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Statistical Mechanics of Quantum Mechanical Particles with Hard Cores

I. The Thermodynamic Pressure

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Abstract. The definition of the thermodynamic pressure of a quantum mechanical system of hard core particles is considered for a wide variety of boundary conditions and a large class of interactions. It is shown that the pressure can be defined for elastic walls and that in the limit of an infinite system the thermodynamic pressure both exists and is independent of the coefficient of elasticity. Similarly if repulsive wall boundary conditions are used the thermodynamic pressure exists. Unfortunately it has not been possible to demonstrate that the two pressures obtained are identical but a number of their properties and interrelationships are established.

1. Introduction

In this, and a subsequent, paper we extend to quantum hard core systems various results which have been obtained for classical [1–3] and quantum [4–6] spin systems and classical hard core systems [7]. In this paper we consider properties of the thermodynamic pressure.

To define the thermodynamic pressure one must first consider a finite system and this leads to a certain ambiguity concerning the choice of boundary conditions, which, in the quantum mechanical formalism, is related to the choice of the Hamiltonian. We consider Hamiltonians with a large class of stable interactions whose domains are specified by conditions of the form

$$\frac{\partial \Psi}{\partial n} = \sigma \Psi$$

on the boundary of the system; $\partial \Psi / \partial n$ denotes the normal derivative across the boundary of a wave function Ψ. The parameter σ introduced in this manner is related to the elasticity of the walls of the system, $\sigma = 0$ is perfect elasticity, $\sigma = \infty$ infinite repulsion, and $\sigma = -\infty$ infinite attraction. We prove that for finite σ the thermodynamic pressure exists and is independent of σ. This generalizes the result obtain by Ruelle [8] in the case $\sigma = +\infty$, i.e. the boundary condition $\Psi = 0$. Unfortunately we have not been able to establish that the pressure we define is identical to that of Ruelle although the former is certainly greater or equal to the latter.

2. General Formalism

Thoughout this, and the following, paper we will consider particles satisfying Bose-Einstein statistics; the discussion of Fermi particles is actually easier and all the results we obtain can be derived in this case.

Let Λ be an open bounded subset of the ν-dimensional Euclidean space R^ν. The set F_a^Λ of physical configurations of a system of bosons, with hard cores of diameter a, contained in Λ is defined by

$$F_a^\Lambda = \{X ; |x-y| \geqq a \quad \text{for} \quad x, y \in X,\ x \neq y \quad \text{where} \quad X \subset \Lambda\};$$

$N(X) = \operatorname{card} X$ takes values $0, 1, \ldots N_a(\Lambda)$, where $N_a(\Lambda)$ is the maximum number of hard core particles which can be confined in Λ. We introduce ϱ_a by

$$\varrho_a = \sup_{\Lambda \subset R^\nu} \frac{N_a(\Lambda)}{V(\Lambda)}$$

where $V(\Lambda)$ denotes the volume, i.e. Lebesgue measure, of Λ.

The Hilbert space $\mathscr{H}_a(\Lambda)$ of vector states describing the finite system is given by the space of square integrable functions over the configurations $X \subset F_a^\Lambda$, i.e. $\Psi(\emptyset)$ is defined to be a complex scalar and if $X = \{x_1, \ldots, x_n\} \subset F_a^\Lambda$ then $\Psi(X) = \Psi(x_1, \ldots, x_n)$ is assumed to be totally symmetric and square integrable; the scalar product on $\mathscr{H}_a(\Lambda)$ is defined by

$$(\Psi, \Phi) = \overline{\Psi(\emptyset)}\, \Phi(\emptyset) + \sum_{n=1}^{N_a(\Lambda)} \int_{F_a^\Lambda} \frac{dx_1 \ldots dx_n}{n!}\, \overline{\Psi(x_1 \ldots x_n)}\, \Phi(x_1 \ldots x_n).$$

Alternatively we can define a measure dX on F_a^Λ by

$$\int_\Lambda dX \cdot = \sum_{n=0}^{N_a(\Lambda)} \int_{F_a^\Lambda} \frac{dx_1 \ldots dx_n}{n!}.$$

and then we have the compact notation

$$(\Psi, \Phi) = \int_\Lambda dX\, \overline{\Psi(X)}\, \Phi(X).$$

Next consider the connections between the Hilbert spaces of different finite systems. If Λ_1 and Λ_2 are disjoint open bounded subsets of R^ν then $\mathscr{H}_a(\Lambda_1)$ and $\mathscr{H}_a(\Lambda_2)$ can be identified as subspaces of $\mathscr{H}_a(\Lambda_1 \cup \Lambda_2)$. For example it is easily seen that the condition $\Psi(X) = 0$ if $X \not\subset F_a^{\Lambda_1}$ defines a subspace of $\mathscr{H}_a(\Lambda_1 \cup \Lambda_2)$ which is isomorphic to $\mathscr{H}_a(\Lambda_1)$.

Further the space $\mathscr{H}_a(\Lambda_1 \cup \Lambda_2)$ can be identified as a subspace of the symmetric tensor product space $\overline{\mathscr{H}_a(\Lambda_1) \otimes \mathscr{H}_a(\Lambda_2)}$. The elements of this latter space are square integrable functions over pairs (X_1, X_2) of configurations $X_1 \subset F_a^{\Lambda_1}$, $X_2 \subset F_a^{\Lambda_2}$ and the subspace of vectors defined by the restriction $\Psi(X_1, X_2) = 0$ if $X_1 \cup X_2 \not\subset F_a^{\Lambda_1 \cup \Lambda_2}$ is isomorphic to $\mathscr{H}_a(\Lambda_1 \cup \Lambda_2)$. These identifications allow us to extend, or conversely restrict, operators from one space to another; these possibilities will be of use in making various estimates.

Finally, let us define a particularly useful operator, the number operator N_Λ on $\mathscr{H}_a(\Lambda)$ by

$$(N_\Lambda \Psi)(X) = \sum_{x \in X} \Psi(X) = N(X)\, \psi(X),$$

i.e. $N(X)$ is the number of points in the set X. Clearly N_Λ is a bounded self-adjoint operator with $N_\Lambda \geqq 0$ and $\|N_\Lambda\| = N_a(\Lambda)$. If $\Lambda_1 \cap \Lambda_2 = \emptyset$, then the number operators N_{Λ_1}, N_{Λ_2} can be extended to operators acting on $\mathscr{H}_a(\Lambda_1 \cup \Lambda_2)$, which we will also denote by N_{Λ_1} and N_{Λ_2}, by the definitions

$$(N_{\Lambda_1} \Psi)(X) = \sum_{x \in X \cap \Lambda_1} \Psi(X)$$

$$(N_{\Lambda_2} \Psi)(X) = \sum_{x \in X \cap \Lambda_2} \Psi(X)$$

and we have then

$$N_{\Lambda_1 \cup \Lambda_2} = N_{\Lambda_1} + N_{\Lambda_2}.$$

3. Hamiltonians of Finite Systems

The description of a finite system of particles presents us with a wide choice of possible boundary conditions. In quantum mechanics the specification of boundary conditions is closely allied to the specification of the Hamiltonian of the system and in particular the choice of kinetic energy operator. We next consider the problem of defining Hamiltonians with various choices of boundary conditions.

To fix our ideas, let us first introduce a kinetic energy operator S_Λ for the finite system of hard core particles confined to Λ. We assume here, and in the following, that the surface of Λ is smooth in the sense of [9], and define S by

$$(S_\Lambda \Psi)(X) = -\sum_{x \in X} \nabla_x^2 \Psi(X);$$

∇_x^2 denotes the Laplacian and the domain $D(S_\Lambda)$ of S_Λ is taken to be the infinitely often differentiable functions with compact support in F_a^Λ. On this domain, S_Λ is symmetric but not essentially self-adjoint. A self-adjoint of S_Λ would determine a possible dynamics of the system of non-interacting particles and this of course entails the specification of the behaviour of the particles at the boundaries of F_a^Λ, i.e. specification of boundary conditions is equivalent to the choice of a particular self-adjoint extension of S_Λ.

