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2005 J. Phys. A: Math. Gen. 38 6293

(http://iopscience.iop.org/0305-4470/38/28/003)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 6293–6310 doi:10.1088/0305-4470/38/28/003

Onsager's inequality, the Landau–Feynman ansatz and superfluidity

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Received 15 March 2005, in final form 1 June 2005
Published 29 June 2005
Online at stacks.iop.org/JPhysA/38/6293

Abstract

We revisit an inequality due to Onsager, which states that the (quantum) liquid structure factor has an upper bound of the form (const) $\times$ $|\vec{k}|$, for not too large modulus of the wave vector $\vec{k}$. This inequality implies the validity of the Landau criterion in the theory of superfluidity with a definite, nonzero critical velocity. We prove an auxiliary proposition for general Bose systems, together with which we arrive at a rigorous proof of the inequality for one of the very few solvable examples of an interacting Bose fluid, Girardeau's model. The latter proof demonstrates the importance of the thermodynamic limit of the structure factor, which must be taken initially at $\vec{k} \neq \vec{0}$. It also substantiates very well the heuristic density functional arguments, which are also shown to hold exactly in the limit of large wavelengths. We also briefly discuss which features of the proof may be present in higher dimensions, as well as some open problems related to superfluidity of trapped gases.

PACS numbers: 67.40.−w, 67.40.Db

1. Introduction

The properties of the Fourier transform of the pair (or density–density) correlation—in particular its extrapolation to zero angle, and the corresponding relation to the isothermal compressibility—have been thoroughly studied in connection with the critical behaviour of classical fluids (see M E Fisher's early review [1]). The situation is very different regarding the corresponding quantity—which we shall call the liquid structure factor—for quantum Bose fluids [2]. Even for the impenetrable Bose gas—a prototype of one-dimensional systems with on-site repulsion—very few results on correlation functions exist, notably on the Fourier transform of the one-particle density matrix, a mathematical tour-de-force by Lenard [3]. Some results on higher-order correlations exist as well [4], in connection with the so-called Fisher–Hartwig conjecture [5], but they are restricted to Dirichlet or Neumann boundary conditions (b.c.).

The quantum liquid structure factor plays a crucial role in the Feynman variational ansatz [6], but periodic b.c. are essential in this context, because the corresponding wavefunction must have definite momentum.

In this paper we present a rigorous proof of Onsager's inequality [2] for the liquid structure factor in the one-dimensional impenetrable Bose gas (Girardeau's model [7]). This inequality implies the validity of Landau's criterion of superfluidity [8] with a definite, nonzero critical velocity. Some features of the proof hold—others are expected to hold—in higher dimensions, as discussed in the conclusion.

2. Onsager's inequality, the Landau criterion and the Feynman ansatz: summary

Several criteria for superfluidity exist in the literature [9]. By one of the standard criteria [9], the free Bose gas is a superfluid, while by the Landau criterion (see, e.g., [8]), it is not. Landau postulated a spectrum of elementary excitations (see, e.g., figure 13.11 of [10]), which leads, by a well-known argument, to the startling property of superfluidity of the Bose fluid, i.e., the fact that under certain conditions its viscosity (e.g., of liquid He-II) vanishes, i.e., the liquid is capable of flowing without dissipation through very thin capillaries, as long as the velocity $\vec{v}$ of the liquid has an absolute value below a certain critical speed v_c:

$$|\vec{v}| \leqslant v_c. \tag{1}$$

In general, v_c increases as the diameter of the capillary decreases. See [10] or [11] as excellent introductory texts.

The Hamiltonian of a system of N particles in a cube Λ of side L, upon which periodic b.c. are imposed, may be written (we use units such that $\hbar = m = 1$, where m is the mass of the particles):

$$H_\Lambda = -\frac{1}{2}\sum_{j=1}^{N} \Delta_j + V(\vec{x}_1, \ldots, \vec{x}_N). \tag{2}$$

The momentum operator may be written as

$$\vec{P}_\Lambda = -\mathrm{i}\sum_{j=1}^{N} \nabla_j. \tag{3}$$

Above,

$$V = \sum_{1\leqslant i<j\leqslant N} \Phi(\vec{x}_i - \vec{x}_j), \tag{4}$$

where Φ is the interparticle potential, which we assume to satisfy the conditions appropriate to existence of the thermodynamic limit [12]. Let

$$U_{\vec{v}} \equiv \mathrm{e}^{\mathrm{i}\vec{v}\cdot(\vec{x}_1+\cdots+\vec{x}_N)} \tag{5a}$$

be the unitary operator which implements Galilean transformations. The operator implementing unitary Galilean transformation has actually the form

$$U_{\vec{v}}^t = \mathrm{e}^{\mathrm{i}\vec{v}\cdot[(\vec{x}_1+\cdots+\vec{x}_N)-t\vec{P}_\Lambda]}. \tag{5b}$$

However we may restrict ourselves to $t = 0$ in (5*b*), and use (5*a*) instead, just for the purpose of obtaining the transformed Hamiltonian (energy), which indeed yields the correct formula (7). The reason for the latter is that the commutator of the generator of $U_{\vec{v}}$ in (5*b*) with H_Λ is independent of t, because

$$[H_\Lambda, \vec{P}_\Lambda] = 0. \tag{6}$$

The operators are defined on the Hilbert space $\mathcal{H}_\Lambda = L^2_{\text{sym}}(\Lambda^N)$ of symmetric square integrable wavefunctions over the N-fold Cartesian product of the cube Λ with itself, satisfying periodic b.c. on Λ. We shall disregard the spin variable. We have

$$\widetilde{H}^{\vec{v}}_\Lambda \equiv U^*_{\vec{v}} H_\Lambda U_{\vec{v}} = H_\Lambda + \vec{v} \cdot \vec{P}_\Lambda + \tfrac{1}{2} N \vec{v}^2. \tag{7}$$

Suppose the fluid moves with constant velocity $\vec{v}$ with respect to some fixed inertial frame F. In the rest frame of the fluid the Hamiltonian is H_Λ, and by (6) $\widetilde{H}^{\vec{v}}_\Lambda$ is the Hamiltonian with respect to the frame F. In the rest frame of the fluid, it possesses a unique ground state Ω_Λ, with energy $E_0(N, L)$ say, and zero momentum:

$$H_\Lambda \Omega_\Lambda = E_0(N, L)\Omega_\Lambda, \tag{8a}$$

$$\vec{P}_\Lambda \Omega_\Lambda = \vec{0}. \tag{8b}$$

The fact that the ground state is simple, i.e., nondegenerate, is a property of bosons only which will be used later (see, e.g., [11] for a popular textbook account: for precise conditions on Φ in (4) see [13], where a proof is given). By (6)–(8),

$$H^{\vec{v}}_\Lambda \Omega_\Lambda = \left(E_0(N, L) + \tfrac{1}{2} N \vec{v}^2\right)\Omega_\Lambda. \tag{9a}$$

Thus the energy eigenvalue of Ω_Λ in frame F is

$$E^F_0 \equiv E_0(N, L) + \tfrac{1}{2} N \vec{v}^2. \tag{9b}$$

Because of (6), there exist common eigenstates of H_Λ and $\vec{P}_\Lambda$, which we denote by $\psi^{\vec{k}}_\Lambda$, i.e.,

$$H_\Lambda \psi^{\vec{k}}_\Lambda = E_\Lambda(\vec{k})\psi^{\vec{k}}_\Lambda, \tag{10}$$

$$\vec{P}_\Lambda \psi^{\vec{k}}_\Lambda = \vec{k}\psi^{\vec{k}}_\Lambda, \tag{11}$$

where $\vec{k} \in \Lambda^*$, and

$$\Lambda^* \equiv \left\{ \frac{2\pi}{L}\vec{n}, \vec{n} \equiv (n_1, n_2, n_3), n_i \in \mathbb{Z}, i = 1, 2, 3 \right\}. \tag{12}$$

