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FREE ENERGY OF GRAVITATING FERMIONS

par Walter THIRRING

ABSTRACT

We calculate rigorously, in a suitable thermodynamic limit, the free energy of a system of nonrelativistic fermions which interact with attractive r^{-1} - potentials. It is shown that the effective field approximation becomes exact in this limit and results in the temperature-dependent Thomas-Fermi equations.

1. INTRODUCTION

The quantum mechanical Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\vec{P}_i^2}{2M_i} + \sum_{1\leq i<j\leq N} \frac{e_i e_j - \kappa M_i M_j}{|\vec{x}_i - \vec{x}_j|} \tag{1.1}$$

describing N particles interacting with r^{-1} potentials is the relevant quantity if weak and nuclear interactions as well as relativistic effects can be neglected. In spite of the vast domain of applicability only few results have been rigorously derived from it, if $N > 2$. Dyson and Lenard [1] have shown that, for $\kappa = 0$, $\sum_i e_i = 0$ and certain combinations of statistics, the ground state energy of (1.1) for large N is proportional to N. Lebowitz and Lieb [2] announced a proof that the free energy F_N then is well-behaved.

Lévy-Leblond [3] proved that, for $\kappa > 0$ and $\sum_i e_i = 0$, the ground state energy for identical fermions is proportional to $N^{7/3}$ for large N.

We propose to calculate exactly the limit $N \to \infty$ of $N^{-7/3} F_N$ for nonrelativistic identical fermions interacting with their gravitational forces. The reason why this can be done is that, owing to the long range of the force, the temperature-dependent Thomas-Fermi equations become exact.

The system exhibits an interesting thermic behaviour which resembles certain features of stars and which has been discussed previously for simplified models [4].

There is a region where the microcanonical heat capacity is negative. In the canonical ensemble that region is bridged by a phase transition.

In this paper we shall concentrate on the mathematical problem of the asymptotic equality of the exact and the Thomas-Fermi free energy.

We denote by $F(N,\beta,R)$ the free energy of a system of N identical fermions enclosed within a spherical volume $\frac{4\pi}{3}R^3$ at temperature $T = 1/k\beta$ (k = Boltzmann's constant). The fermions interact with their gravitationl forces only. We will choose units $\hbar = 1$, Fermion mass = 1, and κ = gravitation constant = 1.

The free energy is defined by

$$e^{-\beta F(N,\beta,R)} = \mathrm{Tr}_{\mathcal{H}(N,R)}\, e^{-\beta\{\frac{1}{2}\sum_{i=1}^{N} \vec{p}_i^{\,2} - \frac{1}{2}\sum_{i\neq j=1}^{N} |\vec{x}_i - \vec{x}_j|^{-1}\}} \tag{1.2}$$

where $\mathcal{H}(N,R)$ is the Hilbert space of square integrable, complex valued, totally antisymmetric wave functions of N arguments $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N$ which vanish if at least one $|\vec{x}_i| \geqslant R$. By the unitary transformation $x \to R^{-1}x$, $p \to Rp$ expression (1.2) can be rewritten as

$$e^{-\beta F(N,\beta,R)} = \mathrm{Tr}_{\mathcal{H}(N,1)}\, e^{-\beta\{\frac{1}{2}R^{-2}\sum_{i=1}^{N} \vec{p}_i^{\,2} - \frac{1}{2}R^{-1}\sum_{i\neq j=1}^{N} |\vec{x}_i - \vec{x}_j|^{-1}\}} \tag{1.3}$$

We will investigate the limit $\lambda \to \infty$ of

$$\lambda^{-7/3}\, F(\lambda N, \lambda^{-4/3}\beta, \lambda^{-1/3}R) \tag{1.4}$$

for fixed N, β, R and for $\lambda N \in \mathbb{N}$.
The limit along the particular "ray" (1.4) is dictated by the Thomas-Fermi equations and their law of corresponding states. It means that the system becomes hotter and contracts if N is increased. The usual limit (β constant, $R \sim N^{1/3}$) could be taken if we would choose $\kappa \sim N^{-2/3}$. It should also be noted that for non-interacting particles the two limits coincide since

$$\lambda^{-1}\, F_{\kappa=0}\, (\lambda N, \beta, \lambda^{1/3}R) = \lambda^{-7/3}\, F_{\kappa=0}\, (\lambda N, \lambda^{-4/3}\beta, \lambda^{-1/3}R)$$

holds.

We define

$$f(\lambda,V) = -\frac{1}{\beta\lambda} \log \mathrm{Tr}_{\mathcal{H}(\lambda N,1)}\; e^{-\beta\lambda(K + V)} \tag{1.5}$$

with

$$K = \tfrac{1}{2}\,\lambda^{-5/3}\,R^{-2} \sum_{i=1}^{\lambda N} \vec{P}_i^{\,2} \tag{1.6}$$

and for various interactions V.

For

$$V_{\mathcal{N}} = -\tfrac{1}{2}\,\lambda^{-2}\,R^{-1} \sum_{\substack{i,j=1\\ i\neq j}}^{\lambda N} |\vec{x}_i - \vec{x}_j|^{-1} \tag{1.7}$$

we have

$$f(\lambda,V_{\mathcal{N}}) = \lambda^{-7/3}\,F(\lambda N,\lambda^{-4/3}\beta,\lambda^{-1/3}R) \tag{1.8}$$

i.e. the function of which we want to study the limit $\lambda \to \infty$. If N has been chosen sufficiently large, β and R small [6] the limit is the desired free energy since then

$$\lim_{\lambda\to\infty} f(\lambda,V_{\mathcal{N}}) \simeq f(1,V_{\mathcal{N}}) = F(N,\beta,R) \tag{1.9}$$

