qquad (4.30)
$$

Chemical equilibrium is then characterized by

$$\mu_q \text{ Hadron side} = \mu_q \text{ Plasma side}$$

$$\mu_s \text{ Hadron side} = \mu_s \text{ Plasma side} \quad . \qquad (4.31)$$

With these relations the phase transition is still a function of the three variables T, μ_q and μ_s. It turns out that the phase transition is very insensitive to the choice of μ_s as was verified by calculating the phase transition curve including and excluding all particles containing strange quarks. Particles containing strange quarks are rare in the system (see Ch.(4.3.3)). The dominant particles at the phase transition are the pion for small μ_q and the nucleon for small T. Both pion and nucleon do not contain strange quarks. For other values of T and μ, pion and nucleon are still the main constituents of the hadron gas. The most important particle carrying strangeness is the kaon (K). The next most abundant species of particle, ρ and Δ, does not contain any strange quarks. The presence of a few particles containing strange quarks leads to a small increase of the energy density. This reflects the fact that the pressure is mainly due to the light particles whereas all particles contribute to the energy density. The insensitivity of the phase transition to particles containing strange quarks has also been found in calculations using the "ε-correction" [33]. In the following calculation I will set μ_s=0. This is justified because it is assumed that a QGP created in a high energy heavy ion collision will have no net strangeness, as normal matter contains no strange quarks and strange quarks are always created as strange-antistrange pairs. For μ_s=0 there will be no net strangeness in the QGP. This exactly describes the conditions expected at the beginning of the phase transition QGP→HG or at the end of a phase transition HG→QGP. For the hadron phase however, μ_s must be different from zero except for some special conditions [92], and for T=0. This means that during the phase transition μ_s has to change, leading to a separation of strangeness between the two phases during the transition. Some interesting suggestions for the experimental detection of the phase transition are based on this fact [36,37,92]. As discussed above the influence of μ_s on the phase transition is small. I have therefore restricted my calculations to μ_s=0.

4.4.3 The calculation procedure

In order to calculate the properties of the phase transition with the pressure ensemble used to describe the hadron phase, the computer program has to work at four levels. Starting from the lowest one they are:

1. Calculation of the integrals in eq.(3.34) and eq.(3.38) for a given set of variables P,T,μ,v. This was done with a Gaussian integration routine or by interpolation of the before tabulated integral (see appendix A).

2. Calculation of the pressure in the thermodynamic limit (eq.2.15) by finding the pole of the grand canonical pressure partition function (eq.(3.31)) i.e. the zero of the denominator of the grand canonical partition function for given values of T,μ,v (see appendix B).

3. Determination of the maximum of the pressure P as a function of v (see appendix C) for given T,μ i.e. the value of v which will be chosen by the system.

4. Balancing the pressure in both phases. This is done by either changing T for fixed μ_q or changing μ_q for fixed T. Doing the calculation for different values of the fixed variable leads to the critical curve (pairs of T and μ_q at the phase transition) in the T-μ_q plane. The balance of the pressures was calculated numerically by searching for the root of $F = P_{\text{Plasma phase}} - P_{\text{Hadron phase}}$ (see Appendix B).

The numerical calculation of such a hierarchical problem is difficult. For the balance of the pressure and the adjustment of T or μ_q to a certain accuracy (level 4) the pressure in the thermodynamic limit of the hadron phase obtained from level 3 has to be calculated to a higher accuracy than requested on level 4. The accuracy has to increase again from level 3 to level 2. The numerical solution of the integrals on level 1 necessary to find the optimal particle size in level 2 have to be done with the highest accuracy. If the accuracy change from one level to the next level is too small, the program fails to satisfy all the conditions. If the increase in accuracy is too high, the accuracy to balance the pressure must be low. Otherwise the computer time necessary to do the calculation is enormous because a calculation of the integrals on level 1 to a higher accuracy leads to a rapid increase in CPU (central processor unit) time. The calculation was only possible with a rootfinding program (Appendix B) and a minimum search program (Appendix C) specially written for this purpose.

For all calculations the particles listed in table 4.1 (Ch.4.3.3) are taken into account as long as their contribution to the total particle density ρ exceeds 0.5% and if the particle species does not contribute to the volume occupied by all particles by less than 0.5%. It was verified that this does not alter the presented results.

4.4.4 Phase transition curves for different strange quark mass

Fig.(4.18) shows the phase transition in the T-μ_q plane at $B^{\frac{1}{4}}$= 170 MeV for different values of the strange quark mass used to calculate the QGP phase.

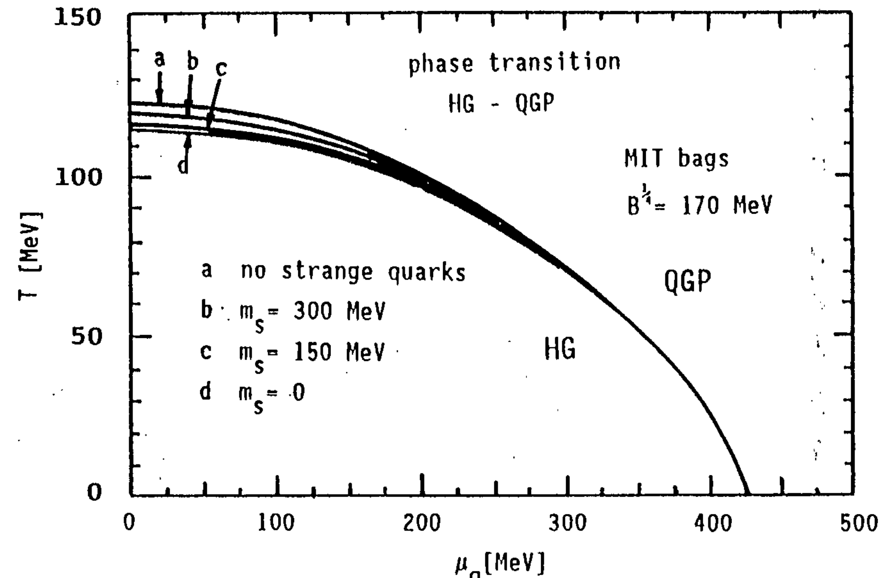

Figure 4.18: Dependence of the phase transition on the choice of m_s

The effect of the strange quark mass is only significant for small μ_q. The pressure of the strange quarks adds to the pressure of the light quarks and gluons. For the same chemical potential, a higher pressure is obtained if the strange quarks are included. The phase transition will occur at a smaller temperature because a smaller temperature leads to a stronger reduction of the pressure in the plasma phase than in the hadron phase. An equilibrium of both phases can again be achieved. The higher the mass of the strange quarks, the lower the reduction of the critical temperature as compared to the case where no strange quarks have been taken into account in the plasma phase. This reduction is due to the mass suppression. For increasing values of the light quark chemical potential μ_q, the number of quarks in the plasma phase increases while the amount of strange quarks with chemical potential $\mu_s=0$ decreases due to the lower temperature of the phase transition point. The fraction of strange quarks becomes negligible.

4.4.5 Dependence of the phase transition on the bag constant

The dependence of the phase transition on the bag constant B is shown in fig.(4.19).

