A Rigorous Derivation of the Gross-Pitaevskii Energy Functional for a Two-dimensional Bose Gas

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Abstract

We consider the ground state properties of an inhomogeneous two-dimensional Bose gas with a repulsive, short range pair interaction and an external confining potential. In the limit when the particle number N is large but $\bar{\rho}a^2$ is small, where $\bar{\rho}$ is the average particle density and a the scattering length, the ground state energy and density are rigorously shown to be given to leading order by a Gross-Pitaevskii (GP) energy functional with a coupling constant $g \sim 1/|\ln(\bar{\rho}a^2)|$. In contrast to the 3D case the coupling constant depends on N through the mean density. The GP energy per particle depends only on Ng. In 2D this parameter is typically so large that the gradient term in the GP energy functional is negligible and the simpler description by a Thomas-Fermi type functional is adequate.

1 Introduction

Motivated by recent experimental realizations of Bose-Einstein condensation the theory of dilute, inhomogeneous Bose gases is currently a subject of intensive studies. Most of this work is based on the assumption that the ground state properties are well described by the Gross-Pitaevskii (GP) energy functional (see the review article [10]). A rigorous derivation of this functional from the basic many-body Hamiltonian in an appropriate limit is not a simple matter, however, and has only been achieved recently for bosons with a short range, repulsive interaction in three spatial dimensions [1].

The present paper is concerned with the justification of the GP functional in two spatial dimensions. Several new issues arise. One is the form of the nonlinear interaction term in the energy functional for the GP wave function Φ. In three dimensions this term is $4\pi a \int |\Phi|^4$, where a is the scattering length of the interaction potential. The rationale is the well known formula for the energy density of a homogeneous Bose gas, which, for dilute gases with particle density ρ, is $4\pi a\rho^2$. This fact has been 'known' since the early 50's but a rigorous proof is fairly recent [3]. In two dimensions the corresponding formula is $4\pi\rho^2|\ln(\rho a^2)|^{-1}$ as proved in [2] by extension of the method of [3]. The formula was first stated by Schick [4]; other early references to this formula are [5, 6, 7, 8, 9]. It would seem natural to consider $4\pi \int |\Phi|^4 |\ln(|\Phi|^2 a^2)|^{-1}$ as the interaction term in the GP functional, and this has indeed been suggested in [11]. Such a term, however, is unnecessarily complicated for the purpose of leading order calculations. In fact, since the logarithm varies only slowly it turns out that one can use the *same* form as in the three dimensional case, but with an appropriate dimensionless coupling constant g replacing the scattering length, and still retain an exact theory (to leading order in ρ).

The functional we shall consider is thus

$$\mathcal{E}^{\rm GP}[\Phi] = \int \left(|\nabla\Phi(\mathbf{x})|^2 + V(\mathbf{x})|\Phi(\mathbf{x})|^2 + 4\pi g|\Phi(\mathbf{x})|^4\right) \mathrm{d}^2\mathbf{x}, \tag{1.1}$$

where V is the external confining potential and all integrals are over $\mathbb{R}^2$.

The choice of g is an issue on which there has not been unanimous opinion in the recent papers [11, 12, 13, 14, 15, 16, 17] on this subject. We shall prove that a right choice is $g = |\ln(\bar\rho a^2)|^{-1}$ where $\bar\rho$ is a mean density that will be defined more precisely below. This mean density depends on the particle number N, which implies that the scaling properties of the GP functional are quite different in two and three dimensions. In the three-dimensional case the natural parameter is $Na/a_{\rm osc}$, with $a_{\rm osc}$ being the length scale defined by the external confining potential. If $a/a_{\rm osc}$ is scaled like $1/N$ as $N\to\infty$ this parameter is fixed and the gradient term $\int|\nabla\Phi|^2$ in the GP functional is of the same order as the other terms. In two dimensions the corresponding parameter is $N|\ln(\bar\rho a^2)|^{-1}$. For a quadratic external potential $\bar\rho$ behaves like $N^{1/2}/a_{\rm osc}^2$ and hence the parameter can only be kept fixed if $a/a_{\rm osc}$ decreases exponentially with N. A slower decrease means that the parameter tends to infinity. This corresponds to the so-called Thomas Fermi (TF) limit where the gradient term has been dropped altogether and the functional is

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int \left(V(\mathbf{x})\rho(\mathbf{x}) + 4\pi g \rho(\mathbf{x})^2 \right) \mathrm{d}^2\mathbf{x}, \tag{1.2}$$

defined for nonnegative functions ρ. Our main result, stated in Theorems 1.3 and 1.4 below, is that minimization of (1.2) reproduces correctly the ground state energy and density of the many-body Hamiltonian in the limit when $N \to \infty$, $\bar{\rho}a^2 \to 0$, but $N|\ln(\bar{\rho}a^2)|^{-1} \to \infty$. Only in the exceptional situation that $N|\ln(\bar{\rho}a^2)|^{-1}$ stays bounded is there need for the full GP functional (1.1), cf. Theorems 1.1 and 1.2.