Let $\psi^{(0),\vec{k}}_\Lambda$ be common eigenstates of H_Λ and $\vec{P}_\Lambda$ of the smallest energy above $E_0(N, L)$, which we denote by $E^\Lambda_0(\vec{k})$. Under certain conditions, seen to be realized in soluble models [7, 14, 15], it may be expected that

$$E^\Lambda_0(\vec{k}) = E_0(N, L) + \epsilon_\Lambda(\vec{k}), \tag{13}$$

where $\epsilon_\Lambda(\vec{k})$ is the energy of an 'elementary excitation' (see [15] for a better definition of this important concept, which should not be confused with 'quasiparticle'—the latter dissipate). By (7) and (13), the energy of the lowest energy excitations above the ground state in frame F is given by

$$E_0(N, L) + \epsilon_\Lambda(\vec{k}) + \vec{v} \cdot \vec{k} + \tfrac{1}{2} N \vec{v}^2. \tag{14}$$

There will be dissipation if this energy is smaller than the energy of Ω_Λ in frame F, which is given by (9b); thus, by (9b) and (14), there is no dissipation, i.e., there is superfluidity, if

$$\epsilon_\Lambda(\vec{k}) + \vec{v} \cdot \vec{k} \geqslant 0, \tag{15}$$

which is expected to hold if (1) is satisfied. This is Landau's criterion. It is satisfied (with a calculable v_c) in the two remarkable models [7, 14, 15]. Relation (15) also provides the condition for Ω_Λ to be the ground state in the moving frame.

In order to formulate Landau's criterion more precisely, we have to define the thermodynamic limit of $\epsilon_\Lambda(\vec{k})$ for any $\vec{k}$, not only those in (12). Let $\{\Lambda_n\}$ be an increasing sequence of periodic boxes,

$$\vec{k}_n \in \Lambda_n^* \qquad \text{and} \qquad \vec{k}_n \longrightarrow \vec{k} \neq \vec{0}. \tag{16a}$$

Since any real number can be expressed as a limit of rational numbers, we may define

$$\widetilde{\epsilon}(\vec{k}) = \lim_n \epsilon_{\Lambda_n}(\vec{k}_n). \tag{16b}$$

On the above-defined $\widetilde{\epsilon}(\vec{k})$ we formulate then

Assumption 1. *$\widetilde{\epsilon}(\vec{k}) > 0$ for $\vec{k} \neq \vec{0}$ is independent of the sequence in (16b) and is a continuous function of $\vec{k}$ when the limit on the rhs of (16b) exists.*

By (15), (16) and assumption 1, the following inequality holds for all $\vec{k} \in \mathbb{R}^3$:

$$\widetilde{\epsilon}(\vec{k}) + \vec{v} \cdot \vec{k} \geqslant 0. \tag{17}$$

The above may look too pedantic, but we shall see that the thermodynamic limit will play an important role later on. With the above assumptions, we shall drop the tilde on $\epsilon(\vec{k})$ from now on. We remark that assumption 1 has been proved in at least one case, that of magnons (or spin-waves) in quantum ferromagnets [16, 17].

An important attempt to 'explain' (17), i.e., to derive (17) from microscopic laws, was undertaken by Bogoliubov (see [8] for an excellent review), assuming the existence of Bose Einstein condensation (BEC). As remarked by Leggett in his beautiful review [18], 'while extremely suggestive, Bogoliubov's result referred to a dilute system, which is rather far from real-life liquid He-II'. What seems to be usually not emphasized is that Bogoliubov's model, even in the version which conserves particle number [8], is not Galilean-covariant, i.e., does not satisfy (7), and, thus, does not satisfy local mass conservation, an essential physical requirement (this seems to be well known but, for a proof, see [19]). Bogoliubov's seminal work led, however, to the genesis of an understanding of $e_0(\rho)$ (defined by (26)) through later work (see [20] and references given there). One of its important byproducts was the realization that it is the repulsive part of the potential which plays the major role in superfluidity. This is vindicated in the remarkable one-dimensional models of Girardeau [7] and Lieb and Liniger [14, 15]. The latter, however, illustrate an important fact: superfluidity is independent of BEC, because these models display superfluidity in the sense of Landau [15], but no BEC (this was proved in [3] for Girardeau's model, and is presumably also true for the Lieb–Liniger model).

As remarked by Leggett in [18], a particular successful attack on the full He-II problem (i.e., not only the dilute case) was made by Feynman [6] and Feynman–Cohen [21] (see also Lieb's remarkable early review [20]) through a variational wavefunction (in our notation (8), (10), (11)):

$$\psi_\Lambda^{\vec{k}}(\vec{x}_1, \ldots, \vec{x}_N) \equiv \sum_{i=1}^{N} \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{x}_i}\, \Omega_\Lambda(\vec{x}_1, \ldots, \vec{x}_N), \tag{18}$$

(the Feynman–Cohen ansatz [21] leads to somewhat better results, but we shall not consider it in this paper). By using partial integration, and the periodic b.c. (see, e.g., [11], exercise p 262, or [6]), we obtain

$$\frac{\langle \psi_\Lambda^{\vec{k}} | H_\Lambda \psi_\Lambda^{\vec{k}} \rangle}{\langle \psi_\Lambda^{\vec{k}} | \psi_\Lambda^{\vec{k}} \rangle} = E_0(N, L) + \mathcal{E}_\Lambda(\vec{k}), \tag{19}$$

where

$$\mathcal{E}_\Lambda(\vec{k}) \equiv \frac{N\vec{k}^2}{2\langle\psi_\Lambda^{\vec{k}}|\psi_\Lambda^{\vec{k}}\rangle} = \frac{\vec{k}^2}{2\mathcal{S}_\Lambda(\vec{k})} \tag{20}$$

and

$$\mathcal{S}_\Lambda(\vec{k}) = \frac{1}{N}\langle\psi_\Lambda^{\vec{k}}|\psi_\Lambda^{\vec{k}}\rangle = \frac{1}{N}\int_{\Lambda^N} \mathrm{d}\vec{x}_1\cdots\mathrm{d}\vec{x}_N \left|\sum_{i=1}^N \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}_i}\right|^2 \Omega_\Lambda^2(\vec{x}_1,\ldots,\vec{x}_N). \tag{21}$$

(As follows from the Perron–Frobenius theorem, Ω_Λ is unique, and may be taken to be positive [13]). Except for a factor $\rho = \frac{N}{V}$, (21) defines the liquid structure factor, which may—in the case of liquid He-II—be measured independently of the excitation spectrum, by x-ray scattering (see [10], figure 13.10).

By (21), $\mathcal{S}_\Lambda(\vec{k})$ has a direct physical interpretation: it is—for $\vec{k} \neq \vec{0}$—the Fourier transform of the pair correlation function in the ground state ([1], p 951).

Equation (18) and the min–max principle imply that, for $\vec{k} \neq \vec{0}$, (19) is an upper bound to the energies of the 'elementary excitations', i.e., the lowest eigenvalues of H_Λ which are larger than the ground state energy. The following assumption will be made:

Assumption 2. *The Feynman ansatz (18) yields a (qualitatively) good approximation to the energy of the elementary excitations.*

The above assumption is widely accepted today [18], because it is confirmed by experiment both for liquid He-II [10] and for trapped gases [22].

Assumptions 1 and 2 imply, together with (20), that

Assumption 1′. *Under (16a), the limit*

$$\mathcal{S}(\vec{k}) \equiv \lim_n \mathcal{S}_{\Lambda_n}(\vec{k}_n), \tag{22}$$

exists and is a continuous function of $\vec{k}$.