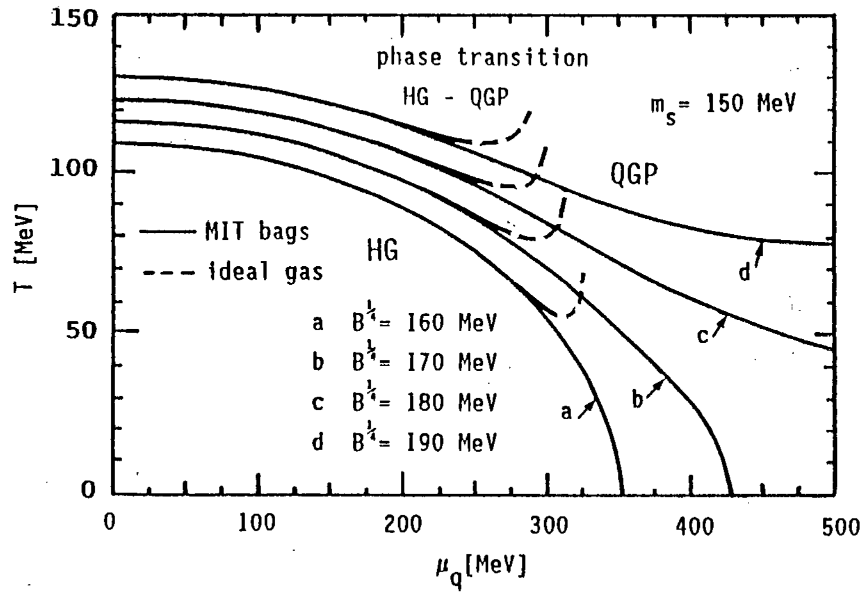

Figure 4.19: Phase transition HG-QGP for different bag constants

To demonstrate the influence of the volume correction on the phase transition, the phase transition resulting if the hadron side is described as a gas of ideal particles, is also indicated (broken lines). For small values of μ_q the difference is very small. Under these conditions it should be sufficient to describe the hadron gas as an ideal gas. The free space at the phase transition (fig.(4.20)) confirms this assumption. At T=0, more than 95% of the total volume is available to the particles. For constant baryon density less volume is taken up by the particles if the bag constant is increased. The particles are smaller if a higher bag constant is chosen.

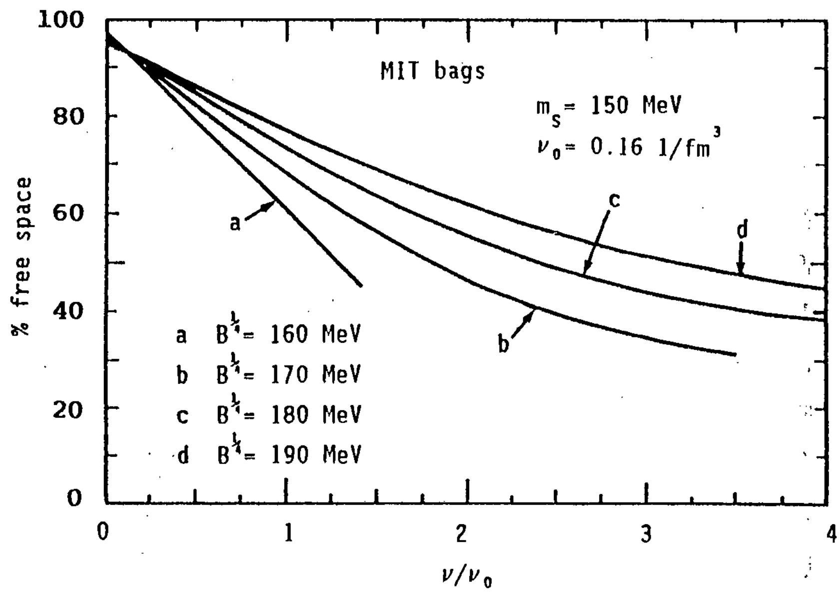

Figure 4.20: Free space at the phase transition HG-QGP

Only for a baryon density close to zero, the higher temperature at the phase transition for larger bag constant leads to a greater total number of particles (particles + antiparticles), so that even though the particles are smaller, more space is filled up. The strong increase of the critical temperature with the bag constant B is an effect not caused by the volume correction.

Fig.(4.21) shows the pressure of both hadron gas and QGP at μ_q=0 for increasing temperature to different values of the bag constant B.