For technical reasons we cannot directly prove our assertion for the singular Newton potential

$$v_{\mathcal{N}}(\vec{x},\vec{y}) = |\vec{x} - \vec{y}|^{-1}. \tag{1.10}$$

We shall have to replace it by

$$v_{\mu s}(\vec{x},\vec{y}) = \sum_{a=1}^{s} \nu_a \varphi_a(\vec{x}) \varphi_a(\vec{y}) \tag{1.11}$$

where φ_a are the normalized and real eigenfunctions appearing in the expansion of the continuous potential $(\mu > 0)$

$$\frac{1 - e^{-\mu|\vec{x}-\vec{y}|}}{|\vec{x} - \vec{y}|} = \sum_{a=1}^{\infty} \nu_a \varphi_a(\vec{x}) \varphi_a(\vec{y}) \tag{1.12}$$

considered as an integral kernel operator.
The φ_a satisfy the equation

$$\int_{|y|\leqslant 1} d^3y \, \frac{1 - e^{-\mu|\vec{x}-\vec{y}|}}{|\vec{x} - \vec{y}|} \varphi_a(\vec{y}) = \nu_a \varphi_a(\vec{x}) \tag{1.13}$$

with positive eigenvalues ν_a.
Again for technical reasons we include the self-interaction and define

$$V_{\mu s} = - \tfrac{1}{2} \lambda^{-2} R^{-1} \sum_{i,j=1}^{\lambda N} v_{\mu s}(\vec{x}_i,\vec{x}_j) = - \lambda^{-1} \sum_{a=1}^{s} J_a^{\,2} \tag{1.14}$$

where

$$J_a = \left(\frac{\nu_a}{2R\lambda}\right)^{\frac{1}{2}} \sum_{i=1}^{\lambda N} \varphi_a(\vec{x}_i) \, . \tag{1.15}$$

In chapter 2 we shall prove that these approximations are arbitrarily good in the sense that

$$\lim_{\mu\to\infty} \lim_{s\to\infty} \lim_{\lambda\to\infty} \{f(\lambda,V_{\mu s}) - f(\lambda,V_{\mathcal{N}})\} = 0 \tag{1.16}$$

holds. This also shows that our result does not depend on the singularity but on the long range of the Newton potential. In particular, the addition of sufficiently short range forces will not affect it.

Next we add to $V_{\mu s}$ a term

$$W_{\mu s}[\sigma] = \lambda^{-1} \sum_{a=1}^{s} (J_a - \sigma_a)^2 \qquad (1.17)$$

where $(\sigma_1, \sigma_2, \ldots, \sigma_s) \in \mathbb{R}^s$.

It will turn out that for suitable σ's the effect of this term is negligible: we prove in chapter 3 that

$$\lim_{\lambda\to\infty} \{ \inf_{\sigma\in\mathbb{R}^s} f(\lambda, V_{\mu s} + W_{\mu s}[\sigma]) - f(\lambda, V_{\mu s})\} = 0 \qquad (1.18)$$

is true.

The interaction $V_{\mu s} + W_{\mu s}[\sigma]$ is linear in the operators J_a, it describes a system of non-interacting particles in the external field generated by σ. We will demonstrate in chapter 4 that the barometric formula results in the limit $\lambda \to \infty$: If the external field $U: [0,1] \to \mathbb{R}$ is a regulated function (i.e. the uniform limit of step functions, see ref. 9) and

$$V = \lambda^{-1} \sum_{i=1}^{\lambda N} U(|\vec{x}_i|) \qquad (1.19)$$

the corresponding interaction then

$$\lim_{\lambda\to\infty} f(\lambda, V) = -\frac{N\alpha}{\beta} - \frac{1}{\beta} R^3 \int_0^1 dr 4\pi r^2 g_\beta(-\alpha - \beta U(r)) \qquad (1.20)$$

where

$$g_\beta(z) = \int \frac{d^3p}{(2\pi)^3} \ln(1 + e^{-\frac{1}{2}\beta p^2 + z}) \qquad (1.21)$$

and α is the solution of

$$R^3 \int_0^1 dr\ 4\pi r^2\ g'_\beta(-\alpha-\beta U(r)) = N. \tag{1.22}$$

α is unique since $g'(z)$ is strictly monotonic.
In chapter 5 it will be shown that $\lim\limits_{\lambda\to\infty}$ and $\inf\limits_{\sigma\varepsilon S}$ in (1.18) can be interchanged, that the infimum is actually attained for a $\sigma^{\mu s}\varepsilon\ S$, and that this $\sigma^{\mu s}$ is a solution of the self-consistency equation, i.e.

$$U^{\mu s}(\vec{x}) = \sum_{a=1}^{s} \sigma_a^{\mu s}\ \nu_a\ \varphi_a(\vec{x}) \quad \text{satisfies}$$

$$U^{\mu s}(\vec{x}) = -\int d^3y\ v_{\mu s}(\vec{x},\vec{y})\ g'_\beta(-\beta R^2 U^{\mu s}(\vec{y}) - \alpha^{\mu s}) \tag{1.23}$$

with

$$R^3 \int d^3x\ g'_\beta(-\beta R^2\ U^{\mu s}(\vec{x}) - \alpha^{\mu s}) = N.$$

These are the well known temperature dependent Thomas-Fermi equations for particles interacting with the potential $v_{\mu s}$. In ref. 5 we discuss uniqueness and properties of its solutions. In particular, we demonstrate that the solution is insensitive to small changes of v (and can therefore be calculated on a computer): we shown that $U^{\mu s}$ tends with $\mu, s \to \infty$ to a solution U of the Thomas-Fermi equation with the Newton potential. α and F converge to the corresponding values.