In the case of hard core particles the boundary ∂F_a^Λ of the space of configurations is complicated but consists of an external boundary Ω_Λ^e defined by

$$\Omega_\Lambda^e = \{X; X \cap \partial\Lambda \neq \emptyset\}$$

and an internal boundary $\Omega_\Lambda^i = \partial F_a^\Lambda \backslash \Omega_\Lambda^e$. We will now consider a variety of self-adjoint extensions of S_Λ each of which has the property that their eigenfunctions vanish on the internal boundary but which satisfy different conditions on the external boundary. We introduce and study these operators by the use of semi-bounded forms (for a brief review of the theory of positive forms and the associated positive operators see the appendix). This method of studying self-adjoint differential operators is quite standard and a good introduction to the subject is provided in [9].

We begin by introducing a form t_Λ^0 as follows. The domain $D(t_\Lambda^0)$ of t_Λ^0 is specified to be the functions which are continuously differentiable in the closure $\bar{F}_a^\Lambda$ of F_a^Λ and vanish in a neighbourhood of Ω_Λ^i. On this domain we take

$$t_\Lambda^0(\Psi) = \int_\Lambda dX \sum_{x \in X} |\nabla_x \Psi(X)|^2 .$$

The form t_Λ^0 is positive, densely defined, and can be proved to be closable. For notational simplicity we also denote the closure by t_Λ^0. By proposition $A1$ there exists a positive self-adjoint operator T_Λ^0 such that

$$t_\Lambda^0(\Psi) = (T_\Lambda^{0\frac{1}{2}} \Psi, T_\Lambda^{0\frac{1}{2}} \Psi)$$

for $\Psi \in D(t_\Lambda^0)$ and further $D(t_\Lambda^0) = D(T_\Lambda^{0\frac{1}{2}})$. The operator defined in this manner is the self-adjoint extension of S_Λ whose domain is specified by the boundary condition $\Psi = 0$ on Ω_Λ^i but $\partial\Psi(X)/\partial n_x = 0$ if $x \in \partial\Lambda$ where $\partial/\partial n_x$ denotes the inward normal derivative.

Next let us define t_Λ^σ, for σ real, by $D(t_\Lambda^\sigma) = D(t_\Lambda^0)$ and

$$t_\Lambda^\sigma(\Psi) = t_\Lambda^0(\Psi) + \sigma s_\Lambda(\Psi)$$

where

$$s_\Lambda(\Psi) = \int_{\Omega_\Lambda^e} dS |\Psi|^2, \qquad \Psi \in D(t_\Lambda^0) .$$

The last integral is taken over the external surface[1] of F_a^A. Although t_A^σ is densely defined it is not clear that it is lower semi-bounded for $\sigma < 0$. A standard calculation shows however that s_A is relatively t_A^0-bounded with relative bound 0 (we will reproduce this calculation below in an improved form). Accepting this result we deduce that t_A^σ is lower semi-bounded and closable and the domain of the closure coincides with the domain of t_A^0. Further there is a self-adjoint extension T_A^σ of S_A associated with t_A^σ in the canonical fashion. The domain of T_A^σ is specified by the boundary condition $\Psi = 0$ on Ω_A^i and $\partial \Psi(X)/\partial n_x - \sigma \Psi(X) = 0$ for $x \in \partial A$ (cf. for example [9]).

Finally we introduce the form t_A by specifying the domain $D(t_A)$ to be the infinitely often differentiable functions with compact support in F_a^A and then taking

$$t_A(\Psi) = \int_A dX \sum_{x \in X} |\nabla_x \Psi(X)|^2, \qquad \psi \in D(t_A).$$

This form is the minimal form associated with S_A and is closable. We again denote its closure by t_A. The self-adjoint operator T_A associated with t_A is the Friederichs extension of S_A and its domain is specified by the boundary condition $\Psi = 0$ on ∂F_a^A.

We next consider order relations between the various forms introduced above and for this purpose it is necessary to examine the form s_A in more detail.

Let $x = (x_1, \ldots, x_\nu) \to \xi(x) = (\xi_1(x_1), \ldots, \xi_\nu(x_\nu))$ be a real-vector-valued function continuously differentiable in the closed region $\bar{A}$ and satisfying the boundary condition $\boldsymbol{n} \, . \, \xi + 1 = 0$ on ∂A where $\boldsymbol{n}$ denotes the inward normal. The integral representation

$$s_A(\Psi) = \int_A dX \sum_{x \in X} \nabla_x . (\xi(x) \, |\Psi(X)|^2)$$

follows straightforwardly by integration. However we now have

$$\begin{aligned} &s_A(\Psi) \\ &= \int_A dX \sum_{x \in X} \{(\nabla_x . \xi(x)) |\Psi(X)|^2 + \xi(x) . (\nabla_x \overline{\Psi(X)}) \Psi(X) + \overline{\Psi(X)} \xi(x) . \nabla_x \Psi(X)\}. \end{aligned}$$

Now denoting the support of $|\xi|$ by A_ξ and using the inequality

$$|(\xi(x) . \nabla_x \overline{\Psi(X)}) \Psi(X) + \overline{\Psi(X)} (\xi(x) . \nabla_x \Psi(X))| \leqq \frac{1}{\varepsilon} |\nabla_x \Psi(X)|^2 + \varepsilon |\xi(x) \Psi(X)|^2, \qquad \varepsilon > 0$$

[1] In the above definition we could introduce σ as a C^∞ function on the surface of A and then introduce this function in the integral. Our subsequent results generalize easily to this case. Alternatively we could consider different choices of boundary conditions on the internal boundaries and still obtain our main results, existence of the thermodynamic pressure, etc.

we find

$$
\begin{aligned}
0 &\leqq s_\Lambda(\Psi) \\
&\leqq \int_\Lambda dX \sum_{x \in X \cap \Lambda_\xi} \left\{ \frac{1}{\varepsilon} | \nabla_x \Psi(X) \|^2 + \varepsilon |\xi(x)\, \Psi(X)|^2 + | \nabla_x \cdot \xi(x) \| \, \Psi(X)|^2 \right\}.
\end{aligned}
$$

Thus s_Λ is relatively t_Λ^0-bounded as stated above but we are still free to choose ξ and this allows us to obtain various interesting relations.