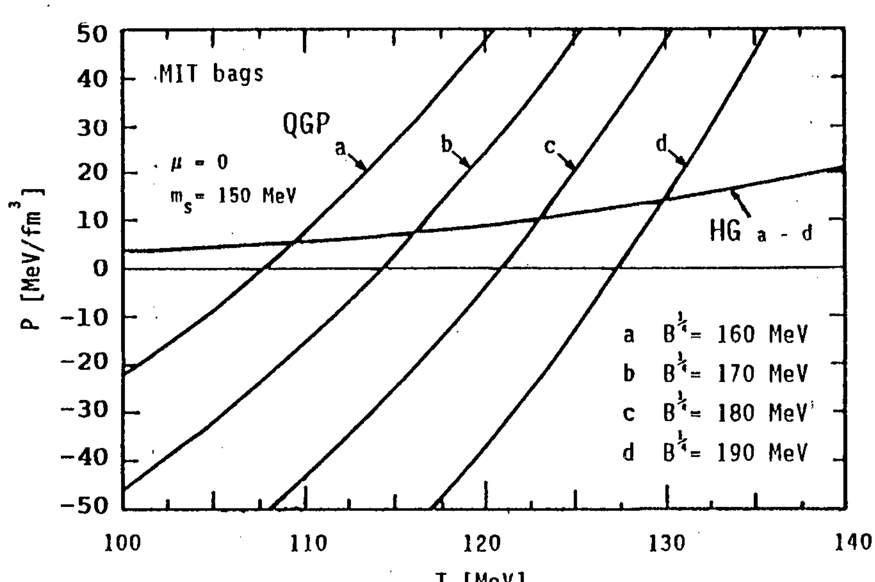

Figure 4.21: Pressure at μ=0 as function of T to different bag constants

The critical temperature moves to higher values mainly because the pressure of the QGP is lower for larger bag constants, i.e. interpreting the bag constant as the vacuum pressure, the higher pressure of the vacuum reduces the pressure of the quarks and gluons in the plasma when seen from the hadron side (see eq.(4.25)). The behaviour of the phase transition curve for increasing μ is interesting. For bag constants lower than $B^{\frac{1}{4}}$= 170 MeV a phase transition for T=0 is found. For larger bag constants there is no phase transition at T=0. Looking at the phase transition curves where the hadron gas is calculated as an ideal gas, a very steep increase of the phase transition temperature with increasing μ_q occurs after an initial drop. This is found for any value of the bag constant (higher than $B^{\frac{1}{4}}$= 148 MeV, for lower values there is no phase transition at all, see Ch.(4.3.1) and [21]). With the volume correction a phase transition is possible for much smaller values of T. For bag constants $B^{\frac{1}{4}}$< 170 MeV the correction due to the particle size is so strong that a phase transition is found for T=0. For larger bag constants the hadrons described here with the basic MIT bag equation (eq.(4.12)) are not only smaller (see fig.(4.7b) in Ch.(4.3.1)), they are also "softer" in the sense that the same type of particle will always have a lower mass when compressed to the same size (see fig.(4.7d) in Ch.(4.3.1)). It is easier to compress them further. I have already shown that a soft particle system goes over into an ideal pointlike gas at high densities (see Ch.(4.3.4) fig.(4.15b) showing P/ε for μ=0). If the bag constant is higher the relativistic behaviour occurs at lower μ_q because the particles are smaller and lighter if compressed to the same size. P/ε for different values of B along the phase transition shown in fig.(4.22) verifies this. For small μ_q we find the opposite. Low bag constants lead to a larger value of P/ε. The general increase for small μ_q arises from the change in composition. Pions dominate at low values of μ_q. Compared to the nucleons which dominate at low temperature the pions are more relativistic because they are lighter. Furthermore a higher temperature at the phase transition leads to a more relativistic system. This explains the general increase of P/ε for small values of μ_q. Nevertheless the system with the highest bag constant and the highest critical temperature is not the most relativistic system. This is due to the fact that for higher temperature more particles with a high mass are present. For μ=0 and $B^{\frac{1}{4}}$= 160 MeV, 22% of all particles are not pions. For $B^{\frac{1}{4}}$= 190 MeV, 35% are not pions.

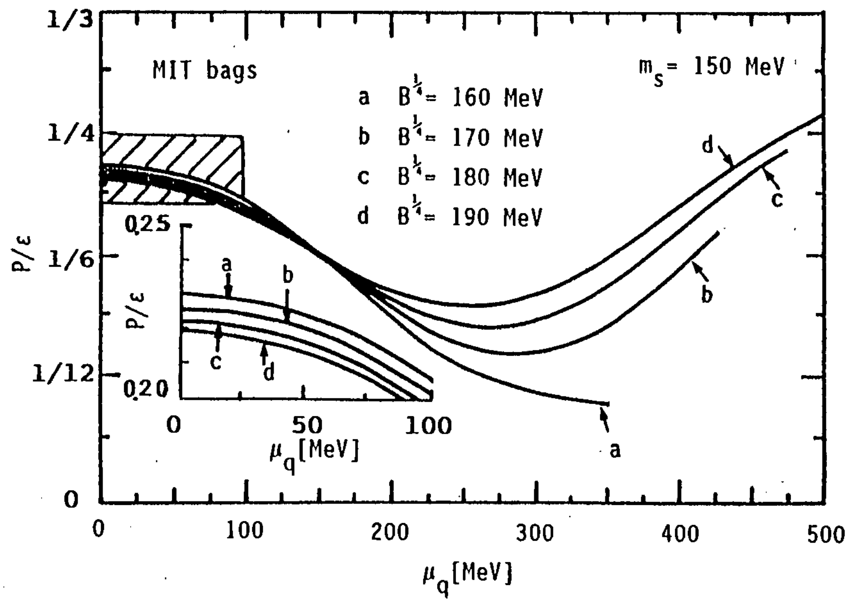

Figure 4.22: P/ε at the phase transition HG-QGP to different values of B

The increase in the amount of heavy particles causes the system to be less relativistic for higher bag constants. As shown earlier, the particles are more pointlike if the bag constant is increased. Therefore it is not surprising that the system calculated with a high bag constant will take up the behaviour found for an ideal gas description, and that from a certain value of μ_q the phase transition temperature increases for increasing μ_q. No phase transition for T=0 exists. The nucleons (remember: for a calculation using the pressure ensemble, there are only nucleons at T=0, see Ch.(4.3.2)) are too small and soft. The reduction of the pressure due to the volume correction is too small. In addition the pressure of the QGP is lower for higher bag constants B. Fig.(4.23a and b) shows the pressure in both phases at T=0 for two different values of the bag constant.

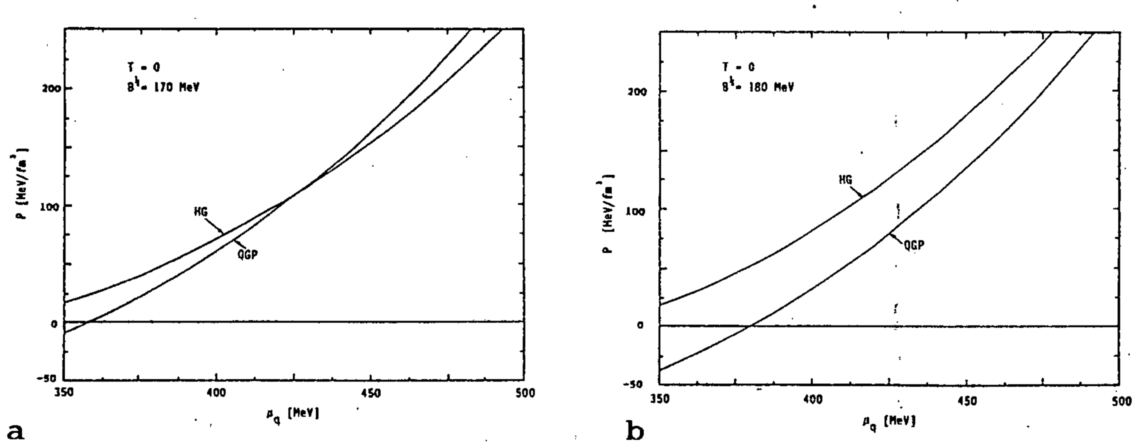

Figure 4.23: Pressure at T=0 for $B^{1/4}$= 170 MeV and $B^{1/4}$= 180 MeV

Already for $B^{1/4}$= 170 MeV a slight change in the slope of one of the pressure curves has a strong effect on μ_q where the curves cross (phase transition). For $B^{1/4}$= 180 MeV the slopes of the pressure in both phases is so similar that they will not cross. Because a phase transition is generally expected to also take place at zero temperature my model description leads to an upper limit of the bag constant. In general we find that the phase transition depends on the volume correction only at low temperatures (see the following paragraph). In my calculation "compressible" particles (hadrons obeying the basic MIT bag equation) were introduced. A change in the size of the particles and their "intrinsic" behaviour must lead to a different result for small temperatures. A change from $B^{1/4}$= 160 MeV to $B^{1/4}$= 180 MeV in this model already means that the size of an isolated nucleon changes from 2.73 fm^3 to 1.72 fm^3. It turns out that the basic form of the bag equation cannot be used to do calculations for any bag constant. If the basic form of the MIT bag equation is used, values for the bag constant close to the value originally obtained ($B^{1/4}$= 145 MeV) [73-75] should be chosen. For too high bag constants the particles become too small in this description (a nucleon radius smaller than 0.5 fm is expected to be unrealistic). It is also unrealistic that the particles are "softer" if we give them a smaller size. If the size of the particles used only describes the "hard core" it should be hard to compress them. For the basic MIT bag equation I found just the opposite behaviour. This behaviour should change if a chiral bag model [93-95] is used; the introduction of a pion cloud leads to an additional contribution to the mass proportional to $1/r^3$. Including this term will lead to "harder" EOS. It is interesting to see that more recent modifications of the "basic" MIT bag equation predict nearly the same size for the particles obtained here at a bag constant of $B^{1/4}$= 170 MeV for much higher bag constants (e.g. $B^{1/4}$= 220 MeV) [90]. Independent of the volume correction this also leads to higher phase transition temperatures at μ_q= 0 (critical temperature). Higher critical temperatures seem more realistic than the values around T_c= 120 MeV for $B^{1/4}$= 170 MeV. For a bag constant of $B^{1/4}$= 220 MeV the critical temperature is around $T_c \approx$ 150 MeV.

