On the Relation Between Classical and Quantum Statistical Mechanics

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Abstract. Classical and quantum statistical mechanics are compared in the high temperature limit $\beta = 1/kT \to 0$. While this limit is rather trivial for spin systems, we obtain some rigorous results which suggest (and sometimes prove) different asymptotics for continuous systems, depending on the behaviour of the two-body potential for small distances: the difference between suitable classical and quantum variables vanishes as β^2 for smooth potentials and as $\sqrt{\beta}$ for potentials with hard cores.

I. Introduction

Although nature is governed by quantum mechanics, there is still much interest in classical statistical mechanics. This comes from the belief that for not too low temperatures the structural differences between the two are small. In fact, several deep similarities between classical and quantum *lattice* systems with regard to phase transitions are apparent [1]. Rigorous results on the low temperature behaviour of even the simplest quantum lattice systems from the point of view of ground state properties, namely, ferromagnetic quantum spin systems, are as yet incomplete [2]. For quantum continuous systems the situation is much worse, at least concerning rigorous results: very little is known on phase transitions for interacting systems, and low temperature properties are studied for just a few one-dimensional models.

Another reason for interest in classical statistics is the fact that it is an approximation to quantum statistics in a precise sense. There is an extensive literature on the classical $\hbar \to 0$ limit of quantum statistics (see [3–5] and references given there). It is a weakness of these studies that no correction terms are provided. Then the limit $\hbar \to 0$ remains mathematical, because physically $\hbar$ cannot be varied. A reasonable statement for continuous systems would be: the difference between

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quantum and classical quantities is small if the thermal wavelength $\lambda = \left(2\pi\hbar^2 \frac{\beta}{m}\right)^{1/2}$ is small with respect to a characteristic length of the potential. The physical parameter which is then actually varied is the (inverse) temperature $\beta \to 0$. For this interpretation of the $\hbar \to 0$ limit it is, of course, essential that it commutes with the thermodynamic limit. This causes difficulties, for example: the upper bound for the difference of the quantum $f^Q(v, \beta)$ and classical $f^{Cl}(v, \beta)$ canonical free energies (which we multiply by β for reasons explained shortly),

$$\Delta f(v, \beta) = \beta[f^Q(v, \beta) - f^{Cl}(v, \beta)], \tag{I.1a}$$

in [5] involves an attractive (temperature dependent) potential in the Bose case, which simulates the statistical exchange attraction, and taking the thermodynamic limit *first* requires, for reasons of stability, a singular repulsive (e.g. hard-core) potential. For such potentials, however, the lower bound of [4, 5] is not applicable, because it employs (plane-wave) eigenfunctions of the free Hamiltonian, which are not in the domain of the full Hamiltonian. Hence, at least with present methods, there is an essential gap in the classical $\hbar \to 0$ limit for bosons. For a class of bounded (and therefore, by stability, necessarily positive) potentials, the problem is solved by Simon's microstability condition [4].

In this paper we are primarily concerned with the physical form of the classical limit: $\beta \to 0$, keeping $\hbar$ fixed. For lattice systems, the high-temperature behaviour of Δf, defined by (I.1a), follows trivially from Lieb's paper [3] on the classical limit of quantum spin systems (Appendix B). The corresponding result for continuous systems has been obtained only on a heuristic level using the Zassenhaus formula [14, Chap. 10.2]. A rigorous analysis shows that there is a marked difference in the high temperature asymptotics between bounded positive and hard core potentials. This can already be seen in the low-density region where the virial expansion is applicable. In Sect. 1 we present some estimates on the difference,

$$\Delta b_2(\beta) = b_2^Q(\beta) - b_2^{Cl}(\beta), \tag{I.1b}$$

between the quantum and classical (direct) second-order virial coefficients [14], both for bounded positive and pure hard-core potentials. In the former case we show that

$$\left| -\frac{\Delta b_2(\beta)}{b_2^{Cl}(\beta)} \right|_{\beta \downarrow 0} \leqq c\beta. \tag{I.2}$$

Throughout the paper, c denotes a strictly positive constant, which may vary from inequality to inequality. The reason for considering $-\Delta b_2$, rather than Δb_2, in the estimates above and below, will be explained shortly. The exchange part of Δb_2 is known to decay exponentially as $\beta \downarrow 0$ [16, 17], and does not, therefore, affect the leading behaviour above. For a pure hard-core potential we find (for β sufficiently small),

$$-c\sqrt{\beta} \leqq -\Delta b_2(\beta) \leqq 0 \tag{I.3}$$

with

$$-\Delta b_2(\beta) \underset{\beta \downarrow 0}{\sim} -c\sqrt{\beta}, \quad v = 1 \tag{I.4}$$

in dimension $v = 1$. Indeed, on the basis of [12, 13], we expect

$$- \Delta b_2(\beta) \underset{\beta \downarrow 0}{\sim} - c \sqrt{\beta} \quad \text{(all } v) \tag{I.5}$$

in any dimension v, but the computations found in the literature (see, especially, [13]) rely on summation of various series involving phase-shifts $\delta_\ell(k)$ over all angular momenta (see also [14]). Indeed, for potentials with singularity of type $r^{-m}, m > 2$ as $r \to 0$ (r denoting the radial distance from the origin), it is found that [15]

$$\delta_\ell(k) \to A k^{1 - 2/m}, \, k \to \infty, \, \ell \text{ fixed}.$$

As emphasized in [15], this conclusion leaves open the asymptotic behaviour of $\delta_\ell(k)$ as both ℓ and k diverge. This is the main difficulty in obtaining rigorous estimates for $\Delta b_2(\beta)$ as $\beta \downarrow 0$ [which depend on the behaviour of all $\delta_\ell(k)$ for $k \to \infty$] by the phase-shift method. Nevertheless, the results of [12, 13] are believed to be exact. As a matter of fact, the dimensionality should not play a significant role as $\beta \downarrow 0$, affecting only the value of c in (I.5). Therefore, we have not studied the problem for $v > 1$. Indeed, the computed value of c in (I.4) (Sect. II) is just one third of the coefficient in [13] for $v = 3$.

The above results are consistent with the following asymptotic behaviour of $\Delta f(v, \beta)$ defined by (I.1 a),

$$\left| \frac{\Delta f(v, \beta)}{f^{Cl}(v, \beta)} \right|_{\beta \downarrow 0} \leqq c\beta \quad \text{(positive bounded potential)}, \tag{I.6a}$$

$$\frac{\Delta f(v, \beta)}{f^{Cl}(v, \beta)} \underset{(\beta \downarrow 0)}{\cong} - c\sqrt{\beta} \quad \text{(hard-core system)}. \tag{I.6b}$$

A nonrigorous, but probably asymptotically correct estimate suggests

$$\frac{\Delta f(v, \beta)}{f^{Cl}(v, \beta)} = + c\beta^3$$

in (I.6a), see Sect. II. We first explain the correspondence between (I.2) and (I.6a), as well as (I.3) and (I.6b).

Denoting by $p^Q(v, \beta)$ [respectively $p^{Cl}(v, \beta)$] the canonical pressure, we have

$$\beta(p^Q(v, \beta) - p^{Cl}(v, \beta)) = \left(\frac{\partial \Delta f(v, \beta)}{\partial v} \right)_\beta \tag{I.7a}$$

(as is well known [19, 21], this formula holds for almost all $v > v_c$, where v_c is the close-packing specific volume). The virial expansion of the right-hand side of (I.7) is [14, 19]

$$\beta(p^Q(v, \beta) - p^{Cl}(v, \beta)) = \sum_{i \geqq 2} \frac{\Delta b_i(\beta)}{v^i}, \tag{I.7b}$$

where $\Delta b_i(\beta)$ are differences between i^{th} order quantum and classical virial coefficients, defined as in (I.1 b). By (I.7b) we find

$$\Delta f(v, \beta) = \sum_{i \geqq 2} \frac{\Delta \tilde{b}_i(\beta)}{v^{i-1}},$$

with

$$\Delta \tilde{b}_i(\beta) = -i \Delta b_i(\beta),$$

and hence

$$\Delta \tilde{b}_2(\beta) = -2 \Delta b_2(\beta).$$

This explains the change of sign in the estimates (I.2), (I.3), and (I.4), to keep the correspondence with (I.6), as well as multiplication by β in (I.1 a).

A formal calculation using the Zassenhaus formula [14, Chap. 10.2] suggests that

$$|\Delta f(v, \beta)/f^{\mathrm{Cl}}(v, \beta)| \underset{\beta \downarrow 0}{\sim} c\beta. \tag{I.7c}$$

This behaviour agrees with (I.6a) but not (I.6b). If the nonrigorous asymptotic estimate of Sect. II, Remark II.1, is true, the (I.7c) disagrees with the expected behaviour of both types of potential.

One might expect more than (I.6), for instance an asymptotic series in powers of $\sqrt{\beta}$ for hard core systems (in which case f^{Cl} is analytic in β in a neighbourhood of $\beta = 0$ [18]), eventually Borel-summable. This does not follow from the estimates in Ginibre's classic work (see [16] and references given there) and remains as the most interesting, but probably hardest, open question.

In Sect. III we derive some estimates for $\Delta f(v, \beta)$ for fixed finite, but arbitrary, density (smaller than close-packing). In (III.1) the upper bound of [5] is generalized to cover hard-core potentials, yielding the result that

$$\Delta f(v, \beta) \leqq c \exp(-\alpha/\beta), c \geqq 0, \alpha > 0. \tag{I.8}$$

For positive bounded pair potentials, it is easy to show by the methods of [5], that

$$\lim_{\beta \downarrow 0} \Delta f(v, \beta) = 0 \quad \text{(bounded positive potentials)} \tag{I.9}$$

in two cases (Fermi-Dirac and Maxwell-Boltzmann statistics). No correction term was obtained, so that (I.2) remains as the only precise indication of the validity of (I.6a). In III.2 we derive a lower bound for $\Delta f(v, \beta)$ holding for a class of hard-core potentials. For a complete proof of (I.9) and correction terms, we need some information on the classical pure hard-core free energy $f_{\mathrm{Cl}}^{\mathrm{h.c.}}(v)$, which is only available for $v = 1$ and, in order not to clutter the argument with additional assumptions, we restrict ourselves to this case. It should be emphasized, however, that very similar, if not identical, arguments are expected to hold in higher dimensions. Indeed, in Sect. III.2.1 we provide, using methods of functional integration [11], a lower bound on the partition function for a class of hard-core systems which is useful in the thermodynamic limit and valid for all dimensions. As a corollary, we prove in Sect. III.2.2 that, if $v = 1$,

$$\Delta f(v, \beta) \geqq -c\beta^{\frac{1}{2} - \varepsilon} \tag{I.10}$$

for sufficiently small β, and any $\varepsilon > 0$. The reader will easily recognize what general properties of $f_{\mathrm{Cl}}^{\mathrm{h.c.}}(v)$ are necessary for the validity of the proof of (III.2.2). Finally, we remark that even for pure hard cores and $v = 1$ our result is nontrivial, because the one-dimensional quantum mechanical hard core problem is *not* solvable (for

$a \neq 0$). In Sect. III.2.3 we show that Baumgartner's method [5] using the Thirring coherent states yield the weaker bound

$$\Delta f(v, \beta) \geq -c\beta^{1/3}. \tag{I.11}$$

The above holds, however, for a class of interactions larger than the one we treat in (III.2.1).

Finally, in Appendix C we study the (equivalent) highenergy limit of the entropy, using the well-known method of Dirichlet-Neumann bracketing [10, Chap. XIII-15]. Although only bounded *external* fields are analysed there, the method is instructive, because, taking the thermodynamic limit *first* involves estimates of a completely different nature than those of [10, Chap. XIII, 15] for finite systems. It also yields correction terms of the expected type.

In Appendix A we collect some technical results used in the main text.

II. High Temperature Behaviour of the Second Virial Coefficient

In this section, we study the direct second order virial coefficient in two cases:

(A) for a positive infinitely differentiable potential of compact support $V \in C_0^\infty(\mathbb{R}^3)$;

(B) for a pure hard-core potential

$$V(x) = \begin{cases} \infty & \text{if } |x| \leq a \\ 0 & \text{otherwise}. \end{cases}$$

Since our aim is to obtain qualitative results, we did not try to determine the largest class of potentials for which the results of this section are expected to hold. For brevity, we refer to potentials of the above types as of class A and B, respectively.