Lemma 1. *Let Λ be a parallelepiped with surface area $S(\Lambda)$ then the following inequality is valid*

$$0 \leqq s_\Lambda \leqq \varrho_a S(\Lambda).$$

Hence t_Λ^0 is lower semi-bounded with bound given by

$$t_\Lambda^\sigma \geqq \varrho_a S(\Lambda) \min\{0, \sigma\}.$$

Further if $\sigma_1 > \sigma_2$, then the following ordering of forms is valid

$$t_\Lambda \geqq t_\Lambda^{\sigma_1} \geqq t_\Lambda^{\sigma_2} \geqq t_\Lambda^{\sigma_1} - (\sigma_1 - \sigma_2)\, \varrho_a S(\Lambda).$$

Proof. Let Λ be given by

$$\Lambda = \{x; 0 \leqq x_i < L_i, i = 1, 2, \dots \nu\}$$

and choose ξ_i as follows

$$
\begin{aligned}
&\xi_i(x_i) = \varepsilon^2 x_i - 1, \quad 0 \leqq x_i \leqq 1/\varepsilon^2, \\
&\xi_i(x_i) = 0, \quad 1/\varepsilon^2 \leqq x_i \leqq L_i - 1/\varepsilon^2, \\
&\xi_i(x_i) = 1 - \varepsilon^2 (L_i - x_i), \quad L_i - 1/\varepsilon^2 \leqq x_i \leqq L_i,
\end{aligned}
$$

where we take $\varepsilon^2 L_i \geqq 2$. With this choice of ξ the above inequality for s_Λ is valid and referring to the discussion of the number operator given in the previous section we find

$$0 \leqq s_\Lambda \leqq \frac{1}{\varepsilon} t_\Lambda^0 + \varrho_a S(\Lambda) \left(1 + \frac{1}{\varepsilon}\right).$$

Thus in the limit $\varepsilon \to \infty$ we have

$$0 \leqq s_\Lambda \leqq \varrho_a S(\Lambda).$$

Now the lower bound for t_Λ^σ follows from this inequality and

$$t_\Lambda^\sigma = t_\Lambda^0 + \sigma s_\Lambda \geqq \sigma s_\Lambda.$$

Similarly the order relationship between $t_\Lambda^{\sigma_1}$ and $t_\Lambda^{\sigma_2}$ follows by noting that

$$t_\Lambda^{\sigma_1} = t_\Lambda^{\sigma_2} + (\sigma_1 - \sigma_2)\, s_\Lambda.$$

Finally t_Λ^σ is an extension of t_Λ and hence the relation $t_\Lambda \geqq t_\Lambda^\sigma$ follows by definition.

After this discussion of the kinetic energy let us consider the definition of the interaction Hamiltonians.

The interaction between particles of the finite system is defined in terms of an operator U_Λ on $\mathscr{H}_a(\Lambda)$ which we will assume to be bounded with a bound of the form

$$\|U_\Lambda\| \leqq B N_a(\Lambda) \leqq B \varrho_a V(\Lambda)$$

where $B > 0$ and independent of Λ. Further let $\Lambda_1 \cap \Lambda_2 = \emptyset$ and consider $U_{\Lambda_1 \cup \Lambda_2}$, U_{Λ_1} and U_{Λ_2}, as operators on $\mathscr{H}_a(\Lambda_1 \cup \Lambda_2)$. We assume that

$$\|U_{\Lambda_1 \cup \Lambda_2} - U_{\Lambda_1} - U_{\Lambda_2}\| \leqq C(S(\Lambda_1) + S(\Lambda_2))\, \varrho_a$$

where $S(\Lambda_1)$ and $S(\Lambda_2)$ are the surface areas of Λ_1 and Λ_2 respectively and $C(\geqq 0)$ is independent of Λ_1 and Λ_2. Finally we assume that U_Λ is translationally invariant. To explain this notion we introduce the unitary operator $V_{\Lambda,x}$ from $\mathscr{H}_a(\Lambda)$ to $\mathscr{H}_a(\Lambda + x)$ by

$$(V_{\Lambda,x}\Psi)(X) = \Psi(X - x).$$

Then we demand that the interaction operators satisfy

$$U_{\Lambda + x} = V_{\Lambda,x} U_\Lambda V_{\Lambda,x}^{-1}.$$

The above conditions on the interactions are rather strong but are characteristic of the topological space of interactions introduced by Gallavotti and Miracle-Sole in the study of classical hard core systems [7].

Now with the interaction U_Λ we can associate a bounded form u_Λ by the definition $D(u_\Lambda) = \mathscr{H}_a(\Lambda)$ and

$$u_\Lambda(\Psi) = (\Psi, U_\Lambda \Psi)$$

Similarly we can associate the form n_Λ with the number operator N_Λ, i.e.

$$n_\Lambda(\Psi) = (\Psi, N_\Lambda \Psi), \qquad D(n_\Lambda) = \mathscr{H}_a(\Lambda).$$

With these definitions we introduce the following forms

$$h_\Lambda^\sigma(\Psi) = t_\Lambda^\sigma(\Psi) + u_\Lambda(\Psi) - \mu n_\Lambda(\Psi),$$
$$h_\Lambda(\Psi) = t_\Lambda(\Psi) + u_\Lambda(\Psi) - \mu n_\Lambda(\Psi),$$

and note that these forms determine the operators

$$H_\Lambda^\sigma = T_\Lambda^\sigma + U_\Lambda - \mu N_\Lambda,$$
$$H_\Lambda = T_\Lambda + U_\Lambda - \mu N_\Lambda$$

respectively. H_Λ^σ and H_Λ correspond to the grand canonical Hamiltonians of our interacting system with μ interpretable as the chemical potential.

Note that T_Λ^σ, N_Λ, etc. reduce to zero on the zero particle subspace of $\mathscr{H}_a(\Lambda)$. We will further assume for convenience that U_Λ is normalized, by addition of a multiple of the identity, such that $H_\Lambda^\sigma = 0 = H_\Lambda$ on the zero particle subspace.

4. The Thermodynamic Pressure

We now examine the definition of the thermodynamic pressure. As a preliminary to this study we consider properties of the local partition functions and local pressures defined with the Hamiltonians introduced in the previous section. It should perhaps be emphasized that the majority of the properties we derive are obtained by application of the minimax theorem (cf. Proposition A2 of the Appendix), i.e. by monotonicity arguments, or by use of convexity.

For simplicity we will throughout this section restrict Λ to be a parallelepiped.

Lemma 2. *The spectra of the local Hamiltonians H_Λ^σ and H_Λ consist of discrete eigenvalues of finite multiplicity. The operators* $\exp\{-\beta H_\Lambda^\sigma\}$ *and* $\exp\{-\beta H_\Lambda\}$ *are of trace class for all $\beta > 0$.*

Proof. The above properties of H_Λ have been already proved by Ruelle [8]. Note however that from Lemma 1 we have $h_\Lambda \geqq h_\Lambda^\sigma$ and h_Λ^σ is lower semi-bounded. Thus applying the minimax theorem we can conclude that if H_Λ^σ has the stated properties then these properties are automatically shared by H_Λ.

Next note that from the definition of the interaction and from Lemma 1 we have:

$$\begin{aligned} h_\Lambda^\sigma &\geqq t_\Lambda^\sigma - (B + |\mu|)\, \varrho_a V(\Lambda) \\ &\geqq \begin{cases} t_\Lambda^0 - (B + |\mu|)\, \varrho_a V(\Lambda) & \text{if} \quad \sigma \geqq 0 \\ t_\Lambda^0 - (B + |\mu|)\, \varrho_a V(\Lambda) + \sigma \varrho_a S(\Lambda) & \text{if} \quad \sigma \leqq 0 \,. \end{cases} \end{aligned}$$

Thus appealing to the minimax theorem once again we conclude that if T_Λ^0 has the desired properties then these properties are guaranteed for H_Λ^σ, and hence H_Λ.

Next introduce the space $\mathscr{H}(\Lambda)$ by

$$\mathscr{H}(\Lambda) = \bigoplus_{n=0}^{N_a(\Lambda)} L_+^2(\Lambda^n)$$

We can define a closed extension $\hat{t}_\Lambda^0$ of t_Λ^0 on $\mathscr{H}(\Lambda)$ by using the definition of t_Λ^0 but omitting the domain requirement $\Psi(X) = 0$ if $X \notin F_a^\Lambda$ and the restriction that Ψ must vanish in the neighbourhood of Ω_Λ^i. By definition we have $t_\Lambda^0 \geqq \hat{t}_\Lambda^0$ and hence if $\hat{T}_\Lambda^0$ is the operator, on $\mathscr{H}(\Lambda)$, associated with $\hat{t}_\Lambda^0$ then we see that the proof of the lemma is complete if we can show that $\exp\{-\beta\hat{T}_\Lambda^0\}$ is of trace class for $\beta > 0$. But this last property can be checked by explicit calculation.

