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Thermodynamic Limit of Correlation Functions in a System of Gravitating Fermions

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Abstract. We show that the correlation functions in a system of gravitating fermions converge as tempered distributions in the thermodynamic limit, if the system is not at the point of phase-transition. The densities converge to the density of the Thomas-Fermi-theory and are not correlated in the limit.

I. Introduction

It has been shown by P. Hertel et al. ([1, 2]) that non-relativistic gravitating fermions have a kind of thermodynamic limit and that in the limit the system is governed by temperature-dependent Thomas-Fermi- (T.F.-) equations. What is unusual in this limit is the dependence of parameters on the particle-number N: the system is confined to a region, the linear dimensions of which vary as $N^{-1/3}$ and the temperature is set proportional to $N^{4/3}$ or the energy proportional to $N^{7/3}$, if one works with the microcanonical ensemble.) The free energy divided by $N^{7/3}$ has then a definite finite limit when N tends to infinity. To make things conceptually simpler and to obtain a certain similarity to the usual thermodynamic formulas, we transform the Hamiltonian

$$H_N=\sum_{i=1}^{N} p_i^2/2m-\kappa\sum_{i<j}|x_i-x_j|^{-1} \tag{1}$$

with the unitary transformation

$$x\mapsto N^{-1/3}x,\ p\mapsto N^{1/3}p \tag{2}$$

and divide it by $N^{4/3}$.

The resulting Hamiltonian,

$$\tilde{H}_N=N^{-2/3}\sum_{i=1}^{N} p_i^2/2m-\kappa/N\sum_{i<j}|x_i-x_j|^{-1} \tag{3}$$

with Dirichlet boundary-conditions in $L^2(V)$, (V does not depend on N) serves to define a canonical ensemble with temperature β^{-1} (which is also N-independent).

We thus obtain a sequence of ensembles, for which there exists the "thermodynamic" limit of the free energy per particle

$$f(N,\beta)=-(\beta N)^{-1}\log \operatorname{Tr}\exp(-\beta\tilde{H}_N)\,. \tag{4}$$

In this paper we investigate the corresponding thermodynamic limit of the local density and correlation-functions.

II. The Strategy

The density at a point $\varrho(x)$ cannot be obtained as an expectation value of an operator, it is only a quadratic form [3]. Therefore, we shall deal with integrated densities

$$\varrho(w)=\int d^3x\varrho(x)w(x),\ w \text{ is any test-function in } \mathscr{S}(R^3)\,. \tag{5}$$

We normalize the density so that its integral over all space equals 1. In a system with N particles, (5) is then the expectation value of the operator

$$\hat{\varrho}_N(w)=N^{-1}\sum_{i=1}^{N} w(x_i)\,. \tag{6}$$

With the help of the symmetrized product of n test functions

$$S(x_1\dots x_n)=n!^{-1}\sum_{\text{Permutations } p(\alpha)}\prod_{\alpha=1}^{n} w_\alpha(x_{p(\alpha)}) \tag{7}$$

we define the operator for integrated correlation functions:

$$\hat{\varrho}_N(w_1\dots w_n)=N^{-n}\sum_{i_1\dots i_n} S(x_{i_1}\dots x_{i_n})\,. \tag{8}$$

All operators of the form (6) or (8) are bounded. Their equilibrium values can therefore be written as derivatives of concave functions ([4, 5]):

$$\begin{aligned}\langle\hat{\varrho}_N(w_1\dots w_n)\rangle_\beta &=\operatorname{Tr}\{\hat{\varrho}_N(w_1\dots w_n)\exp(-\beta\tilde{H}_N)\}\exp\beta N f(N,\beta,0) \\ &=\frac{\partial}{\partial\lambda}f(N,\beta,\lambda)|_{\lambda=0}\end{aligned} \tag{9}$$

$$f(N,\beta,\lambda)=-(\beta N)^{-1}\log\operatorname{Tr}\exp[-\beta(\tilde{H}_N+\lambda N\hat{\varrho}_N(w_1\dots w_n))]\,. \tag{10}$$

The basic concept we shall follow is to show that the thermodynamic limit exists for $f(N,\beta,\lambda)$ and the limit of derivatives equals the derivative of the limiting function $\phi(\beta,\lambda)$ (which is also concave in λ).