4.4.6 Comparison to the "excluded volume correction" and the "ε-correction"

In the "excluded volume correction" the bag constant and the particle size can be used as independent parameters. In a description with the pressure ensemble particle size and the bag constant are related through the bag equation. In the "ε-correction" the particle size does not appear at all. Because this model "originates" from the bootstrap model (Ch.(2.3)) the size of the particles was "substituted" by the energy density because at the bootstrap singularity the entire space is filled with matter of energy density 4BV (one huge cluster). Fig.(4.24) and fig.(4.25) show the phase transition in the T-μ_q plane and the corresponding free space as a function of μ_q.

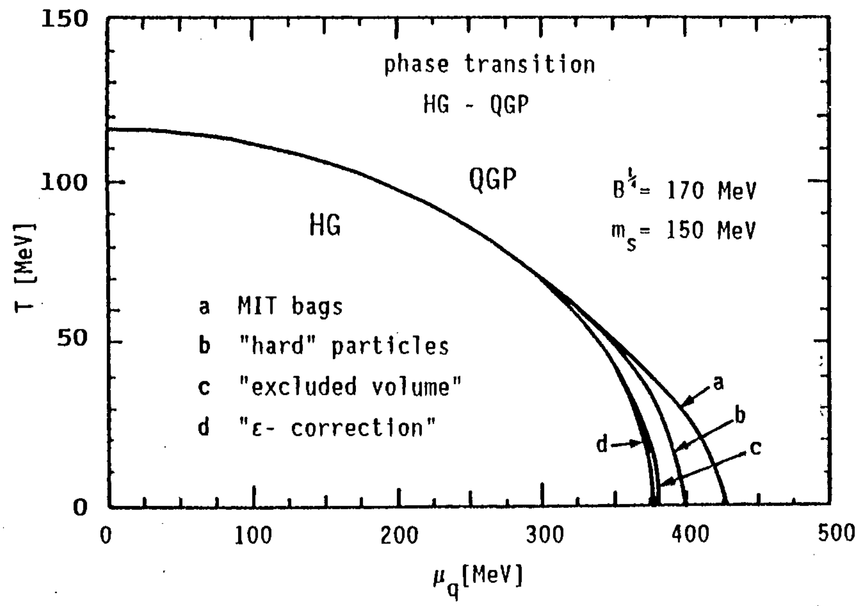

Figure 4.24: Phase transition for different types of models

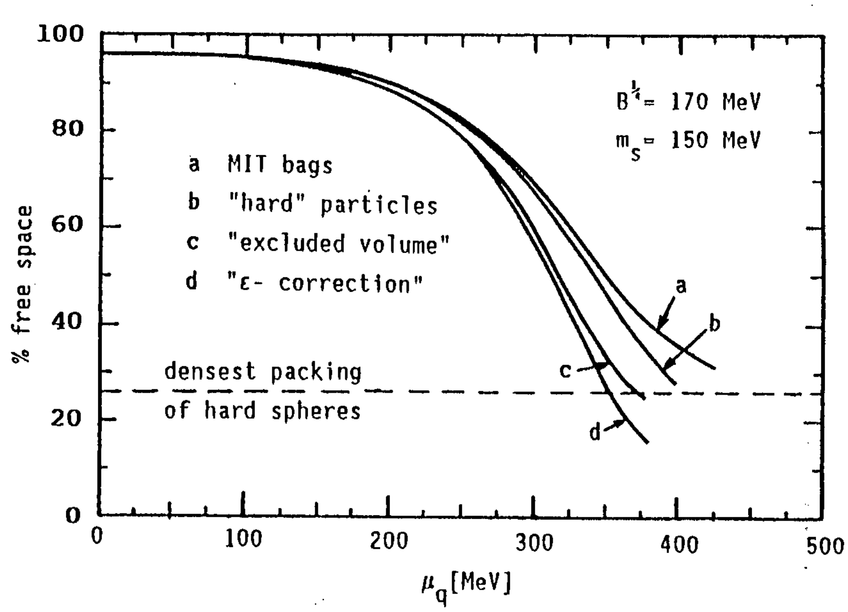

Figure 4.25: Free space at the phase transition HG-QGP

I have shown the results of calculations with the pressure ensemble assuming soft and hard particles, the "extended volume correction" and the "ε-correction", using hard particles with a bag constant $B^{\frac{1}{4}}$= 170 MeV. The particle size chosen for the hard particles is the volume the particles will have at infinite dilution in the calculation using the pressure ensemble for soft particles, i.e. the volume at the minimum of the MIT bag equation (see fig.(4.17a). As shown the volume is filled to a great extent at low temperatures only. The free space for T=0 is

31.4 % (-----) soft particles pressure ensemble
28.0 % (16.7%) hard particles pressure ensemble
15.9 % (1.6 %) hard particles "excluded volume correction"
25.0 % (22.1%) hard particles "ε-correction" .

The values in brackets are the free space if a bag constant of $B^{\frac{1}{4}}$= 235 MeV (B = 397 MeV/fm^3) is used. Note that a free space of 26% belongs to the densest packing of spheres. For lower values of the free space as obtained with the "excluded volume correction" and the "ε-correction" the model is only consistent under the assumption that the particles are deformed. The baryon density ν for the hadron phase and the plasma phase for the different models with $B^{\frac{1}{4}}$= 170 MeV are shown in fig.(4.26).

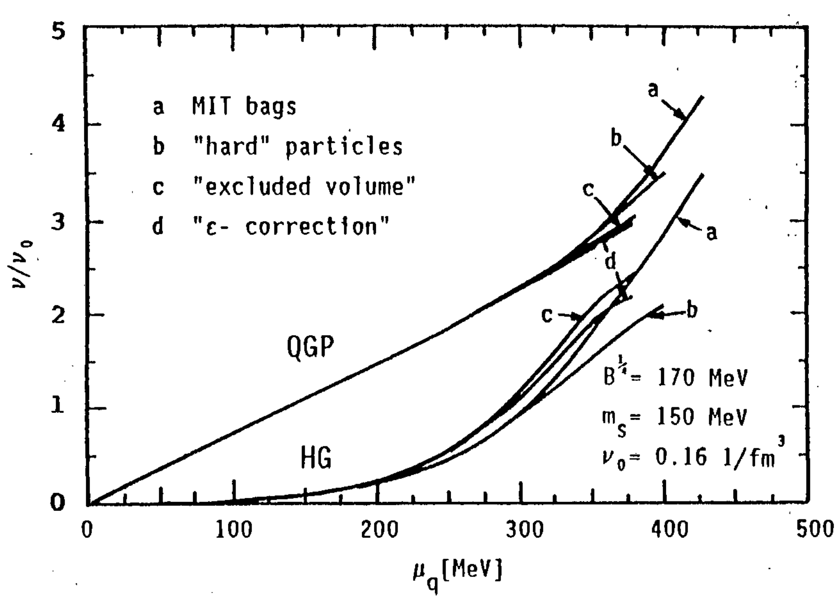

Figure 4.26: Baryon density ν at the phase transition HG-QGP

The QGP phase has always the higer density, as expected. The curves end where T=0. At this point the jump in the baryon density is

ν_{HG}/ν_0	ν_{QGP}/ν_0	model
3.5 (---)	4.3 (----)	soft particles pressure ensemble
2.1 (8.8)	3.5 (20.0)	hard particles pressure ensemble
2.4 (8.4)	3.0 (9.7)	hard particles "excluded volume correction"
2.2 (6.4)	3.0 (9.0)	hard particles "ε-correction" .