Case (A). The classical second order virial coefficient $b_2^{Cl}(\beta)$ is analytic in β and

$$b_2^{Cl}(\beta) = \tfrac{1}{2} \int d^3x [1 - e^{-\beta V(x)}]. \tag{II.1}$$

The two-body quantum Hamiltonian is given on $L^2(\mathbb{R}^3)$ by

$$H = H_0 + V, \tag{II.2a}$$

$$H_0 = -\tfrac{1}{2}\Delta \tag{II.2b}$$

($h = m^* = 1$, where $m^* = m/2$ is the "reduced mass"). Let

$$A(\beta) \equiv e^{-\beta H} - e^{-\beta H_0}. \tag{II.3}$$

When $A(\beta)$ is trace-class, we shall assume that the thermodynamic limit of the direct quantum second-order virial coefficient per particle (see, e.g., [14] for the definitions in finite volume) exists independently of the boundary conditions and equals

$$b_2^Q(\beta) = -\tfrac{1}{2}\lambda^3 \operatorname{tr} A(\beta), \tag{II.4}$$

where

$$\lambda = (2\pi\beta)^{1/2} \tag{II.5}$$

is the thermal wave-length. In case (A), $A(\beta)$ is trace-class by [11, Theorem 21.4, p. 228], and for case (B) we shall comment later in the section. Let $dv_{a,c;t}$ denote the *probability* measure formally associated to Wiener measure $d\mu_0$ by

$$P_t(a,c)^{-1} \, \delta(\omega(0)-a) \, \delta(\omega(t)-c) \, d\mu_0 \qquad \text{(II.6)}$$

(see definition, p. 39 of [11]), where $P_t(a,c)$ is defined below in (II.11); it corresponds to restriction to brownian paths $b(\cdot)$ [with $\omega(\cdot)=x+b(\cdot)$], with preassigned positions at time zero and time t. Let $E_{0,a;t,c}$ denote expectation with respect to dv and $P_{0,a;t,c}(A) \equiv E_{0,a;t,c}\{\chi(A)\}$, where $\chi(A)$ denotes the characteristic function of the event A.

Proposition II.1. *Let V belong to class* (A). *Then*

$$\Delta b_2(\beta) = b_2^Q(\beta) - b_2^{Cl}(\beta)$$

$$= \tfrac{1}{2} \int d^3x \, E_{0,x;\beta,x} \left\{ \exp[-\beta V(x)] - \exp\left[-\int_0^\beta ds \, V(\omega(s)) \right] \right\}. \qquad \text{(II.7)}$$

Proof. Let

$$f(x,\beta) \equiv E_{0,x;\beta,x} \left\{ \exp[-\beta V(x) - \exp\left[-\int_0^\beta ds \, V(\omega(s)) \right] \right\}. \qquad \text{(II.8)}$$

Suppose $x \notin \operatorname{supp} V$. Then, the only Brownian paths $b(\cdot)$ which contribute in the above expectation are those which start at x and intersect $\operatorname{supp} V$ at least once before returning to x. As in [16], let

$$F'(\beta,\varepsilon,\delta) = \{b \,|\, \exists t \text{ and } t' \text{ in } [0,\beta] \text{ such that } |t-t'| \leq \delta,$$
$$\text{and } |b(t)-b(t')| > 4\varepsilon\} \,.$$

Clearly

$$F'(\beta,\varepsilon,\beta) \supseteq F''(\beta,\varepsilon) \equiv \{b \,|\, \exists t \in [0,\beta] \text{ such that}$$
$$|b(t)-x| > 4\varepsilon\} \,. \qquad \text{(II.9a)}$$

Setting $x = y$ in ((1.31) of [16, p. 343]), and taking into account the normalization in (II.6), we obtain

$$P_{0,x;\beta,x}(F'(\beta,\varepsilon,\beta)) \leq 16\sqrt{2} \, \chi\left(\frac{\varepsilon}{2},\beta\right), \qquad \text{(II.9b)}$$

where

$$\chi(\varepsilon,\delta) \equiv \int_{|x|>\varepsilon} P_\delta(x,0) \, d^3x \,, \qquad \text{(II.10)}$$

$$P_\delta(x,y) = (2\pi\delta)^{-3/2} \exp(-|x-y|^2/2\delta) \,. \qquad \text{(II.11)}$$

Hence, by (II.8), (II.9), (II.10) and the boundedness of V, there exist positive constants c, d, and M such that

$$|f(x,\beta)| \leq c \exp(\beta M) \, P_{0,x;\beta,x}(F''(\beta,d|x|))$$

$$\leq 4c \exp(\beta M) \, \chi\left(\frac{d|x|}{2},\beta\right), \qquad \text{(II.12)}$$

which is exponentially decreasing in $|x|$ in view of (II.10). Hence, f is integrable in x for each β. Let $\{f_n\}_{n\in\mathbb{Z}_+}$ be a sequence of functions in $C_0^\infty(\mathbb{R}^3)$ increasing monotonically to 1. Then

$$\tfrac{1}{2}\lambda^3\,\mathrm{tr}(f_n e^{-\beta H}f_n)=\tfrac{1}{2}\int d^3x\,f_n^2(x)E_{0,x;\beta,x}\left\{\exp\left[-\int_0^\beta V(\omega(s))\,ds\right]\right\} \qquad \text{(II.13)}$$

[11, Theorem 6.6], and similarly

$$\tfrac{1}{2}\lambda^3\,\mathrm{tr}(f_n e^{-\beta H_0}f_n)=\tfrac{1}{2}\int d^3x\,f_n^2(x). \qquad \text{(II.14)}$$

Let

$$b_2^{Cl}(\beta,f_n)\equiv\tfrac{1}{2}\int d^3x\,f_n(x)\,(1-e^{-\beta V(x)})\,f_n(x). \qquad \text{(II.15)}$$

Clearly,

$$b_2^{Cl}(\beta,f_n)\xrightarrow[n\to\infty]{} b_2^{Cl}(\beta). \qquad \text{(II.16)}$$

Since $V\geqq 0$, [11, Theorem 21.4, p. 228] implies that $\mathrm{tr}(e^{-\beta H}-e^{-\beta H_0})<\infty$. Hence, by Lemma A.1 of Appendix A,

$$\mathrm{tr}(f_n(e^{-\beta H}-e^{-\beta H_0})f_n)\xrightarrow[n\to\infty]{}\mathrm{tr}(e^{-\beta H}-e^{-\beta H_0}),$$

and therefore, by (II.4), (II.13), and (II.14),

$$b_2^Q(\beta)=\lim_{n\to\infty}\tfrac{1}{2}\int d^3x\,f_n^2(x)\,E_{0,x;\beta,x}\Big\{1-e^{-\int_0^\beta V(\omega(s))ds}\Big\}. \qquad \text{(II.17)}$$

By (II.15) and (II.16),

$$\Delta b_2(\beta)=\tfrac{1}{2}\lim_{n\to\infty}\int d^3x\,f_n^2(x)\,E_{0,x;\beta,x}\Big\{e^{-\beta V(x)}-e^{-\int_0^\beta V(\omega(s))}\Big\}ds. \qquad \text{(II.18)}$$

By (II.12) the expectation occurring in (II.18) is uniformly bounded (in x) by an integrable function. Hence, (II.18) and the Lebesgue dominated convergence theorem yield (II.7). $\square$

Proposition II.2. *Let V belong to class (A). Then (I.2) holds.*

Proof. The boundedness of V and (II.7) allow us to write

$$\Delta b_2(\beta)=\tfrac{1}{2}\int d^3x\,e^{-\beta V(x)}\,E_{0,x;\beta,x}\left\{1-\exp\left[-\int_0^\beta ds(V(\omega(s))-V(x))\right]\right\}$$

$$=-\tfrac{1}{2}\int d^3x\,e^{-\beta V(x)}\,E_{0,x;\beta,x}\left\{\frac{\displaystyle\sum_{n=1}^\infty\left(-\int_0^\beta ds(V(\omega(s))-V(x))\right)^n}{n!}\right\}. \qquad \text{(II.19)}$$

Equation (II.19) may be justified in the same way as the steps leading to (II.18):

$$\left|E_{0,x;\beta,x}\left\{\frac{\displaystyle\sum_{n=1}^\infty\left(-\int_0^\beta ds\,V(\omega(s))-V(x)\right)^n}{n!}\right\}\right|\leqq c_1\chi\left(\frac{d_1|x|}{2},\beta\right)e^{\beta M_1}$$

for some positive constants c_1, d_1, M_1. Let, now, $\mathrm{supp}\, V \subseteq \{|x| \le a\}$. By (II.19)

$$\Delta b_2(\beta) = I_1 + I_2, \tag{II.20}$$

where

$$I_1 \equiv \tfrac{1}{2} \int\limits_{|x| \le 2a} d^3 x\, e^{-\beta V(x)}\, E_{0,x;\beta,x} \left\{ \frac{\sum\limits_{n=1}^{\infty} \left(-\int\limits_0^{\beta} ds(V(\omega(s)) - V(x)) \right)^n}{n!} \right\}, \tag{II.21a}$$

and

$$I_2 \equiv \tfrac{1}{2} \int\limits_{|x| > 2a} d^3 x\, E_{0,x;\beta,x} \left\{ 1 - \exp\left[-\int\limits_0^{\beta} ds\, V(\omega(s)) \right] \right\}. \tag{II.21b}$$

By the argument of Proposition II.1,

$$|I_2| \le c \int\limits_{|x| > 2a} d^3 x\, \chi\left(d\left(\frac{|x| - a}{2} \right), \beta \right), \tag{II.22}$$

where χ is defined by (II.10). For β sufficiently small,

$$\chi\left(\frac{d(|x| - a)}{2}, \beta \right) \le c\beta^{-1} \exp[-d^2(|x| - a)^2/4\beta]. \tag{II.23}$$

The estimate above is not optimal but suffices for our purposes. Inserting (II.23) into (II.22) we see that

$$|I_2| \le c\beta^{-1} \int\limits_{r > 2a} dr\, r^2\, e^{-d^2(r-a)^2/4\beta}, \tag{II.24}$$

and therefore I_2 is exponentially small in β^{-1}, for β sufficiently small. Hence, by (II.20), in order to establish (I.2), it suffices to prove that

$$|I_1| \le c\beta^2. \tag{II.25}$$

Let

$$I_1' \equiv \tfrac{1}{2} \int\limits_{|x| \le 2a} d^3 x \exp[-\beta V(x)]\, E_{0,x;\beta,x} \left\{ \sum_{n=2}^{\infty} \left(-\int\limits_0^{\beta} ds(V(\omega(s)) - V(x)) \right)^n \Big/ n! \right\}.$$

By the boundedness of V,

$$|I_1'| \le c\beta^2. \tag{II.26}$$

Now,

$$I_1 = I_1' + I_2', \tag{II.27a}$$

where

$$I_2' = -\tfrac{1}{2} \int\limits_{|x| \le 2a} d^3 x\, e^{-\beta V(x)} E_{0,x;\beta,x} \left\{ \int\limits_0^{\beta} ds(V(\omega(s)) - V(x)) \right\}. \tag{II.27b}$$

We now use the explicit covariance formulae (see, e.g., [11, pp. 40, 41])

$$E_{0,x;\beta,x}\{b_i(s)\} = 0, \qquad 0 \le s \le \beta, \tag{II.28a}$$

$$E_{0,x;\beta,x}\{b_i(s)\, b_j(t)\} = \delta_{ij}[s(\beta - t)], \qquad 0 \le s \le t \le \beta, \tag{II.28b}$$

where $i, j = 1, 2, 3$. In order to see the argument more clearly, consider the case $v = 1$. Then

$$V(x + b(s)) - V(x) = \sum_{n=1}^{2N-1} \frac{V^{(n)}(x)}{n!} b(s)^n + \frac{V^{(2N)}(x + \theta b(s))}{(2N)!} b(s)^{2N}, \quad \text{(II.28 c)}$$

where $\theta \in [0, 1]$ depends on N and $b(s)$ and $V^{(n)}(x) \equiv \dfrac{d^n V(x)}{dx^n}$. In correspondence to (II.28 c), let

$$I_2' = -\frac{1}{2} \int_{|x| \leq 2a} d^3x \, e^{-\beta V(x)} (\alpha_1(x) + \alpha_2(x)), \quad \text{(II.28 d)}$$

where

$$\alpha_1(x) = \sum_{n=1}^{2N-1} \frac{V^{(n)}(x)}{n!} E_{0, x; \beta, x} \left\{ \int_0^\beta ds \, b(s)^n \right\}, \quad \text{(II.28 e)}$$

and

$$|\alpha_2(x)| \leq \frac{V^{(2N)}(x + \theta b(s))}{(2N)!} b(s)^{2N}. \quad \text{(II.28 f)}$$