The fact that it is necessary to take the thermodynamic limit with $\vec{k} \neq \vec{0}$ is shown in appendix A for the free Bose gas: the limits $\vec{k} \to \vec{0}$ and the thermodynamic limit do not commute. This procedure also has a physical reason: it is necessary to eliminate the (infinite) forward scattering peak, i.e., by considering $\vec{k} \neq \vec{0}$, before probing the density–density correlations for the infinite system ([1], p 951).

2.1. Onsager's inequality

Inequality (23) (with condition (24)) will be referred to as Onsager's inequality [2]:

$$\mathcal{S}(\vec{k}) \leqslant c|\vec{k}|, \qquad \vec{k} \neq \vec{0}, \tag{23}$$

where

$$0 < c < \infty \tag{24}$$

is a constant independent of N, L, but possibly dependent on ρ.

We see from the above definition that Onsager's inequality, taken together with Feynman's ansatz (assumption 2 and (18)) implies Landau's condition (17), with v_c (defined by (1)) given by

$$v_c = (2c)^{-1}. \tag{25}$$

For the free Bose gas $S_\Lambda(\vec{k})$, given by (21), equals 1 (see (A.2) of appendix A), which is, of course, necessary in order to be compatible with (20).

Let $e_0(\rho)$ denote the ground-state energy per particle in the thermodynamic limit

$$e_0(\rho) = \lim_{L\to\infty} \frac{E_0(\rho L^3, L)}{(\rho L^3)}. \tag{26}$$

By [12] $e_0(\rho)$ is a convex function of ρ. Thus, when $e_0''(\rho) \equiv \mathrm{d}^2 e_0(\rho)/\mathrm{d}\rho^2$ exists,

$$e_0''(\rho) \geqslant 0.$$

We assume that

$$0 < e_0''(\rho) < \infty. \tag{27}$$

Equations (23) and (24) constitute a precise formulation of Onsager's inequality [2], with

$$c \equiv \left(\frac{1}{\rho e_0''(\rho)}\right)^{1/2}. \tag{28}$$

Note that (24) and (28) are consistent due to (27) if we assume $0 < \rho < \infty$ which we do henceforth.

In this paper we derive (23) and (24) for a soluble model, Girardeau's model [7], defined in section 4, which is believed to be a prototype of a class of one-dimensional Bose fluids with pointwise repulsive interactions. We believe that several aspects of the derivation are relevant to higher dimensions and discuss this in section 5. In particular, proposition 1 of section 3 is of general validity, as shown in [2]. Our derivation in section 3 'rounds off' some points left over in [2], such as emphasizing the important role of nondegeneracy of the ground state—which leads to nondegenerate perturbation theory—and the vanishing of some mixed terms (36). In section 4 we conclude the proof of (23) and (24) for Girardeau's model.

It is important to realize the intrinsically nonperturbative nature (in $\vec{k}$) of the bound (23) on $\mathcal{S}_\Lambda(\vec{k})$ in the thermodynamic limit. Writing in (21),

$$\left|\sum_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}_i}\right|^2 = 1 + \sum_{\substack{i,j=1\\ i\neq j}}^{N} \mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{x}_i - \vec{x}_j)}, \tag{29}$$

it becomes clear that the double sum above would contribute a term $O(N^2)/N = O(N)$ to $\mathcal{S}_\Lambda(\vec{k})$ if the configurations $\vec{x}_i \approx \vec{x}_j, \forall i \neq j$ were not suppressed: due to the strong repulsion at short distances, such configurations are highly improbable in $\Omega(\vec{x}_1, \ldots, \vec{x}_N)$ (think of hard cores). But the linear term in the perturbative expansion (in $\vec{k}$) of (29) is identically zero by symmetry, thus suggesting $\mathcal{S}_\Lambda(\vec{k}) = O(|\vec{k}|^2)$!

3. Proof of an auxiliary proposition

We now provide a proof of an auxiliary proposition (proposition 1). The derivation in [2] is incomplete in some details. Let $P_{0,\Lambda}$ denote the projector onto the orthogonal complement $\Omega_\Lambda^\perp$ of the unique ground state Ω_Λ, $\psi_\Lambda^{(\vec{k})}$ be given by (18), and

$$A_\Lambda \equiv P_{0,\Lambda}(H_\Lambda - E_0(N, L))^{1/2} P_{0,\Lambda}, \tag{30}$$

$$B_\Lambda \equiv P_{0,\Lambda}(H_\Lambda - E_0(N, L))^{-1/2} P_{0,\Lambda}. \tag{31}$$

Since, by (8) and (18), $\psi_\Lambda^{\vec{k}}$ is an eigenfunction of $\vec{P}_\Lambda$ with eigenvalue $\vec{k}$, and $\vec{k} \neq \vec{0}$, $\psi_\Lambda^{\vec{k}} \in P_{0,\Lambda}\mathcal{H}_\Lambda$, and thus, by the Schwarz inequality

$$\langle\psi_\Lambda^{\vec{k}}|\psi_\Lambda^{\vec{k}}\rangle^2 = \langle A_\Lambda\psi_\Lambda^{\vec{k}}|B_\Lambda\psi_\Lambda^{\vec{k}}\rangle^2 \leqslant \langle A_\Lambda\psi_\Lambda^{\vec{k}}|A_\Lambda\psi_\Lambda^{\vec{k}}\rangle\langle B_\Lambda\psi_\Lambda^{\vec{k}}|B_\Lambda\psi_\Lambda^{\vec{k}}\rangle \tag{32}$$

but

$$\begin{aligned}\langle A_\Lambda\psi_\Lambda^{\vec{k}}|A_\Lambda\psi_\Lambda^{\vec{k}}\rangle &= \langle P_{0,\Lambda}\psi_\Lambda^{\vec{k}}|(H_\Lambda - E_0(N,L))P_{0,\Lambda}\psi_\Lambda^{\vec{k}}\rangle\\ &= \langle\psi_\Lambda^{\vec{k}}|(H_\Lambda - E_0(N,L))\psi_\Lambda^{\vec{k}}\rangle\\ &= N\frac{\vec{k}^2}{2}\end{aligned} \tag{33}$$

by partial integration and use of the periodic b.c. We also have that

$$\begin{aligned}\langle B_\Lambda\psi_\Lambda^{\vec{k}}|B_\Lambda\psi_\Lambda^{\vec{k}}\rangle &= \langle\psi_\Lambda^{\vec{k}}|(H_\Lambda - E_0(N,L))^{-1/2}P_{0,\Lambda}(H_\Lambda - E_0(N,L))^{-1/2}\psi_\Lambda^{\vec{k}}\rangle\\ &= \langle\Omega_\Lambda|W_N^{\vec{k}\,*}(H_\Lambda - E_0(N,L))^{-1}P_{0,\Lambda}W_N^{\vec{k}}\Omega_\Lambda\rangle.\end{aligned} \tag{34}$$

In (34), $W_N^{\vec{k}}$ is the multiplication operator

$$\left(W_N^{\vec{k}}\varphi\right)(\vec{x}_1,\ldots,\vec{x}_N) = \sum_{i=1}^N e^{i\vec{k}\cdot\vec{x}_i}\varphi(\vec{x}_1,\ldots,\vec{x}_N). \tag{35}$$