We shall now describe the setting more precisely. The starting point is the Hamiltonian for N identical bosons in an external potential V and with pair interaction v,

$$H^{(N)} = \sum_{i=1}^{N} \left(-\nabla_i^2 + V(\mathbf{x}_i) \right) + \sum_{i<j} v(\mathbf{x}_i - \mathbf{x}_j), \tag{1.3}$$

acting on the totally symmetric wave functions in $\otimes^N L^2(\mathbb{R}^2)$. Units have been chosen so that $\hbar = 2m = 1$, where m is the particle mass. We assume that v is nonnegative and spherically symmetric with a finite scattering length a. (For the definition of scattering length in two dimensions see [2]). The external potential should be continuous and tend to ∞ as $|\mathbf{x}| \to \infty$. It is then possible and convenient to shift the energy scale so that $\min_{\mathbf{x}} V(\mathbf{x}) = 0$. For the TF limit theorem we shall require some additional properties of V to be specified later.

The ground state energy ω of the one particle operator $-\nabla^2 + V$ is a natural energy unit and gives rise to a length unit $a_{\mathrm{osc}} \equiv \omega^{-1/2}$. Writing $V(\mathbf{x}) = \omega\hat{V}(\mathbf{x}/a_{\mathrm{osc}})$ it is experimentally feasible to let a_{osc} vary with N, keeping $\hat{V}$ fixed. The dimensionless interaction potential $\hat{v}$, defined by $v(\mathbf{x}) = \omega\hat{v}(\mathbf{x}/a_{\mathrm{osc}})$ has the dimensionless scattering length a/a_{osc} if a is the scattering length of v. Varying a_{osc} at fixed external potential $\hat{V}$ is equivalent to scaling $\hat{v}$ for fixed v and hence varying the scattering length. In the dilute limit when a/a_{osc} is much smaller than the mean particle distance the ground state energy depends only on a/a_{osc} and not on other features of v.

We shall measure all energies in terms of ω and lengths in terms of a_{osc}. The notation $E^{\mathrm{QM}}(N,a)$ for the ground state energy of (1.3) is then justified, but it should be kept in mind that a here really stands for a/a_{osc} and varying a with N is equivalent to varying a_{osc} at fixed v.

The quantum mechanical particle density is defined by

$$\rho^{\rm QM}_{N,a}(\mathbf{x}) = N\int |\Psi^{(N)}(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_N)|^2 {\rm d}^2\mathbf{x}_2\ldots{\rm d}^2\mathbf{x}_N, \tag{1.4}$$

where $\Psi^{(N)}$ is a ground state for (1.3).

The GP functional (1.1) has an obvious domain of definition (cf. Eq. (2.1) in [1]). The infimum of $\mathcal{E}^{\rm GP}[\Phi]$ under the condition $\int|\Phi|^2 = N$ will be denoted by $E^{\rm GP}(N,g)$. The infimum is obtained for a unique, positive function, denoted $\Phi^{\rm GP}_{N,g}$, and the GP density is defined as $\rho^{\rm GP}_{N,g}(\mathbf{x}) = \Phi^{\rm GP}_{N,g}(\mathbf{x})^2$.

The ground state energy of the TF functional (1.2) with the subsidiary condition $\int\rho = N$ is denoted $E^{\rm TF}(N,g)$. The corresponding minimizer can be written explicitly; it is

$$\rho^{\rm TF}_{N,g}(\mathbf{x}) = \frac{1}{8\pi g}[\mu^{\rm TF} - V(\mathbf{x})]_+, \tag{1.5}$$

where $[t]_+\equiv\max\{t,0\}$ and $\mu^{\rm TF}$ is chosen so that the normalization condition $\int\rho^{\rm TF}_{N,g} = N$ holds.