By (II.28 a, b), the Gaussian nature of the process and Wick's theorem (see, e.g., [11, Lemma 20.4, p. 217]),

$$E_{0, x; \beta, x}\{b(s)^n\} = \begin{cases} \dfrac{(2m)!}{m! \, 2^m} s^m (\beta - s)^m & \text{if} \quad n = 2m \\ 0 & \text{otherwise}. \end{cases} \quad \text{(II.29 a)}$$

We have

$$\int_0^\beta ds \, s^m (\beta - s)^m = \beta^{2m+1} B(m+1, m+1) = \frac{\beta^{2m+1} m!^2}{(2m+1)!}. \quad \text{(II.29 b)}$$

Let

$$G_n \equiv \sup_{x \in \mathbb{R}} |V^{(n)}(x)|. \quad \text{(II.29 c)}$$

Then, by (II.28 e) and (II.29)

$$|\alpha_1(x)| \leq \sum_{m=1}^{N-1} \frac{G_{2m} m!}{(2m+1)! \, 2^m} \beta^{2m+1} \leq c\beta^3 \quad \text{(II.30 a)}$$

for β sufficiently small. By the same procedure applied to (II.28 f),

$$|\alpha_2(x)| \leq \frac{\beta^{2N+1} G_{2N} N!}{(2N+1)! \, 2^N}. \quad \text{(II.30 b)}$$

By (II.26), (II.27), (II.28 d–f), (II.30 a), and (II.30 b), we obtain (II.25). $\quad \square$

Remark II.1. Unfortunately, expansion of $V(x + b(s)) - V(x)$ in each term of the series in (II.19) leads to a divergent, possibly asymptotic, series. Since (I.2) and (I.4) suffice to display the qualitative difference between potentials of classes (A) and (B), we do not pursue this question further here, but remark that (II.19) yields the

following *formal* result. The leading contribution to (II.19) stems from

$$\Delta b_2(\beta) = -\frac{1}{2}\int d^3x\, e^{-\beta V(x)}\frac{1}{2}\sum_{i=1}^{3}\left(\frac{\partial^2 V}{\partial x_i^2}\right)\int_0^\beta ds\, E(b_i(s)^2)$$

$$+\frac{1}{2}\int d^3x\, E_{0,x;\beta,x}\left\{\frac{\left(\left(\int_0^\beta ds\left(\sum_{i=1}^{3}\frac{\partial V}{\partial x_i}\right)b_i(s)\right)^2\right]}{2}\right\}$$

$$\cong -\frac{\beta^3}{24}\sum_{i=1}^{3}\int d^3x(1-\beta V(x))\sum_{i=1}^{3}\left(\frac{\partial^2 V}{\partial x_i^2}\right)$$

$$+\frac{\beta^4}{24}\cdot\frac{1}{2}\int d^3x\sum_{i=1}^{3}\left(\frac{\partial V}{\partial x_i}\right)^2 = -\frac{\beta^4}{48}\int d^3x\sum_{i=1}^{3}\left(\frac{\partial V}{\partial x_i}\right)^2.$$

Notice that this term is strictly negative, in contrast with the sign in case (B), see below. If this result is asymptotically correct, and reflects the behaviour of $\Delta f(v,\beta)$, then, according to (I.6b), neither potentials of class (A) nor of class (B) agree with (I.7c).

Case (B). In this case (II.7) yields

$$\Delta b_2(\beta) = \tfrac{1}{2}\int d^3x\, E_{0,x;\beta,x}\{\chi(|x|>a) - \chi(|x+b(s)|>a; 0\le s\le \beta)\}$$

(where χ is the characteristic function). The integrand above expresses the probability that the brownian motion during time $0\le s\le\beta$ starting at x (with $|x|>a$) get into the ball of radius a. In the following, we present some results pertaining to $\Delta b_2(\beta)$.

Proposition II.3. *Let $v=1$. Then*

$$-\Delta b_2(\beta) \underset{\beta\downarrow 0}{\sim} -c\sqrt{\beta}, \tag{II.31}$$

with $c=\dfrac{\sqrt{\pi}}{2\sqrt{2}}$.

Proof. In case (B),

$$b_2^{Cl}(\beta) = a \tag{II.32}$$

by (II.1) (if $v=1$). Quantum-mechanically, the corresponding Poisson kernel may be written down by the method of images

$$P_\beta(x,y) = \frac{1}{\sqrt{2\pi\beta}}\begin{cases} e^{-\frac{1}{2\beta}(x-y)^2} - e^{-\frac{1}{2\beta}(x+y-2a)^2} & \text{for} \quad x,y>a, \\ e^{-\frac{1}{2\beta}(x-y)^2} - e^{-\frac{1}{2\beta}(x+y+2a)^2} & \text{for} \quad x,y<-a, \\ 0 & \text{otherwise}. \end{cases}$$

This yields

$$\lambda\,\mathrm{tr}(e^{-\beta H} - e^{-\beta H_0}) = \left\{-\int_{-a}^{a}dx - \int_{a}^{\infty}e^{-\frac{1}{2\beta}(2x-2a)^2}dx\right.$$

$$\left. -\int_{-\infty}^{-a}e^{-\frac{1}{2\beta}(2x+2a)^2}dx\right\} = -\left(2a+\sqrt{\frac{\pi\beta}{2}}\right),$$

and hence by (II.32), we obtain (II.31). $\square$

The three-dimensional result, believed to be exact, is [13]

$$b_2^Q(\beta) = b_2^{Cl}(\beta)\left(1 + \frac{\lambda}{a}\frac{3}{4} + \dots\right).$$

Comparing with (II.31) and (II.32), we see that the correction to the classical result is expected to be proportional to $\sqrt{\beta}$, with a factor three times larger as the corresponding one in one dimension. In three-dimensions, a rigorous lower bound of the above form may be derived as follows. Let $H = H_0^D = -\frac{1}{2}\Delta^D$, with $(-\Delta^D)$ the Dirichlet Laplacian for the region $\mathbb{R}^3\backslash S$, where $S \equiv \{x \in \mathbb{R}^3 : |x| \leq a\}$, that is, the operator on $L^2(\mathbb{R}^3\backslash S)$ which is the Friedrichs extension of $(-\Delta)$ on $C_0^\infty(\mathbb{R}^3\backslash S)$. Let $(e^{-\beta H_0} - e^{-\beta H_0^D})(x, y)$ denote the kernel of the operator $(e^{-\beta H_0} - e^{-\beta H_0^D})$.

Proposition II.4.

$$-c\sqrt{\beta} \leqq -\Delta b_2(\beta) \leqq 0 \tag{II.33}$$

for β sufficiently small and $c > 0$.

Proof. A nice and simple application of the functional method [11, Lemma 21.3, p. 227] yields

$$0 \leqq (e^{-\beta H_0} - e^{-\beta H_0^D})(x, y) \leqq (2\pi\beta)^{-3/2}\exp\left\{-\frac{[\text{dist}(x, S)^2 + \text{dist}(y, S)^2]}{4\beta}\right\} \tag{II.34}$$

if $x, y \in \Omega$, the unbounded component of $\mathbb{R}^3\backslash S$. It is proved (although not formally stated there) in Theorem 21.4, p. 228, of [11] that $(e^{-\beta H_0} - e^{-\beta H_0^D})$ is trace class. We have then

$$b_2^Q(\beta) = -\frac{1}{2}\lambda^3\,\text{tr}(e^{-\beta H_0^D} - e^{-\beta H_0})$$
$$= \frac{1}{2}(2\pi\beta)^{3/2}\,\text{tr}(e^{-\beta H_0} - e^{-\beta H_0^D}). \tag{II.35}$$

From (II.1),

$$b_2^{Cl}(\beta) = \frac{2}{3}\pi a^3. \tag{II.36}$$

By (II.34), (II.35), and (II.36):

$$b_2^Q(\beta) = \frac{1}{2}(2\pi\beta)^{3/2}\left\{\int\limits_{|x|\leqq a} d^3x(e^{-\beta H_0})(x, x)\right.$$

$$+ \int\limits_{|x|\geqq a} d^3x[e^{-\beta H_0}(x, x) - (e^{-\beta H_0^D})(x, x)]\bigg\}$$

$$\leqq b_2^{Cl}(\beta) + \frac{4\pi}{2}\int\limits_a^\infty dr\, r^2\, e^{-(r-a)^2/2\beta}$$

$$= b_2^{Cl}(\beta) + c_1\sqrt{\beta} + c_2\beta + c_3\beta^{3/2},$$

with c_1, c_2, and c_3 strictly positive constants. This implies (II.33). □

Notice that (II.31) and (II.33) are, respectively, (I.4) and (I.3) of the introduction.

As a final remark, it is an open problem to prove that the estimates in the present section yield the corresponding estimates (I.6) for the free energy even for

sufficiently small density by the methods of [16], except in case (A). In the latter case, (I.6a) follows rigorously from Proposition II.2 or II.3 if the density is sufficiently small [16]. We are, however, interested in *fixed* (but arbitrary) density and β sufficiently small. This motivated our search for direct bounds on the free energy in the next sections.

III. Upper and Lower Bounds for $\Delta f(v, \beta)$

III.1. Upper Bound for $\Delta f(v, \beta)$

In this section we generalize the upper bound of [5] to hard-core systems. We consider N particles in a v-dimensional hypercube Λ^v and the corresponding Hilbert space $\mathcal{H}_\Lambda^{(N)} = L^2(\Lambda^{vN})$. To each particle is associated a momentum p_i, $i = 1, \dots, N$, which acts as a differential operator on $\mathcal{H}_\Lambda^{(N)}$:

$$(p_j \psi)(x_1, \dots, x_N) = -i\hbar \nabla_x \psi(x_1, \dots, x_N), \tag{III.1}$$

where $D(p_j) = C_0^\infty(\Lambda^{vN})$. Define the free Dirichlet Hamiltonian (kinetic energy) as the self-adjoint operator $H_{0,\Lambda}$ associated with the closure of the quadratic form

$$h_0(\psi) = \sum_{i=1}^N \|p_i \psi\|^2, \quad D(h_0) = C_0^\infty(\Lambda^{vN}). \tag{III.2}$$

The Hilbert space $\mathcal{H}_{\Lambda,a}^{(N)}$ for N particles with spherical hard cores of diameter a is a closed subspace of $\mathcal{H}_\Lambda^{(N)}$ spanned by $\psi \in \mathcal{H}_\Lambda^{(N)}$ which vanish on the set

$$S_a^{(N)} = \{(x_1, \dots, x_N); x_i \in \mathbb{R}^v, |x_i - x_j| \leq a \text{ for some } i \neq j \in \{1, 2, \dots, N\}\}. \tag{III.3}$$

We now define the free energy for hard-core systems $H_{0,\Lambda}^a$ as the (positive, self-adjoint) operator corresponding to the Friedrichs extension associated to the positive quadratic form

$$h_0^a(\psi) = \sum_{i=1}^N \|p_i \psi\|^2, \quad (h_0^a) = C_0^\infty(\Lambda^{vN} \setminus S_a^{(N)}). \tag{III.4}$$

In order to extend the upper bound of [5] to hard-core systems, some problems arise. The main proof in [5] is valid only on the whole Hilbert space $\mathcal{H}_\Lambda^{(N)}$. Let V be an interparticle interaction, given as a multiplication by a real potential:

$$(V\psi)(x_1, \dots, x_N) = v(x_1, \dots, x_N)\, \psi(x_1, \dots, x_N). \tag{III.5}$$

We assume that

$$v \in L^\infty(\Lambda^{Nv}). \tag{III.6}$$

Under the above assumption, the Friedrichs extension and the form sum extension of $(H_{0,\Lambda}^a + V)$ are equal. Let, now, $\{U_m\}_{m \geq 0}$ be a set of interactions on $\mathcal{H}_\Lambda^{(N)}$ defined by the potentials

$$U_m(x_1, \dots, x_N) = \begin{cases} m & \text{if } (x_1, \dots, x_N) \in S_a^{(N)} \\ 0 & \text{if } (x_1, \dots, x_N) \notin S_a^{(N)} \end{cases}. \tag{III.7}$$

Under the above assumptions on V, it follows from Lemma A.2 of Appendix A that $H_{0,\Lambda} + U_m + V$ is self-adjoint on $D(H_{0,\Lambda})$ and converges to the Friedrichs extension H_Λ^a of $H_{0,\Lambda}^a + V$ in the strong resolvent sense as $m \to \infty$.