We now write $W_N^{\vec{k}} = \sum_{i=1}^N \cos(\vec{k}\cdot\vec{x}_i) + i\sum_{i=1}^N \sin(\vec{k}\cdot\vec{x}_i)$ in (34). For finite N, L, $(H_\Lambda - E_0(N,L))$ has a nonzero lower bound on $P_{0,\Lambda}\mathcal{H}_\Lambda$, and insertion of a basis of eigenstates $|\phi_i\rangle$ of $(H_\Lambda - E_0(N,L))$ in $P_{0,\Lambda}\mathcal{H}_\Lambda$ is rigorously justified because Ω_Λ is a normalized state. Furthermore, because H_Λ is a real operator, we may choose this basis of eigenstates $|\phi_i\rangle$ as consisting of real functions. The 'mixed terms' in (34)

$$\sum_j \frac{-i}{E_j - E_0}\langle\Omega_\Lambda|\sum_{i=1}^N \sin(\vec{k}\cdot\vec{x}_i)|\phi_j\rangle\langle\phi_j|\sum_{i=1}^N \cos(\vec{k}\cdot\vec{x}_i)|\Omega_\Lambda\rangle \tag{36a}$$

and

$$\sum_j \frac{i}{E_j - E_0}\langle\phi_j|\sum_{i=1}^N \cos(\vec{k}\cdot\vec{x}_i)|\Omega_\Lambda\rangle\langle\Omega_\Lambda|\sum_{i=1}^N \sin(\vec{k}\cdot\vec{x}_i)|\phi_j\rangle \tag{36b}$$

thus add to zero, and we obtain from (34) and analytic perturbation theory [23]:

Proposition 1.

$$\langle\psi_\Lambda^{\vec{k}}|\psi_\Lambda^{\vec{k}}\rangle^2 \leqslant \frac{N\vec{k}^2}{2}\langle B_\Lambda\psi_\Lambda^{\vec{k}}|B_\Lambda\psi_\Lambda^{\vec{k}}\rangle \tag{37a}$$

where

$$\langle B_\Lambda\psi_\Lambda^{\vec{k}}|B_\Lambda\psi_\Lambda^{\vec{k}}\rangle = \frac{1}{2}\left(-\frac{\partial^2}{\partial\lambda^2}E_{0,1}(N,L,\lambda)\right)_{\lambda=0} + \frac{1}{2}\left(-\frac{\partial^2}{\partial\lambda^2}E_{0,2}(N,L,\lambda)\right)_{\lambda=0} \tag{37b}$$

Above, $E_{0,1}(N,L,\lambda)$ is the ground-state energy of the Hamiltonian

$$H_\Lambda^{(1)}(\lambda) \equiv H_\Lambda - E_0(N,L) + \lambda\sum_{i=1}^N \cos(\vec{k}\cdot\vec{x}_i) \tag{38a}$$

and $E_{0,2}(N,L,\lambda)$ is the ground-state energy of the Hamiltonian

$$H_\Lambda^{(2)}(\lambda) \equiv H_\Lambda - E_0(N,L) + \lambda\sum_{i=1}^N \sin(\vec{k}\cdot\vec{x}_i). \tag{38b}$$

By (34) and the argument following it the two quantities on the rhs of (37) are also the second-order energy terms in analytic perturbation theory [23, 24]. The boson nature of the particles is used to the sole extent that the ground state is nondegerate [13]. The radius of convergence of the perturbation series in λ is expected to tend to zero as $(1/N)$, for our N-particle system, but this is no source of trouble as long as λ is taken to go to zero in (37) for fixed, finite N and L. What is remarkable in (37) and (38) is the fact that the perturbation is an external potential.

4. Onsager's inequality and Girardeau's model

A heuristic but appealing argument due to Onsager (see [2] and appendix B) yields

$$\lim_{\substack{N\to\infty \\ L\to\infty \\ \frac{N}{L^3}=\rho}} \left[\frac{1}{N}\langle B_\Lambda \psi_\Lambda^{\vec{k}} | B_\Lambda \psi_\Lambda^{\vec{k}}\rangle\right] \leqslant c_1 \tag{39}$$

where

$$c_1 \equiv \frac{1}{\rho e_0''(\rho)} \tag{40}$$

whenever the limit on the lhs of (39) exists. Putting together (21), (32), (33), (39) and (40), we arrive at (25) and (28) with $c = (c_1/2)^{1/2}$.

Other arguments (see, e.g., (A.97)–(A.103) of [10], 'longitudinal sum rules') which yield $\mathcal{S}(\vec{k}) \sim c|\vec{k}|$ for $|\vec{k}|$ sufficiently small, all depend on the argument in appendix B. This is a density-functional type of argument, which, in general, is not generally justifiable for fermions, whenever the ground state is degenerate [25]. For bosons, the ground state is nondegenerate, and density-functional theory looks the same as for fermions, but it has been rigorously established recently that, even in the dilute limit, a semiclassical description of bosons is impossible (see, e.g., [26], remarks after (2.12)). Thus, the derivation of (39) and (40) given in [2] (a somewhat better version of which, with corrections, is given in appendix B) is conceptually open to question. But, perhaps most importantly, the derivation has a 'miraculous' character, because in (34) the contribution of intermediate states is expected to yield (const) $\times\, |\vec{k}|^{-1}$ due to the denominator $(H_\Lambda - E_0(N, L))^{-1}$ and the fact that the lowest states are expected to have energy $\epsilon_\Lambda(\vec{k}) \sim c|\vec{k}|$ above the ground state! These matters are dealt with in a different way in the appendix of [21]: there, the argument relies on the study of the terms of a perturbation theory which likely diverges.

We now examine (39) and (40) in the light of one of the very few soluble models of a superfluid, the Girardeau model (the Lieb–Liniger model [14, 15] is expected to yield similar results). We shall see that the results confirm (39) and (40) surprisingly well, and formula (B.11), derived from density functional theory, holds exactly, in the limit $\vec{k} \to \vec{0}$.

We start by the Hamiltonian of the Lieb–Liniger model [14]

$$H_{N,L}^d = -\frac{1}{2}\sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + 2d \sum_{1\leqslant i<j\leqslant N} \delta(x_i - x_j) \tag{41}$$

with $d > 0$, with periodic b.c. on a box of length L. In the limit $d \to \infty$ one obtains a model of impenetrable bosons, with the impenetrable core shrunk to a point, previously treated by Girardeau [7], and called Girardeau's model. Both models exhibit two branches of Bogoliubov excitations which satisfy Landau's criterion [15], and which recently have been seen experimentally [27]. Since the results on Girardeau's model may be obtained from the Lieb–Liniger model (41) by continuity as $d \to \infty$ [14, 15], we expect that our results are also true for the richer model (41), and are, thus, prototypical of this class of models.

One of the basic features of Girardeau's model is that, due to the repulsive interaction, the system acquires a finite compressibility (proportional to $(e_0''(\rho))^{-1}$), in contrast to the free Bose gas, for which, e.g., with Dirichlet b.c.,

$$E_0(\rho L^3, L) = f\rho L$$

where f is a constant, and thus, by (28), $e_0(\rho) = 0$ for all ρ. Thus $e_0''(\rho)$ is also identically zero, i.e., $c_1 = +\infty$ in (39) and (40). Thus inequality (23) (with c given by (28)) is trivially true by (A.2).