We now define the mean density $\bar\rho$ as the average of the TF density $\rho^{\rm TF}_{N,1}$ at coupling constant $g=1$, weighted with $N^{-1}\rho^{\rm TF}_{N,1}$, i.e.,

$$\bar\rho = \frac{1}{N}\int \rho^{\rm TF}_{N,1}(\mathbf{x})^2{\rm d}^2\mathbf{x}. \tag{1.6}$$

It is clear that $\bar\rho$ depends on N and when we wish to emphasize this we write $\bar\rho_N$. The definition (1.6) has the advantage that $\bar\rho$ is easily computed; for instance, if $V(\mathbf{x})\sim|\mathbf{x}|^s$ for some $s>0$, then $\bar\rho_N\sim N^{s/(s+2)}$. It may appear more natural to define $\bar\rho$ self-consistently as $\bar\rho = \frac{1}{N}\int\rho^{\rm TF}_{N,g}(\mathbf{x})^2{\rm d}^2\mathbf{x}$ with $g = |\ln(\bar\rho a^2)|^{-1}$, which amounts to solving a nonlinear equation for $\bar\rho$. Also, the TF density could be replaced by the GP density. However, since $\bar\rho$ will only appear under a logarithm such sophisticated definitions are not needed for the leading order result we are after. The simple formula (1.6) is adequate for our purpose, but it should be kept in mind that the self-consistent definition may be relevant in computations beyond the leading order.

With this notation we can now state the two dimensional analogue of Theorem I.1 in [1].

Theorem 1.1 (GP limit for the energy). *If, for $N\to\infty$, $a^2\bar\rho_N\to 0$ with $N/|\ln(a^2\bar\rho_N)|$ fixed, then*

$$\lim_{N\to\infty}\frac{E^{\rm QM}(N,a)}{E^{\rm GP}(N,1/|\ln(a^2\bar\rho_N)|)} = 1. \tag{1.7}$$

The corresponding theorem for the density, c.f. Theorem I.2 in [1], is

Theorem 1.2 (GP limit for the density). *If, for $N \to \infty$, $a^2\bar\rho_N \to 0$ with $\gamma \equiv N/|\ln(a^2\bar\rho_N)|$ fixed, then*

$$\lim_{N\to\infty} \frac{1}{N}\rho^{\rm QM}_{N,a}(\mathbf{x}) = \rho^{\rm GP}_{1,\gamma}(\mathbf{x}) \tag{1.8}$$

in the sense of weak convergence in $L^1(\mathbb{R}^2)$.

These theorems, however, are not particularly useful in the two dimensional case, because the hypothesis that $N/|\ln(a^2\bar\rho_N)|$ stays bounded requires an exponential decrease of a with N. As remarked above, the TF limit, where $N/|\ln(a^2\bar\rho_N)| \to \infty$, is much more relevant. Our treatment of this limit requires that V is asymptotically homogeneous and sufficiently regular in a sense made precise below. This condition can be relaxed, but it seems adequate for most practical applications and simplifies things considerably.

Definition 1.1. We say that V is *asymptotically homogeneous* of order $s > 0$ if there is a function W with $W(\mathbf{x}) \neq 0$ for $\mathbf{x} \neq \mathbf{0}$ such that

$$\frac{\lambda^{-s}V(\lambda\mathbf{x}) - W(\mathbf{x})}{1 + |W(\mathbf{x})|} \to 0 \quad \text{as} \quad \lambda \to \infty \tag{1.9}$$

and the convergence is uniform in $\mathbf{x}$.

The function W is clearly uniquely determined and homogeneous of order s, i.e., $W(\lambda\mathbf{x}) = \lambda^s W(\mathbf{x})$ for all $\lambda \geq 0$.

Theorem 1.3 (TF limit for the energy). *Suppose V is asymptotically homogeneous of order $s > 0$ and its scaling limit W is locally Hölder continuous, i.e., $|W(\mathbf{x}) - W(\mathbf{y})| \leq (\text{const.})|\mathbf{x}-\mathbf{y}|^\alpha$ for $|\mathbf{x}|, |\mathbf{y}| = 1$ for some fixed $\alpha > 0$. If, for $N \to \infty$, $a^2\bar\rho_N \to 0$ but $N/|\ln(a^2\bar\rho_N)| \to \infty$, then*

$$\lim_{N\to\infty} \frac{E^{\rm QM}(N,a)}{E^{\rm TF}(N, 1/|\ln(a^2\bar\rho_N)|)} = 1. \tag{1.10}$$

To state the corresponding theorem for the density we need the minimizer of (1.2) with $g = 1$, V replaced by W, and normalization $\int\rho = 1$. We shall denote this minimizer by $\tilde\rho^{\rm TF}_{1,1}$; an explicit formula is

$$\tilde\rho^{\rm TF}_{1,1}(\mathbf{x}) = \frac{1}{8\pi}[\tilde\mu^{\rm TF} - W(\mathbf{x})]_+, \tag{1.11}$$

where $\tilde\mu^{\rm TF}$ is determined by the normalization condition.