Explicitly,

$$\lim_{m \to \infty} \| [(H_{0,\Lambda} + U_m + V + E)^{-1} - (H_\Lambda^a + E)^{-1}] \psi \| = 0, \psi \in \mathcal{H}_{\Lambda,a}^{(N)}, \quad \text{(III.8a)}$$

$$\lim_{m \to \infty} \| (H_{0,\Lambda} + U_m + V + E)^{-1} \psi \| = 0, \psi \in \mathcal{H}_{\Lambda,a}^{(N)\perp}, \quad \text{(III.8b)}$$

for all $E > 0$ (if $V \geqq 0$ — otherwise add a constant to V). We are now able to state the main result of this section. Let $Z_{\Lambda,B}(\beta)$, $Z_{\Lambda,F}(\beta)$, and $Z_{\Lambda,MB}(\beta)$ denote the canonical partition functions for Bose-Einstein, Fermi-Dirac, and Maxwell-Boltzmann statistics, defined in the usual way [19] for hard-core systems satisfying the assumptions stated above.

Theorem III.1. a) $Z_{\Lambda,B}(\beta) \leqq \tilde{Z}_\Lambda^{Cl}(\beta)$,

b) $Z_{\Lambda,F}(\beta) \leqq Z_\Lambda^{Cl}(\beta)$,

c) $Z_{\Lambda,MB}(\beta) \leqq Z_\Lambda^{Cl}(\beta)$,

where

$$Z_\Lambda^{Cl}(\beta) = \frac{1}{N!} \int_{x \in \Lambda^{N\nu} \setminus S_a^{(N)}} \frac{d^{N\nu}x \, d^{N\nu}p}{(2\pi\hbar)^{N\nu}} \exp[-\beta H_\Lambda^{Cl}(p,x)], \quad \text{(III.9)}$$

with

$$H_\Lambda^{Cl}(p,x) = \sum_{i=1}^{N} p_i^2 + v(x_1, \ldots, x_N) \quad \text{(III.10)}$$

is the classical partition function, and $\tilde{Z}_\Lambda^{Cl}$ is the classical partition function corresponding to the Hamiltonian

$$\tilde{H}_\Lambda^{Cl}(p,x) = H_\Lambda^{Cl}(p,x) + v_B(x_1, \ldots, x_N), \quad \text{(III.11)}$$

$$v_B(x_1, \ldots, x_N) = \sum_{1 \leqq i < j \leqq N} v_B(|x_i - x_j|), \quad \text{(III.12)}$$

$$\tilde{v}_B(|x|) = -\frac{1}{\beta} \exp\left(-\frac{1}{4\beta\hbar^2}|x|^2\right). \quad \text{(III.13)}$$

(Note a sign misprint in (30) of [5].) As in [5], we took $2m = 1$ for simplicity).

Proof. Let T_β be defined on $\mathcal{H}_\Lambda^{(N)}$ by

$$T_\beta \psi = \begin{cases} e^{-\beta H_\Lambda^0} \psi & \text{if} \quad \psi \in \mathcal{H}_{\Lambda,a}^{(N)} \\ 0 & \text{if} \quad \psi \in \mathcal{H}_{\Lambda,a}^{(N)\perp}, (\beta > 0) \end{cases}. \quad \text{(III.14)}$$

By (III.8), (III.14), and Lemma A.3 of Appendix A,

$$\exp[-\beta(H_{0,\Lambda} + U_m + V)]\psi \xrightarrow[m \to \infty]{} T_\beta \psi \quad \forall \psi \in \mathcal{H}_\Lambda^{(N)}. \quad \text{(III.15)}$$

By (III.15) and Proposition A.1 of Appendix A:

$$Z_{\Lambda,B}(\beta) = \mathrm{tr}_{\mathcal{H}_{\Lambda,a}^{(N)}} P_\beta \exp(-\beta H_\Lambda^a) = \mathrm{tr}_{\mathcal{H}_\Lambda^{(N)}}(P_B T_\beta)$$
$$= \lim_{m \to \infty} \mathrm{tr}_{\mathcal{H}_\Lambda^{(N)}} P_B \exp[-\beta(H_{0,\Lambda} + U_m + V)]. \quad \text{(III.16)}$$

As in [5], P_B denotes the projector onto the symmetric (Boson) subspace. We may now follow the proof of [5, p. 33], based on the Golden-Thompson inequality, to find:

$$\operatorname{tr}_{\mathscr{H}_\Lambda^{(N)}} P_B \exp\left[-\beta(H_0 + U_m + V)\right]$$

$$\leq \int \frac{d^{N\nu}x \, d^{N\nu}p}{(2\pi\hbar)^{N\nu}} \exp\left[-\beta\left(\sum_{i=1}^N p_i^2 + U_m(x_1, \ldots, x_N)\right.\right.$$

$$\left.\left. + v(x_1, \ldots, x_N) + v_B(x_1, \ldots, x_N)\right)\right]. \tag{III.17}$$

Taking now the limit of the right-hand side of (III.17), as $m \to \infty$, and using the monotone convergence theorem, we finally obtain a). The proofs of b) and c) are similar. $\quad\square$

In order to prove (I.8), let V_Λ be the volume of Λ and define the "free energies":

$$f_{\Lambda,\mathrm{B}}^{\mathrm{Q}}(\beta) = \frac{1}{V_\Lambda} \log Z_{\Lambda,\mathrm{B}}(\beta) \tag{III.18a}$$

with similar definitions for $f_{\Lambda,\mathrm{F}}^{\mathrm{Q}}(\beta)$ and $f_{\Lambda,\mathrm{MB}}^{\mathrm{Q}}(\beta)$, and

$$f_\Lambda^{\mathrm{Cl}}(\beta) = \frac{1}{V_\Lambda} \log Z_\Lambda^{\mathrm{Cl}}(\beta). \tag{III.18b}$$

We also denote the thermodynamic limit [19, 21] of $f_\Lambda(\beta)$ by $f(v, \beta)$, as in Sect. I, where $v = \lim\limits_{(V_\Lambda, N \to \infty)} \dfrac{V_\Lambda}{N}$ is the specific volume. Note that by (III.18) our $f(v, \beta)$ differs from the usual canonical free energy by a factor $(-\beta)$, conforming to the definition (I.1) already discussed in that section.

Theorem III.2. *Under the assumptions of this section for hard-core systems, (I.8) holds.*

Proof. According to b) and c) of Theorem III.1, (I.8) holds for Fermi-Dirac and Maxwell-Boltzmann statistics, with $c = 0$. We now concentrate on the Bose case. We have, by (III.18), (III.12) and a) of Theorem III.1,

$$f_{\Lambda,\mathrm{B}}^{\mathrm{Q}}(\beta) - f_\Lambda^{\mathrm{Cl}}(\beta) = \frac{1}{V_\Lambda} \log \frac{Z_{\Lambda,\mathrm{B}}(\beta)}{Z_\Lambda^{\mathrm{Cl}}(\beta)}$$

$$\leq \varrho \sup_N \sup_{\substack{x_i \in \mathbb{R}^\nu \\ i=1,\ldots,N \\ |x_i - x_j| \geq a, i \neq j}} \left[\frac{|\beta v_B(x_1, \ldots, x_N)|}{N}\right], \tag{III.19}$$

where $\varrho = \dfrac{1}{v}$ is the density. Now, by [21, Appendix A], and (III.13),

$$\sup_{\substack{x_i \in \mathbb{R}^\nu, i=1,\ldots,N \\ |x_i - x_j| \geq a, i \neq j}} |\beta v_B(x_1, \ldots, x_N)| \leq \beta B N, \tag{III.20a}$$

where

$$\beta B = \sum_{t \neq 0} \sup_{x \in \Delta(t)} |\beta \tilde{v}_B(x)|, \tag{III.20b}$$

and the sum is over all cubic cells $\Delta(t)$ centered at the points $t = nd$, with $d = \dfrac{a}{\sqrt[3]{v}}$ and $n \in \mathbb{Z}^\nu$. Let

$$f(\ell) = \exp - \left[\frac{1}{4\beta\hbar^2}(\ell - \tfrac{1}{2})^2 d^2 \right], \quad \ell = 1, 2, 3, \ldots. \tag{III.21}$$

Then, by (III.20b) and (III.21), and setting $v = 3$:

$$\beta B \leq 3.2 \sum_{\ell = 1}^{\infty} f(\ell) + 3.4 \left(\sum_{\ell = 1}^{\infty} f(\ell) \right)^2 + 8 \left(\sum_{\ell = 1}^{\infty} f(\ell) \right)^3. \tag{III.22}$$

Above, we considered separately the cells centered at points on the three coordinate axes, as well as those centered at points on the three coordinate planes, and disregarded double or multiple countings. A similar estimate holds for general v. Equation (I.8) follows immediately from [(III.19)–(III.22)] and the Euler summation formula (see, e.g., [22, Appendix]) applied to the function f.   □

Remark III.1. The constant α in (I.8) may be evaluated

$$\alpha = \left(\frac{d}{8\hbar} \right)^2 = \left(\frac{a}{8\sqrt{3}\hbar} \right)^2.$$

The thermal wavelength is $\lambda = \sqrt{\pi\beta}\hbar$. Hence the right-hand side of (I.8) is exponentially small in the ratio a/λ, a precise version of the condition $v^{1/3}(>a) \gg \lambda$ [14, Chap. 10.2].   □

III.2. Lower Bound for Hard-Core System

III.2.1. Lower Bound for the Partition Function. In this section we derive a lower bound for the partition function, using methods of functional integration [11, 16]. We assume a positive bounded potential v in (III.5) in addition to a hard core of diameter a, satisfying

$$v(x_1, \ldots, x_N) = \sum_{1 \leq i < j \leq N} \tilde{v}(|x_i - x_j|), \tag{III.23}$$

$$\tilde{v}(|x|) = 0 \quad \text{if} \quad |x| < a, \tag{III.24}$$

$$0 \leq \tilde{v}(|x|) \quad \forall x \in \mathbb{R}^\nu. \tag{III.25}$$

For some $\varepsilon > 0$ and

$$0 < D < \infty, \tilde{v}(|x|) \leq D/(1 + |x|)^{\nu + \varepsilon} \quad \forall x \in \mathbb{R}^\nu, \tag{III.26}$$

$$\tilde{v}(\lambda|x|) \leq \tilde{v}(|x|) \lambda \geq 1 \quad \forall x \in \mathbb{R}^\nu. \tag{III.27}$$

Condition (III.26) suffices for stability [21]. Assumption (III.27) of monotone decrease is, as we shall see, essential. We first approximate the full Hamiltonian by $(H_{0,\Lambda} + U_m + V)$ on $\mathcal{H}_\Lambda(N)$ as in Sect. III.1.