Putting (1.16), (1.18), (1.20), and the results of chapter 6 together, we arrive at the final result:

For all $N \varepsilon \mathbb{N}$, $\beta > 0$ and $R > 0$ we have

$$\lim_{\lambda\to\infty} \lambda^{-7/3} F(\lambda N, \lambda^{-4/3}\beta, \lambda^{-1/3}R) =$$

$$- \frac{R^5}{2} \int_{|\vec{x}|\leq 1} d^3x \, U(x) \int \frac{d^3p}{(2\pi)^3} \frac{1}{1 + e^{\beta(\frac{p^2}{2} + R^2U(x)) + \alpha}} - \frac{N\alpha}{\beta}$$

$$- \frac{R^3}{\beta} \int_{|\vec{x}|\leq 1} d^3x \int \frac{d^3p}{(2\pi)^3} \ln(1 + e^{- \beta(\frac{p^2}{2} + R^2U(x)) - \alpha}) \qquad (1.24)$$

where $U(x)$ and α are determined by

$$U(\vec{x}) = - \int_{|\vec{x}|\leq 1} \frac{d^3x'}{(\vec{x}-\vec{x}')} \int \frac{d^3p}{(2\pi)^3} \frac{1}{1 + e^{\beta(\frac{p^2}{2} + R^2U(x)) + \alpha}} \qquad (1.25)$$

and

$$R^3 \int_{|\vec{x}|\leq 1} d^3x \int \frac{d^3p}{(2\pi)^3} \frac{1}{1 + e^{\beta(\frac{p^2}{2} + R^2U(x)) + \alpha}} = N. \qquad (1.26)$$

If (1.25) and (1.26) admit, as is actually the case, for some values N, β, R several solutions, that one for which the right-hand side of (1.24) is smallest is to be chosen.

2. REPLACING $V_{\mathcal{N}}$ BY $V_{\mu s}$

The operator $V_{\mathcal{N}}$ of (1.7) is bounded with respect to K of (1.6) : for all $\Psi \epsilon \mathcal{D}_K$ - $\mathcal{D}_K$ is the standard domain of K such that K is self-adjoint [7] - there exist positive numbers a and b such that

$$||V_{\mathcal{N}} \Psi|| \leqslant a \, || \Psi || + b || K \Psi || \qquad (2.1)$$

holds. The infimum of all such b, the K-bound of $V_{\mathcal{N}}$, is zero [7]. Therefore, according to an investigation by Maison [8], $f(\lambda, \kappa V_{\mathcal{N}})$ of (1.5) exists, is entire in κ, and holomorphic in β in the half-plane $\mathrm{Re}\, \beta > 0$. The derivative with respect to κ can be expressed as an expectation value of the interaction:

$$\frac{d}{d\kappa} f(\lambda, \kappa V_{\mathcal{N}}) = \langle V_{\mathcal{N}} \rangle_{\kappa V_{\mathcal{N}}} \qquad (2.2)$$

where

$$\langle A \rangle_V = \frac{\mathrm{Tr}_{\mathcal{H}(\lambda N,1)} \, A \, e^{-\lambda\beta(K+V)}}{\mathrm{Tr}_{\mathcal{H}(\lambda N,1)} \, e^{-\lambda\beta(K+V)}} \, . \qquad (2.3)$$

The domain of the self-adjoint operator $K + V_{\mathcal{N}}$ is also $\mathcal{D}_K$. The eigenfunctions φ_a of (1.13) are continuous, hence the operators J_a are bounded, and so is $V_{\mu s}$. Thus, $f(\lambda, V_{\mu s})$ exists as well.

The difference between $V_{\mu s}$ and $V_{\mathcal{N}}$ is

$$V_{\mu s} - V_{\mathcal{N}} = V_Y - \tfrac{1}{2} \lambda^{-1} R^{-1} N\mu + \tfrac{1}{2} \lambda^{-2} R^{-1} \sum_{i,j=1}^{\lambda N} \sum_{a=s+1}^{\infty} \nu_a \varphi_a(\vec{x}_i) \varphi_a(\vec{x}_j) \qquad (2.4)$$

with

$$V_Y = \tfrac{1}{2}\lambda^{-2}R^{-1}\sum_{i\neq j=1}^{\lambda N}\frac{e^{-\mu|\vec{x}_i-\vec{x}_j|}}{|\vec{x}_i-\vec{x}_j|}\,. \tag{2.5}$$

By Mercer's theorem [9] the sum (1.12) converges uniformly in $S_1 \times S_1$, consequently the norm of the last term in (2.4) converges to zero uniformly with respect to λ if $s\to\infty$. Therefore,

$$\lim_{s\to\infty}\lim_{\lambda\to\infty}\left[f(\lambda,V_{\mu s}) - f(\lambda,V_{\mathcal{N}}+V_Y)\right] = 0 \tag{2.6}$$

holds for all $\mu > 0$ in virtue of the general property

$$|f(\lambda,A+B) - f(\lambda,A)| \leqslant \|B\|\,. \tag{2.7}$$

Now, V_Y is smaller than $-V_{\mathcal{N}}$ thus the $(K+V_{\mathcal{N}})$ - bound of V_Y is also zero. Consequently, the mapping $t \to f(\lambda,V_{\mathcal{N}} + t\,V_Y)$ is entire. For real t it increases with t since $V_Y \geqslant 0$ and it is concave (this is a general property of $f(\lambda,A+tB)$). We then find

$$\begin{aligned} 0 &\leqslant f(\lambda,V_{\mathcal{N}}+V_Y) - f(\lambda,V_{\mathcal{N}}) \\ &\leqslant \frac{d}{dt}f(\lambda,V_{\mathcal{N}}+t\,V_Y)_{t=0} = \langle V_Y\rangle_{V_{\mathcal{N}}}\,. \end{aligned} \tag{2.8}$$

It is now our task to show that the expectation value of the Yukawa-interaction V_Y vanishes uniformly in λ if $\mu\to\infty$. For this we will calculate a lower bound of $\mu^{-1/5}K - V_Y$.

Following Dyson [1] we decompose this Hamiltonian as follows:

$$\mu^{-1/5}K - V_Y = \sum_{i=1}^{n} h_i;\qquad h_i = \sum_{\substack{j=1\\ j\neq i}}^{n}\left(\frac{\vec{p}_j^{\,2}}{2M} - \alpha\,\frac{e^{-\mu|\vec{x}_i-\vec{x}_j|}}{|\vec{x}_i-\vec{x}_j|}\right) \tag{2.9}$$

where

$$n = \lambda N, \quad M = \mu^{1/5} \lambda^{5/3} R^2 (\lambda N - 1) \quad \text{and}$$

$$\alpha = \tfrac{1}{2} \lambda^{-2} R^{-1}.$$

Each of the h_i is an Hamiltonian describing the motion of n-1 particles of mass M in the attractive Yukawa-potential of the n'th. The particles do not interact. The ground state of h_i is obtained if the n particles are filled into the n lowest states (recall that we deal with fermions).