Theorem 1.4 (TF limit for the density). *Let V satisfy the same hypothesis as in Theorem 1.3. If, for $N \to \infty$, $a^2\bar{\rho}_N \to 0$ but $\gamma = N/|\ln(a^2\bar{\rho}_N)| \to \infty$, then*

$$\lim_{N\to\infty} \frac{\gamma^{2/(s+2)}}{N}\rho^{\mathrm{QM}}_{N,a}(\gamma^{1/(s+2)}\mathbf{x}) = \tilde{\rho}^{\mathrm{TF}}_{1,1}(\mathbf{x}) \tag{1.12}$$

in the sense of weak convergence in $L^1(\mathbb{R}^2)$.

Remark 1.1. For large N, $\bar{\rho}_N$ behaves like (const.)$N^{s/(s+2)}$. Moreover, prefactors are unimportant in the limit $N \to \infty$, because $\bar{\rho}_N$ stands under a logarithm. Hence Theorems 1.3 and 1.4 could also be stated with $N^{s/(s+2)}$ in place of $\bar{\rho}_N$.

The proofs of these theorems follow from upper and lower bounds on the ground state energy $E^{\mathrm{QM}}(N,a)$ that are derived in Sections 3 and 4. For these bounds some properties of the minimizers of the functionals (1.1) and (1.2), discussed in the following section, are needed.

2 GP and TF theory

In this section we consider the functionals (1.1) and (1.2) with an arbitrary positive coupling constant g. Existence and uniqueness of minimizers is shown in the same way as in Theorem II.1 in [1]. The GP energy $E^{\mathrm{GP}}(N,g)$ has the simple scaling property $E^{\mathrm{GP}}(N,g) = NE^{\mathrm{GP}}(1,Ng)$. Likewise, $N^{-1/2}\Phi^{\mathrm{GP}}_{N,g} \equiv \phi^{\mathrm{GP}}_{\gamma}$ depends only on

$$\gamma \equiv Ng \tag{2.1}$$

and satisfies the normalization condition $\int |\phi^{\mathrm{GP}}_{\gamma}|^2 = 1$. The variational equation (GP equation) for the GP minimization problem, written in terms of $\phi^{\mathrm{GP}}_{\gamma}$, is

$$-\Delta\phi^{\mathrm{GP}}_{\gamma} + V\phi^{\mathrm{GP}}_{\gamma} + 8\pi\gamma(\phi^{\mathrm{GP}}_{\gamma})^3 = \mu^{\mathrm{GP}}(\gamma)\phi^{\mathrm{GP}}_{\gamma}, \tag{2.2}$$

where the Lagrange multiplier (chemical potential) $\mu^{\mathrm{GP}}(\gamma)$ is determined by the subsidiary normalization condition. Multiplying (2.2) with $\phi^{\mathrm{GP}}_{\gamma}$ and integrating we obtain

$$\mu^{\mathrm{GP}}(\gamma) = E^{\mathrm{GP}}(1,\gamma) + 4\pi\gamma\int \phi^{\mathrm{GP}}_{\gamma}(\mathbf{x})^4 \mathrm{d}^2\mathbf{x}. \tag{2.3}$$

For the upper bound on the quantum mechanical energy in the next section we shall need a bound on the absolute value of the minimizer $\phi^{\mathrm{GP}}_{\gamma}$.

Lemma 2.1 (Upper bound for the GP minimizer).

$$\|\phi_\gamma^{\rm GP}\|_\infty^2 \leq \frac{\mu^{\rm GP}(\gamma)}{8\pi\gamma} \tag{2.4}$$

Proof. $\phi_\gamma^{\rm GP}$ satisfies the variational equation

$$-\Delta\phi_\gamma^{\rm GP} + U\phi_\gamma^{\rm GP} = \mu^{\rm GP}\phi_\gamma^{\rm GP} \tag{2.5}$$

with $U = V + 8\pi\gamma(\phi_\gamma^{\rm GP})^2$. By a superharmonicity argument one easily sees that $U(\mathbf{x}) \leq \mu^{\rm GP}$ where $\phi_\gamma^{\rm GP}$ achieves its maximum. Since $V \geq 0$ this yields $8\pi\gamma\|\phi_\gamma^{\rm GP}\|_\infty^2 \leq \mu^{\rm GP}$. □