The operator $\hat{T}_\Lambda^0$ is the kinetic energy operator of a finite number of free point particles and the eigenvalues of $\hat{T}_\Lambda^0$ can be computed. On $L_+^2(\Lambda)$ the eigenvalues are given by

$$\varepsilon(\boldsymbol{n}) = \sum_{i=1}^{\nu} \left(\frac{n_i \pi}{L_i}\right)^2$$

where L_i denotes the lengths of the edges of Λ and n_i takes the values 0, 1, 2, ... On the higher particle subspaces $L_+^2(\Lambda^m)$ the eigenvalues are given by all possible sums of m single particle eigenvalues. Using Ruelle's estimation procedure [8] we find that for $0 < z < 1$

$$\frac{1}{V(\Lambda)} \log Tr_{\mathscr{H}(\Lambda)}(e^{-\beta T_\Lambda}) \leqq \frac{z}{1-z}\left(\frac{1}{(4\pi\beta)^{\frac{1}{2}}} + \frac{1}{L_0}\right)^{\nu} - \varrho_a \log z$$

where L_0 denotes the minimum of L_i, $i = 1, \ldots, \nu$. (The L_0-dependence arises because the operator we are considering differs from that considered by Ruelle insofar the value $n_i = 0$ is allowed in the eigenvalues, i.e. we have different boundary conditions.)

The properties derived in the foregoing lemma allow us to introduce the local pressures by the definitions

$$P_\Lambda(\beta, \mu, \sigma) = \frac{1}{V(\Lambda)} \log Tr_{\mathscr{H}_a(\Lambda)}(e^{-\beta H_\Lambda^\sigma}),$$

$$P_\Lambda(\beta, \mu) = \frac{1}{V(\Lambda)} \log Tr_{\mathscr{H}_a(\Lambda)}(e^{-\beta H_\Lambda}).$$

Theorem 1. a) *P_Λ is non-negative and bounded uniformly in Λ*[2].

b) *P_Λ is a convex continuous function of β and μ and the continuity is uniform in Λ*[2].

c) *For $\sigma_1 > \sigma_2$ the following relation is valid*

$$0 \leqq P_\Lambda(\beta, \mu, \sigma_1) - P_\Lambda(\beta, \mu, \sigma_2) \leqq \beta(\sigma_1 - \sigma_2)\, \varrho_a \frac{S(\Lambda)}{V(\Lambda)}.$$

d) *The two pressures are interconnected as follows*

$$P_\Lambda(\beta, \mu) = \lim_{\sigma \to \infty} P_\Lambda(\beta, \mu, \sigma) = \inf_\sigma P_\Lambda(\beta, \mu, \sigma).$$

[2] Λ is assumed to be a parallelepiped with edges of length, $L_1, \ldots, L_\nu$ and the uniformity is in the variables L_i for $L_i \geqq 1$, $i = 1, \ldots, \nu$; the last restriction is assumed to avoid possible singular behaviour for small Λ.

Proof. Due to our normalization of the interaction we have $H_\Lambda^\sigma = 0 = H_\Lambda$ on the zero-particle subspace of $\mathscr{H}_a(\Lambda)$. It immediately follows that P_Λ is non-negative. A bound on $P_\Lambda(\beta, \mu, \sigma)$, and consequently on $P_\Lambda(\beta, \mu)$, which is uniform in Λ is given by the estimates used in the proof of Lemma 2. The convexity of $P_\Lambda(\beta, \mu)$ has been established by Ruelle [8] and the same argument applies to $P_\Lambda(\beta, \mu, \sigma)$ (cf. Proposition A3 of the appendix). The continuity of P_Λ follows from the convexity and the uniformity in Λ is a consequence of the uniform boundedness. Explicitly if $x > 0 \to f(x) \geqq 0$ is a non-negative convex function then for $h \geqq 0$, $1 > a > 0$, and $b > 0$ we have

$$-\frac{h}{ax} f((1-a)\,x) \leqq f(x+h) - f(x) \leqq \frac{h}{bx} f((1+b)\,x).$$

These inequalities follow from the convexity inequality

$$f(\lambda x_1 + (1-\lambda)\,x_2) \leqq \lambda f(x_1) + (1-\lambda) f(x_2), \qquad 0 < \lambda \leqq 1.$$

by the choices $x_1 = x$, $x_2 = (1+b)\,x$, $\lambda = 1 - h/bx$, and $x_1 = x + h$, $x_2 = (1-a)\,x$, $\lambda = ax/(ax+b)$, respectively. From Lemma 1 we have

$$0 \leqq h_\Lambda^{\sigma_1} - h_\Lambda^{\sigma_2} \leqq (\sigma_1 - \sigma_2)\,\varrho_a S(\Lambda), \qquad \sigma_1 > \sigma_2$$

and part *c* of the theorem then follows form Proposition A3 and the definition of P_Λ. It remains to prove part *d*.

Let λ_n and λ_n^σ be the eigenvalues of H_Λ and H_Λ^σ, respectively, arranged in increasing order repeated according to multiplicity. As $\sigma \to h_\Lambda^\sigma$ is a monotonically increasing function we deduce that $\sigma \to \lambda_n^\sigma$ is also monotonically increasing. Hence we can introduce $\overline{\lambda_n}$ by

$$\overline{\lambda_n} = \lim_{\sigma \to \infty} \lambda_n^\sigma = \sup_\sigma \lambda_n^\sigma.$$

Further we have $h_\Lambda \geqq h_\Lambda^\sigma$ and hence

$$\lambda_n \geqq \overline{\lambda_n} \geqq \lambda_n^\sigma.$$

We will prove that $\lambda_n = \overline{\lambda_n}$ and then statement *d* is a consequence of the fact that P_Λ is a continuous function of the eigenvalues.

Let $(\Phi_n^\sigma)_{n \geqq 1}$ be a complete orthonormal set of eigenfunctions of H_Λ^σ corresponding to the eigenvalues $(\lambda_n^\sigma)_{n \geqq 1}$. Due to the normalization we can for each value of n choose a sequence σ_i such that $\sigma_i \to \infty$ and $\Phi_n^{\sigma_i}$ is weakly convergent to a vector Φ_n. We first prove that $\Phi_n^{\sigma_i}$ converges strongly to Φ_n. Let E_λ^σ be the projector on the subspace of $\mathscr{H}_a(\Lambda)$ spanned by all eigenfunctions of H_Λ^σ with eigenvalues less than λ. We have

$$4\overline{\lambda_n} \geqq h_\Lambda^\sigma(\Phi_n^{\sigma_i} - \Phi_n^{\sigma_j}) \geqq h_\Lambda^\sigma((1 - E_\lambda^\sigma)(\Phi_n^{\sigma_i} - \Phi_n^{\sigma_j})) \geqq \lambda \,\|(1 - E_\Lambda^\sigma)(\Phi_n^{\sigma_i} - \Phi_n^{\sigma_j})\|^2.$$

Hence

$$\|\Phi_n^{\sigma_i} - \Phi_n^{\sigma_j}\|^2 \leqq 4\overline{\lambda}_n/\lambda + \|E_\lambda^\sigma(\Phi_n^{\sigma_i} - \Phi_n^{\sigma_j})\|^2 .$$

Now we can choose λ such that $\overline{\lambda}_n/\lambda < \varepsilon$ for any $\varepsilon > 0$. But E_Λ^σ is finite dimensional and $\Phi_n^{\sigma_i}$ is weakly convergent thus the strong convergence follows immediately. Next we wish to prove that $\Phi_n^{\sigma_i}$ is h_Λ^σ-convergent for all σ and hence deduce that Φ_n is in the domain of all h_Λ^σ.