We choose U_m of the form:

$$U_m(x_1, \ldots, x_N) = \sum_{1 \leq i < j \leq N} u_m(|x_i - x_j|), \tag{III.28a}$$

where

$$u_m(|x|) = \begin{cases} m & \text{if } |x| < a \\ 0 & \text{otherwise} \end{cases}. \tag{III.28b}$$

Although U_m is not of the form (III.7), a modification of Lemma A.3 and the proof in Sect. III.1 applies to yield (in this section we consider for simplicity Maxwell Boltzmann statistics only)

$$Z_{A,\text{MB}}(\beta) = \lim_{m \to \infty} Z_A^{(m)}(\beta), \tag{III.29a}$$

$$Z_A^{(m)}(\beta) = \frac{1}{N!} \operatorname{tr}_{\mathscr{H}_A^{(N)}} e^{-\beta(H_{0,A} + U_m + V)}. \tag{III.29b}$$

We write

$$U_m + V = \sum_{1 \leq i < j \leq N} w_m(|x_i - x_j|), \tag{III.30a}$$

where

$$w_m(|x|) = u_m(|x|) + \tilde{v}(|x|), \tag{III.30b}$$

and choose m so large such that w_m also satisfies (III.27). Let dx denote as usual Lebesgue measure on $\mathbb{R}^\nu$ and let (B, β, Db) be the measure space for ν-dimensional Brownian motion [11, p. 38]. We follow the same notation of [11] except for denoting vectors by a special (bold-faced) symbol. As in [11, p. 38], define Wiener measure as the measure $d\mu_0$ on $\mathbb{R}^\nu \times B$ given by $dx \otimes Db$, and let $\omega(t) = x + b(t)$. As in [11, p. 39], let $d\mu_{0,a,c}(\omega)$ denote conditional Wiener measure [which corresponds formally, to setting $\omega(0) = a$, and $\omega(t) = c$]. Let

$$\chi_A(\omega) = \begin{cases} 1 & \text{if } \omega(t) \in A \quad \text{for all } t \in [0, \beta] \\ 0 & \text{otherwise}. \end{cases}$$

Then [23, Theorem 6.3.9] (conditional) Wiener measure corresponding to Dirichlet boundary conditions on A is obtained from the free measure $d\mu_{0,a,c;t}$ by multiplication with the characteristic function χ_A of A. In particular, let $\{\alpha(s)\}_{0 \leq s \leq 1}$ denote Brownian bridge [11, p. 40], related to ω by $\omega(t) = x + \sqrt{\beta}\, \alpha(t/\beta)$. Then the Feynman-Kac formula, together with (4.13) of [11, Chap. II.4], yields the following representation for $Z_A^{(m)}(\beta)$ in (III.29a):

$$Z_A^{(m)}(\beta) = \frac{1}{N!} (2\pi\beta)^{-\nu N/2} \int_{A^{N\nu}} dx \int D\alpha_1, \ldots, D\alpha_N \exp\left\{ -\int_0^\beta dt \sum_{1 \leq i < j \leq N} w_m\left(\left| x_i - x_j \right.\right.\right.$$

$$\left.\left.\left. + \sqrt{\beta}\left[\alpha_i\left(\frac{t}{\beta}\right) - \alpha_j\left(\frac{t}{\beta}\right) \right] \right| \right) \right\} \chi_A\left(x_1 + \sqrt{\beta}\, \alpha_1\left(\frac{t}{\beta}\right) \right) \times \ldots \times \chi_A\left(x_N + \sqrt{\beta}\, \alpha_N\left(\frac{t}{\beta}\right) \right).$$

$$\tag{III.31}$$

Above, $D\alpha_i$ $(i=1,\ldots,N)$ is a copy of the measure corresponding to Brownian bridge. Notice that the trace corresponds to setting $a=c$ in (4.13) of [11].

Let

$$\varrho_i(t) = \sqrt{\beta}\,\alpha_i\!\left(\frac{t}{\beta}\right).$$

If $|\varrho_i(t) - \varrho_j(t)| \leq \delta |x_i - x_j|$, then $(\delta < 1)$,

$$|x_i - x_j + \varrho_i(t) - \varrho_j(t)| \geq (1-\delta)|x_i - x_j|,$$

and by the monotone-decrease property of w_m:

$$w_m(|x_i - x_j + \varrho_i(t) - \varrho_j(t)|) \leq w_m[(1-\delta)|x_i - x_j|]. \qquad \text{(III.32)}$$

Notice that if A, B, C denote the events

$$A = \left\{ \sup_{0 \leq s \leq 1} |\alpha_i(s) - \alpha_j(s)| \leq \frac{\delta}{\sqrt{\beta}}|x_i - x_j|;\ \ \forall i,j = 1,\ldots,N,\ i \neq j; \right.$$

$$\left. x_i + \sqrt{\beta}\,\alpha_i(s) \in \Lambda^\nu,\ \forall i = 1,\ldots,N,\ \forall s \in [0,1] \right\},$$

$$B = \left\{ \sup_{0 \leq s \leq 1} |\alpha_i^{(k)}(s) - \alpha_j^{(k)}(s)| \leq \frac{\delta}{\sqrt{\nu}\sqrt{\beta}}|x_i - x_j|;\ \ \forall i,j = 1,\ldots,N; \right.$$

$$\left. i \neq j,\ \forall k = 1,\ldots,\nu;\ x_i + \sqrt{\beta}\,\alpha_i(s) \in \Lambda^\nu,\ \forall i = 1,\ldots,N,\ \forall s \in [0,1] \right\},$$

$$C = \left\{ \sup_{\substack{i \in [1,N] \\ k \in [1,\nu]}} \sup_{0 \leq s \leq 1} |\alpha_i^{(k)}(s)| \leq \frac{\delta}{2\sqrt{\nu}\sqrt{\beta}}|x_i - x_j|;\ \ \forall i,j = 1,\ldots,N, i \neq j; \right.$$

$$\left. x_i + \sqrt{\beta}\,\alpha_i(s) \in \Lambda^\nu,\ \forall i = 1,\ldots,N,\ s \in [0,1] \right\},$$

then $A \supseteq B \supseteq C$. Now, by (III.31) and (III.32):

$$Z_\Lambda^{(m)}(\beta)$$

$$\geq \frac{1}{N!}(2\pi\beta)^{-\nu N/2} \int_{\Lambda^{N\nu}} dx_1 \ldots dx_N \exp\left\{ -\beta \sum_{1 \leq i < j \leq N} w_m[(1-\delta)|x_i - x_j|] \right\} \cdot E_N(A),$$

$$\text{(III.33)}$$

where $E_N(\cdot)$ denotes expectation with respect to the measure $D\alpha_1 \ldots D\alpha_N$. Taking now the limit $m \to \infty$ on (III.33) and using the monotone convergence theorem, we obtain by (III.29a) and $A \supseteq C$:

$$Z_{\Lambda,\mathrm{MB}}(\beta) \geq \frac{1}{N!}(2\pi\beta)^{-N\nu} \int_{\Lambda^{\nu N}\backslash S_{a_1}^{(N)}} dx_1 \ldots dx_N \exp\left\{ -\beta \sum_{1 \leq i < j \leq N} \tilde{v}(|x_i - x_j|) \right\} \cdot E_N(C),$$

$$\text{(III.34a)}$$

where

$$a_1 \equiv \frac{a}{1-\delta}. \qquad \text{(III.34b)}$$

Now, given that $(x_1, \ldots, x_N) \notin S_{a_1}^{(N)}$, then $C \supseteq D$, where

$$D = \left\{ \sup_{0 \le s \le 1} |\alpha_i^{(k)}(s)| \le \frac{\delta a_1}{2\sqrt{\nu}\sqrt{\beta}}, \quad \forall i = 1, \ldots, N, \ \forall k = 1, \ldots, \nu; \right.$$

$$\left. x_i + \sqrt{\beta}\, \alpha_i(s) \in \Lambda^\nu, \ \forall i = 1, \ldots, N, \ \forall s \in [0, 1] \right\}.$$

Let

$$\Lambda'^\nu \equiv \left\{ x \in \Lambda^\nu; |x^{(k)}| \le \ell - \frac{\delta a_1}{2\sqrt{\nu}}, k = 1, \ldots, \nu \right\}, \tag{III.35}$$

where $\Lambda^\nu = [-\ell, \ell]^\nu$. Then $x \in \Lambda'^\nu$ and $|\alpha^{(k)}(s)| \le \frac{\delta a_1}{2\sqrt{\nu}\sqrt{\beta}}$, $\forall s \in [0, 1]$, imply $(x + \sqrt{\beta}\, \alpha(s)) \in \Lambda^\nu$.

Therefore, given that $x \in (\Lambda')^{\nu N} \setminus S_{a_1}^{(N)}$, it follows that $D \supseteq F$, where

$$F \equiv \left\{ \sup_{0 \le s \le 1} |\alpha_i^{(k)}(s)| \le \frac{\delta a_1}{2\sqrt{\nu}\sqrt{\beta}}, \quad \forall i = 1, \ldots, N, \ \forall k = 1, \ldots, \nu \right\}. \tag{III.36}$$

Hence, we finally get

$$Z_{\Lambda, \mathrm{MB}}(\beta) \ge \frac{1}{N!} (2\pi\beta)^{-\nu N/2} \int_{\Lambda'^{N\nu} \setminus S_{a_1}^{(N)}} dx_1 \ldots dx_N$$

$$\cdot \exp\left\{ -\beta \sum_{1 \le i < j \le N} \tilde{v}(|x_i - x_j|) \right\} \cdot E_N(F). \tag{III.37}$$

Now, the components of $\alpha_i^{(k)}$ are independent, for $i = 1, \ldots, N$ and $k = 1, \ldots, \nu$.

If $i \in [1, N]$ and $k \in [1, \nu]$ are fixed and

$$F_i^{(k)} \equiv \left\{ \sup_{0 \le s \le 1} |\alpha_i^{(k)}(s)| \le \alpha \right\}, \tag{III.38}$$

then [24, Chap. 13.7, p. 29]:

$$E(F_i^k) = 1 - e^{-2\alpha^2}, \quad \forall i \in [1, N], \ \forall k \in [1, \nu], \tag{III.39}$$

where E denotes expectation with respect to one-dimensional Brownian bridge. Inserting (III.39) into (III.37), we obtain

$$Z_{\Lambda, \mathrm{MB}}(\beta) \ge \frac{1}{N!} (2\pi\beta)^{-\nu N/2} \int_{\Lambda'^{\nu N} \setminus S_{a_1}^{(N)}} dx_1 \ldots dx_N$$

$$\cdot \exp\left[-\beta \sum_{1 \le i < j \le N} \tilde{v}(|x_i - x_j|) \right] \cdot \left(1 - e^{-\frac{2\delta^2 a_1^2}{4\beta\nu}} \right)^{\nu N}. \tag{III.40}$$

Write, now

$$\int_{\Lambda'^{\nu N} \setminus S_{a_1}^{(N)}} dx_1 \ldots dx_N \exp\left[-\beta \sum_{1 \le i < j \le N} \tilde{v}(|x_i - x_j|) \right] = \left(\int_{\Lambda'^{N\nu} \setminus S_{a_1}^{(N)}} dx_1 \ldots dx_N \right) \cdot I_N,$$

$$\tag{III.41a}$$

$$I_N \equiv \frac{\int_{\Lambda'^{N\nu} \setminus S_{a_1}^{(N)}} dx_1 \ldots \ldots dx_N \exp\left[-\beta \sum_{1 \le i < j \le N} \tilde{v}(|x_i - x_j|) \right]}{\int_{\Lambda'^{N\nu} \setminus S_{a_1}^{(N)}} dx_1 \ldots dx_N}. \tag{III.41b}$$

By (III.41 b), (III.26) and Fisher's method [21, Appendix A], already used in the proof of Theorem III.2, it is easy to obtain the bound

$$\frac{1}{V_A}\log I_N \geqq -\beta\varrho Dp(a_1),\tag{III.42}$$

where D is the constant in (III.26) and $p(\cdot)$ is a function of the hard-core diameter a, regular in the neighbourhood of any $a \neq 0$; in particular:

$$p(a_1)\xrightarrow[a_1\to a\neq 0]{} p(a).\tag{III.43}$$

Equations (III.40), (III.41), and (III.42) yield, together with definition (III.18):

$$f_{A,\mathrm{MB}}(\beta)\geqq v\varrho\log\left(1-e^{-\frac{\delta^2 a_1^2}{2\beta v}}\right)-\beta\varrho Dp(a_1)+f^{\mathrm{Cl}}_{A',a_1}(\beta)-v\varrho/2\log(2\pi\beta).\tag{III.44}$$