Again the brackets contain the values for ν to a bag constant $B^{\frac{1}{4}}$= 235 MeV. Fig.(4.27) shows the energy density ε in both phases.

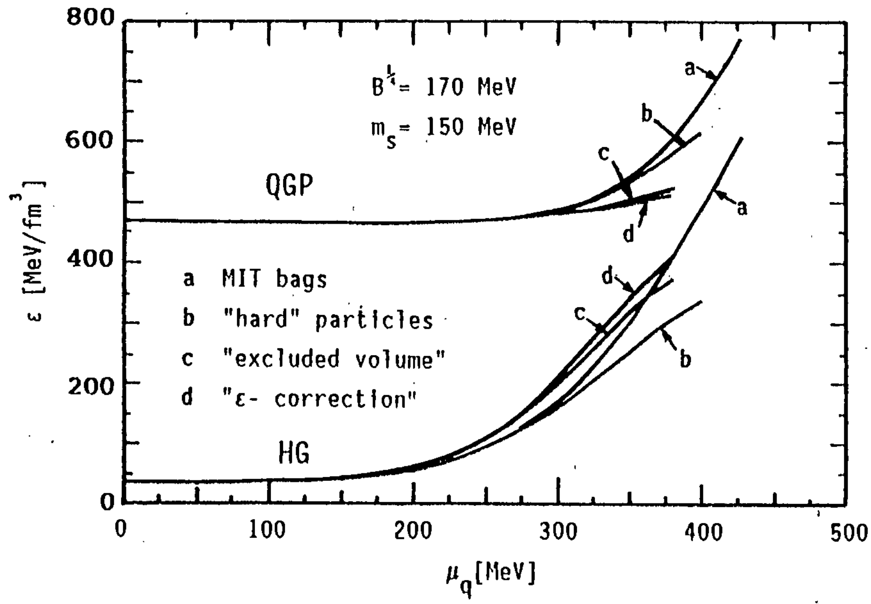

Figure 4.27: Energy density at the phase transition HG-QGP

The difference between the curves is the latent heat. For higher bag constants the latent heat increases. This is caused mainly because the energy density of the vacuum B adds to the energy density of the quarks and gluons (see Ch.(4.4.1)). A large value of the latent heat is consistent with the assumption of a first order phase transition. This does not exclude the possibility of a higher order phase transition. In fig.(4.28) the entropy per baryon is shown as a function of the temperature. The entropy per baryon at the phase transition for both phases intersect. For values of S/b smaller than S/b ≈ 17 a reheating of the system will occur if the phase transition QGP→HG is isentropic [34,36,37,99]. For higher values of S/b the temperature in the system has to decrease. Higher bag constants shift the intersection to higher values of S/b and to higher temperatures.

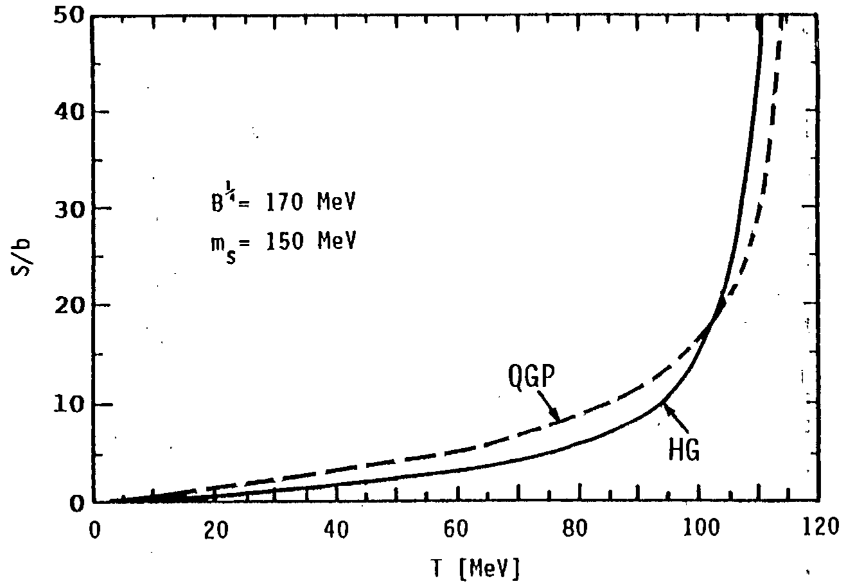

Figure 4.28: Entropy per baryon as function of the temperature at the phase transition HG-QGP

4.4.7 Dependence of the phase transition on α_s corrections

α_s corrections are introduced to describe quantum chromodynamic interactions between quarks and gluons. In both the plasma and the hadron phase, this interaction should be accounted for. In the hadron phase α_s corrections enter because quarks and gluons are the constituents of the hadrons. Various approaches exist on the dependence of α_s on Λ (QCD scale parameter),r_i,μ,T [34,89,90]. In the following calculation I will assume that the basic form of the MIT bag model includes the effect of the α_s corrections. For the plasma phase I will use α_s as a constant to demonstrate the influence of such a correction. Fig.(4.29) shows the phase transition in the T-μ plane calculated for α_s= 0 and α_s= 0.3. The dependence of the phase transition on the value of α_s results from the reduction of the pressure in the plasma phase. A constant finite value of α_s can be interpreted as a reduction of the degeneracy of the QGP (see eq.(4.25)). Because the pressure increases stronger in the QGP than in the hadron phase if T (μ_q) is increased, a finite value of α_s leads to a higher phase transition temperature (value of μ_q). The higher temperature leads to higher baryon and energy density in the hadron phase at the phase transition.