Performing the limit $d \to \infty$ on (41) is equivalent to impose the subsidiary condition:

$$\psi(x_1, \ldots, x_N) = 0 \qquad \text{if} \qquad x_j = x_l, \quad 1 \leqslant j < l \leqslant N. \tag{42}$$

The Bose eigenfunctions ψ^B satisfying (42) and periodic b.c. with period L are given [7] as

$$\psi^B = \psi^F \mathcal{A} \tag{43a}$$

where

$$\mathcal{A}(x_1, \ldots, x_N) = \prod_{j>l} \operatorname{sgn}(x_j - x_l). \tag{43b}$$

Above, $\operatorname{sgn}(x)$ is the algebraic sign of x, and ψ^F are Fermi energy eigenfunctions satisfying (42), which are just the eigenfunctions of a free Fermi gas. For odd N we fill the 'Fermi sphere'

$$-\tfrac{1}{2}(N-1) \leqslant p \leqslant \tfrac{1}{2}(N-1) \tag{44}$$

and the ground-state energy is

$$E_0(N, L) = \sum_{p=1}^{\frac{1}{2}(N-1)} \left(\frac{2\pi p}{L}\right)^2 = \frac{1}{6}(N - N^{-1})(\pi\rho)^2. \tag{45}$$

Thus the ground-state energy density in the thermodynamic limit equals

$$e_0(\rho) = \tfrac{1}{6}\pi^2\rho^3 \tag{46}$$

and thus

$$e_0''(\rho) = \pi^2\rho \tag{47}$$

which satisfies (27).

By (37), (38), (44) $\langle B_\Lambda \psi_\Lambda^k | B_\Lambda \psi_\Lambda^k \rangle$ may be calculated by the formula (N odd)

$$\langle B_\Lambda \psi_\Lambda^k | B_\Lambda \psi_\Lambda^k \rangle = \frac{1}{2}\left\{\left(-\frac{\partial^2}{\partial\lambda^2} E_{0,1}(N, L, \lambda)\right)_{\lambda=0} + \left(-\frac{\partial^2}{\partial\lambda^2} E_{0,2}(N, L, \lambda)\right)_{\lambda=0}\right\} \tag{48}$$

$$E_{0,1}(N, L, \lambda) = \sum_{p=-\frac{1}{2}(N-1)}^{\frac{1}{2}(N-1)} E_1(p, \lambda) \tag{49}$$

$$E_{0,2}(N, L, \lambda) = \sum_{p=-\frac{1}{2}(N-1)}^{\frac{1}{2}(N-1)} E_2(p, \lambda) \tag{50}$$

where $E_1(p, \lambda)$ are the energy levels of the one-particle Hamiltonian

$$H = H_0 + \lambda H_1 \tag{51}$$

with

$$H_0 = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{52}$$

and

$$H_1 = \cos(kx) \tag{53}$$

on $\mathcal{H} = L^2_{\text{per}}[0, L]$, with $k \in \Lambda^* = \left\{\frac{2\pi}{L}n, n \in \mathbb{Z} \setminus \{0\}\right\}$ and the zeroth-order level of H_0 corresponding to $E_1(p, \lambda)$ is

$$E_1^{(0)}(p) = \frac{1}{2}\left(\frac{2\pi p}{L}\right)^2 \tag{54}$$

with p satisfying (44). The levels $E_2(p,\lambda)$ are the same, just replacing H_1 by $H_2 = \sin(kx)$. The level $p = 0$ of H_0 is nondegenerate, all the others in (44) are doubly degenerate, with energies (54) and eigenfunctions

$$\varphi_{p,\alpha=1} = \frac{1}{\sqrt{L}}\,\mathrm{e}^{\mathrm{i}\frac{2\pi p}{L}x}, \qquad \varphi_{p,\alpha=2} = \frac{1}{\sqrt{L}}\mathrm{e}^{-\mathrm{i}\frac{2\pi p}{L}x}; \qquad p \in \left\{1, 2, \ldots, \frac{N-1}{2}\right\}. \tag{55}$$

By Kato degenerate perturbation theory [23], ([24], (10.88)) we find the levels up to second order by solving the equation

$$\det\left\{\lambda\langle\varphi_{p,\beta}|H_1|\varphi_{p,\alpha}\rangle + \lambda^2\langle\varphi_{p,\beta}|H_1 S_p H_1|\varphi_{p,\alpha}\rangle - \left(E_1(p,\lambda) - E_1^{(0)}\right)\delta_{\beta,\alpha}\right\} = 0 \tag{56}$$

where

$$S_p \equiv \frac{Q_p^{(0)}}{E_1^{(0)}\mathbb{I} - H_0}, \qquad Q_p^{(0)} = \mathbb{I} - P_p^{(0)} \tag{57}$$

and

$$P_p^{(0)} = |\varphi_{p,1}\rangle\langle\varphi_{p,1}| + |\varphi_{p,2}\rangle\langle\varphi_{p,2}|. \tag{58}$$

Using (55), (57) and (58) and plane-waves as intermediate states to calculate the second term in (56), we find that equation (56) may be written as

$$\det\begin{pmatrix} a-\mu & c \\ c & a-\mu \end{pmatrix} = 0 \tag{59}$$

with

$$\mu \equiv E_1(p,\lambda) - E_1^{(0)} \tag{60}$$

$$a = \frac{-\lambda^2}{k^2 - 4\left(\frac{2\pi}{L}p\right)^2}\delta_{\frac{2\pi}{L}p \neq \frac{k}{2}} \tag{61}$$

$$c = \frac{\lambda}{2}\delta_{k,\frac{4\pi}{L}p} + \frac{\lambda^2}{4\varepsilon_k}\delta_{\frac{2\pi}{L}p,k}; \qquad \varepsilon_k = \frac{k^2}{2}. \tag{62}$$

The discriminant of (59) is $4a^2 - 4(a^2 - c^2) = 4c^2 > 0$, and thus the eigenvalues for μ are

$$\mu_\pm = a \pm c. \tag{63}$$

The cases $p = 0$, $\frac{2\pi p}{L} = k$, and $\frac{2\pi p}{L} = \frac{k}{2}$ are isolated values which by (48) and (49) do not affect the thermodynamic limit on the lhs of (39). Disregarding these, we see by (63) that the eigenvalues remain doubly degenerate and equal to a, given by (61). Thus, by (48), (49) and (61), and the fact that the second term in (48) is equal to the first, which may be proved, we find

$$e_\Lambda(k) \equiv \frac{1}{N}\left\langle B_\Lambda\psi_\Lambda^k\middle|B_\Lambda\psi_\Lambda^k\right\rangle = 4\left(\frac{L}{2\pi N}\right)\left(\frac{2\pi}{L}\right)\sum_{\substack{p=-\frac{1}{2}(N-1)\\ p\neq 0\\ \frac{2\pi p}{L}\neq\pm\frac{k}{2}}}^{\frac{1}{2}(N-1)} \frac{1}{k^2 - 4\left(\frac{2\pi p}{L}\right)^2}. \tag{64}$$

Clearly the rhs of (64) has a natural extension $\widetilde{e}_\Lambda(k)$ to all $k \neq 0$, obtained by interpreting k in (64) as a real variable. We now find, from (64), the following proposition proved in appendix C:

Proposition 2.

$$\widetilde{e}(k) \equiv \lim_{\substack{N\to\infty\\ L\to\infty\\ \frac{N}{L}=\rho}} \widetilde{e}_\Lambda(k) = \frac{4}{2\pi\rho}Pv\int_{-\pi\rho}^{\pi\rho}\frac{1}{k^2 - 4x^2}\,\mathrm{d}x. \tag{65}$$

Remark 1. The principal value on the rhs of (65) may computed, with the result

$$Pv\int_{-\pi\rho}^{\pi\rho}\frac{1}{k^2-4x^2}\,\mathrm{d}x=\frac{1}{|k|}\operatorname{arccoth}\left(\frac{2\pi\rho}{|k|}\right). \tag{66}$$

The limit $k\to 0$ on the rhs of (66) can be performed by l'Hôpital's rule or more simply by noting that $\operatorname{arccoth}(2\pi\rho/|k|)\approx|k|/2\pi\rho$, so that

$$\lim_{k\to 0}\frac{1}{|k|}\operatorname{arccoth}\left(\frac{2\pi\rho}{|k|}\right)=\frac{1}{2\pi\rho}. \tag{67}$$