For $\varepsilon > 0$ we can choose i_ε such that

$$\|\Phi_m^{\sigma_i} - \Phi_m^{\sigma_j}\|^2 < \varepsilon$$

for $i, j > i_\varepsilon$ and for $m = 1, 2, \ldots M$. It follows that

$$\begin{aligned}\left\|\frac{\Phi_m^{\sigma_i} + \Phi_m^{\sigma_j}}{2}\right\|^2 &= \frac{1}{2}\|\Phi_m^{\sigma_i}\|^2 + \frac{1}{2}\|\Phi_m^{\sigma_j}\|^2 - \left\|\frac{\Phi_m^{\sigma_i} - \Phi_m^{\sigma_j}}{2}\right\|^2 \\ &\geqq 1 - \frac{\varepsilon}{4} .\end{aligned}$$

Thus assuming $\sigma < \sigma_i < \sigma_j$ we have

$$\begin{aligned} h_\Lambda^\sigma(\Phi_m^{\sigma_i} - \Phi_m^{\sigma_j}) &\leqq 2h_\Lambda^{\sigma_i}(\Phi_m^{\sigma_i}) + 2h_\Lambda^{\sigma_j}(\Phi_m^{\sigma_j}) - 4h_\Lambda^{\sigma_i}\left(\frac{\Phi_m^{\sigma_i} + \Phi_m^{\sigma_j}}{2}\right) \\ &\leqq 2(\lambda_m^{\sigma_i} + \lambda_m^{\sigma_j}) - 4h_\Lambda^{\sigma_i}\left(\frac{\Phi_m^{\sigma_i} + \Phi_m^{\sigma_j}}{2}\right).\end{aligned}$$

Now let Ψ be a normalized vector in the subspace spanned by $\Phi_m^{\sigma_j}$, $m = 1, 2, \ldots M - 1$, then

$$\left|\left(\frac{\Phi_M^{\sigma_i} + \Phi_M^{\sigma_j}}{2}, \Psi\right)\right|^2 = \frac{1}{4}|(\Phi_M^{\sigma_i} - \Phi_M^{\sigma_j}, \Psi)|^2 \leqq \frac{\varepsilon}{4} .$$

Thus we have a decomposition of the form

$$\frac{\Phi_M^{\sigma_i} + \Phi_M^{\sigma_j}}{2} = \chi + c\Psi$$

With $(\chi, \Phi_M^{\sigma_j}) = 0$, $m = 1, 2, \ldots, M - 1$ and

$$1 \geqq \|\chi\|^2 \geqq 1 - \varepsilon/2 \quad |c|^2 \leqq \varepsilon/4 .$$

Hence

$$\begin{aligned} h_\Lambda^{\sigma_i}\left(\frac{\Phi_M^{\sigma_i} + \Phi_M^{\sigma_j}}{2}\right) &\geqq \left(\sqrt{h_\Lambda^{\sigma_i}(\chi)} - |c|\sqrt{h_\Lambda^{\sigma_i}(\Psi)}\right)^2 \\ &\geqq \lambda_M^{\sigma_i}\left(\sqrt{1 - \varepsilon/2} - \sqrt{\varepsilon/4}\right)^2, \qquad \varepsilon < 1 \end{aligned}$$

where the last inequality follows from the minimax theorem. Thus

$$h_\Lambda^\sigma(\Phi_M^{\sigma_i} - \Phi_M^{\sigma_j}) \leqq 2(\lambda_M^{\sigma_j} - \lambda_M^{\sigma_i}) + \lambda_M^{\sigma_i}\left[\varepsilon + 4\sqrt{\varepsilon(1 - \varepsilon/2)}\right]$$

Alternatively we have

$$h_\Lambda^\sigma(\Phi_M^{\sigma_i} - \Phi_M^{\sigma_j}) \geqq -\varrho_a[(B+|\mu|)\,V(\Lambda) - \sigma S(\Lambda)]\ \|\Phi_M^{\sigma_i} - \Phi_M^{\sigma_j}\|^2 .$$

Thus we can conclude that $(\Phi_m^{\sigma_i})_{i\geqq 1}$ is h_Λ^σ convergent and each of the limit vectors Φ_m is in the domain of each h_Λ^σ.

Finally we have

$$\begin{aligned} 0 \leqq s_\Lambda(\Phi_m) &= (h_\Lambda^\sigma(\Phi_m) - h_\Lambda^0(\Phi_m))/\sigma, \quad \sigma > 0 \\ &= \lim_{\sigma\to\infty} (h_\Lambda^\sigma(\Phi_m) - h_\Lambda^0(\Phi_m))/\sigma \\ &= 0 . \end{aligned}$$

Thus Φ_m is in the domain of h_Λ. But $(\Phi_m)_{m\geqq 1}$ is a complete orthonormal family and hence a last application of the minimax theorem allows us to deduce that

$$\begin{aligned} \lambda_m \leqq h_\Lambda(\Phi_m) &= h_\Lambda^\sigma(\Phi_m) \\ &= \lim_{i\to\infty} h_\Lambda^\sigma(\Phi_m^{\sigma_i}) . \end{aligned}$$

But we also have

$$\begin{aligned} \lim_{i\to\infty} h_\Lambda^\sigma(\Phi_m^{\sigma_i}) &\leqq \lim_{i\to\infty} \sup h_\Lambda^{\sigma_i}(\Phi_\Lambda^{\sigma_i}) \\ &= \overline{\lambda}_m \\ &\leqq \lambda_m . \end{aligned}$$

Hence $\lambda_m = \overline{\lambda}_m$ and $h_\Lambda(\Phi_m) = \lambda_m$, i.e. the Φ_m form a complete orthonormal set of eigenfunctions of H_Λ, and the proof of the theorem is complete.

Note that the only essential property of the interaction that we have used to derive the results given up to this point is the stability condition

$$U_\Lambda \geqq -BN_a(\Lambda) .$$

Next we turn our attention to the properties of P_Λ as a function of Λ.

Theorem 2. *Let Λ_1 and Λ_2 be disjoint. The following inequalities are valid*

$$\begin{aligned} P_{\Lambda_1\cup\Lambda_2}(\beta,\mu,\sigma) \leqq \frac{V(\Lambda_1)}{V(\Lambda_1\cup\Lambda_2)}\, P_{\Lambda_1}(\beta,\mu,\sigma) \\ + \frac{V(\Lambda_2)}{V(\Lambda_1\cup\Lambda_2)}\, P_{\Lambda_2}(\beta,\mu,\sigma) + \beta\varrho_a(C+\sigma_m)\left(\frac{S(\Lambda_1)+S(\Lambda_2)}{V(\Lambda_1)+V(\Lambda_2)}\right) \end{aligned}$$

where $\sigma_m = \max(0,\sigma)$ and

$$\begin{aligned} &P_{\Lambda_1\cup\Lambda_2}(\beta,\mu) \\ &\geqq \frac{V(\Lambda_1')}{V(\Lambda_1\cup\Lambda_2)}\, P_{\Lambda_1'}(\beta,\mu) + \frac{V(\Lambda_2')}{V(\Lambda_1\cup\Lambda_2)}\, P_{\Lambda_2'}(\beta,\mu) - 2\beta\varrho_a C\left(\frac{S(\Lambda_1)+S(\Lambda_2)}{V(\Lambda_1)+V(\Lambda_2)}\right) \end{aligned}$$

where $\Lambda'_1(\Lambda'_2)$ is the set of points in $\Lambda_1(\Lambda_2)$ at a distance greater than $a/2$ from $\partial\bar{\Lambda}_2(\partial\bar{\Lambda}_1)$.

Proof. The second inequality is due to Ruelle [8]; we have included it for the sake of comparison. We will prove the first inequality and then discuss the proof of the second to illustrate why the inequalities are in opposite sense.