The ground state energy $E^{\rm TF}(N,g)$ of the TF functional (1.2) scales in the same way as $E^{\rm GP}(N,g)$, i.e., $E^{\rm TF}(N,g) = NE^{\rm TF}(1,Ng)$, and the corresponding minimizer $\rho_{N,g}^{\rm TF}$ is equal to $N\rho_{1,Ng}^{\rm TF}$. For short, we shall denote $\rho_{1,\gamma}^{\rm TF}$ by $\rho_\gamma^{\rm TF}$. By (1.5) we have

$$\rho_\gamma^{\rm TF}(\mathbf{x}) = \frac{1}{8\pi\gamma}[\mu^{\rm TF}(\gamma) - V(\mathbf{x})]_+, \tag{2.6}$$

with the chemical potential $\mu^{\rm TF}(\gamma)$ determined by the normalization condition $\int \rho_\gamma^{\rm TF} = 1$. In the same way as in (2.3) we have

$$\mu^{\rm TF}(\gamma) = E^{\rm TF}(1,\gamma) + 4\pi\gamma\int \rho_\gamma^{\rm TF}(\mathbf{x})^2 {\rm d}^2\mathbf{x}. \tag{2.7}$$

The chemical potential can also be computed from a variational principle:

Lemma 2.2 (Variational principle for $\mu^{\rm TF}$).

$$\mu^{\rm TF}(\gamma) = \inf_{\rho\geq 0,\int\rho=1}\int V\rho + 8\pi\gamma\|\rho\|_\infty \tag{2.8}$$

Proof. Obviously, the infimum is achieved for a multiple of a characteristic function for some region $\mathcal{R}\subset\mathbb{R}^2$. If $|\mathcal{R}|$ denotes the area of $\mathcal{R}$, then

$$\begin{aligned}
&\inf_{\int\rho=1}\int V\rho + 8\pi\gamma\|\rho\|_\infty \\
&= \inf_{\mathcal{R}}\left(\int_{\mathcal{R}} V + 8\pi\gamma\right)\frac{1}{|\mathcal{R}|} &(2.9)\\
&= \inf_{\mathcal{R}}\left(\int_{\mathcal{R}}\big(V - \mu^{\rm TF}(\gamma)\big) + 8\pi\gamma + \mu^{\rm TF}(\gamma)|\mathcal{R}|\right)\frac{1}{|\mathcal{R}|}. &(2.10)
\end{aligned}$$

Now $\int_{\mathcal{R}}(V - \mu^{\rm TF}(\gamma)) \geq -8\pi\gamma$, with equality for

$$\left\{\mathbf{x}|V(\mathbf{x}) < \mu^{\rm TF}(\gamma)\right\} \subseteq \mathcal{R} \subseteq \left\{\mathbf{x}|V(\mathbf{x}) \leq \mu^{\rm TF}(\gamma)\right\}. \tag{2.11}$$

□

Corollary 2.1 (Properties of $\mu^{\rm TF}(\gamma)$). *$\mu^{\rm TF}(\gamma)$ is a concave and monotonously increasing function of γ with $\mu^{\rm TF}(0)=0$. Hence $\mu^{\rm TF}(\gamma)/\gamma$ is decreasing in γ. Moreover, $\mu^{\rm TF}(\gamma)\to\infty$ and $\mu^{\rm TF}(\gamma)/\gamma\to 0$ as $\gamma\to\infty$.*

Proof. Immediate consequences of Lemma (2.2), using that $\min_{\mathbf{x}} V(\mathbf{x})=0$ and $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x})=\infty$. $\square$

Note that since $E^{\rm TF}(1,\gamma)\geq \frac{1}{2}\mu^{\rm TF}(\gamma)$ we also see that $E^{\rm TF}(1,\gamma)\to\infty$ with γ. In this limit the GP energy converges to the TF energy, provided the external potential satisfies a mild regularity and growth condition:

Lemma 2.3 (TF limit of the GP energy). *Suppose for some constants $\alpha>0$, L_1 and L_2*

$$|V(\mathbf{x})-V(\mathbf{y})|\leq L_1|\mathbf{x}-\mathbf{y}|^\alpha e^{L_2|\mathbf{x}-\mathbf{y}|}(1+V(\mathbf{x})). \tag{2.12}$$

Then

$$\lim_{\gamma\to\infty}\frac{E^{\rm GP}(1,\gamma)}{E^{\rm TF}(1,\gamma)}=1. \tag{2.13}$$

Proof. It is clear that $E^{\rm TF}(1,\gamma)\leq E^{\rm GP}(1,\gamma)$. For the other direction, we use $(j_\epsilon*\rho^{\rm TF}_\gamma)^{1/2}$ as a test function for $\mathcal{E}^{\rm GP}$, where

$$j_\epsilon(\mathbf{x})=\frac{1}{2\pi\epsilon^2}\exp\left(-\frac{1}{\epsilon}|\mathbf{x}|\right). \tag{2.14}$$