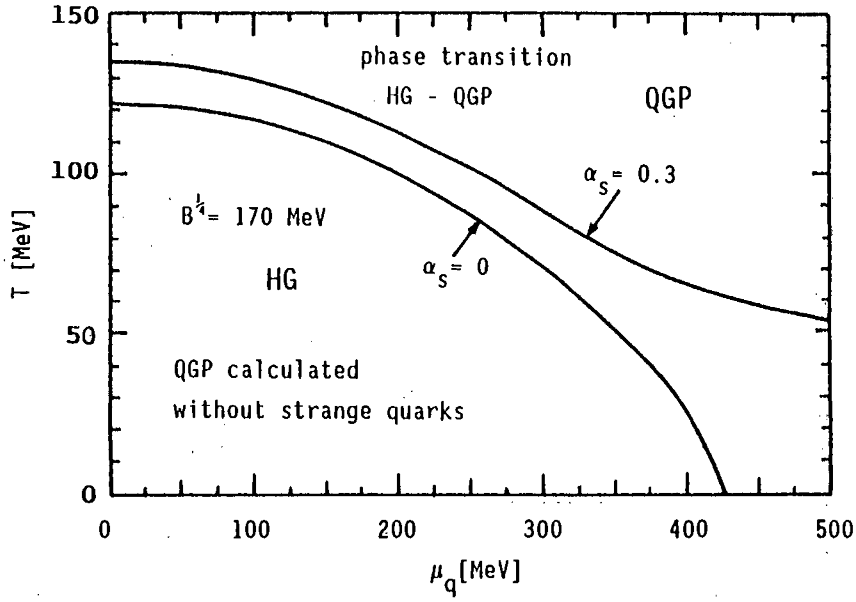

Figure 4.29: Dependence of the phase transition HG-QGP on α_s

The same effect as for increasing the bag constant is seen. At low temperature the particles become so compressed that they develop a relativistic behaviour. No phase transition for T = 0 can be found if $\alpha_s = 0.3$. This is analogous to the case of increasing the bag constant (see Ch.(4.4.5). Once again $m_i \sim 1/r_i$ for small particle radii (compressed particles) in the basic MIT bag equation leads to unrealistically small particles. The knowledge of the higher order term of 1/r is necessary for a proper description at high densities when the particles are compressed. These terms are normally negligible for noncompressed particles (the exceptions are pion contributions to the particle mass which have been included in chiral bag models [93-95]). In contrast to an increase of the bag constant which leads to a strong increase of the latent heat, the latent heat is nearly unchanged if α_s corrections are applied. For the example of $\mu_q=0$ and $B^{1/4} = 170$ MeV

	ε_{HG}	ε_{QGP}	Latent Heat
$\alpha_s=0$	33 MeV/fm^3	459 MeV/fm^3	426 MeV/fm^3 ,
$\alpha_s=0.3$	76 Mev/fm^3	486 MeV/fm^3	410 MeV/fm^3 .

Note that this effect and the increase of the critical temperature is independent of the particular finite size correction. As in all other cases the particles in the hadron phase occupy less than 10% of the total volume at $\mu_q=0$.

5 CONCLUDING REMARKS

The objective of this thesis is a quantitative assessment of the influence of the finite size of hadrons on the EOS of nuclear matter and on the expected phase transition HG-QGP. Different quantum statistical approaches of finite size corrections found in the literature were reviewed. An improved model was developed. In this model the theory of the grand canonical pressure ensemble was successfully applied to a system of different particles (hadrons) including their proper statistics and corrections due to their finite size. The effects of the finite size of the particles was discussed under several different conditions. It was concluded that a description of the hadrons as "hard" particles is not suitable to describe the properties of dense nuclear matter. Instead the MIT bag equation was employed to obtain an EOS of "soft" particles; soft in the sense that the hadrons shrink due to the pressure in the system. The MIT bag equation describes the hadron mass m_i as a function of the volume of the hadron, v_i.

For small temperatures the phase transition is strongly dependent on the finite size of the particles. It was surprising to find that for small μ_q the phase transition is nearly independent of the type of volume correction. The critical temperature T_c depends strongly on the choice of the bag constant B and the application of α_s corrections. Even though I have, with $B^{\frac{1}{4}}$= 170 MeV, chosen a much higher bag constant than $B^{\frac{1}{4}}$= 145 MeV obtained from the MIT bag model, the critical temperature of $T_c \approx 120$ MeV at α_s=0 is rather low. The bag constant of $B^{\frac{1}{4}}$= 170 MeV is considered an upper limit in the chiral bag model (F.Myhrer in [94] page 360). Other bag models [96-98] use even higher bag constants (up to $B^{\frac{1}{4}}$= 235 MeV, by fitting dibaryon states only). Higher bag constants lead to higher critical temperatures and particle densities. With higher particle densities the volume correction also becomes important at μ=0, and will act by reducing the critical temperature, compared to that obtained in an ideal gas description. This is independent of the specific model used to do the volume correction. Higher critical temperatures and densities are also achieved if α_s corrections are applied. Both B and α_s are "input" to the thermodynamic calculation. The phase transition obtained in a thermodynamic description is, as shown, sensitive to the choice of these parameters. Prediciting power can only be achieved if these inputs are accurately known. With the possible range of values for B and α_s this is impossible. Therefore I had to restrict myself to principle effects that occur when finite size corrections are applied. I conclude that a "hard" particle description for nuclear matter at high densities is not reasonable. A description with the pressure ensemble shows that the increase of P/ε with higher densities leads to unphysical sound velocities. Within the "excluded volume correction" or the "ε-correction" similar problems occur (see fig.(4.6) in Ch.(4.2)). Therefore, it seems clear that the hadron should shrink due to the pressure in the system. The new model using the MIT bag equation to describe the "intrinsic" behaviour of the hadrons is promising. It leads to a more consistent description. As expected a change in composition towards the smaller particles is found which is in contrast to earlier models ("excluded volume correction" and "ε-correction").

It is not surprising that the model developed in this thesis is sensitive to the size and the "intrinsic" behaviour of the particles. Therefore, the next step is to improve the model description of the particles (hadrons). It is essential to know the properties of the particles when confined to a small volume. I found that the basic form of the MIT bag equation with a 1/r behaviour is insufficient because for certain choices of B and α_s no phase transition at T=0 can be found.

One of the most difficult questions is: What are the relevant radii of the particles? Quark core? rms? ...?. These questions go even further. Is the size of the particles so small that the particles should be described by wave functions? How to incorporate the finite size of the particles in a completely quantum mechanical description is still an open question. Even if an ansatz is found the question arises whether the problem can be solved, or not. There is no hope of an analytical solution. For the model developed the numerical work was very time-consuming. The FORTRAN programs written to obtain the presented results are about ~10 000 lines altogether (a print-out is available on request).

I would like to close with some critical remarks on the expected phase transition HG-QGP:

If the critical temperature is high (>200 MeV) the volume of the hadrons will be important at the phase transition for any value of μ. A big fraction of the total volume will be taken up by the particles. I cannot exclude the possibility that there is a continuous phase transformation rather than a phase transition. Bigger clusters, i.e. multi-hadrons, not taken into account in the present calculation, could be formed and fill up more and more of the total space. The EOS inside these big "bubbles" could go over continuously into the EOS of the QGP as the "bubble" increases by having more and more quarks, antiquarks and gluons inside. Up to now no description for such "bubbles" (quark matter droplets) exists, i.e. there is no EOS for a finite size system of N particles. Even without the possibility of "bubbles" the calculation presented here indicates that the latent heat decreases when the volume correction becomes important (see Fig.(4.27) in Ch.4.4.6)).

If the properties of the QGP are calculated and the points with equal energy density are drawn in the T-μ plane a curve is obtained which looks like the phase transition curve expected. There may be a physical explanation that the QGP cannot exist for an energy density lower than a critical value nearly independent of T and μ.