In (III.44),

$$f^{\mathrm{Cl}}_{A',a_1}(\beta)=\frac{1}{V_A}\log Z^{\mathrm{Cl}}_{A',a_1}(\beta),$$

where $Z^{\mathrm{Cl}}_{A',a_1}(\beta)$ is the classical partition function of *pure* hard cores in region A'^v, without the kinetic term, which we separated out as the last term in (III.44). Performing the same splitting of (III.41) for the classical partition function, using the positivity of $\tilde{v}$ and again separating out the kinetic term, we find:

$$f^{\mathrm{Cl}}_A(\beta)\leqq f^{\mathrm{Cl}}_{A,a}+\frac{v\varrho}{2}\log(2\pi\beta),\tag{III.45}$$

where $f^{\mathrm{Cl}}_{A,a}$ denotes the classical free energy of *pure* hard cores of diameter a. By (III.44) and (III.45) we find in the thermodynamic limit [noticing that by (III.35) f^{Cl}_{A',a_1} has the same thermodynamic limit $f^{\mathrm{Cl}}_{a_1}$ as f^{Cl}_{A,a_1}]:

$$\Delta f(v,\beta)\geqq\frac{v}{v}\log\left(1-e^{-\frac{\delta^2 a_1^2}{2\beta v}}\right)+f^{\mathrm{Cl}}_{a_1}-f^{\mathrm{Cl}}_a-\beta\cdot\varrho\cdot Dp(a_1).\tag{III.46}$$

III.2.2. The Bound (I.10) *for* $v=1$. Let now $0<\varepsilon<\frac{1}{2}$, $\beta\in[0,\beta_0]$, for some fixed β_0 sufficiently small, and

$$\delta=\delta_\beta=\beta^{\frac{1}{2}-\varepsilon}\tag{III.47}$$

in (III.46) $\left[\text{more properly, }\delta=\left(\frac{\lambda}{a}\right)^{1-2\varepsilon},\text{ where }\lambda=\hbar\sqrt{\beta}\text{ is the thermal wavelength}\right]$. Then the first term in (III.46) is still $O(\exp(-\beta^{2\varepsilon}))$, for β sufficiently small. Since $a_1=a_1(\beta)=\dfrac{a}{1-\delta_\beta}$ by (III.34b), then (III.43) implies that the term $(-\beta\varrho Dp(a_1))$ in (III.46) is of order $O(\beta)$. To see what happens with

$$\Delta f^{\mathrm{Cl}}(\beta)\equiv f^{\mathrm{Cl}}_{a_1(\beta)}-f^{\mathrm{Cl}}_a,\tag{III.48}$$

consider $v=1$, where [25]

$$f^{\mathrm{Cl}}_a=\varrho[1+\log(v-a)].\tag{III.49}$$

We shall assume that

$$v \geqq \xi a_1(\beta), \quad \forall \beta \in [0, \beta_0] \tag{III.50}$$

for some fixed ξ satisfying

$$1 < \xi < \tfrac{3}{2}. \tag{III.51}$$

$\left(\text{Clearly } v > a_1(\beta) = \dfrac{a}{1 - \delta_\beta} \text{ is necessary for } f^c_{a_1(\beta)} \text{ to be defined.} \right)$ On δ_β we impose

$$\delta_\beta \leqq 2(\xi - 1) \quad \text{for all} \quad \beta \in [0, \beta_0]. \tag{III.52}$$

Then, by (III.48) and (III.49):

$$\Delta f^{Cl}(\beta) = \varrho \log \left[1 - \frac{\delta_\beta \cdot a}{(1 - \delta_\beta)(v - a)} \right],$$

with

$$\frac{\delta_\beta a}{(1 - \delta_\beta)(v - a)} \leqq \frac{\delta_\beta}{(\xi - 1) + \delta_\beta} \leqq \frac{2}{3}.$$

Using now the inequality

$$\log(1 - x) \geqq -\alpha x \quad \text{if} \quad x \leqq 1 - \frac{1}{\alpha}, \quad (\alpha > 1)$$

with $\alpha = 3$, we obtain

$$\Delta f^{Cl}(\beta) \geqq -3\varrho \frac{\delta_\beta a}{(1 - \delta_\beta)(v - a)} \geqq -\frac{3a\varrho}{(3 - 2\xi)(v - a)} \delta_\beta, \tag{III.53}$$

if, by (III.50) and (III.52):

$$v \geqq \frac{\xi}{3 - 2\xi} a. \tag{III.54}$$

Clearly, by (III.54), we may choose v arbitrarily close to a (from above) by choosing ξ arbitrarily close to one, but the interval of variation of β shrinks in correspondence, as (III.52) shows. We have thus proved

Proposition III.1. *Given ξ satisfying (III.51) and $0 < \varepsilon < \tfrac{1}{2}$, then (I.10) holds for $v = 1$ if (β, v) is such that $\beta \in [0, \beta_0]$, where $\beta_0 \leqq 2^{\frac{2}{(1 - 2\varepsilon)}} (\xi - 1)^{\frac{2}{(1 - 2\varepsilon)}}$, and v satisfies (III.54).* $\square$

Notice that (III.47) shows that an integrable potential outside the hard core provides a contribution to the free energy of order $O(\beta^{1/2})$ with respect to the hard core term. This agrees with the intuition that for $\beta \downarrow 0$ only the behaviour of the potential near the origin plays a role – see also the introduction.

III.2.3. Lower Bound for $\Delta f(v, \beta)$ Using Coherent States. Assumption (III.27) of monotone decrease of the potential excludes several interesting cases, for instance, potentials which are negative (attractive) at large distances. In this section we

sketch a derivation of the weaker bound (I.11), which is valid, however, for any stable hard-core potential, based on inequalities due to Baumgartner [5, Sect. 2c]. The latter involve an ingenious form of the coherent states which was introduced by Thirring [26]. Since there is no novelty in method, we shall be rather cursory in exposition, referring the reader to [5] for details. The present application reveals, however, the flexibility of the Thirring coherent states, when the wave-function is appropriately chosen.

We assume a two-body interaction (for clarity in this section we use a vector notation):

$$V(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|),$$

with

$$v(|\mathbf{x}|) = \begin{cases} \infty & \text{if} \quad |\mathbf{x}| \leq a \\ \tilde{v}(|\mathbf{x}|) & \text{if} \quad |\mathbf{x}| > a \end{cases}, \tag{III.55}$$

where $\tilde{v}$ is such that V is thermodynamically stable. As in Sect. (III.2) $\tilde{v}$ will not play any significant role for small β. Let $v = 3$ (just to agree with [5]). Then [5, (25) et seq.] [$Z_\Lambda(\beta)$ stands for $Z_{\Lambda,\mathrm{B}}(\beta)$ or $Z_{\Lambda,\mathrm{F}}(\beta)$]:

$$Z_\Lambda(\beta) \geq \frac{1}{N!} \int_{\Lambda^{3N} \setminus S_a^{(N)}} \frac{d^{3N}p \, d^3x}{(2\pi\hbar)^{3N}} \exp[-\beta \hat{H}(\mathbf{p}, \mathbf{x})], \tag{III.56}$$

where

$$\hat{H}(\mathbf{p}, \mathbf{x}) = \sum_{i=1}^{N} (\mathbf{p}_i^2 + 2\mathbf{p}_i \hbar \cdot \langle \phi | \mathbf{p} \phi \rangle + \hbar^2 \langle \phi | \mathbf{p}^2 \phi \rangle)$$

$$+ \sum_{1 \leq i < j \leq N} \hat{v}(|\mathbf{x}_i - \mathbf{x}_j|), \tag{III.57}$$

and

$$\hat{v}(|\mathbf{x}|) = \begin{cases} \int d^3z \, d^3y \, v(|\mathbf{x} - \mathbf{y}|) \, |\phi(\mathbf{z} - \mathbf{y})|^2 \, |\phi(-\mathbf{z})|^2, & |\mathbf{x}| > a \\ \infty, & |\mathbf{x}| \leq a \end{cases}. \tag{III.58}$$

Above, ϕ is a C^∞ function of compact support $\operatorname{supp}\phi$ satisfying
  a) $\int |\phi(\mathbf{x})|^2 \, d^3x = 1$ (normalization)
  b) $\operatorname{supp}\phi \subseteq \{\mathbf{x} \in \mathbb{R}^3; |\mathbf{x}| < a\}$
and

$$\langle \phi | \mathbf{p}^2 \phi \rangle \equiv \int d^3p \, |\tilde{\phi}(\mathbf{p})|^2 \, \mathbf{p}^2, \tag{III.59}$$

$$\langle \phi | \mathbf{p} \phi \rangle \equiv \int d^3p \, |\tilde{\phi}(\mathbf{p})|^2 \, \mathbf{p}, \tag{III.60}$$

where $\tilde{\phi}$ denotes the Fourier transform of ϕ. We choose the hard-core diameter ("ℓ" in [5]) equal to the hard-core diameter a of the original potential. We were also rather informal in definitions such as (III.55) and (III.58), but mathematical details (involving suitable limiting procedures) may be filled in as in Sect. III.1. We now choose ϕ as follows. Let $h(x)$ be a C^∞-function of one real variable, such that $\operatorname{supp}h \subseteq [-1, 1]$, $\int_{-\infty}^{\infty} dx \, h(x) = 1$, and define for $0 < \alpha < \dfrac{a}{\sqrt{3}}$,

$$h_\alpha(x) = \frac{1}{\alpha} h\left(\frac{x}{\alpha}\right).$$

Then $h_\alpha \in C^\infty$, $\mathrm{supp}\, h_\alpha \subseteq [-\alpha, \alpha]$ and $\int\limits_{-\infty}^{\infty} dx\, h_\alpha(x) = 1$. Let, now

$$\phi(\mathbf{x}) = \phi_\alpha(\mathbf{x}) = \prod_{i=1}^{3} \sqrt{h_\alpha(x_i)} = \prod_{i=1}^{3} \frac{1}{\sqrt{\alpha}} \sqrt{h\left(\frac{x_i}{\alpha}\right)}, \mathbf{x} = (x_i)_{i=1}^{3}. \qquad \text{(III.61)}$$

We also assume that $\sqrt{h}$ is C^∞. This is satisfied, for instance, by the standard example of a C^∞ function of compact support

$$h(x) = \begin{cases} c\exp\left(+\dfrac{1}{x^2-1}\right) & |x| \leq 1 \\ \\ 0 & \text{otherwise} \end{cases} \qquad \left(\text{with } c \text{ such that } \int\limits_{-1}^{1} h(x)\, dx = 1\right).$$

$$\text{(III.62)}$$

Condition a) is clearly satisfied, and b) follows from $\alpha < \dfrac{a}{\sqrt{3}}$ assumed above. Further, since ϕ is C^∞, both quantities (III.59) and (III.60) are finite. Since ϕ is real-valued, (III.60) shows that

$$\langle \phi | \mathbf{p}\phi \rangle = \mathbf{0}. \qquad \text{(III.63)}$$

With the choices above, the function ψ defined by

$$\psi(\mathbf{y}) = \int d^3z\, |\phi(\mathbf{z}-\mathbf{y})|^2\, |\phi(-\mathbf{z})|^2 \qquad \text{(III.64)}$$

is of compact support, and

$$\mathrm{supp}\,\psi \subseteq \{\mathbf{y} \in \mathbb{R}^3; |\mathbf{y}| \leq 2\sqrt{3}\,\alpha\}. \qquad \text{(III.65)}$$

Hence, by (III.55), (III.58), and (III.65),

$$\hat{v}(|\mathbf{x}|) = \tilde{v}(|\mathbf{x}|) \quad \text{if} \quad |\mathbf{x}| > a_1 = a + 2\sqrt{3}\,\alpha. \qquad \text{(III.66)}$$

By (III.56), (III.63), (III.66), and definition (III.18) [where $f_A(\beta)$ stands for either $f_{A,\mathrm{B}}(\beta)$ or $f_{A,\mathrm{F}}(\beta)$]:

$$f_A(\beta) \geq \varrho \log \int \frac{d^3p}{(2\pi\hbar)^3} \exp(-\beta p^2) - \beta\varrho\hbar^2 \langle \phi | \mathbf{p}^2\Phi \rangle$$

$$+ \frac{1}{V_A} \log \frac{1}{N!} \int\limits_{A^{3N}\setminus S_{a_1}^{(N)}} d^{3N}x \exp\left[-\beta \sum_{1 \leq i < j \leq N} \tilde{v}(|\mathbf{x}_i - \mathbf{x}_j|)\right]. \qquad \text{(III.67)}$$