We finally have

Theorem 1. *For Girardeau's model, under assumption 1′ $\mathcal{S}(k)$ satisfies Onsager's inequality (23) and (24), with*

$$c=\frac{1}{\sqrt{2}}\frac{1}{\pi\rho}t \tag{68a}$$

where

$$t\simeq 1.0481. \tag{68b}$$

Proof. By proposition 2, for any sequence $\{\Lambda_n\}$ of periodic boxes, the limit $\lim_n e_{\Lambda_n}(k)$ is a continuous function of $k\in[0,\pi\rho]$ and it follows from appendix C that the convergence $\widetilde{e}_\Lambda(k)\to\widetilde{e}(k)$ is uniform in Λ for k in compact subsets of $(0,\pi\rho]$, i.e., not containing the origin. Thus, by (16a) and assumption 1', for all $k\neq 0$,

$$\begin{aligned}\mathcal{S}_\Lambda(k)&=\lim_n S_{\Lambda_n}(k_n)\leqslant\frac{k}{\sqrt{2}}\lim_n e_{\Lambda_n}(k_n)=\frac{k}{\sqrt{2}}\lim_n\widetilde{e}_{\Lambda_n}(k_n)\\&=\frac{k}{\sqrt{2}}\lim_n\widetilde{e}_{\Lambda_n}(k)=\frac{k}{\sqrt{2}}\widetilde{e}(k)\leqslant c|k|\end{aligned} \tag{69}$$

where

$$c\equiv\sup_{k\in[-\pi\rho,\pi\rho]}\left\{\frac{1}{\sqrt{2}}\sqrt{\frac{2}{\pi\rho|k|}\operatorname{arccoth}\left(\frac{2\pi\rho}{|k|}\right)}\right\}=\frac{1}{\sqrt{2}}\frac{1}{\pi\rho}t \tag{70}$$

where $t\simeq 1.0481$, corresponding to the value $k=\pi\rho$, by appendix D. This is Onsager's inequality (23), (24), with c given by (68). □

Remark 2. The result of density functional theory (appendix B) holds as an equality, only in the limit $k\to 0$, because, from (65), (66) and (67)

$$\lim_{k\to 0}\lim_{\substack{N\to\infty\\ L\to\infty\\ \frac{N}{L}=\rho}}\left[\frac{1}{N}\langle B_\Lambda\psi_\Lambda^k|B_\Lambda\psi_\Lambda^k\rangle\right]=\frac{1}{(\pi\rho)^2} \tag{71}$$

which agrees with (B.11). However, from appendix D, we see that (B.11) holds in very good approximation for all k. We shall comment on the reasons for that *a priori* unexpected behaviour in the conclusion.

Remark 3. Equations (64) and (65) show explicitly the importance of performing the limit $k\to 0$ after the thermodynamic limit. Indeed, putting $k=0$ in (64) we obtain a Pv on the rhs which diverges. More precisely, the proof of proposition 2 given in appendix C becomes invalid.

5. Conclusions and outlook

The Feynman variational ansatz is widely accepted today [18]. There is a good reason for that: when compared with experiment, it leads to the famous phonon–roton spectrum of superfluid ^{4}He (see, e.g., figure 13.11 of [10]). The ansatz is only expected to hold for not too large $|\vec{k}|$ ($|\vec{k}| \leqslant k_c \approx 3.5$ Å^{-1}), becoming unstable with respect to the decay into several other types of excitations with lower energies [28]. It is also well established for trapped gases [22].

In this paper we assumed the validity of the ansatz (assumption 3) and attempted to derive a precise connection between it and Landau's criterion of superfluidity (17). This is achieved through the use of Onsager's inequality (23) and (24), whose first part was proved in section 3, proposition 1, which 'rounds off' the 'almost rigorous proof' (see [20]) presented in [2]. The second part was proved in section 4, proposition 2 and theorem 1, for Girardeau's model, a prototype of a one-dimensional Bose fluid with pointwise repulsive interactions. Some features of this proof—in particular the importance of taking $k \to 0$ only after the thermodynamic limit and the role of the one-site repulsion to guarantee the existence of the latter—will be present in higher dimensions. Indeed, as remarked by Lieb in [15], the fact that "the potential is effectively a kinetic energy barrier for large $\gamma = d/\rho$ (where d is defined by (41))—a result that also holds in three dimensions—means that it is really immaterial to the particles whether they can 'get around each other' or merely 'through each other'." The double spectrum predicted in [15] has been found experimentally [27], substantiating the above conjectures to some extent.

For trapped gases, a recent remarkable proof establishes superfluidity according to one of the standard criteria [29]. The latter is, however—as asserted by the authors of [29]—also satisfied by the free Bose gas—in contrast to the Landau criterion. The criteria are therefore inequivalent and it should therefore be most interesting to prove (23) and (24) for trapped gases, in the limit considered in [26] (a review where further references can be found) by which the range of the potential also tends to zero. A first step is the result ([26], remarks after theorem 7.1, in particular (7.2), (7.3) and (7.4)) that there is 100% condensation for all n-particle reduced density matrices, and ([26], corollary 7.2) (convergence of momentum distribution for the one-particle density matrix), but the momentum behaviour of the two-particle density matrix remains to be studied.

It seems rather difficult to show (23) and (24) directly for Girardeau's model: a study of correlation functions in the model is at present restricted to Dirichlet and Neumann b.c. [4]. Thus, our bound for $\mathcal{S}_\Lambda(\vec{k})$ (with periodic b.c.) is new even for Girardeau's model.

Finally, it is gratifying that our result (69) agrees exactly with (B.11) of density-functional theory in the limit $k \to 0$, because the latter is, in a sense, like the Thomas–Fermi theory, of semiclassical nature, which is then expected to hold in the limit of large wavelengths. However, appendix D even shows excellent agreement for all $k \in [-\pi\rho, \pi\rho]$, which may be intuitively understood from (37) (proposition 1) whereby the lhs of (B.11) depends only on the variation of certain energies with respect to the interaction with an external field. The latter is taken care of exactly in density functional theory (first term on the rhs of (B.3)) and is thus a very special case, which is not affected by the problems pointed out in [25] and ([26], remarks after (2.12)). Since the arguments in appendix B are independent of the dimension, this agreement is very strong evidence that (23) and (24) hold for any dimension.

Acknowledgments

One of us (WW) is very grateful to Ph A Martin and V A Zagrebnov for fruitful discussions, and, in particular, to Ph A Martin for emphasizing the importance of taking the limit (23) for $\vec{k} \neq \vec{0}$. We also thank the referees for valuable critical comments. WFW was partially supported by CNPq. MAdaS was supported by a grant from CNPq.