Note that $\int j_\epsilon=1$ and $|\nabla j_\epsilon|=\epsilon^{-1}j_\epsilon$. Therefore

$$\begin{aligned} E^{\rm GP}(1,\gamma) &\leq \int\left(\frac{1}{4j_\epsilon*\rho^{\rm TF}_\gamma}|\nabla j_\epsilon*\rho^{\rm TF}_\gamma|^2+V(j_\epsilon*\rho^{\rm TF}_\gamma)+4\pi\gamma(j\epsilon*\rho^{\rm TF}_\gamma)^2\right)\\ &\leq \frac{1}{4\epsilon^2}+\int\left((j_\epsilon*V)\rho^{\rm TF}_\gamma+4\pi\gamma(\rho^{\rm TF}_\gamma)^2\right), \end{aligned} \tag{2.15}$$

where we have used convexity for the last term. Moreover,

$$\begin{aligned} \int(j_\epsilon*V-V)\rho^{\rm TF}_\gamma &= \int\int {\rm d}^2\mathbf{x}{\rm d}^2\mathbf{y}\, j_\epsilon(\mathbf{x}-\mathbf{y})\left(V(\mathbf{x})-V(\mathbf{y})\right)\rho^{\rm TF}_\gamma(\mathbf{x})\\ &\leq \frac{L_1}{2\pi\epsilon^2}\int\int {\rm d}^2\mathbf{x}{\rm d}^2\mathbf{y}|\mathbf{x}-\mathbf{y}|^\alpha e^{(-\epsilon^{-1}+L_2)|\mathbf{x}-\mathbf{y}|}(1+V(\mathbf{x}))\rho^{\rm TF}_\gamma(\mathbf{x})\\ &\leq (\text{const.})\,\epsilon^\alpha\left(1+E^{\rm TF}(1,\gamma)\right), \end{aligned} \tag{2.16}$$

as long as $\epsilon<L_2^{-1}$. So we have

$$E^{\rm GP}(1,\gamma)\leq(1+(\text{const.})\,\epsilon^\alpha)E^{\rm TF}(1,\gamma)+\frac{1}{4\epsilon^2}+(\text{const.})\,\epsilon^\alpha. \tag{2.17}$$

Optimizing over ϵ gives as a final result

$$E^{\rm GP}(1,\gamma)\leq E^{\rm TF}(1,\gamma)\left(1+({\rm const.})E^{\rm TF}(1,\gamma)^{-\alpha/(\alpha+2)}\right). \tag{2.18}$$

$\square$

Condition (2.12) is in particular fulfilled if V is homogeneous of some order $s>0$ and locally Hölder continuous. In this case,

$$E^{\rm TF}(1,\gamma)=\gamma^{s/(s+2)}E^{\rm TF}(1,1) \tag{2.19}$$

and

$$\gamma^{2/(s+2)}\rho_\gamma^{\rm TF}(\gamma^{1/(s+2)}\mathbf{x})=\rho_{1,1}^{\rm TF}(\mathbf{x}). \tag{2.20}$$

By (2.7) we also have

$$\mu^{\rm TF}(\gamma)=\gamma^{s/(s+2)}\mu^{\rm TF}(1). \tag{2.21}$$

If V is asymptotically homogeneous with a locally Hölder continuous limiting function W, we can prove corresponding formulas for the limit $\gamma\to\infty$. This is the content of the next theorem, where we have included results on the GP $\to$ TF limit as well:

Theorem 2.1 (Scaling limits). *Suppose V satisfies the condition of Theorem 1.3. Let $\tilde{E}^{\rm TF}(1,1)$ be the minimum of the TF functional (1.2) with $g=1$ and $N=1$ and V replaced by W, and let $\tilde{\rho}_{1,1}^{\rm TF}$ be the corresponding minimizer. Then*

(i) $\lim_{\gamma\to\infty}E^{\rm GP}(1,\gamma)/\gamma^{s/(s+2)}=\lim_{\gamma\to\infty}E^{\rm TF}(1,\gamma)/\gamma^{s/(s+2)}=\tilde{E}^{\rm TF}(1,1)$.

(ii) $\lim_{\gamma\to\infty}\gamma^{2/(s+2)}\rho_{1,\gamma}^{\rm GP}(\gamma^{1/(s+2)}\mathbf{x})=\tilde{\rho}_{1,1}^{\rm TF}(\mathbf{x})$, *strongly in* $L^2(\mathbb{R}^2)$.

(iii) $\lim_{\gamma\to\infty}\gamma^{2/(s+2)}\rho_\gamma^{\rm TF}(\gamma^{1/(s+2)}\mathbf{x})=\tilde{\rho}_{1,1}^{\rm TF}(\mathbf{x})$, *uniformly in* $\mathbf{x}$.