Let, now

$$S_\alpha(x) \equiv \sqrt{h_\alpha(x)}.$$

Then, by (III.61)

$$\langle \phi | \mathbf{p}^2\phi \rangle = \frac{3}{2\pi} \int\limits_{-\infty}^{\infty} dp\, p^2 |\tilde{S}_\alpha(p)|^2, \qquad \text{(III.68)}$$

where

$$\tilde{S}_\alpha(p) = \int_{-\infty}^{\infty} dx \, e^{ipx} \sqrt{h_\alpha(x)} = \sqrt{\alpha} \int_{-\infty}^{\infty} dx \, e^{ip\alpha x} \sqrt{h(x)}.$$

Upon substituting this expression for $\tilde{S}_\alpha(p)$ into (III.68) one obtains

$$\langle \phi | \mathbf{p}^2 \phi \rangle = \frac{3}{2\pi\alpha^2} \int_{-\infty}^{\infty} dp \, p^2 \widetilde{(h^{1/2})}(p)^2 ,$$

and hence

$$\langle \phi | \mathbf{p}^2 \phi \rangle \leqq c\alpha^{-2}. \tag{III.69}$$

We may now handle the third term in (III.67) exactly as in Sect. (III.2). The leading term in β will be due to the difference Δf^{Cl} in classical free energies corresponding to hard core diameters a_1 and a. Assuming that the classical free energy for $v = 3$ behaves as the one-dimensional case, i.e., like the right-hand side of (III.49); (for a discussion of this assumption in the context of mean-field models, see [25, p. 93])

$$f_a^{\mathrm{Cl}} = \varrho[1 + \log(v^{1/3} - a)] \tag{III.70}$$

(with $\varrho = 1/v$ the three-dimensional density and a the hard core radius as before), we have

$$\begin{aligned}
\Delta f^{\mathrm{Cl}} &= \varrho[1 + \log(v^{1/3} - a_1)] - \varrho[1 + \log(v^{1/3} - a)] \\
&= (v^{1/3} > a_1 > a) = \varrho \log[1 - (a_1 - a)/(v^{1/3} - a)] \\
&\geqq -3\varrho(a_1 - a)/(v^{1/3} - a),
\end{aligned}$$

if $(a^1 - a)/(v^{1/3} - a) < \frac{2}{3}$, as in Sect. III.2.2. Now, $a_1 - a = 2\sqrt{3}\,\alpha$ by (III.66). Take

$$\frac{\alpha}{v^{1/3} - a} = \alpha^{-2}\beta\hbar^2 \Rightarrow \alpha = (\beta\hbar^2)^{1/3}(v^{1/3} - a)^{1/3}.$$

Then

$$\frac{a_1 - a}{v^{1/3} - a} = 2\sqrt{3}\,\frac{(\beta\hbar^2)^{1/3}(v^{1/3} - a)^{1/3}}{v^{1/3} - a} < \frac{2}{3},$$

which may be written in terms of the thermal wave-length $\lambda = \sqrt{\pi\beta}\,\hbar$:

$$(\lambda/\sqrt{\pi}(v^{1/3} - a))^{2/3} < 1/(3\sqrt{3})$$

or $\lambda < \dfrac{\sqrt{\pi}}{(3\sqrt{3})^{3/2}}(v^{1/3} - a)$. Under this condition

$$\Delta f^{\mathrm{Cl}} \geqq -3\varrho \frac{2\sqrt{3}\,\alpha}{v^{1/3} - a} = -3\varrho 2\sqrt{3}\,\frac{(\lambda/\sqrt{\pi})^{2/3}}{(v^{1/3} - a)^{2/3}},$$

which is of the form (I.11).

Appendix A

In this appendix, we collect some lemmas used in the main text.

Lemma A.1.

$$\mathrm{tr}(f_n(e^{-\beta H} - e^{-\beta H_0})f_n) \xrightarrow[n \to \infty]{} \mathrm{tr}(e^{-\beta H} - e^{-\beta H_0}). \tag{A.1}$$

Proof. It suffices to show the following general result. If A is a trace-class operator and $\{B_n\}$ a uniformly bounded sequence of operators converging weakly to B, then

$$\lim_n \mathrm{tr}[A(B_n - B)] = 0.$$

Let $\{e_p\}$ denote a complete orthonormal set of eigenvectors of A^*A with eigenvalues $\{\lambda_p\}$, $\lambda_p \geq 0$, and let $f_p \equiv \lambda_p^{-1/2} A e_p$ for $\lambda_p \neq 0$. Then $\sum \lambda_p^{1/2} = \|A\|_{\mathrm{tr}} < \infty$ and

$$\mathrm{tr}[A(B_n - B)] = \sum_p \lambda_p^{1/2}(e_p, (B_n - B)f_p).$$

By the uniform boundedness of B_n, the sum over $p > p_0$ is bounded by

$$\left(\sup_n \|B_n - B\|\right) \sum_{p > p_0} \lambda_p^{1/2},$$

which can be made arbitrarily small for a suitable choice of p_0. The finite sum over $p \leq p_0$ for any fixed p_0 tends to zero by the weak convergence $B_n - B \to 0$. $\quad\square$

Lemma A.2. *Let $v \in L^\infty(\Lambda^{\nu N})$ and $\{U_m\}_{m \geq 0}$ be the set of interactions on $\mathcal{H}_\Lambda^{(N)}$ defined in (III.7). Then $(H_{0,\Lambda} + U_m + V)$ is self-adjoint on $D(H_{0,\Lambda})$ and converges to the Friedrichs extension of $(H_{0,\Lambda}^a + V)$ in the strong resolvent sense, i.e., (III.8) holds.*

Proof. The proof is almost identical to the proof of Theorem 1.6, p. 224, of [17]. Slight alterations due to the extra Dirichlet condition on $\partial \Lambda$ are straightforward. Assumption $v \neq 2$ of [27] is not required because under our assumption on v the Friedrichs extension and the form sum extension are equal. $\quad\square$

Lemma A.3. *Assume (III.8). Then (III.15) holds, i.e.,*

$$\exp[-t(H_{0,\Lambda} + U_m + V)]\psi \xrightarrow[m \to \infty]{} T_t\psi \quad \forall \psi \in \mathcal{H}_\Lambda^{(N)}, \tag{A.2}$$

uniformly in any finite interval of $t \geq 0$ (in the main text we use β for t).

Proof. By the assumption (III.5) et seq. both $(H_{0,\Lambda} + U_m + V)$ and $H_\Lambda^a \equiv$ Friedrichs extension of $(H_{0,\Lambda}^a + V)$ belong to $\mathcal{G}(M, \beta)$ for some fixed M, β (independent of m), in the notation of [28, p. 485]. Hence Theorem 2.16, p. 502 of [28] applies to yield (A.2). $\quad\square$

Proposition A.1.

$$\mathrm{tr}_{\mathcal{H}_\Lambda^{(N)}}(P_B \exp[-\beta(H_{0,\Lambda} + U_m + V)]) \xrightarrow[m \to \infty]{} \mathrm{tr}_{\mathcal{H}_\Lambda^{(N)}}(P_B \exp - \beta H_\Lambda^a), \quad (\beta > 0) \tag{A.3}$$

(see Sect. III.1).

Proof. By a variation of Theorem 6.6 of [11] (the variation being for the restriction to a finite volume Λ with the Dirichlet condition), the operator $\exp[-\beta(H_{0,\Lambda}+U_m+V)]$ has a continuous positive kernel which we denote by $K_m(x,y)$, where $x=(x_1,\ldots,x_N)$, $x_j\in\mathbb{R}^\nu$, and similarly for y. Hence $P_B\exp[-\beta(H_{0,\Lambda}+U_m+V)]$ has the kernel

$$\tilde{K}_m(x,y)=N!^{-1}\sum_P K(Px,y).$$

By the Feynman-Kac formula (in the proof of Theorem 6.6 of [11]) $K_m(x,y)$ and hence $\tilde{K}_m(x,y)$ are monotone decreasing functions of m for each fixed x,y. Therefore we have the following limits

$$\lim_{m\to\infty}K_m(x,y)=K_\infty(x,y)$$

$$\lim_{m\to\infty}\tilde{K}_m(x,y)=\tilde{K}_\infty(x,y).$$

Since, by (III.15), $\exp[-\beta(H_{0,\Lambda}+U_m+V)]$ converges strongly to T_β, as $m\to\infty$, $K_\infty(x,y)$ is the kernel of T_β and $\tilde{K}_\infty(x,y)$ that of P_BT_β. If we establish the fact that $\exp[-\beta(H_{0,\Lambda}+U_m+V)]$ and $\exp(-T_\beta)$ are in the trace class, then we can use the lemma, p. 65 of [20] to obtain

$$\operatorname{tr}P_B\exp[-\beta(H_{0,\Lambda}+U_m+V)]=\int\tilde{K}_m(x,x)\,dx,$$

$$\operatorname{tr}P_B\exp(-T_\beta)=\int\tilde{K}_\infty(x,x)\,dx,$$

and therefore

$$\lim_{m\to\infty}\operatorname{tr}P_B\exp[-\beta(H_{0,\Lambda}+U_m+V)]=\operatorname{tr}P_B\exp(-T_\beta),$$

which is (A.3). In order to prove that the above operators are trace class, we may use a variant of Theorem 21.4 of [11] and reduce the problem to the case without potential and without hard core. For a cube Λ, $\exp(-\beta H_{0,\Lambda})$ is trace class by exact computation. $\square$

Appendix B

In this appendix we show that $\Delta f(\beta)\underset{\beta\downarrow0}{\sim}\beta$, where $\Delta f(\beta)$ is, for purposes of comparison, the same quantity defined in (I.1a), in the case of quantum spin systems. This follows from a trivial application of Lieb's inequalities [3]:

$$Z_\Lambda^{\mathrm{Cl}}(S)\leqq Z_\Lambda^{\mathrm{Q}}(S)\leqq Z_\Lambda^{\mathrm{Cl}}(S+1) \tag{B.1}$$

(with the same notation as [3]). In order to avoid unnecessary notational complications, assume that

$$H_\Lambda^{\mathrm{Q}}=\sum_{x,y\in\Lambda}J(x-y)\mathbf{S}_x\cdot\mathbf{S}_y, \tag{B.2}$$

with

$$\sum_{x\in\mathbb{Z}^\nu}|J(x)|<\infty \quad\text{(stability)}$$

and **S** spin operators corresponding to spin quantum number S. Then (B.1) and (B.2) together imply

$$f_A^{Cl}(\beta, S) - f_A^{Cl}(\beta, 1) \leqq f_A^Q(\beta, S) - f_A^{Cl}(\beta, 1) \equiv \Delta f(\beta)$$
$$\leqq f_A^{Cl}(\beta, S+1) - f_A^{Cl}(\beta, 1), \tag{B.3}$$

where $f_A^Q(\beta, S)$ [respectively $f_A^{Cl}(\beta, S)$] is the quantum (respectively classical) free energy per particle, defined as in (III.18). The latter corresponds to the classical Hamiltonian

$$H_A^{Cl} = \sum_{x,y \in A} J(x-y)(S\mathbf{t}_x \cdot S\mathbf{t}_y),$$

where $\mathbf{t}_x$ are three-dimensional unit vectors. From (B.3) we obtain immediately, in the thermodynamic limit

$$-c\beta|S^2 - 1| \leqq \Delta f(\beta) \leqq c\beta[(S+1)^2 - 1], \tag{B.4}$$

where $c \equiv \sum_{x \in \mathbb{Z}^\nu} |J(x)|$.