Appendix A

In this appendix we study the liquid structure factor (21) for the free Bose gas, where

$$\Omega_\Lambda = \frac{1}{L^{3/2}} \otimes \cdots \otimes \frac{1}{L^{3/2}}.$$

For $\vec{k} \neq \vec{0}$

$$\begin{aligned} \mathcal{S}_\Lambda(\vec{k}) &= \frac{1}{NL^{3N}} \int_{\Lambda^N} \mathrm{d}\vec{x}_1 \cdots \mathrm{d}\vec{x}_N \left| \sum_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}_i} \right|^2 \\ &= 1 + \frac{1}{NL^{3N}} \sum_{1\leqslant i\neq j\leqslant N} \int_{\Lambda^N} \mathrm{d}\vec{x}_1 \cdots \mathrm{d}\vec{x}_N \, \mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{x}_i - \vec{x}_j)} \\ &= 1 + \frac{N(N-1)}{NL^{3N}} L^{3(N-2)} \int_{\Lambda^2} \mathrm{d}\vec{x}_1 \, \mathrm{d}\vec{x}_2 \, \mathrm{e}^{-\mathrm{i}\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)} \\ &= 1 + (N-1)L^{-6} \left(\int_\Lambda \mathrm{d}\vec{x} \, \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}} \right)^2. \end{aligned} \tag{A.1}$$

By (A.1)

$$\mathcal{S}_\Lambda(\vec{k}) = 1 \qquad \text{if} \quad \vec{k} \neq \vec{0}, \quad \vec{k} \in \Lambda^* \tag{A.2}$$

while

$$\mathcal{S}_\Lambda(\vec{0}) = N \qquad \text{if} \quad \vec{k} = \vec{0}. \tag{A.3}$$

Thus,

$$\lim_{\substack{N\to\infty \\ L\to\infty \\ \frac{N}{L^3}=\rho}} \mathcal{S}_\Lambda(\vec{0}) = +\infty. \tag{A.4}$$

Equations (A.2)–(A.4) show that it is crucial to take the thermodynamic limit with $\vec{k} \neq \vec{0}$, and only thereafter the limit $\vec{k} \to \vec{0}$, in order to find the behaviour of the liquid structure factor for large wavelength. Note that (A.2) must hold in order to be compatible with (20) in the free case.

Appendix B

In this appendix we present in some detail a more precise, albeit nonrigorous, variant of Onsager's derivation of (39) and (40) [2]. Note that there are misprints and some incorrectness in the derivation in [2].

By the variational principle, for the Hamiltonian (38*a*) ((38*b*) is, of course, treated the same way); the ground-state energy is

$$E(N, L, \lambda) = \inf_\psi \langle \psi | H_\Lambda^{(1)}(\lambda)\psi \rangle. \tag{B.1}$$

In (B.1), ψ are normalized test functions, for N bosons in a periodic cube Λ of side L. Each test function corresponds to a test-one-particle density

$$\rho(\vec{x}) = N \int_{\Lambda^N} \mathrm{d}\vec{x}_2 \, \mathrm{d}\vec{x}_3 \cdots \mathrm{d}\vec{x}_N |\psi(\vec{x}, \vec{x}_2, \ldots, \vec{x}_N)|^2. \tag{B.2}$$

We compute the infimum (B.1) in two steps [25]: first, we *fix* a test-function $\rho(\vec{x})$ and denote by $\{\psi_\rho^\alpha\}_\alpha$ the class of test functions with this ρ. Define the constrained energy minimum, with fixed ρ, as

$$E_\Lambda\{\rho\} \equiv \inf_\alpha \langle \psi_\rho^\alpha | H_\Lambda^{(1)}(\lambda) \psi_\rho^\alpha \rangle = \int_\Lambda v_\lambda(\vec{x}) \rho(\vec{x})\, \mathrm{d}\vec{x} + F_\Lambda\{\rho\} \tag{B.3}$$

where

$$v_\lambda(\vec{x}) \equiv \lambda \cos(\vec{k} \cdot \vec{x}) \tag{B.4}$$

and

$$F_\Lambda\{\rho\} \equiv \inf_\alpha \langle \psi_\rho^\alpha | H_\Lambda - E_0(N, L) | \psi_\rho^\alpha \rangle \tag{B.5}$$

is a universal functional of the density. In the second stage, we find the infimum over all ρ:

$$E_0(N, L, \lambda) = \inf_\rho E_\Lambda\{\rho\}. \tag{B.6}$$

Let $\rho_\lambda^\Lambda(\vec{x})$ correspond to the infimum in (B.6), and $\rho^\Lambda(\vec{x})$ to the infimum in (B.6) for $\lambda = 0$, which we assume are attained in a suitable space.

By the definition (28) of e_0, it is reasonable to assume from (B.5), for large Λ, that

$$F_\Lambda\{\rho\} = \int_\Lambda \left[e_0\{\rho_\lambda^\Lambda(\vec{x})\} - e_0\{\rho^\Lambda(\vec{x})\}\right] \mathrm{d}\vec{x} \tag{B.7}$$

for some functional $e_0\{\rho\}$, such that in the thermodynamic limit $\rho^\Lambda(\vec{x}) \to \rho$, and $e_0(\rho)$ is given by (28). By (B.3), (B.4), (B.6) and (B.7):

$$\begin{aligned} E_0(N, L, \lambda) &\equiv \int_\Lambda \mathrm{d}\vec{x} \left[e_0\{\rho_\lambda^\Lambda(\vec{x})\} - e_0\{\rho^\Lambda(\vec{x})\}\right] + \lambda \int_\Lambda \mathrm{d}\vec{x}\, \rho_\lambda^\Lambda(\vec{x}) \cos(\vec{k} \cdot \vec{x}) \\ &\cong \frac{1}{2} e_0''(\rho) \int_\Lambda \mathrm{d}\vec{x} \left[\rho_\lambda^\Lambda(\vec{x}) - \rho^\Lambda(\vec{x})\right]^2 + \lambda \int_\Lambda \mathrm{d}\vec{x}\, \rho_\lambda^\Lambda(\vec{x}) \cos(\vec{k} \cdot \vec{x}) \end{aligned}$$

for Λ 'sufficiently large' and λ 'sufficiently small'. Equating the functional derivative with respect to ρ_λ^Λ in (B.8) to find the minimum, we obtain, under assumption (29)

$$e_0''(\rho)\left[\rho_\lambda^\Lambda(\vec{x}) - \rho^\Lambda(\vec{x})\right] + \lambda \cos(\vec{k} \cdot \vec{x}) = 0$$

and

$$\rho_\lambda^\Lambda(\vec{x}) - \rho^\Lambda(\vec{x}) = -\frac{\lambda}{e_0''(\rho)} \cos(\vec{k} \cdot \vec{x}). \tag{B.9}$$

Inserting (B.9) into (B.8) we find for the actual minimum value

$$\begin{aligned} E_0(N, L, \lambda) = \frac{\lambda^2}{2} (e_0''(\rho))^{-1} \int_\Lambda \mathrm{d}\vec{x} \cos^2(\vec{k} \cdot \vec{x}) - \lambda^2 (e_0''(\rho))^{-1} \int_\Lambda \mathrm{d}\vec{x} \cos^2(\vec{k} \cdot \vec{x}) \\ + \lambda\rho \int_\Lambda \mathrm{d}\vec{x} \cos(\vec{k} \cdot \vec{x}) = -\frac{\lambda^2}{2} (e_0''(\rho))^{-1} \int_\Lambda \mathrm{d}\vec{x} \cos^2(\vec{k} \cdot \vec{x}) \end{aligned} \tag{B.10}$$

for $\vec{k} \neq \vec{0}$. Repeating the calculation for (38*b*), we obtain the same result as the rhs of (B.10) except for the replacement of $\cos^2(\vec{k} \cdot \vec{x})$ by $\sin^2(\vec{k} \cdot \vec{x})$. Finally, for the rhs of (39) we get

$$\frac{1}{N} \langle B_\Lambda \psi_\Lambda^{\vec{k}} | B_\Lambda \psi_\Lambda^{\vec{k}} \rangle = (e_0''(\rho))^{-1} \frac{L^3}{N} = \frac{1}{\rho e_0''(\rho)} \tag{B.11}$$

from which (39) and (40) follow as an equality. It should be clear to the reader that the above derivation, while appealing, is far from rigorous. Indeed, (B.11) does not hold as an