In this thesis the corrections to the EOS for nuclear matter due to the finite size of the hadrons, was improved by introducing a new model. In contrast to the other volume corrections discussed, all thermodynamic properties are calculated in the usual thermodynamic limit. It was found that the phase transition HG-QGP is strongly dependent on the value of the bag constant, the application of α_s corrections and the model describing the properties of the hadrons. Before being able to further improve on the calculations it is essential that a reliable value for the bag constant is established and a better description of the α_s corrections and the hadrons is developed.

Acknowledgements

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APPENDIX A: Numerical Solution of the Integrals

The integrals in this work are of the type

$$\int_0^\infty p^2 \; f(E) \; dp \qquad \text{with } E=(p^2+m^2)^{\frac{1}{2}} \; . \qquad \text{(A1)}$$

They appear in connection with the calculation of pressure P, energy density ε and particle density n. These integrals were all solved by the same procedure outlined below for the general form of all these equations (A1). At the end the three different functions f(E) appearing in the expressions for P,n and ε in the pressure ensemble as the most complicated case are given. It is easy to extract all other cases from these three examples by simple manipulations.

For the numerical solution of the integral of type (A1) it is advantageous to first do some mathematical manipulations to change the infinite integration limits of the integral to finite values. There are two reasons for doing so:

1. The construction of the digital computers leads to a biggest, lowest (negative) and smallest (i.e near 0) number due to the finite resolution of the numbers. Trying to solve (A1) in the given form with any numerical integration routine available will fail when pushing the upper integration boundary to the biggest number available. The contribution to the integral of the infinite tail of the function in the argument is finite. This means that the function decreases with increasing momentum or energy (in all our cases like $e^{-E/T}$) and will fall into the "gap" around 0. Random numbers will be integrated long before the upper boundary reaches the biggest possible number. On the other hand the step size for the integration has to be reduced to a very small value in order to resolve the main contribution at the lower integration limit. This leads to a very long calculation time.

2. When the problems mentioned under 1. are avoided by a realistic finite upper integration limit there is no way to ensure that the integral calculated is accurate to the required number of digits. It is impossible to say how far one can push the upper integration limit before the limit of the computer is reached. One also does not know how far one must integrate to obtain a sufficiently accurate result.

A better way to solve the integral numerically is to change the variables from p to E

$$\int_0^\infty p^2 \; f(E) \; dp = \int_m^\infty E \; (E^2-m^2)^{\frac{1}{2}} \; f(E) \; dE \qquad \text{(A2)}$$

and substitute the high energy behaviour $x=e^{-E/T}$ which leads to

$$\int_m^\infty E \; (E^2-m^2)^{\frac{1}{2}} \; f(E) \; dE = -T^3 \int_0^{e^{-\beta m}} \frac{\ln x \; (\ln^2 x - (\beta m)^2)^{\frac{1}{2}}}{x} \; f(E) \; dx$$

$$\text{with } E = - T \ln x \quad . \qquad \text{(A3)}$$

The infinite upper integration limit is thus converted into a finite value. However the argument now has a singularity at x=0 (ln 0). The substitution "squeezes" the infinite tail into this singularity. Because the contribution of the singularity is finite (improper integral) and is located at the boundary of the integration it is possible to use a Gaussian integration routine or any other method which does not use the function value at the boundary. Only routines which split the given interval in more and more subdivisions until the required accuracy is reached must be used. This ensures that an error will occur during the computing if the contribution of the singularity is not finite and the integral is not an improper integral. In this case the interval next to the singularity will be split until the function is requested so close to the singularity that an overflow occurs. It was verified with some analytical improper integrals, that the accuracy given to the Gauss routine used here (CERN computer library D109 DGAUSS) is really reached if the upper boundary in eq.(A3) is not too small i.e. temperatures should be >20 MeV.

Three different functions f(E) appear in connection with the pressure ensemble. Inserting them into the equation above leads to

$$\text{a)} \quad \pm \int_0^\infty p_j^2 \; \ln(1 \pm e^{-\beta(E_j - \mu_j + Pkv_j)}) \; dp_j$$

$$= \mp \; T^3 \int_0^{a_j} \frac{\ln x}{x} \; \ln(1 \pm \frac{x}{b_j}) \; (\ln^2 x - \ln^2 a_j)^{\frac{1}{2}} \; dx \qquad \text{(A4)}$$

b) $$\pm \int_0^\infty p_j^2 \frac{1}{1 \pm e^{\beta(E_j-\mu_j+Pkv_j)}} dp_j$$

$$= \mp T^3 \int_0^{a_j} \frac{\ln x}{x \pm b_j} (\ln^2 x - \ln^2 a_j)^{\frac{1}{2}} dx \qquad (A5)$$

c) $$\pm \int_0^\infty p_j^2 \frac{E_j}{1 \pm e^{\beta(E_j-\mu_j+Pkv_j)}} dp_j$$

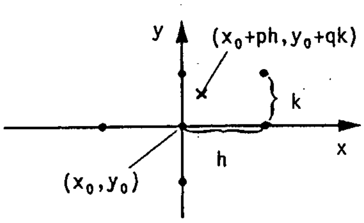
$$= \pm T^4 \int_0^{a_j} \frac{\ln^2 x}{x \pm b_j} (\ln^2 x - \ln^2 a_j)^{\frac{1}{2}} dx \qquad (A6)$$

where I have used the abbreviations

$$a_j = e^{-\beta m_j} \quad \text{and} \quad b_j = e^{\mu_j+Pkv_j}.$$

It turned out that for finding the pressure in the thermodynamic limit the integral eq.(A4) had to be calculated frequently and caused a very long running time on the computer. The program was much faster after tabulating the integral as a function of the two parameters a and b for the most important areas of the two parameters. The value of the integral was then interpolated (when the parameters were inside the table area) by the six point bivariate interpolation formula [100]:

$$f(x_0+ph,y_0+qk) = \frac{1}{2} [\ p(p-1)\ f_{-1,0} + q(q-1)\ f_{0,-1} + p(p-2q+1)\ f_{1,0} + q(q-2p+1)\ f_{0,1}\ ] + (1+pq-p^2-q^2)\ f_{0,0} + pq\ f_{1,1}$$



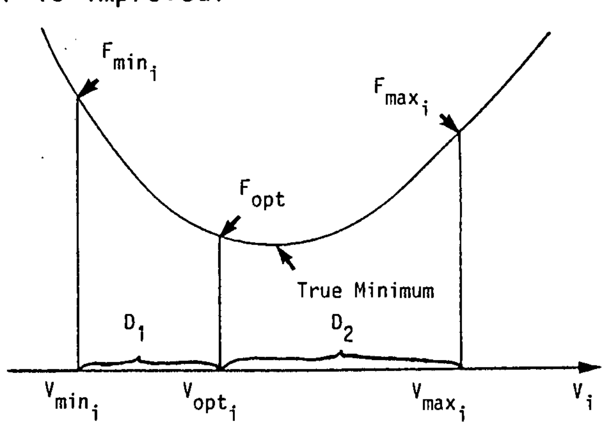
with $f_{i,j} = f(x_0+ih,y_0+jh)$.