The single particle bound states lie certainly higher than those of the hydrogen atom, namely $\varepsilon_\nu = -M\alpha^2/2\nu^2$ with multiplicity $\nu^2 (\nu = 1,2,\ldots)$. However, the Yukawa-potential can bind at most n_o states, for which number the upper bound

$$\begin{aligned} n_o &\leqslant 2\left\{\int_0^\infty dr\ r\ 2M\alpha \frac{e^{-\mu r}}{r}\right\} \cdot \left\{\sup_{r\geqslant 0} r^2\ 2M\alpha \frac{e^{-\mu r}}{r}\right\}^{\frac{1}{2}} \\ &\leqslant 2 \left(\frac{2M\alpha}{\mu}\right)^{3/2} \end{aligned} \tag{2.10}$$

is known [10]. n_o corresponds to a hydrogen atom principal quantum number ν_o with $\nu_o^3/3 = n_o$, therefore the ground state of h_i is higher than

$$-\tfrac{1}{2} M\alpha^2 \sqrt[3]{3n_o} \geqslant -2\alpha^2 M(M\alpha/\mu)^{\frac{1}{2}}.$$

We conclude that $\mu^{-1/5} K - V_Y$ is bounded from below by $-2n\alpha^2 M(M\alpha/\mu)^{\frac{1}{2}}$ so that we obtain

$$0 \leqslant V_Y \leqslant \mu^{-1/5}(K + R^{\frac{1}{2}} N^{5/2}). \tag{2.11}$$

It remains to show that $\langle K \rangle_{V_{\mathcal{N}}}$ is bounded independently of λ.

The mapping

$$t \to -\frac{2}{\beta\lambda} \log \mathrm{Tr}_{\mathcal{H}(\lambda N,1)}\, e^{-\frac{\beta\lambda}{2}(tK+2V_{\mathcal{N}})} \tag{2.12}$$

is analytic in the half-plane $\mathrm{Re}\, t > 0$, increases with real t and is concave. Hence the derivative with respect to t for $t=2$, which is just $\langle K \rangle_{V_{\mathcal{N}}}$, is smaller than

$$2f(\lambda,V_{\mathcal{N}}) - 2f(\lambda,2V_{\mathcal{N}})_{\beta/2}$$

where the suffix $\beta/2$ means that definition (1.5) applies with β being replaced by $\beta/2$.

The first term can be bounded above by

$$-\frac{1}{\beta\lambda}\log \mathrm{Tr}_{\mathcal{H}(\lambda N,1)}\, e^{-\beta\lambda K} = -\frac{1}{\beta\lambda} \log \mathrm{Tr}_{\mathcal{H}(\lambda N,\lambda^{1/3}R)}\, e^{-\beta\sum_{i=1}^{\lambda N}\frac{\vec{p}_i^{\,2}}{2}}$$

which is nothing else but the usual free energy for non-interacting fermions. It is known [11)] that the free energy of a system of λN non-interacting particles within a spherical volume $\lambda \frac{4\pi}{3} R^3$, if divided by λ, converges with $\lambda\to\infty$ towards the well-known limit. Since $\lambda N \in \mathbb{N}$ there is an upper and a lower bound, $f_L(N,\beta,R) \leqslant f(\lambda,0) \leqslant f_U(N,\beta,R)$, so that

$$f(\lambda,V_{\mathcal{N}}) \leqslant f(\lambda,0) \leqslant f_U(N,\beta,R) \tag{2.13}$$

holds for all λ.

The second term can be bounded from below since with Lévy-Leblond's estimate [3)] for the ground state of identical fermions with gravitational interaction, we find $K + 2\kappa V_{\mathcal{N}} \geqslant -\kappa^2 N^{7/3}$ for all R and λ so that

$K + 2V_{\mathcal{N}} \geqslant \frac{1}{2}K - 2N^{7/3}$ and

$$f(\lambda, 2V_{\mathcal{N}})_{\beta/2} \geqslant \tfrac{1}{2}\, f(\lambda, 0)_{\beta/4} - 2N^{7/3} \geqslant \tfrac{1}{2}\, f_L(N, \tfrac{\beta}{4}, R) - 2N^{7/3} \qquad (2.14)$$

holds for all λ.

With (2.13) and (2.14) we have established an λ-independent bound for $\langle K \rangle_{V_{\mathcal{N}}}$. This result together with (2.11), (2.8) and (2.6) complete the proof of equation (1.16):

$$\lim_{\mu\to\infty} \lim_{s\to\infty} \lim_{\lambda\to\infty} \{f(\lambda, V_{\mu s}) - f(\lambda, V_{\mathcal{N}})\} = 0.$$

3. THE EFFECTIVE FIELD APPROXIMATION

It has been demonstrated in the preceding section that, for the purpose of calculating the free energy, the original interaction $V_{\mathcal{N}}$ can be approximated by a finite sum of squares of bounded hermitian operators J_a. In this chapter we shall show how a further simplification is achieved if a product of operators is replaced by the product of the operator and its expectation value. The justification of replacing a field by what is usually called the effective field was originally demonstrated by Bogoliubov jr. [12] in connection with the BCS theory of superconductivity.

Let us define

$$\phi(t,j) = -\frac{1}{\beta} \ln \mathrm{Tr}\, e^{-\beta\{\lambda K + \sum_{a=1}^{s} [-J_a^2 + t(J_a^2 - \langle J_a \rangle_j)^2 + j_a J_a]\}} \tag{3.1}$$

where

$$\langle A \rangle_j = \frac{\mathrm{Tr}\, A\, e^{-\beta\{\lambda K + \sum_{a=1}^{s} [-J_a^2 + j_a J_a]\}}}{\mathrm{Tr}\, e^{-\beta\{\lambda K + \sum_{a=1}^{s} [-J_a^2 + j_a J_a]\}}} \tag{3.2}$$

for $j \in \mathbb{R}^s$.