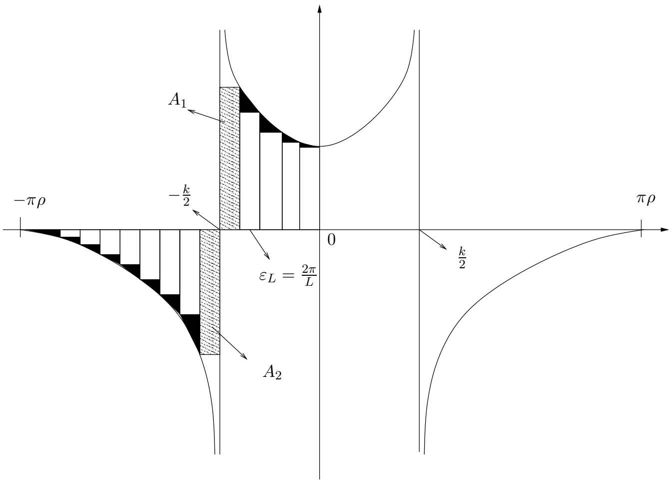

Figure 1. Graph of $f : x \to \frac{1}{(\frac{k}{2})^2 - x^2}$.

equality, as proved in the main text, but, as shown in appendix D, it is very close to the exact result. Indeed, by (47), the rhs of (B.11) is $(1/\pi^2\rho^2) = (1/\pi^2)$ for $\rho = 1$. By (65), it must be compared with $(2/\pi) f(x)$, where $f(x)$ is the function plotted in appendix D. The value plotted for $x = 0$ is $(1/2\pi)$, which yields the rhs of (B.11), but we see from that table that the value plotted even for $x = \pi$ is very close to the value for $x = 0$.

Appendix C

Proof of proposition 2. We must prove that the rhs of (64) is, in the thermodynamic limit,

$$I \equiv \frac{8}{2\pi\rho} P v \int_{-\pi\rho}^{\pi\rho} \frac{\mathrm{d}x}{k^2 - 4x^2} = \frac{8}{2\pi\rho} \lim_{\varepsilon\to 0} \left(\int_{-\pi\rho}^{-\varepsilon} \frac{\mathrm{d}x}{k^2 - 4x^2} + \int_{\varepsilon}^{\pi\rho} \frac{\mathrm{d}x}{k^2 - 4x^2} \right). \tag{C.1}$$

The difficulty lies in the fact that, in the rhs of (64), the 'integration step' $\varepsilon_L \equiv 2\pi/L$ may not be directly identified with the ε in (C.1), because it depends on L. In figure 1 we show the graph of the function $f : x \to \frac{1}{\left(\frac{k}{2}\right)^2 - x^2}$.

Let us call the finite sum over the $p \leqslant 0$ on the rhs of (64) by Σ_l (the argument for the right side is the same). We have

$$\Sigma_l = A_1 + \Sigma_l^1 + A_2 + \Sigma_l^2, \tag{C.2}$$

where Σ_l^1 is the sum of the areas of all inscribed rectangles between $-k/2 + \varepsilon_L$ and zero, and Σ_l^2 is the sum of the areas of all inscribed rectangles between $-\pi\rho$ and $-k/2 - \varepsilon_L$.

We have, by symmetry,

$$A_1 = -A_2 \tag{C.3}$$

while

$$\Sigma_l^1 = \int_{-\frac{k}{2}+\varepsilon_L}^{0} \frac{\mathrm{d}x}{\left(\frac{k}{2}\right)^2 - x^2} + \alpha_L^1 \tag{C.4}$$

and

$$\Sigma_l^2 = \int_{-\pi\rho}^{-\frac{k}{2}-\varepsilon_L} \frac{\mathrm{d}x}{\left(\frac{k}{2}\right)^2 - x^2} - \alpha_L^2 \tag{C.5}$$

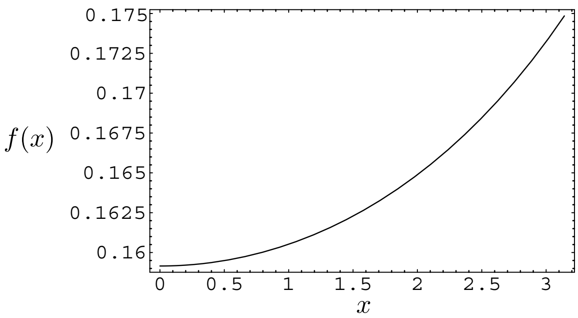

Figure 2. Plot of $f(x)$ for $\rho = 1$.

where

$$\alpha_L^1 - \alpha_L^2 \quad \underset{L\to\infty}{\longrightarrow} 0 \qquad \text{for fixed} \quad k \neq 0. \tag{C.6}$$

In order to prove (C.4), we note that α_L^1 is the sum of the areas of the regions in black in figure 1 which lie to the left of $(-k/2 - \varepsilon_L)$, while α_L^2 is the sum of the areas in black between $(-k/2 + \varepsilon_L)$ and zero:

$$\alpha_L^1 = \left(\int_{-\pi\rho}^{-\frac{k}{2}-\varepsilon_L} f'(x)\,\mathrm{d}x \right) \varepsilon_L[1 + o(1/L)] \tag{C.7}$$

$$\alpha_L^2 = \left(\int_{-\frac{k}{2}+\varepsilon_L}^{0} f'(x)\,\mathrm{d}x \right) \varepsilon_L[1 + o(1/L)]. \tag{C.8}$$

Now

$$\begin{aligned} \varepsilon_L \int_{-\pi\rho}^{-\frac{k}{2}-\varepsilon_L} f'(x)\,\mathrm{d}x &= \varepsilon_L \frac{1}{(-k/2 + x)(-k/2 - x)} \Bigg|_{-\pi\rho}^{-\frac{k}{2}-\varepsilon_L} \\ &= \varepsilon_L \frac{1}{-k - \varepsilon_L} \frac{1}{\varepsilon_L} - \varepsilon_L \frac{1}{(-k/2 - \pi\rho)(-k/2 + \pi\rho)} \\ &= \frac{1}{-k - \varepsilon_L} + \varepsilon_L \frac{1}{(k/2 + \pi\rho)(\pi\rho - k/2)} \end{aligned} \tag{C.9}$$

while

$$\begin{aligned} \varepsilon_L \int_{-\frac{k}{2}+\varepsilon_L}^{0} f'(x)\,\mathrm{d}x &= \varepsilon_L \frac{1}{(-k/2 + x)(-k/2 - x)} \Bigg|_{-\frac{k}{2}+\varepsilon_L}^{0} \\ &= \frac{\varepsilon_L}{(k/2)^2} + \varepsilon_L \frac{1}{-k + \varepsilon_L} \frac{1}{\varepsilon_L}. \end{aligned} \tag{C.10}$$

For $k \neq 0$, (C.7)–(C.10) establish (C.6). Putting (C.6) into (C.2)–(C.5) we obtain that the thermodynamic limit of the rhs of (64) indeed equals I, given by (C.1). □

Appendix D

In this appendix, we show the behaviour of the function on the rhs of (66):

$$f(x) = \frac{1}{x} \operatorname{arccoth}\left(\frac{2\pi\rho}{x}\right),$$

defined for $x \geqslant 0$.

Setting $\rho = 1$, we construct the following table:

x	$f(x)$
0	0.159 155 (∗)
$\pi/10$	0.159 288
$\pi/5$	0.159 689
$3\pi/10$	0.160 365
$2\pi/5$	0.161 329
$\pi/2$	0.162 601
$3\pi/5$	0.164 205
$7\pi/10$	0.166 178
$4\pi/5$	0.168 565
$9\pi/10$	0.171 428
π	0.174 850

where (∗) is the limit (67).

In figure 2, we plot $f(x)$ for $\rho = 1$.

We thus see that in the interval $[0, \pi]$, f is monotonically increasing, and thus the largest value for c, given by the rhs of (68), is the square root of the ratio $f(\pi)/f(0) \equiv t^2 \simeq 0.174\,850/0.159\,155 \simeq 1.0986$, which equals $t \simeq 1.0481$.

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