III. The Thomas-Fermi-Equations

Following [1], we have to approximate $V(x,y)=\kappa/|x-y|$ by $V_s(x,y)=\kappa(1-\exp(-s|x-y|)/|x-y|$, then we have to divide the Volume V into cells $\Lambda_a(a=1\dots g)$ and to approximate again $V_s(x,y)$ from below by potentials $V_{s,g}(x,y)$, which are constant in each pair of cells. In the same manner we define $S_{s,g}(x_1 \dots x_n)$ to be step functions, which are constant in each n-tuple of cells and approximate $S(x_1 \dots x_n)$. S_s can be taken equal to S.

In analogy to (3) and (4) we define:

$$H_{N,\sigma}(\lambda) = N^{-2/3} \sum p_i^2/2m - \frac{1}{N} \sum_{i<j} V_\sigma(x_i, x_j) + \lambda N^{-n+1} \sum_{i_1 \dots i_n} S_\sigma(x_{i_1} \dots x_{i_n}), \quad (11)$$

$$f_\sigma(N, \beta, \lambda) = -(\beta N)^{-1} \log \operatorname{Tr} \exp[-\beta H_{N,\sigma}(\lambda)]. \quad (12)$$

The index σ stands for either s, g or s or none.
Without complications, the results of [1] for $\lambda = 0$ may be generalized:

$$\exists \lim_{N \to \infty} f_{s,g}(N, \beta, \lambda) = \phi_{s,g}(\beta, \lambda), \quad (13)$$

$$\exists \lim_{N \to \infty} f(N, \beta, \lambda) = \lim_{s \to \infty} \lim_{g \to \infty} \phi_{s,g}(\beta, \lambda). \quad (14)$$

$\phi_{s,g}$ is the free energy of the T.F.-theory:

$$\begin{aligned} \phi_\sigma = \mu_\sigma + \int_V d^3x \varrho_\sigma(x)[\tfrac{1}{2} U_\sigma(x) - \lambda(n-1)/n S_\sigma(x)] \\ -\beta^{-1} \int_V d^3x \int d^3p (2\pi)^{-3} \log\{1 + \exp[-\beta(p^2/2m - \mu_\sigma(x))]\}, \end{aligned} \quad (15)$$

$$U_\sigma(x) = \int_V V_\sigma(x, y) \varrho_\sigma(y) d^3y, \quad (16)$$

$$S_\sigma(x) = n \int_{V^{n-1}} S_\sigma(x_1 x_2 \dots x_n) \prod_{i=2}^n \varrho_\sigma(x_i) d^3x_i. \quad (17)$$

The ϱ's and μ's are solutions of T.F.-equations:

$$\mu_\sigma(x) = \mu_\sigma + U_\sigma(x) - \lambda S_\sigma(x), \quad (18)$$

$$\varrho_\sigma(x) = \int d^3p (2\pi)^{-3} \{1 + \exp[\beta(p^2/2m - \mu_\sigma(x))]\}^{-1}. \quad (19)$$

The value of the constant μ_σ has to be chosen such that

$$\int_V \varrho_\sigma(x) d^3x = 1.$$

Consider:

$$\begin{aligned} \Psi_\sigma(\varrho, \beta, \lambda) = -\tfrac{1}{2} \int_{V \times V} d^3x d^3y \varrho(x) V_\sigma(x, y) \varrho(y) + \lambda \int_{V^n} S_\sigma(x_1 \dots x_n) \prod_{i=1}^n \varrho(x_i) d^3x_i \\ + \int_V d^3x \varrho(x) \mu(x) - \beta^{-1} \int_V d^3x \int d^3p (2\pi)^{-3} \log\{1 + \exp[-\beta(p^2/2m - \mu(x))]\}. \end{aligned} \quad (20)$$

$\mu(x)$ is here a function of $\varrho(x)$, implicitly defined by Equation (19). One verifies easily the validity of the variational principle:

$$\phi_\sigma(\beta, \lambda) = \min_{\varrho \in \Omega} \Psi_\sigma(\varrho, \beta, \lambda), \quad (21)$$

$$\Omega = \{\varrho \in L^1(V) : \varrho(x) \geqq 0, \int_V \varrho(x) d^3x = 1\}.$$

IV. Behavior of the T.F.-Theory When g and s Tend to Infinity

Our aim is to show that $\phi(\beta, \lambda) = \lim_{s\to\infty} \lim_{g\to\infty} \phi_{s,g}(\beta, \lambda)$. The proof follows [2], but we have to be careful about technicalities, since rotational invariance is broken by $S_\sigma(x_1 \ldots x_n)$.