$\phi(t,j)$ is increasing and concave in t, hence

$$0 \leqslant \phi(1,j) - \phi(0,j) \equiv \delta(j) \leqslant \sum_{a=1}^{s} \langle (J_a - \langle J_a \rangle_j)^2 \rangle_j \tag{3.3}$$

holds.

The fluctuation on the right-hand side can be further estimated [13] by

$$\delta(j) \leqslant \sum_{a=1}^{s} \left\{ \frac{1}{\beta}\left(- \frac{\partial^2 \phi(0,j)}{\partial j_a{}^2}\right) + \sqrt{\left(- \frac{\partial^2 \phi(0,j)}{\partial j_a{}^2}\right) < [J_a, [\lambda K, J_a]] >_j} \right\}. \quad (3.4)$$

Now, the integral

$$\delta(\xi) = \int_0^1 dj_1 \ldots \int_0^1 dj_s \; \delta(j) \quad (3.5)$$

defines a $\xi \in \mathbb{R}^s$ with $0 \leqslant \xi_a \leqslant 1$, and since $\left|\frac{\partial \delta(j)}{\partial j_a}\right| \leqslant 2 \;||J_a||$ holds - recall that $\delta(j)$ is the difference between two ϕ's the derivative of which with respect to j_a is an expectation value of J_a - we arrive at

$$\delta(0) \leqslant \delta(\xi) + \sum_{a=1}^{s} 2 \, ||J_a|| \, . \quad (3.6)$$

$\delta(\xi)$ can now easily be estimated by

$$\delta(\xi) \leqslant \sum_{a=1}^{s} \{\frac{1}{\beta} 2 \, ||J_a|| + \sqrt{2 \, ||J_a|| \cdot || [J_a, [\lambda K, J_a]] ||} \} \quad (3.7)$$

so that

$$0 \leqslant \phi(1,0) - \phi(0,0) \quad (3.8)$$

$$\leqslant \sum_{a=1}^{s} \{ 2^{\frac{1}{2}} \; \frac{1+\beta}{\beta} \; \nu_a^{\frac{1}{2}} \; R^{-\frac{1}{2}} N \varphi_a \lambda^{\frac{1}{2}}$$

$$+ \; 2^{-\frac{1}{4}} \nu_a^{3/4} \; R^{-7/4} \; N \varphi_a^{\frac{1}{2}} \; \varphi_a' \; \lambda^{-1/12} \}$$

has been established. We have used that the double commutator is equal to $\frac{1}{2} \lambda^{-5/3} R^{-3} \nu_a \sum_{i=1}^{\lambda N} (\vec{\nabla} \varphi_a(x_i))^2$ and that

$$\varphi_a = \sup_{\vec{x} \varepsilon S_1} |\varphi_a(\vec{x})| \quad (3.9)$$

$$\varphi_a' = \sup_{\vec{x} \varepsilon S_1} |\vec{\nabla} \varphi_a(\vec{x})| \quad (3.10)$$

are both finite since the eigenfunctions φ_a are continuous and continuously differentiable in S_1 (cf. equation (1.13)).

With the positive definite operator $W_{\mu s}[\sigma]$ as defined in (1.17) one finds by comparing (1.5) with (3.1)

$$\lambda^{-1}\ \phi(0,0) = f(\lambda, V_{\mu s}) \tag{3.11}$$

$$\leq \inf_{\sigma\varepsilon \mathbb{R}^s} f(\lambda, V_{\mu s} + W_{\mu s}[\sigma])$$

$$\leq f(\lambda, V_{\mu s} + W_{\mu s}[\langle J\rangle_o]) = \lambda^{-1}\ \phi(1,0)$$

which, together with (3.8) proves equation (1.18), namely

$$\lim_{\lambda\to\infty} \{ \inf_{\sigma\varepsilon \mathbb{R}^s} f(\lambda, V_{\mu s} + W_{\mu s}[\sigma]) - f(\lambda, V_{\mu s})\} = 0.$$

4. THE BAROMETRIC FORMULA

With

$$\sigma(\vec{x}) = \sum_{a=1}^{s} \sqrt{\frac{2}{R^5 \lambda \nu_a}}\, \sigma_a \varphi_a(\vec{x}) \tag{4.1}$$

and

$$U(\vec{x}) = - \sum_{a=1}^{s} R^2 \nu_a \sqrt{\frac{2}{R^5 \lambda \nu_a}}\, \sigma_a \varphi_a(\vec{x}) \tag{4.2}$$

we may write for the interaction appearing in equation (1.18):

$$V_{\mu s} + W_{\mu s}\underline{\bar{\sigma}} = - \tfrac{1}{2} R^3 \int_{S_1} d^3x\, \sigma(\vec{x})\, U(\vec{x}) + \lambda^{-1} \sum_{i=1}^{\lambda N} U(\vec{x}_i). \tag{4.3}$$

The first term on the r.h.s. of (4.3) is a c-number and will appear as an additive contribution to the free energy. It presents no problem for the limit $\lambda \to \infty$. In this chapter we concentrate on the second term, in particular, we want to study the limit $\lambda \to \infty$ of

$$\phi(\lambda,U,N) = f(\lambda, \lambda^{-1} \sum_{i=1}^{\lambda N} U(\vec{x}_i)) \tag{4.4}$$

$$= - \frac{1}{\beta\lambda} \log \mathrm{Tr}_{\mathcal{H}(\lambda N,1)}\, e^{-\beta\left[\lambda K + \sum_{i=1}^{\lambda N} U(\vec{x}_i)\right]}$$

$$= - \frac{1}{\beta\lambda} \log \mathrm{Tr}_{\mathcal{H}(\lambda N,\lambda^{1/3}R)}\, e^{-\beta \sum_{i=1}^{\lambda N}\left[\frac{\vec{p}_i^{\,2}}{2} + U\left(\frac{\vec{x}_i}{\lambda^{1/3}R}\right)\right]}$$

for fixed β, R and various λ-independent external potentials $U(\vec{x})$.

Note that fixed U corresponds to $\sigma_a \sim \lambda^{\frac{1}{2}}$, but this is no difficulty for equation (1.18) since the infimum there extends over all of $\mathbb{R}^s$.