We begin by noting that from the second condition placed on our interactions and Lemma 1, we have

$$h^\sigma_{\Lambda_1\cup\Lambda_2} \geqq h^\sigma_{\Lambda_1} + h^\sigma_{\Lambda_2} - \varrho_a(C+\sigma_m)\,(S(\Lambda_1)+S(\Lambda_2))$$

where $h^\sigma_{\Lambda_1}$ and $h^\sigma_{\Lambda_2}$ are now understood to be forms defined on $\mathcal{H}_a(\Lambda_1\cup\Lambda_2)$, e.g.

$$h^\sigma_{\Lambda_1}(\Psi) = \int_{\Lambda_1\cup\Lambda_2} dX \sum_{x\in X\cap\Lambda_1} |\nabla_x\Psi(X)|^2 + \int dS_{\Lambda_1}|\Psi|^2 + (\Psi, U_{\Lambda_1}\Psi) - \mu(\Psi, N_{\Lambda_1}\Psi)$$

for $\Psi\in D(h^\sigma_{\Lambda_1\cup\Lambda_2})$. Now noting that $\mathcal{H}_a(\Lambda_1\cup\Lambda_2)\subset\overline{\mathcal{H}_a(\Lambda_1)\otimes\mathcal{H}_a(\Lambda_2)}$ we can define extensions $\hat{h}^\sigma_{\Lambda_1}$ and $\hat{h}^\sigma_{\Lambda_2}$, of $h^\sigma_{\Lambda_1}$ and $h^\sigma_{\Lambda_2}$, on the latter space by

$$\hat{h}^\sigma_{\Lambda_1}(\Psi) = \int_{\Lambda_1} dX \int_{\Lambda_2} dY \sum_{x\in X} |\nabla_x\Psi(X\cup Y)|^2 + \int dS_{\Lambda_1}|\Psi|^2 + (\Psi, U_{\Lambda_1}\Psi) \text{ etc.}$$

Thus the sum $\hat{h}^\sigma_{\Lambda_1}+\hat{h}^\sigma_{\Lambda_2}$ is on extension of $h^\sigma_{\Lambda_1}+h^\sigma_{\Lambda_2}$ and we have

$$h^\sigma_{\Lambda_1\cup\Lambda_2} + \varrho_a(C+\sigma_m)\,(S(\Lambda_1)+S(\Lambda_2)) \geqq h^\sigma_{\Lambda_1} + h^\sigma_{\Lambda_2} \geqq \hat{h}^\sigma_{\Lambda_1} + \hat{h}^\sigma_{\Lambda_2}\,.$$

Clearly the operator associated with the last form is $H^\sigma_{\Lambda_1}\otimes 1 + 1\otimes H^\sigma_{\Lambda_2}$. The first statement of the theorem follows immediately from the definition of P_Λ by use of Proposition A3.

Whilst the above proof is a proof by extension the second inequality is proved by restriction. Firstly we use the condition on our interactions to deduce that

$$h_{\Lambda_1\cup\Lambda_2} \leqq h_{\Lambda'_1} + h_{\Lambda'_2} + h_{\Lambda_3} + 2\varrho_a C(S(\Lambda_1)+S(\Lambda_2))$$

where $\Lambda_3 = \Lambda_1\cup\Lambda_2\backslash\Lambda'_1\cup\Lambda'_2$ and the forms $h_{\Lambda'_1}$, $h_{\Lambda'_2}$ and h_{Λ_3} are understood to be forms on $D(h_{\Lambda_1\cup\Lambda_2})$ as above. Now $D(h_{\Lambda'_1})\otimes D(h_{\Lambda'_2})\subset D(h_{\Lambda_1\cup\Lambda_2})$ and consists of vectors Ψ with the property that $\Psi(X)=0$ if $X\not\subset\Lambda'_1\cup\Lambda'_2$. The restriction of h_{Λ_3} to this domain is zero whilst we denote the restrictions of $h_{\Lambda'_1}$ and $h_{\Lambda'_2}$ by $\hat{h}_{\Lambda'_1}$ and $\hat{h}_{\Lambda'_2}$. We have

$$h_{\Lambda_1\cup\Lambda_2} \leqq \hat{h}_{\Lambda'_1} + \hat{h}_2 + 2\varrho_a C(S(\Lambda_1)+S(\Lambda_2))\,.$$

But the operator associated with $\hat{h}_{\Lambda'_1}+\hat{h}_{\Lambda'_2}$ is clearly $H_{\Lambda'_1}\otimes 1 + 1\otimes H_{\Lambda'_2}$ acting on $D(H_{\Lambda'_1})\otimes D(H_{\Lambda'_2})$ and the second inequality follows, by application of the minimax theorem, in a similar manner to the first.

It should be noted that there is one significant difference in the information we have used to derive the inequalities of the above theorem.

The first inequality depends upon the interactions satisfying the condition of the form

$$U_{\Lambda_1 \cup \Lambda_2} - U_{\Lambda_1} - U_{\Lambda_2} \geqq -\varrho_a C(S(\Lambda_1) + S(\Lambda_2)) \tag{$*$}$$

whilst the second inequality is based upon the converse condition

$$U_{\Lambda_1 \cup \Lambda_2} - U_{\Lambda_1} - U_{\Lambda_2} \leqq \varrho_a C(S(\Lambda_1) + S(\Lambda_2)) . \tag{$**$}$$

Thus the first inequality can be derived for a large class of interactions. For example if U_Λ is given in the usual manner by a potential function then the first inequality immediately follows for positive potentials with no condition of decrease at infinity.

Theorem 3. *The following limit, over the net of increasing parallelepipeds, exists*

$$P(\beta, \mu) = \lim_{\Lambda \to \infty} P_\Lambda(\beta, \mu, \sigma) \qquad \beta > 0$$

and is independent of σ. P is a convex continuous function of β and μ. Secondly the limit

$$P_\infty(\beta, \mu) = \lim_{\Lambda \to \infty} P_\Lambda(\beta, \mu) = \lim_{\Lambda \to \infty} \lim_{\sigma \to \infty} P_\Lambda(\beta, \mu, \sigma)$$

exists and defines a convex continuous function of β and μ and in general

$$P_\infty(\beta, \mu) \leqq P(\beta, \mu)$$

P and P_∞ take values in the interval

$$\left[0, 2\sqrt{\left(\varrho_a + \frac{1}{2(4\pi\beta)^{\nu/2}}\right)^2 - \varrho_a^2 + (B + \mu_m)\,\beta\varrho_a}\,\right]$$

where $\mu_m = \max(0, \mu)$.

Proof. The proof of the existence of the limits is a standard argument based upon the sub-additivity and super-additivity properties of Theorem 2 combined with the boundedness properties of theorem 1a and the assumed invariance of the interactions. We will not repeat the details. The upper bound on P and P_∞ are given by minimizing the bound obtained in the proof of Lemma 2 with respect to the parameter z which occurs in this bound. All other properties are a direct consequence of Theorem 1.

5. Conclusion

There are two positive features and one negative feature of the foregoing results. Firstly we have established that the thermodynamic pressure exists for elastic boundary conditions by establishing a sub-additivity property for the local pressure. Secondly we have established that the thermodynamic pressure obtained in this manner is independent of the elasticity. Thirdly we have failed to establish that the thermodynamic pressure obtained in this manner is identical to the pressure obtained with infinitely repulsive walls. We would like to comment on these points in turn and mention obvious generalizations.