As functions of x, all $V_\sigma(x, y)$ are in a uniformly bounded set in $L^p(V)$ $(p<3)$:

$$\|V_{s,g}(x, y)\|_p \leqq \|V_s(x, y)\|_p \leqq \|\kappa|x-y|^{-1}\|_p \leqq \|\kappa|x|^{-1}\|_p =: c_p \,. \tag{22}$$

The $U_\sigma(x)$ are convex combinations of the $V_\sigma(x, y)$; hence, its p-norms are also bounded by c_p. The S_σ's are bounded in all L^p's by some constant k.

It is more difficult to find a bound to the set of constants μ_σ. We study the function

$$g(\beta, \mu) = \int d^3p (2\pi)^{-3} (1 + \exp \beta(p^2 - \mu))^{-1} \,. \tag{23}$$

With this function, (19) can be written as $\varrho_\sigma(x) = (2m)^{3/2} g(\beta, \mu_\sigma(x))$. $g(\beta, \mu)$ has the properties:

$$0 < \frac{\partial}{\partial\mu} g(\beta, \mu) \leqq \beta g(\beta, \mu) \qquad \text{(monotonicity in } \mu\text{)}, \tag{24}$$

$$\begin{aligned} g(\beta, \mu) = \beta^{-3/2} g(1, \beta\mu) \leqq \theta(1-\beta\mu)\beta^{-3/2} g(1, 1) + \theta(\beta\mu - 1)(6\pi^2)^{-1}(\mu^{3/2} \\ + \tfrac{3}{2}\mu\beta^{-3/2} + \tfrac{3}{2}\beta^{-3/2}) \,. \end{aligned} \tag{25}$$

Because of the L^p-boundedness of the potentials, there exists a number b such that

$$\int_V d^3x \theta(|\mu_\sigma(x) - \mu_\sigma| - b) < v/2 \left(v = \int_V d^3x\right).$$

And with $A_\sigma = \{x : \varrho_\sigma(x) > (2m)^{3/2} g(\beta, \mu_\sigma - b)\}$, this implies

$$\int_{V - A_\sigma} d^3x < v/2 \,.$$

We can define $\hat{\mu}$ by $\frac{1}{2}v(2m)^{3/2} g(\beta, \hat{\mu} - b) = 1$, and the inequality $\mu_\sigma < \hat{\mu}$ follows from the monotonicity (24) and

$$1 = \int_V \varrho_\sigma(x) d^3x > \int_{A_\sigma} \varrho_\sigma(x) d^3x > \tfrac{1}{2}v(2m)^{3/2} g(\beta, \mu_\sigma - b) \,.$$

Up to now we know that all $\mu_\sigma(x)$ form a bounded set in each L^p if $p<3$. (25) tells us that $\varrho(\mu)$ does not grow stronger than $\mu^{3/2}$ so that the $\varrho_\sigma(x)$ are in a bounded set in every $L^{2p/3}$:

$$q < 2 \Rightarrow \exists d_q : \|\varrho_\sigma(x)\|_q \leqq d_q \,. \tag{27}$$

Now we use Hölders inequality:

$$\max_{x\in V} |\int V_\sigma(x, y) \varrho_\sigma(y) d^3y| \leqq \max_{x\in V} \|V_\sigma(x, y)\|_p \|\varrho_\sigma(y)\|_q \leqq c_p d_q \,, \tag{28}$$

where the following relations must hold:

$$2 < p < 3, \; 3/2 < q < 2, \; 1/p + 1/q = 1 \,.$$

This gives a uniform L^∞-bound for all densities:

$$|\varrho_\sigma(x)| \leqq (2m)^{3/2} g(\beta, \hat{\mu} + c_p d_q + k). \tag{29}$$

To be able to make statements about convergence, we define, in addition to $U_{s,g}(x)$, functions $W_{s,g}(x) = \int_V d^3y V_s(x, y) \varrho_{s,g}(y)$ and

$$T_{s,g}(x) = n \int_{V^{n-1}} S(x_1 x_2 \dots x_n) \prod_{i=2}^{n} \varrho_{s,g}(x_i) d^3 x_i ,$$

which are uniformly continuous:

$$|\vec{\nabla} W_{s,g}(\vec{x})| = \left| \int_V d^3y \varrho_{s,g}(y) \nabla_x V_s(x, y) \right| \leqq \|\varrho_{s,g}\|_\infty \int_V |\nabla(1/|x|)| d^3 x = \text{const} < \infty . \tag{30}$$

They therefore form two conditionally compact sets (theorem of Ascoli), and have pointwise converging subsequences as $g \to \infty$, which is also true for the $U_{s,g}$, since

$$\lim_{g \to \infty} |U_{s,g}(x) - W_{s,g}(x)| = 0 ,$$

and equally for the $S_{s,g}$.