Another remark concerns rotational symmetry: the truncation of the eigenfunction expansion (1.12) to (1.11) can always be done in such a way that the rotational symmetry of $v_{\mu s}(\vec{x},\vec{y})$ is preserved. Since then $V_{\mu s}$ of (1.14) is also invariant under rotations the expectation value appearing in equation (3.11) of the J's will define a spherically symmetric $\sigma(x)$. Therefore, the infimum in (3.11) needs to be with respect to spherically symmetric $\sigma(x)$ only. Since $U(x)$ of equation (4.2) equals $-R^2 \int d^3y\, v_{\mu s}(\vec{x},\vec{y})\, \sigma(y)$ we have to consider spherically symmetric external potentials only if s is chosen such that $v_{\mu s}$ is spherically symmetric.

The problem thus separates into a radial and an angular part. Correspondingly, the eigenvalues ε of

$$H = \beta\left[\frac{p^2}{2} + U\left(\frac{r}{\lambda^{1/3}R}\right)\right] \tag{4.5}$$

can be labelled by a radial quantum number n and the angular quantum number ℓ. A lower bound for the ε's is readily available

$$\varepsilon_{n,\ell} \geqslant \beta(R^{-2}\ \lambda^{-2/3}\tfrac{1}{2}\ell(\ell+1) + v) \tag{4.6}$$

where

$$v = \inf_{0 \leqslant r \leqslant 1} U(r) \tag{4.7}$$

is finite since U is a finite sum of functions which are continuous in the unit ball S_1.

For this reason U can be approximated by a piecewise constant potential U_T with a finite number g of steps:
for all $\eta > 0$ there is an integer g such that for

$$U_T(r) = U_i = U\left(\frac{i - 1/2}{g}\right) \quad \text{if} \quad \frac{i-1}{g} \leqslant r < \frac{i}{g}, \quad i=1,\dots,g \qquad (4.8)$$

we have

$$\sup_{0 \leqslant r \leqslant 1} |U(r) - U_T(r)| \leqslant \eta \ .$$

We furthermore consider a potential U_W which is U_T + infinite walls at $r=i/g$. This means that we impose in addition the restriction that the wave functions have to vanish at $r=i/g$. Both U_T and U_W are extensions of the same potential U_o defined on the dense set of wave functions vanishing at $r=i/g$. The intersection of this domain with the domain of K gives $\mathcal{D}_o$, the domain of $H_o = \beta(p^2/2 + U_o(r/\lambda^{1/3} R))$. H_o is not self-adjoint but has defect indices (g,g). Its self-adjoint extension H_W and H_T have domains $\mathcal{D}_o + \mathcal{D}_W$ and $\mathcal{D}_o + \mathcal{D}_T$ respectively where $\mathcal{D}_W$ and $\mathcal{D}_T$ are g-dimensional subspaces. Clearly $\varepsilon^W_{n,\ell} \geqslant \varepsilon^T_{n,\ell}$ and from the minimax-principle (E_n is an n-dimensional subspace)

$$\varepsilon^{W,T}_{n,\ell} = \inf_{E_n \subset \mathcal{D}_o + \mathcal{D}_{W,T}} \ \sup_{\chi \varepsilon E_n} (\chi(r)\, Y^m_\ell | H_{W,T}\chi(r) Y^m_\ell) \qquad (4.9)$$

we learn

$$\varepsilon^W_{n-g,\ell} - \eta \leqslant \varepsilon^T_{n,\ell} - \eta \leqslant \varepsilon_{n,\ell} \leqslant \varepsilon^T_{n,\ell} + \eta \leqslant \varepsilon^W_{n,\ell} + \eta \qquad (4.10)$$

$(\forall n > g, \forall \ell)$.

This implies for the partition functions the following inequalities

$$\sum_\nu{}' e^{-\sum_{n,\ell} \nu_{n,\ell}\, \varepsilon^W_{n,\ell} - N\lambda\eta} \leqslant \sum_\nu{}' e^{-\sum_{n,\ell} \nu_{n,\ell}\, \varepsilon_{n,\ell}} \qquad (4.11)$$

$$\leqslant \sum_\nu{}' e^{-\sum_\ell \{\sum_{n=1}^{g} \nu_{n,\ell}\, \varepsilon_{n,\ell} + \sum_{n=g+1}^{\infty} \nu_{n,\ell}\, \varepsilon^W_{n-g,\ell}\} + N\lambda\eta} \ .$$

Σ'_{ν} indicates the sum over all occupation numbers compatible with $\sum_{n,\ell} \nu_{n,\ell} = \lambda N$.

In terms of the corresponding free energies (4.4) we deduce from (4.6) and (4.11)

$$- \phi(\lambda,U_W,N) - N\eta \leq - \phi(\lambda,U,N) \tag{4.12}$$

$$\leq \lambda^{-1} (\beta^{-1} \log g - gv) + N\eta - \inf_{\lambda N-g\leq N'\leq\lambda N} \phi(\lambda,U_W,N') .$$

Now, the eigenfunctions of H_W have their support in one of the shells $(i-1) \leq rg \leq i$, we can therefore replace the radial quantum number n by the pair (i,m) where i labels the shell and m the radial excitation in this shell. We shall require the following estimate later on:

$$\tfrac{1}{2}\beta\, R^{-2}\, \lambda^{-2/3} \left[(\pi mg)^2 + \ell(\ell+1) \left(\tfrac{g}{i}\right)^2 + 2U_i\right] \tag{4.13}$$

$$\leq \varepsilon^W_{i,m,\ell} \leq$$

$$\tfrac{1}{2}\beta R^{-2}\, \lambda^{-2/3} \begin{Bmatrix} (\pi mg)^2 + \ell(\ell+1) \left(\frac{g}{i-1}\right)^2 + 2U_i & \text{for } i > 1 \\ (\pi mg)^2 + 4\ell(\ell+1)g^2 + 2U_1 & \text{for } i = 1 \end{Bmatrix} .$$