Appendix C

In this appendix we show that the high energy limit of the microcanonical entropy of an infinite system of particles in a bounded external potential is classical, by using the technique of Dirichlet-Neumann bracketing [10, Chap. XIII.15]. However, by performing the thermodynamic limit *before* the high-energy limit, we shall see that the corresponding estimates are quite different in character from those of [10, Chap. XIII.15]. We assume that

$$H_A^D = \sum_{i=1}^N h_i, \tag{C.1a}$$

$$h_i = -\Delta_i^D + v(\mathbf{x}_i), \tag{C.1b}$$

$$|v(\mathbf{x})| \leqq \alpha \quad \text{for some} \quad \alpha < \infty, \tag{C.2}$$

where Δ^D is the Laplacian with Dirichlet boundary conditions on a cube $A = [-a, a]^3$ with volume $V = (2a)^3$. We let

$$\mu(E, V, N) = \frac{1}{N!} \ (\# \text{ eigenvalues of } H_A^D \leqq E), \tag{C.3}$$

$$g(E, V, N) = \frac{\tau_{3N}}{(2\pi\hbar)^{3N} N!} \int_{\mathbf{x} \in A; v(\mathbf{x}) \leqq E} d^{3N} x (E - v_T(\mathbf{x}))^{3N/2}, \tag{C.4}$$

where τ_{3N} is the volume of the unit sphere in $3N$-dimensions, and

$$v_T(\mathbf{x}) \equiv \sum_{i=1}^N v(\mathbf{x}_i). \tag{C.5}$$

Let, also

$$\varrho = N/V, \tag{C.6}$$

$$v_{+,T}(N) \equiv \sup_{\mathbf{x} \in A^N} v_T(\mathbf{x}) = N v_{\max}, \tag{C.7a}$$

and

$$v_{-,T}(N) = \inf_{\mathbf{x} \in \Lambda^N} v_T(\mathbf{x}) = N v_{\min}, \tag{C.7b}$$

where, by (C.2)

$$v_{\max} \leqq \alpha, \tag{C.7c}$$

$$v_{\min} \geqq -\alpha. \tag{C.7d}$$

Let

$$g_{\pm}(E, V, N) = \frac{\tau_{3N}}{(2\pi\hbar)^{3N} N!} \int_{\mathbf{x} \in \Lambda; v_{\pm}^T \leqq E} d^{3N}x (E - v_{\pm,T}(N))^{3N/2}, \tag{C.8}$$

$$S(E, V, N) \equiv \frac{1}{V} \log \mu(E, V, N), \tag{C.9}$$

$$S_{\mathrm{Cl}, \pm}(E, V, N) = \frac{1}{V} \log g_{\pm}(E, V, N), \tag{C.10a}$$

$$S_{\mathrm{Cl}}(E, V, N) = \frac{1}{V} \log g(E, V, N), \tag{C.10b}$$

$$\mu_{+}(E, V, N) = \frac{1}{N!} \, (\# \text{ eigenvalues of } H_{+}^D \leqq E), \tag{C.11a}$$

$$\mu_{-}(E, V, N) = \frac{1}{N!} \, (\# \text{ eigenvalues of } H_{-}^N \leqq E), \tag{C.11b}$$

where

$$H_{+}^D \equiv -\Delta^D + v_{+,T}(N); \quad -\Delta^D \equiv \sum_{i=1}^{N} (-\Delta_i^D), \tag{C.12a}$$

$$H_{-}^N \equiv -\Delta^N + v_{-,T}(N); \quad -\Delta^N = \sum_{i=1}^{N} (-\Delta_i^N), \tag{C.12b}$$

and Δ_i^D (respectively Δ_i^N) are the Laplacians with Dirichlet (respectively Neumann) boundary conditions (defined as in [10, Chap. XIII.15]). Finally, let

$$S_{\pm}(E, V, N) = \frac{1}{V} \log \mu_{\pm}(E, V, N). \tag{C.13}$$

Proposition C.1.

$$\lim_{\varepsilon \to \infty} \lim_{\substack{N \to \infty \\ V \to \infty \\ N/V = \varrho}} \sup [(V\varepsilon, V, N) - S_{\mathrm{Cl}}(V\varepsilon, V, N)]$$

$$= \lim_{\varepsilon \to \infty} \lim_{\substack{N \to \infty \\ V \to \infty \\ N/V = \varrho}} \inf [S(V\varepsilon, V, N) - S_{\mathrm{Cl}}(V\varepsilon, V, N)] = 0. \tag{C.14}$$

Proof. We have, by Dirichlet-Neumann bracketing [10, Chap. XIII.15] and (C.11):

$$\mu_{+}(E, V, N) \leqq \mu(E, V, N) \leqq \mu_{-}(E, V, N). \tag{C.15}$$

Let $\varepsilon > \varrho_\alpha$. We have

$$\tau_{3N} = \frac{\pi^{3N/2}}{\Gamma\left(\frac{3N}{2}+1\right)} = \left(\frac{3N}{2}\right)^{-\frac{3N}{2}} \frac{(\pi e)^{3N/2}}{\sqrt{3\pi N}\,(1+o(N^{-1}))} = \left(\frac{3N}{2}\right)^{-\frac{3N}{2}} c_N, \quad \text{(C.16)}$$

$$c_N = \frac{(\pi e)^{3N/2}}{\sqrt{3\pi N}\,(1+o(N^{-1}))}. \quad \text{(C.17)}$$

We may therefore write, by (C.7):

$$\sigma(\varepsilon, V, N) \leqq g_+(E, V, N) \leqq g(E, V, N) \leqq g_-(E, V, N) \leqq \tau(\varepsilon, V, N), \quad \text{(C.18)}$$

where

$$\sigma(\varepsilon, V, N) = \frac{1}{N!}\left[\frac{V}{(2\pi\hbar)^3}\right]^N \exp\left[\frac{3N}{2}\log\left(\frac{2V}{3N}\right)\right](\varepsilon-\varrho\alpha)^{\frac{3N}{2}} c_N, \quad \text{(C.19a)}$$

$$\tau(\varepsilon, V, N) = \frac{1}{N!}\left[\frac{V}{(2\pi\hbar)^3}\right]^N \exp\left[\frac{3N}{2}\log\left(\frac{2V}{3N}\right)\right](\varepsilon+\varrho\alpha)^{\frac{3N}{2}} c_N. \quad \text{(C.19b)}$$

By (C.15) and (C.18)

$$\frac{\mu_+(E, V, N)}{g_-(E, V, N)} \leqq \frac{\mu(E, V, N)}{g(E, V, N)} \leqq \frac{\mu_-(E, V, N)}{g_+(E, V, N)}. \quad \text{(C.20)}$$

Now

$$\frac{\mu_+(E, V, N)}{g_-(E, V, N)} = \frac{\mu_+(E, V, N)/g_+(E, V, N)}{1 + \dfrac{g_-(E, V, N) - g_+(E, V, N)}{g_+(E, V, N)}}, \quad \text{(C.21)}$$

and hence, by (C.10a), (C.13), and (C.21) with $E = V\varepsilon$:

$$\frac{1}{V}\log\frac{\mu_+(E, V, N)}{g_-(E, V, N)} = S_+(E, V, N) - S_{Cl,+}(E, V, N)$$

$$- \frac{1}{V}\log\left[1 + \frac{g_-(E, V, N) - g_+(E, V, N)}{g_+(E, V, N)}\right].$$

By (C.8) and (C.2)

$$0 \leqq g_-(E, V, N) - g_+(E, V, N) \leqq \frac{3N}{2}\frac{\tau_{3N}}{(2\pi\hbar)^{3N} N!} V^{\frac{3N}{2}-1} \cdot V^N (\varepsilon+\varrho\alpha)^{\frac{3N}{2}-1} (2N\alpha),$$

and therefore

$$0 \leqq \frac{g_-(E, V, N) - g_+(E, V, N)}{g_+(E, V, N)} \leqq 3N^2\alpha V^{-1}\left(\frac{\varepsilon+\varrho\alpha}{\varepsilon-\varrho\alpha}\right)^{\frac{3N}{2}-1}(\varepsilon-\varrho\alpha)^{-1}$$

$$= 3\varrho\alpha N\left(\frac{\varepsilon+\varrho\alpha}{\varepsilon-\varrho\alpha}\right)^{\frac{3N}{2}-1}(\varepsilon-\varrho\alpha)^{-1}. \quad \text{(C.22)}$$

Hence, for sufficiently large N

$$1 + \frac{g_- - g_+}{g_+} \leqq 6\varrho\alpha N \left(\frac{\varepsilon + \varrho\alpha}{\varepsilon - \varrho\alpha}\right)^{\frac{3N}{2} - 1} (\varepsilon - \varrho\alpha)^{-1},$$

$$\frac{1}{V} \log\left(1 + \frac{g_- - g_+}{g_+}\right) \leq \frac{1}{V} \log[6\varrho\alpha N(\varepsilon - \varrho\alpha)^{-1}]$$
$$+ \left(\frac{3N}{2} - 1\right) \Big/ V \log\left(\frac{\varepsilon + \varrho\alpha}{\varepsilon - \varrho\beta}\right). \qquad (C.23)$$

By (C.20)–(C.23),

$$S(E, V, N) - S_{\text{Cl}}(E, V, N) \geqq S_+(E, V, N) - S_{\text{Cl}, +}(E, V, N)$$
$$- \frac{1}{V} \log[6\varrho\alpha N(\varepsilon - \varrho\alpha)^{-1}] - \left(\frac{3}{2}\varrho - \frac{1}{V}\right) \log\left(\frac{\varepsilon + \varrho\alpha}{\varepsilon - \varrho\alpha}\right). \qquad (C.24)$$

Similarly, from (C.20),

$$S(E, V, N) - S_{\text{Cl}}(E, V, N) \leqq S_-(E, V, N) - S_{\text{Cl}, -}(E, V, N)$$
$$+ \frac{1}{V} \log\frac{g_-(E, V, N)}{g_+(E, V, N)} \leqq S_-(E, V, N) - S_{\text{Cl}, -}(E, V, N)$$
$$+ \frac{3}{2}\varrho \log\frac{\varepsilon + \varrho\alpha}{\varepsilon - \varrho\alpha} + \frac{1}{V} \log[6\varrho\alpha N(\varepsilon - \varrho\alpha)^{-1}] \qquad (C.25)$$

by (C.18) and (C.19).

By (C.24) and (C.25) we shall have proven Proposition C.1 if we can establish that

$$\lim_{\substack{N \to \infty \\ V \to \infty \\ N/V = \varrho}} \frac{1}{V} \log\frac{\mu_\pm(V\varepsilon, V, N)}{g_\pm(V\varepsilon, V, N)} = 0. \qquad (C.26)$$
$$\varepsilon \text{ arbitrary}.$$

Proof of (C.26). a) Dirichlet-case $(+)$:

$N! \mu_+$ is the number of unit cubes with "right upper" corner inside the sphere S_r, $r = r_0 N^{5/6}$ ("Dirichlet-cubes").

$N! g_+$ is the volume of S_r:

$$N! g_+ = \frac{\tau_{3N}}{h^{3N}} r^{3N}.$$

Let $d_0 = \sqrt{3N}$ be the diagonal of a unit cube, then the sphere $S_{r - d_0}$ is completely filled with Dirichlet-cubes. Therefore

$$N! \mu_+ \geqq \frac{\tau_{3N}}{h^{3N}} (r - d_0)^{3N},$$

$$1 \leqq \frac{g_+}{\mu_+} \leqq \left(1 - \frac{d_0}{r}\right)^{-3N} = \left(1 - \frac{\sqrt{3}}{r_0} \frac{3^{1/3}}{(3N)^{1/3}}\right)^{-3N} \leqq e^{aN^{2/3}},$$

with a suitable constant a. This implies

$$\frac{1}{V}\log\frac{g_+}{\mu_+} \leqq a\frac{N^{2/3}}{V} \xrightarrow[\substack{N\to\infty \\ V\to\infty \\ N/V=\varrho}]{} 0 \,.$$

b) Neumann-case $(-)$:

$N!\,\mu_-$ is the number of unit cubes with "left lower" corner inside the sphere S_r. As above

$$N!\,\mu_- \leqq \frac{\tau_{3N}}{h^{3N}}(r+d_0)^{3N} \,,$$

$$1 \leqq \frac{\mu_-}{g_-} \leqq \left(1+\frac{d_0}{r}\right)^{3N} \leqq e^{a'N^{2/3}} \,. \qquad \square$$

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