The same applies to the limit $s \to \infty$. The densities also have a converging subsequence (say to $\tilde{\varrho}$) since they are well behaved functions of the $U_\sigma(x)$ and $S_\sigma(x)$.

To see that the limits are again solutions of T.F.-equations we observe that the Ψ_σ's are continuous as functionals over $L^1 \cap L^\infty$ and converge pointwise as $g \to \infty$ and $s \to \infty$. Therefore:

$$\lim_{s \to \infty} \lim_{g \to \infty} \Psi_{s,g}(\varrho_{s,g}, \beta, \lambda) = \lim_{s \to \infty} \Psi_s(\varrho_s, \beta, \lambda) = \Psi(\tilde{\varrho}, \beta, \lambda) . \tag{31}$$

On the other hand one certainly has:

$$\min_{\varrho \in \Omega} \Psi(\varrho, \beta, \lambda) \geqq \lim_{s \to \infty} \lim_{g \to \infty} \min_{\varrho \in \Omega} \Psi_{s,g}(\varrho, \beta, \lambda) , \tag{32}$$

so that the minimum is attained at $\tilde{\varrho}$:

$$\Phi(\beta, \lambda) = \Psi(\tilde{\varrho}, \beta, \lambda) = \lim_{s \to \infty} \lim_{g \to \infty} \Phi_{s,g}(\beta, \lambda) = \lim_{N \to \infty} f(N, \beta, \lambda) . \tag{33}$$

V. Taking the Derivative

In order to be able to apply Theorem A2 of the appendix, we have to make sure that the $\tilde{\varrho} = \tilde{\varrho}(\lambda)$ vary continuously with λ at $\lambda = 0$. We can use the same considerations for the limit $\lambda \to 0$ as for $g \to \infty$ and $s \to \infty$: there are converging subsequences $\tilde{\varrho}(\lambda_i) \to \tilde{\varrho}(0)$ as $\lambda_i \to 0$. This implies continuity, if $\tilde{\varrho}(0)$ is unique. We claim the following

Theorem. *If β is not the critical value β_c, then the solutions of the T.F.-Equations* (18) *and* (19) *in a spherical volume and at $\lambda = 0$ are rotation invariant and unique.*

Proof. We characterize classes K_m of densities ϱ by real-valued functions $m(r)$:

$$K_m = \left\{ \varrho \in \Omega : \int_V \theta(r - \varrho(x)) d^3 x = m(r) \, \forall r \right\} . \tag{34}$$

Every term of the form $\int_V F(\varrho(x)d^3x$ is a functional, which depends only on the class K_m of ϱ. In $\Psi(\varrho, \beta, \lambda)$ only the term $\int_{V\times V} d^3xd^3y\varrho(x)V(x-y)\varrho(y)$ is not of this form. But this term is minimized by the unique spherically symmetric and decrasing function in K_m [6]. (We specify now that V shall have the form of a sphere.) For spherically symmteric functions one knows that the solution of (18), (19) at $\lambda=0$ are unique ($\tilde{\varrho}(0)=\varrho_{TF}$) unless the system is at the critical point β_c, where a phase-transition occurs [2]. Q.e.d.

In the last step we use (9), (33), Griffith's Lemma [7] and Theorem A2. The result is:

$$\lim_{N\to\infty} \langle\hat{\varrho}_N(w_1\dots w_n)\rangle_\beta=\frac{\partial}{\partial\lambda}f(N,\beta,\lambda)|_{\lambda=0}=\frac{\partial}{\partial\lambda}\Phi(\beta,\lambda)|_{\lambda=0} \tag{35}$$

$$=\frac{\partial}{\partial\lambda}\Psi(\varrho_{TF},\beta,\lambda)|_{\lambda=0}=\prod_{i=1}^{n}\int\varrho_{TF}(x)w_i(x)d^3x\,,\quad\text{if}\quad\beta\neq\beta_c\,.$$

This means that the expectation values of the density converge as tempered distributions to the T.F.-density and are not correlated in the limit. A related result for the T.F.-theory of atoms ([8, 9]) suggests that the densities converge as distributions over the test-function space $L^{5/2}(V)$.