APPENDIX B : Numerical search for the pressure in the thermodynamic limit

In a description using the pressure ensemble, the thermodynamic limit is obtained by finding the pole of the grand canonical pressure partition function (see Ch.(3.2)). A numerical search for a pole is difficult. With eq.(3.34) the problem is converted to the problem of finding the root of the denominator of the grand canonical pressure partition function. Library functions exist for this purpose . Because the library program available, CERN program library C205 RZERO, is written in single precision and sometimes has returned a wrong value (this problem seems to be solved now) a new root finding program for a function f(x) in double precision was written, taking care not to calculate the function at points too close to each other. This avoids errors resulting from the finite accuracy of f(x). (The integrals necessary to calculate f(x) are calculated only to a certain accuracy by a Gaussian integration method). Because this program is frequently used, care was taken to make it fast and to protect it against all possible errors.

APPENDIX C: Numerical search for the size of the soft particles

The size of the particles is determined by the maximum of the pressure P with respect to all particle volumes (eq.(4.23)). To obtain this point it is necessary to calculate a maximum in n dimensions. This was done numerically. Library programs are always written to find a minimum in n dimensions because the problem of the search for a maximum can be converted to a minimum search by changing the sign of the function; in my case, to a search of the minimum of -P. Initially the CERNLIB program package MINUIT D506 was used. It was possible to locate the minimum, but it was almost impossible to improve the minimum to an accuracy of more than 3%. Close to the minimum, the change in the function is very small. If the function is calculated at points close to each other in an area near the minimum, the difference in the function value is very inaccurate because the function itself is calculated to a certain accuracy only. In this case the point calculated for the improved location of the minimum can be completely wrong. To solve the problem of finding the optimal volumes of the particles, a new minimizing program was written, using the fact that the particle volumes of the different particles are not significantly correlated (as seen from the correlation coefficients calculated by MINUIT). For uncorrelated parameters it is possible to improve one parameter at a time without affecting the minimum with respect to the other parameters. The new program improves all parameters (i.e. all particle volumes), one at a time. At first the parameter with the largest error is improved.



The error is defined as the maximum of $\frac{D_1}{v_{opt_i}}$ and $\frac{D_2}{v_{opt_i}}$. In the beginning v_{min}, v_{max}, v_{opt} are set to the values given to the function when it is called. If one parameter is improved so far that the error of another parameter becomes significantly larger, i.e. if the error of the improved parameter drops below 1/5 of the next largest error, this parameter is improved next. The procedure is continued until all parameters are adjusted to better than the required accuracy. Finally it is checked again if the function really has a minimum between the error limits of each parameter. As mentioned, this procedure can only be applied if the parameters are not significantly correlated. Otherwise the minimum will be lost. This is reported by the program. To avoid the problem with the finite accuracy of the function as much as possible, an improved value for a parameter was shifted to 1/4 of the required accuracy if the new point was closer than that to the previous best value of this parameter. For the calculations done in this thesis the program worked well as long as the contribution of one kind of particle to the pressure was high enough, i.e. as long as the pressure is sensitive to this type of particle. A species of particles was excluded from the calculation when their total density and the volume occupied was less than 0.5% and decreasing.

APPENDIX D: Alternative least squares fit to the hadron mass spectrum

A fit of the MIT bag equation (eq(4.10)) to the hadron spectrum is always problematic because we will only accept a fit where the mass obtained for the nucleon is close to the well known experimentally determined value. This is not normally achieved in a least squares fit to all light hadrons. The fitted mass of the unstable particles tends to be too high. It turns out that a better fit can be obtained if the unstable particles are excluded. Even then the MIT bag equation yields an unacceptable high value for the nucleon mass.

An acceptable least square fit was found by modifying the MIT bag equation and introducing additional free parameters [81]. Instead of the four free parameters of the MIT bag equation, eight parameters are fitted. This equation cannot be extended further because it turns out that the free parameters are significantly correlated.

Based on the MIT bag equation and the fit mentioned above, I found that an improved fit can be obtained using the following ansatz:

$$m(v) = E_V + E_0 + E_Q + E_C \qquad \text{(D1)}$$

where E_V, E_0 and E_Q are taken from the MIT bag formulation [74,75] and E_C from [81]. E_C is the colour interaction and accounts for both E_m and E_E of the MIT bag model. E_C distinguishes between the interactions q-q, q-s, and s-s by the introduction of three parameters h_{qq}, h_{qs} and h_{ss}. Instead of the four parameters B, Z_0, m_s and α_c in the MIT bag equation (4.10), I have the six free parameters B, Z_0, m_s, h_{qq}, h_{qs} and h_{ss}. In order to fit all masses with the same relative error, I decided to minimize the relative error (see eq.(4.11)). This ensures that all masses are accurate to the same number of digits.

It turns out that by using eq.(D1), no significant correlations between the parameters are found (it is worth mentioning that even with the MIT bag equation, significant correlations occur).

The results obtained for a fit to the most stable particles including and excluding the pion are shown in Table D1.

TABLE D1 : Results obtained by a fit to eq.(D1)

The particles included into the fit are marked with "+". The mass of the light quarks has been set to m_q=0.

		fit excluding the pion						fit including the pion			
		m_{exp} [MeV]	m_{calc} [MeV]	r_{min} [fm]	v_{min} [fm³]			m_{exp} [MeV]	m_{calc} [MeV]	r_{min} [fm]	v_{min} [fm³]
+	N	939	940	0.87	2.79	+	N	939	939	0.87	2.75
	Δ	1232	1291	0.97	3.82		Δ	1232	1293	0.97	3.79
+	ω	783	783	0.82	2.32	+	ω	783	783	0.82	2.30
+	K	496	496	0.60	0.92	+	K	496	496	0.60	0.91
	K^*	892	913	0.80	2.12		K^*	892	911	0.79	2.10
+	φ	1020	1017	0.76	1.86	+	φ	1020	1016	0.76	1.84
+	Σ	1193	1191	0.89	2.93	+	Σ	1193	1193	0.89	2.91
+	Λ	1116	1114	0.87	2.71	+	Λ	1116	1113	0.86	2.68
	Σ^*	1385	1432	0.95	3.64		Σ^*	1385	1432	0.95	3.60
+	Ξ	1318	1316	0.87	2.72	+	Ξ	1318	1317	0.86	2.69
	Ξ^*	1533	1562	0.94	3.42		Ξ^*	1533	1562	0.93	3.39
+	Ω	1672	1681	0.91	3.18	+	Ω	1672	1682	0.91	3.15
	ρ	769	783	0.82	2.32		ρ	769	783	0.82	2.30
	π	137	145	0.47	0.43	+	π	137	137	0.46	0.40

Fit excluding the pion: $B^{1/4}$= 160 MeV Z_0= 2.20 m_s= 302 MeV, h_{qq}= 0.273 h_{qs}= 0.187 h_{ss}= 0.0540

Fit including the pion: $B^{1/4}$= 160 MeV Z_0= 2.20 m_s= 301 MeV, h_{qq}= 0.275 h_{qs}= 0.186 h_{ss}= 0.0561

The success of eq.(D1) indicates that in future theoretical bag models the colour interaction term should be reviewed and maybe improved.

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