The proof of the first point, the existence of the thermodynamic pressure, can be straightforwardly extended to the case of point particles if $\sigma \leqq 0$ and the essential estimate depends only upon an inverse tempering condition of the form (*), a condition which does not necessarily entail any decrease at infinity of the interaction potentials. Thus we have a significant generalization of the known results which are based upon a tempering condition of the form (**). As it would be out of place to give the statements of the results for point particles in the present paper we merely emphasize that in operator language the important point is the inequality

$$T^{\sigma}_{\Lambda_1 \cup \Lambda_2} \geqq T^{\sigma}_{\Lambda_1} + T^{\sigma}_{\Lambda_2}, \qquad \sigma \leqq 0, \qquad \Lambda_1 \cap \Lambda_2 = \emptyset$$

for the kinetic energy operators. In the case of repulsive wall boundary conditions the kinetic energy operator satisfies the inverse inequality

$$T_{\Lambda_1 \cup \Lambda_2} \leqq T_{\Lambda_1} + T_{\Lambda_2}, \qquad \Lambda_1 \cap \Lambda_2 = \emptyset .$$

To establish the existence of the thermodynamic pressure for point particles with $\sigma > 0$ and to show that it is independent of σ is slightly more complicated. This relies upon an estimate of the form given by Lemma 1 which shows that the effect of changing the boundary conditions can be majorized in terms of the number of particles near the surface of the system. In the case of hard core particles this is of course proportional to the surface area but in the case of point particles is unbounded. Thus more precise estimates have to be made for the configurations of importance.

Finally we have defined two pressures. The first is given by increasing the linear dimension L of our system for fixed elasticity σ and is given in the double limit $\sigma, L \to \infty$ if $\sigma/L \to 0$. The second pressure is given by taking the limit $\sigma \to \infty$ and then $L \to \infty$. To prove that these two pressures are identical it is necessary to obtain some continuity of $P_\Lambda(\beta, \mu, \sigma)$ for large σ which is uniform in L. Note that as $P_\Lambda(\beta, \mu, \sigma)$ behaves quite differently at $\sigma = +\infty$ and $\sigma = -\infty$ it is natural to expect the appearance of a fractional power such as $\sigma^{-\frac{1}{2}}$ in the discussion of analyticity or continuity properties for large σ. We offer this as an interesting problem.

Appendix

Positive Forms and Operators

We briefly review the theory of positive, or more precisely non-negative, forms and their connection with positive self-adjoint operators; this review is extracted from the more general discussion given in [10], Chapter VI.

Let $\mathscr{H}$ be a complex Hilbert space. We consider forms $t(\varphi, \psi)$ defined for $\varphi, \psi \in D(t)$, a linear manifold of $\mathscr{H}$, such that $t(\varphi, \psi)$ is complex valued, linear in ψ, and anti-linear in φ. The manifold $D(t)$ is called the domain of t and t is said to be densely defined if $D(t)$ is dense in $\mathscr{H}$. The form $t(\psi) = t(\psi, \psi)$ is called the quadratic form associated with $t(\varphi, \psi)$; $t(\psi)$ determines $t(\varphi, \psi)$ uniquely by the polarization formula

$$t(\varphi, \psi) = \tfrac{1}{4}\left[t(\varphi + \psi) - t(\varphi - \psi) + it(\varphi + i\psi) - it(\varphi - i\psi)\right].$$

Two forms t_1 and t_2 are equal, $t_1 = t_2$, if and only if they have the same domain D and $t_1(\varphi, \psi) = t_2(\varphi, \psi)$ for all pairs $\varphi, \psi \in D$; t_1 is an extension of t_2, $t_1 \supset t_2$ or $t_2 \subset t_1$, if and only if $D(t_1) \supset D(t_2)$ and $t_1(\varphi, \psi) = t_2(\varphi, \psi)$ for all pairs $\varphi, \psi \in D(t_2)$. The sum $t = t_1 + t_2$ of the forms t_1 and t_2 is defined by

$$t(\varphi, \psi) = t_1(\varphi, \psi) + t_2(\varphi, \psi), \qquad D(t) = D(t_1) \cap D(t_2)$$

and the product αt of t by a scalar α is given by

$$(\alpha t)(\varphi, \psi) = \alpha t(\varphi, \psi), \qquad D(\alpha t) = D(t).$$

A form t is said to be symmetric if

$$t(\varphi, \psi) = \overline{t(\varphi, \psi)}, \qquad \varphi, \psi \in D(t)$$

and from the polarization formula we see that t is symmetric if and only if $t(\psi)$ is real valued.

A symmetric form t is said to be bounded from below if

$$t(\psi) \geqq \gamma \|\psi\|^2, \qquad \psi \in D(t)$$

where $\| \ \|$ denotes the norm on $\mathscr{H}$. The largest number γ with this property is called the lower bound of t and we write $t \geqq \gamma$. In particular if $t \geqq o$ then t is said to be positive (i.e. non-negative). More generally an order relation is introduced between symmetric forms by defining $t_1 \geqq t_2$ if $D(t_1) \subset D(t_2)$ and

$$t_1(\psi) \geqq t_2(\psi), \qquad \psi \in D(t_1).$$

Note that this definition is slightly odd insofar the larger form has the smaller domain thus for example if $t_2 \supset t_1$, then $t_1 \geqq t_2$.

Each positive symmetric form t satisfies the inequalities

$$|t(\varphi, \psi)| \leqq t(\varphi)^{\frac{1}{2}}\, t(\psi)^{\frac{1}{2}},$$
$$t(\varphi+\psi)^{\frac{1}{2}} \leqq t(\varphi)^{\frac{1}{2}} + t(\psi)^{\frac{1}{2}},$$
$$t(\varphi+\psi) \leqq 2t(\varphi) + 2t(\psi).$$

Let t be a positive symmetric form. A sequence (ψ_n) of vectors in $\mathscr{H}$ is said to be t-convergent to ψ in $\mathscr{H}$, in symbols $\psi_n \underset{t}{\to} \psi$ as $n\to\infty$, if $\psi_n \in D(t)$, $\psi_n \to \psi$ strongly, and $t(\psi_n - \psi_m) \to 0$ as $n, m\to\infty$. Note that ψ does not necessarily belong to $D(t)$. The form t is said to be closed if $\psi_n \underset{t}{\to} \psi$ implies that $\psi\in D(t)$ and $t(\psi_n-\psi)\to 0$. Further t is defined to be closable if it has a closed extension. In particular t is closable if and only if $\psi_n \underset{t}{\to} 0$ implies $t(\psi_n)\to 0$. If this latter condition is satisfied then the closure (smallest closed extension) $\tilde{t}$ of t can be defined as follows. The domain $D(\tilde{t})$ is the set of all $\psi\in\mathscr{H}$ such that there exists a sequence (ψ_n) with $\psi_n \underset{t}{\to} \psi$ and $\tilde{t}$ is given by

$$\tilde{t}(\varphi, \psi) = \lim t(\varphi_n, \psi_n)$$

for any $\psi_n \underset{t}{\to} \psi$, $\varphi_n \underset{t}{\to} \varphi$. If t is closed a linear submanifold D' of $D(t)$ is called a core of t if the restriction t' of t with domain D' has the closure t, i.e. if $\tilde{t}' = t$.

The study of positive forms is closely connected to the study of positive self-adjoint operators;

Proposition A 1. *Let t be a densely defined, closed, positive form on $\mathscr{H}$. There exists a positive self-adjoint operator T with domain $D(T)$ dense in $\mathscr{H}$ and such that*

1) $D(T)\subset D(t)$ and $t(\varphi,\psi) = (\varphi, T\psi)$

for every $\varphi\in D(t)$ and $\psi\in D(T)$. The operator T is uniquely determined by this condition.