Introducing the partition function of the i'th shell

$$e^{-\lambda\beta\phi^{(i)}(\lambda,N)} = \Sigma'_{\nu}\, e^{-\sum_{m,\ell} \nu_{m,\ell}\, \varepsilon^W_{i,m,\ell}} \tag{4.14}$$

we obtain for the partition function with walls

$$e^{-\lambda\beta\phi(\lambda,U_W,N)} = \sum_{\substack{(N_1,\dots,N_g) \\ \Sigma N_i=N}} e^{-\lambda\beta \sum_{i=1}^{g} \phi^{(i)}(\lambda,N_i)} . \tag{4.15}$$

Since U_W is constant inside a shell the free energy $\phi^{(i)}(\lambda,N)$ is the free energy of non-interacting particles plus NU_i. One knows[11)] that $\phi^{(i)}(\lambda,N)$ decreases with increasing λ. By standard arguments[11)] one can demonstrate that this property also holds for $\phi(\lambda,U_W,N)$. Since the latter is bounded below by $\phi(\lambda,0,N) - vN$ - which is known to converge for $\lambda \to \infty$ - we conclude that $\phi(\infty,U_W,N) = \lim_{\lambda\to\infty} \phi(\lambda,U_W,N)$ exists.

From (4.12) we deduce that $\phi(\infty,U,N)$ also exists and is arbitrarily close to $\phi(\infty,U_W,N)$ for η sufficiently small.

The explicit form of $\phi(\infty,U_W,N)$ can be calculated by studying the grand canonical ensemble.

The standard proof of the equivalence of the canonical and the grand canonical ensemble can easily be formulated to apply to the case at hand. The grand canonical partition function is the sum of those for the individual shells which are the usual expressions for non-interacting particles (this can be seen by inspecting the limits (4.13) of the eigenvalues). In the limit $\lambda \to \infty$ the sums over eigenvalues approach integrals in momentum space, and with $\eta \to 0$ $(g \to \infty)$ the sum over shells becomes a space integral. We will not write down all the necessary epsilontics since this is an exercise in elementary analysis.

The result is

$$\lim_{\lambda\to\infty} \phi(\lambda,U,N) = -\frac{N\alpha}{\beta} - R^3 \frac{1}{\beta}\int_0^1 dr\, 4\pi r^2 \int_0^1 \frac{d\varepsilon\, \sqrt{\varepsilon}}{\sqrt{2}\,\pi^2} \times \tag{4.16}$$

$$\times \ln\left(1 + e^{-\beta(\varepsilon+U(r)) - \alpha}\right)$$

with α being the unique solution of

$$N = R^3 \int_0^1 dr\, 4\pi r^2 \int_0^1 \frac{d\varepsilon\, \sqrt{\varepsilon}}{\sqrt{2}\,\pi^2} \left(1 + e^{\beta(\varepsilon+U(r)) + \alpha}\right)^{-1} . \tag{4.17}$$

This completes the proof of the barometric formula (1.20) to (1.22) .

5 . THE RESULT FOR $V_{\mu s}$.

It is a by-product of the investigations in the preceding section that $\phi(\lambda,U,N)$ converges from above towards the limit. Therefore, the limit and the infimum operation in equation (1.18) can be interchanged.

We have thus to investigate the infimum of

$$\frac{R^5}{2} \sum_{a=1}^{s} \nu_a \sigma_a^2 - \frac{N\alpha_\sigma}{\beta} - \frac{1}{\beta} R^3 \int_{|x|\leqslant 1} d^3x \; g_\beta(\beta R^2 \sum_{a=1}^{s} \nu_a \sigma_a \varphi_a(x) - \alpha_\sigma) \qquad (5.1)$$

where α_σ is a solution of

$$R^3 \int_{|x|\leqslant 1} d^3x \; g'_\beta(\beta R^2 \sum_{a=1}^{s} \nu_a \sigma_a \varphi_a(x) - \alpha_\sigma) = N \; . \qquad (5.2)$$

Since σ depends on α this solution need no longer be unique.

The derivative of (5.1) with respect to σ_b is

$$R^5 \nu_b \{\sigma_b - \int_{|y|\leqslant 1} d^3y \; g'_\beta(\beta R^2 \sum_{a=1}^{s} \nu_a \sigma_a \varphi_a(y) - \alpha_\sigma) \varphi_b(y)\} . \qquad (5.3)$$

Note that the derivative of α_σ does not appear because of the subsidary condition (5.2).

We see that the free energy (5.1) increases with $|\sigma_b|$ if $|\sigma_b| > R^2 N \varphi_b$.
Hence the infimum in equation (1.18) can be restricted to an infimum over the compact cube $|\sigma_a| \leqslant 2R^2 N \max\limits_{1\leqslant b\leqslant s} \varphi_b$.

Since (5.1) is continuous and continuously differentiable with respect to any σ_b the infimum is attained at a point $\sigma^{\mu s}(x) = \sum_{a=1}^{s} \sigma_a^{\mu s} \varphi_a(x)$ where all partial derivatives (5.3) vanish.

(5.2) and (5.3) are exactly the self-consistency equations (1.23) we referred to in chapter 1 .

6 . THE THOMAS-FERMI EQUATION .

In this section we shall demonstrate that solving the T.F.E. and taking the limit $\mu \to \infty$, $s \to \infty$ are interchangeable operations : In terms of the potential the equation can be written ,

$$\mathcal{U}_{\mu s}(x) = - \int_{S_1} d^3x' \, v_{\mu s}(\vec{x},\vec{x}') \; 2 \int_0^\infty \frac{d\varepsilon \sqrt{\varepsilon}}{\sqrt{2}\,\pi^2} \; \frac{1}{1 + e^{\beta(\varepsilon + \mathcal{U}_{\mu s}(x')) + \alpha_{\mu s}}} \, . \qquad (6.1)$$

A mass distribution which generates this potential is

$$\rho_{\mu s}(x) = 2 \int_0^\infty \frac{d\varepsilon \sqrt{\varepsilon}}{\sqrt{2}\,\pi^2} \; \frac{1}{1 + e^{\beta(\varepsilon + \mathcal{U}_{\mu s}(x)) + \alpha_{\mu s}}} \, . \qquad (6.2)$$

We have

$$\rho_{\mu s}(x) \geqslant 0 \quad \text{and} \quad \int_{S_1} d^3x \, \rho_{\mu s}(x) = N \, . \qquad (6.3)$$

Let η be an arbitrary positive number. Since $v_{\mu s}$ converges uniformly to v_μ there exists $s_0(\mu) \in \mathbb{N}$ such that

$$| v_{\mu s}(\vec{x},\vec{x}') - v_\mu(\vec{x},\vec{x}') | \leqslant \eta \qquad (6.4)$$

is valid for $\vec{x}, \vec{x}' \in S_1, \mu > 0$ and $s \geqslant s_0(\mu)$.