Proof. With the demanded properties of V, (2.13) holds. Using this and (1.9) one easily verifies (i). Moreover, $\gamma^{2/(s+2)}\rho_{1,\gamma}^{\rm GP}(\gamma^{1/(s+2)}\mathbf{x})$ is a minimizing sequence for the functional in question, so we can conclude as in Theorem II.2 in [1] that it converges to $\tilde{\rho}_{1,1}^{\rm TF}(\mathbf{x})$ strongly in L^2, proving (ii). (Remark: In Eq. (2.10) in [1] there is a misprint, instead of $\rho_{1,Na}^{\rm GP}$ one should have $\tilde{\rho}_{1,Na}^{\rm GP}$ on the left side.) To see (iii) let us define

$$\widehat{\rho}_\gamma(\mathbf{x})=\gamma^{2/(s+2)}\rho_\gamma^{\rm TF}\left(\gamma^{1/(s+2)}\mathbf{x}\right). \tag{2.22}$$

We can write

$$\widehat{\rho}_\gamma(\mathbf{x}) = \frac{1}{8\pi}\left[\gamma^{-s/(s+2)}\mu^{\rm TF}(\gamma) - W(\mathbf{x}) - \epsilon(\gamma,\mathbf{x})\right]_+ \tag{2.23}$$

with

$$\epsilon(\gamma,\mathbf{x}) = \gamma^{-s/(s+2)}V(\gamma^{1/(s+2)}\mathbf{x}) - W(\mathbf{x}). \tag{2.24}$$

By assumption, $|\epsilon(\gamma,\mathbf{x})| < \delta(\gamma)(1+W(\mathbf{x}))$ for some $\delta(\gamma)$ with $\lim_{\gamma\to\infty}\delta(\gamma) = 0$. Because $\int\widehat{\rho}_\gamma = 1$ for all γ, we see from Eq. (2.23) that $\mu^{\rm TF}(\gamma)\gamma^{-s/(s+2)}$ converges to some c as $\gamma\to\infty$. Moreover, we can conclude that the support of $\widehat{\rho}_\gamma$ is for large γ contained in some bounded set $\mathcal{B}$ independent of γ. Therefore

$$1 = \lim_{\gamma\to\infty}\int\widehat{\rho}_\gamma = \int(8\pi)^{-1}[c - W(\mathbf{x})]_+ \tag{2.25}$$

by dominated convergence, so c is equal to the $\tilde{\mu}^{\rm TF}$ of Eq. (1.11). Now

$$\widehat{\rho}_\gamma(\mathbf{x}) = \frac{1}{8\pi}\left[\tilde{\mu}^{\rm TF} - W(\mathbf{x}) - \bar{\epsilon}(\gamma,\mathbf{x})\right]_+ \tag{2.26}$$

with

$$\bar{\epsilon}(\gamma,\mathbf{x}) = \epsilon(\gamma,\mathbf{x}) + \tilde{\mu}^{\rm TF} - \gamma^{-s/(s+2)}\mu^{\rm TF}(\gamma). \tag{2.27}$$

Again $|\bar{\epsilon}(\gamma,\mathbf{x})| < \bar{\delta}(\gamma)(1+W(\mathbf{x}))$ for some $\bar{\delta}(\gamma)$ with $\lim_{\gamma\to\infty}\bar{\delta}(\gamma) = 0$. By Eqs. (1.11) and (2.26) we thus have

$$\|\widehat{\rho}_\gamma - \tilde{\rho}^{\rm TF}_{1,1}\|_\infty < C\bar{\delta}(\gamma). \tag{2.28}$$

with $C = (8\pi)^{-1}\sup_{\mathbf{x}\in\mathcal{B}}(1+W(\mathbf{x})) < \infty$. □

The *mean density* for the TF theory is defined by

$$\bar{\rho}_\gamma \equiv N\int\rho^{\rm TF}_\gamma(\mathbf{x})^2{\rm d}^2\mathbf{x}. \tag{2.29}$$

For $\gamma = N$, i.e., $g = 1$ this is the same as (1.6). It satisfies

Lemma 2.4 (Bounds on $\bar{\rho}_\gamma$). *For some constant $C > 0$*

$$N\frac{\mu^{\rm TF}(\gamma)}{8\pi\gamma} \geq \bar{\rho}_\gamma \geq CN\frac{\mu^{\rm TF}(\gamma)}{\gamma}. \tag{2.30}$$