2) *$D(T)$ is a core of t.*

3) *If $\psi\in D(t)$, $\chi\in\mathscr{H}$ and $t(\varphi,\psi) = (\varphi,\chi)$*

holds for every φ in a core of t then $\psi\in D(T)$ and

$$T\psi = \chi.$$

4) *$D(t) = D(T^{\frac{1}{2}})$ and*

$$t(\varphi,\psi) = (T^{\frac{1}{2}}\varphi, T^{\frac{1}{2}}\psi) \qquad \varphi,\psi\in D(t).$$

$D'\subset D(t)$ is a core of t if and only if it is a core of $T^{\frac{1}{2}}$.

These results show that the forms provide a convenient means for constructing positive self-adjoint operators. Typically one is often faced with the problem of constructing positive self-adjoint extensions of a given positive symmetric operator and it is often easy to use this operator to construct symmetric forms. If these forms are closable then they yield, by the above construction, the desired self-adjoint extensions. The only feature which is rather delicate is the closability; we next give three common criteria for this property.

I. Let S be a positive symmetric operator on $\mathscr{H}$ and define t by $D(t)=D(S)$ and

$$t(\varphi, \psi)=(\varphi, S\psi) \quad \varphi, \psi \in D(S)=D(t);$$

then t is positive, symmetric and closable. The self-adjoint operator associated with the closure $\tilde{t}$ of t is referred to as the Friedrichs extension of S.

II. Let S be an arbitrary operator on $\mathscr{H}$ and define t by $D(t)=D(S)$ and

$$t(\varphi, \psi)=(S\varphi, S\psi), \qquad \varphi, \psi \in D(S)=D(t);$$

then t is positive, symmetric, and t is closable if and only if S is closable. (t is closed if and only if S is closed.)

III. Let $(S_i)_{i\geqq 1}$ be a sequence of positive bounded operators on $\mathscr{H}$ and define t by

$$D(t)=\left\{\psi;\ \psi\in\mathscr{H},\ \sum_{i\geqq 1}(\psi, S_i\psi)<\infty\right\}$$

and

$$t(\psi)=\sum_{i\geqq 1}(\psi, S_i\psi), \qquad \psi\in D(t),$$

then t is positive, symmetric, and closed.

Hitherto we have principally discussed positive forms but results similar to the above are valid for forms bounded below. If $t\geqq\gamma$ then t' defined by

$$t'(\varphi, \psi)=t(\varphi, \psi)-\gamma(\varphi, \psi), \qquad D(t')=D(t)$$

is positive. If t is densely defined and closed the same is true of t' and we may then associate the operator T' to t and the operator $T=T'+\gamma 1$ (1 is the identity operator on $\mathscr{H}$) has as consequence the property

$$t(\varphi, \psi)=(\varphi, T\psi), \qquad \psi\in D(T')=D(T).$$

Let us consider the addition of forms in more detail. It is natural to ask what conditions two forms t_1 and t_2 must satisfy to ensure that the sum $t=t_1+t_2$ is bounded below. Clearly, this is the case if t_1 and t_2 are bounded below but this condition is not necessary. One weaker condition can be found by considering the concept of relative boundedness. Let t_1 be bounded from below then t_2 is said to be t_1-bounded from below with bound b if $D(t_2) \supset D(t_1)$ and

$$t_2(\psi) \geqq -a\|\psi\|^2 - b t_1(\psi), \qquad \psi \in D(t_1)$$

with $a, b \geqq 0$. If t_2 is t_1-bounded from below with bound $b \leqq 1$ then

$$(t_1 + t_2)(\psi) \geqq -a\|\psi\|^2 + (1-b)\, t_1(\psi), \qquad \psi \in D(t_1),$$

i.e. $t_1 + t_2$ is bounded from below. Further let t_1 be bounded from below then t_2 is said to be t_1-bounded with bound b if $D(t_2) \supset D(t_1)$ and

$$|t_2(\psi)| \leqq a\|\psi\|^2 + b t_1(\psi), \qquad \psi \in D(t_1)$$

with $a, b \geqq 0$. If t_2 is t_1-bounded with bound $b < 1$ then $t_1 + t_2$ is bounded from below and $t_1 + t_2$ is closable if and only if t_1 is closable in which case $D(\widetilde{t_1 + t_2}) = D(\tilde{t}_1)$.

If t_1 and t_2 are closed forms bounded from below the same is true of $t = t_1 + t_2$. If t is densely defined the associated self-adjoint operators T, T_1 and T_2 are defined and T may be regarded as the sum of T_1 and T_2 in a generalized sense which we write

$$T = T_1 \dot{+} T_2 .$$

Conversely if T_1 and T_2 are self-adjoint operators which are bounded below the associated forms exist and the generalized sum can be defined as the operator associated with $t = t_1 + t_2$ whenever this latter form is densely defined. The generalized sum is an extension of the ordinary sum and in general the two do not coincide.

The following form of the minimax theorem is often useful.

Proposition A 2. *Let t be a densely defined, closed, lower semi-bounded form and let T be the associated self-adjoint operator. Further let D be a core of t and for every finite dimensional subspace $M \subset D$ define*

$$\lambda(M) = \sup_{\psi \in M, \|\psi\| = 1} t(\psi)$$

and for every integer $m \geqq 1$ define

$$\lambda_m = \inf_{\dim M = m} \lambda(M).$$

It follows that $\lambda_m \to \infty$ as $m \to \infty$ if and only if the spectrum of T consists of discrete eigenvalues of finite multiplicity and in this case the eigenvalues are given in increasing order, repeated according to multiplicity by the λ_m.

Let t_1 and t_2 be two forms of the kind considered in the proposition and λ_m^1, λ_m^2, the corresponding numbers defined by the minimax process. If $t_1 \geqq t_2$ in the sense of the order relation introduced earlier we have $\lambda_m^1 \geqq \lambda_m^2$ and in particular if $\lambda_m^2 \to \infty$ as $m \to \infty$ then $\lambda_m^1 \to \infty$.

A large number of existence theorems in statistical mechanics are based on the use of inequalities derived from convexity arguments. We reproduce a standard proposition of this nature phrased in the language of forms

Proposition A 3. *Let t and t' be densely defined, closed, lower semi-bounded forms on $\mathscr{H}$ and let T and T' be the associated self-adjoint operators.*

1) *Let D be a core of t and $\mathscr{F}$ a finite family of orthonormal vectors $\varphi \in D$. The following conditions are equivalent*

a) $$\sup_{\mathscr{F}} \sum_{\varphi \in \mathscr{F}} \exp\{-t(\varphi)\} < +\infty$$

b) $$Tr_{\mathscr{H}}(e^{-T}) < +\infty$$

and if they are satisfied then

$$\sup_{\mathscr{F}} \sum_{\varphi \in \mathscr{F}} \exp\{-t(\varphi)\} = Tr_{\mathscr{H}}(e^{-T}).$$

2) *Consequently if $D(t') \subset D(t)$, $t' \geqq t$, and e^{-T} is of trace class then*

$$Tr_{\mathscr{H}}(e^{-T'}) \leqq Tr_{\mathscr{H}}(e^{-T}).$$

3) *Take $0 < \alpha < 1$ and assume $\alpha t + (1-\alpha) t'$ is densely defined. Let $\alpha T \dot{+} (1-\alpha) T'$ denote the operator associated with the closure of this latter form and assume e^{-T} and $e^{-T'}$ are of trace class. It follows that*

$$Tr_{\mathscr{H}}(e^{-(\alpha T \dot{+} (1-\alpha) T')}) \leqq Tr_{\mathscr{H}}(e^{-T})^{\alpha}\, Tr_{\mathscr{H}}(e^{-T'})^{1-\alpha}.$$

This proposition is extracted from similar statements given in [8]; using the foregoing material the proofs of [8] can be straight-forwardly adapted. Similar statements can of course be made for more general convex functions than the function $x \to e^{-x}$.

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