From (6.1), (6.3) and (6.4) we deduce

$$-\left(\frac{1}{x} + \eta\right) N \leqslant - \int_0^1 dx' \, 4\pi x'^2 \rho_{\mu s}(x') \left\{ \frac{\theta(x-x')}{x} + \frac{\theta(x'-x)}{x'} \right\} - N\eta$$

$$\leqslant - \int_{S_1} d^3x' \, \rho_{\mu s}(x') \, v_\mu(\vec{x},\vec{x}') - N\eta \leqslant \mathcal{U}_{\mu s}(x) \leqslant N\eta \qquad (6.5)$$

for $\mu > 0$ and $s \geqslant s_0(\mu)$.

We define α_0 by solving

$$\int_0^1 dx \, 4\pi x^2 \, 2 \int_0^\infty \frac{d\varepsilon \sqrt{\varepsilon}}{\sqrt{2}\,\pi^2} \; \frac{1}{1 + e^{\beta(\varepsilon + N\eta) + \alpha_0}} = N \qquad (6.6)$$

so that, as a consequence of (2.6), (6.2), (6.5) and (6.6) we obtain

$$\alpha_{\mu s} \geqslant \alpha_0 \qquad (s \geqslant s_0(\mu)) \qquad (6.7)$$

as (μ, s)-independent bound.

Substituting (6.5) and (6.7) into (6.2) we find another bound

$$0 \leq \rho_{\mu s}(x) \leq 2\int_0^\infty \frac{d\varepsilon\,\sqrt{\varepsilon}}{\sqrt{2}\,\pi^2}\;\frac{1}{1+e^{\beta(\varepsilon - x^{-1}N - N\eta)+\alpha_0}} = \rho_0(x) \quad . \qquad (6.8)$$

$\rho_0(x)$ is continuous in $(0,1]$, and since $\lim_{x\to 0} x^{3/2}\rho_0(x)$ exists we deduce

$$0 \leq x^{3/2}\rho_{\mu s}(x) \leq c_0 \qquad (6.9)$$

for $x \in [0,1]$ and with (μ, s)-independent c_0 (if $s \geq s_0(\mu)$).

By inserting (6.9) into (6.1) one obtains

$$-N\eta - 8\pi c_0 \leq U_{\mu s}(x) \leq N\eta \quad , \qquad (6.10)$$

and from this result, (6.7), and (6.2)

$$c_1 \leq \rho_{\mu s}(x) \leq c_2 \qquad (6.11)$$

with c_1 and c_2 also independent on μ and s (if $s \geq s_0(\mu)$).

The potentials $v_{\mu s}: S_1 \times S_1 \to \mathbb{R}$ are continuous and converge with $s \to \infty$ towards v_μ in the supremum norm. According to Ascoli's theorem [10] the family $v_{\mu s}$ (μ fixed, $s \in \mathbb{N}$) is then equi- and uniformly continuous. Because of (6.11) the $U_{\mu s}$ are also equicontinuous. With (6.10) it follows, again according to Ascoli's theorem, that we can choose a uniformly converging sequence out of the family $U_{\mu s}$ (μ fixed) the limit of which we shall call U_μ. The corresponding sequence $\alpha_{\mu s}$ (cf. equ. (2.6)) converges as well to an α_μ.

To these converging sequences of potentials and α's corresponds a sequence of mass distributions which converges to a ρ_μ since (6.2) is a continuous mapping $\mathcal{C}_{\mathbb{R}}(S_1) \longrightarrow \mathcal{C}_{\mathbb{R}}(S_1)$. The limiting functions satisfy the conterpart of (A.4), namely

$$U_\mu(x) = -\int d^3x'\, v_\mu(\vec{x},\vec{x}')\,\rho_\mu(x') \quad . \qquad (6.12)$$

If the family $U_{\mu s}$ has more than one accumulation point it is irrelevant, for the purpose of calculating the free energy, which we choose. They will give rise to the same free energy since $F_{U_{\mu s}}$ decreases with increasing s [11].

That $\lim_{s\to\infty} F_{U_{\mu s}}$ is equal to $F_{\lim_{s\to\infty} U_{\mu s}}$ follows from the fact that the convergence of the potentials is uniform and S_1 is compact.

Because the limit ϱ_μ also satisfies (6.11) we deduce

$$|\vec{\nabla} U_\mu(x)| \leq c_2 \int_{S_1} d^3x' \, \frac{1-(1+\mu|\vec{x}-\vec{x}'|)e^{-\mu|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|^2}$$
$$\leq c_2 \int_{S_2} \frac{d^3z}{z^2} \leq 8\pi c_2 \quad , \tag{6.13}$$

i.e. the U_μ are equicontinuous. Together with (6.10) this implies (using again Ascoli's theorem) that the family of potentials U_μ has an accumulation point which we shall call U [12]. Likewise an accumulation point ϱ exists such that U is the potential generated by ϱ as defined with (2.5). By the same reasoning as for $s\to\infty$ we arrive at the following conclusion:

$$\lim_{\mu\to\infty} \lim_{s\to\infty} F_{U_{\mu s}} = F_U \tag{6.14}$$

where U satisfies (2.9) with α and ϱ being defined by (2.5) and (2.6). If (2.9) allows many solutions only those for which F_U is smallest are to be taken into account since the remaining solutions cannot be accumulation points of U .

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