Appendix: Two Theorems on Concave Functions

Theorem A1. *Let a concave function $f(\lambda)$ be defined by a variational principle:*

$$f(\lambda)=\min_{\varrho\in\Omega}F(\varrho,\lambda)$$

and such that the minimum is attained at some ϱ_λ:

$$f(\lambda)=F(\varrho_\lambda,\lambda)\,.$$

Furthermore, we suppose that the partial derivatives

$$F'(\varrho,\lambda_0)=\frac{\partial}{\partial\lambda}F(\varrho,\lambda)|_{\lambda=\lambda_0}$$

exist for all pairs (ϱ,λ_0). Then the following relation holds:

$$f'_+(\lambda)\leqq F'(\varrho_\lambda,\lambda)\leqq f'_-(\lambda)\,.$$

$f'_+(f'_-)$ is the right- (left-) hand-side derivative, which exists, since f is concave [10]. □

Proof.

$$f'_+(\lambda)=\lim_{\varepsilon\to0}(1/\varepsilon)[F(\varrho_{\lambda+\varepsilon},\lambda+\varepsilon)-F(\varrho_\lambda,\lambda)]\leqq\lim_{\varepsilon\to0}(1/\varepsilon)[F(\varrho_\lambda,\lambda+\varepsilon)-F(\varrho_\lambda,\lambda)]$$

$$=F'(\varrho_\lambda,\lambda)=\lim_{\varepsilon\to0}(1/\varepsilon)[F(\varrho_\lambda,\lambda)-F(\varrho_\lambda,\lambda-\varepsilon)]$$

$$\leqq\lim_{\varepsilon\to0}(1/\varepsilon)[F(\varrho_\lambda,\lambda)-F(\varrho_{\lambda-\varepsilon},\lambda-\varepsilon)]=f'_-(\lambda)\,.$$

Theorem A2. *If it is possible to attach a topology to Ω such that $F'(\varrho, \lambda)$ is a continuous function on $\Omega \times R$ and if there exists a path of minimizing ϱ_λ, continuous at λ_0, then $f(\lambda)$ is differentiable at λ_0 and*

$$f'(\lambda_0) = F'(\varrho_{\lambda_0}, \lambda_0).$$

Proof. Since f is concave, for $x > y$ the relations $f'_+(x) \leqq f'_-(x) \leqq f'_+(y)$ hold. For $\varepsilon > 0$ and with Theorem A1:

$$F'(\varrho_{\lambda_0+\varepsilon}, \lambda_0+\varepsilon) \leqq f'_-(\lambda_0+\varepsilon) \leqq F'(\varrho_{\lambda_0}, \lambda_0) \leqq f_-(\lambda_0) \leqq f'_+(\lambda_0-\varepsilon) \leqq F'(\varrho_{\lambda_0-\varepsilon}, \lambda_0-\varepsilon).$$

The difference between the right- and left-hand-side tends to zero with $\varepsilon \to 0$ because of the continuity. Q.e.d.

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References

1. Hertel, P., Narnhofer, H., Thirring, W.: Commun. math. Phys. **28**, 159—167 (1972)
2. Hertel, P., Thirring, W.: Thermodynamic Instability of a System of Gravitating Fermions. In: Dürr, H. P. (Ed.): Quanten und Felder. Braunschweig: Vieweg 1971
3. Thirring, W.: Vorlesungen über mathematische Physik T7: Quantenmechanik. Lecture notes
4. Narnhofer, H., Thirring, W.: Acta Phys. Austr. **41**, 281—297 (1975)
5. Maison, H. D.: Commun. math. Phys. **22**, 166—172 (1971)
6. Lichtenstein, L.: Math. Z. **3**, 8—10 (1918)
7. Griffiths, R. B.: J. Math. Phys. **5**, 1215—1222 (1964)
8. Baumgartner, B.: The Thomas-Fermi-Theory as Result of a Strong-Coupling-Limit. To be published
9. Thirring, W.: Vorlesungen über mathematische Physik T8: Quantenmechanik großer Systeme. Lecture notes
10. Roberts, A., Varberg, D.: Convex Functions. London: Academic Press 1973

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