Proof. The upper bound is trivial. Because $\widehat{\rho}_\gamma$, defined in (2.22), converges uniformly to $\tilde{\rho}^{\rm TF}_{1,1}$ and $\mu^{\rm TF}(\gamma)\gamma^{-s/(s+2)} \to \tilde{\mu}^{\rm TF}$ as $\gamma \to \infty$, we have the lower bound

$$\frac{\gamma\bar{\rho}_\gamma}{N\mu^{\rm TF}(\gamma)} \geq 8\pi\gamma^{s/(s+2)}\mu^{\rm TF}(\gamma)^{-1}\left(\int(\tilde{\rho}^{\rm TF}_{1,1})^2 - 2\|\tilde{\rho}^{\rm TF}_{1,1} - \widehat{\rho}\|_\infty\right) > C \quad (2.31)$$

for some $C > 0$. □

Remark 2.1. With V asymptotically homogeneous of order s, $\mu^{\rm TF}(\gamma)\gamma^{-s/(s+2)}$ converges as $\gamma \to \infty$, i.e. $\mu^{\rm TF}(\gamma) \sim \gamma^{s/(s+2)}$ for large γ. So the mean TF density for coupling constant $g = 1$, defined in (1.6), has the asymptotic behavior $\bar{\rho} \sim N^{s/(s+2)}$.

3 Upper bound to the QM energy

As in the three dimensional case, cf. Eqs. (3.29) and (3.27) in [1], one has the upper bound

$$\frac{E^{\rm QM}(N,a)}{N} \leq \frac{\int|\nabla\phi^{\rm GP}_\gamma|^2 + V(\phi^{\rm GP}_\gamma)^2}{1 - N\|\phi^{\rm GP}_\gamma\|^2_\infty I} + \frac{NJ\int(\phi^{\rm GP}_\gamma)^4 + \frac{2}{3}N^2(\|\phi^{\rm GP}_\gamma\|^2_\infty K)^2}{(1 - N\|\phi^{\rm GP}_\gamma\|^2_\infty I)^2}, \quad (3.1)$$

where we have implicitly used that $-\Delta\phi^{\rm GP}_\gamma + V\phi^{\rm GP}_\gamma \geq 0$, which is justified by Lemma 2.1. The coefficients I, J and K are given by Eq. (2.4)–(2.10) in [2]. They depend on the scattering length and a parameter b. We choose $\gamma = N/|\ln(a^2\bar{\rho})|$ and $b = \bar{\rho}^{-1/2}$. (Recall that $\bar{\rho}$ is short for $\bar{\rho}_N$.) With this choice we have (as long as $a^2\bar{\rho} < 1$)

$$J = \frac{4\pi}{|\ln(a^2\bar{\rho})|}, \quad (3.2)$$

and the error terms

$$N\|\phi^{\rm GP}_\gamma\|^2_\infty I \leq ({\rm const.})\frac{\mu^{\rm GP}(\gamma)}{\bar{\rho}}\left(1 + O(|\ln(a^2\bar{\rho})|^{-1})\right) \quad (3.3)$$

and

$$K^2N^2\|\phi^{\rm GP}_\gamma\|^4_\infty \leq ({\rm const.})E^{\rm GP}(1,\gamma)\frac{\mu^{\rm GP}(\gamma)}{\bar{\rho}}\left(1 + O(|\ln(a^2\bar{\rho})|^{-1})\right), \quad (3.4)$$

where we have used Lemma 2.1. So we have the upper bound

$$\frac{E^{\rm QM}(N,a)}{E^{\rm GP}(N, 1/|\ln(a^2\bar{\rho})|)} \leq 1 + O\left(\mu^{\rm GP}(\gamma)/\bar{\rho}\right) + O((|\ln(a^2\bar{\rho})|^{-1})). \quad (3.5)$$

Now if γ is fixed as $N \to \infty$

$$\frac{\mu^{\rm GP}(\gamma)}{\bar\rho} \sim \frac{1}{|\ln(a^2\bar\rho)|} \sim \frac{1}{N}. \tag{3.6}$$

If $\gamma \to \infty$ with N we have instead, assuming that the external potential is asymptotically homogeneous of order s,

$$\frac{\mu^{\rm GP}(\gamma)}{\bar\rho} \sim \frac{\mu^{\rm TF}(\gamma)}{\mu^{\rm TF}(N)} \sim \left(\frac{\gamma}{N}\right)^{s/(s+2)}, \tag{3.7}$$

so in any case

$$\frac{E^{\rm QM}(N,a)}{E^{\rm GP}(N,1/|\ln(a^2\bar\rho)|)} \leq 1 + O\left(|\ln(a^2\bar\rho)|^{-s/(s+2)}\right) \tag{3.8}$$

holds as $N\to\infty$ and $a^2\bar\rho \to 0$.

4 Lower bound to the QM energy

Compared to the treatment of the 3D problem in [1] the new issue here is the TF case, i.e., $\gamma = N/|\ln(a^2\bar\rho)| \to \infty$, and we discuss this case first. The GP limit with γ fixed can be treated in complete analogy with the 3D case, cf. Remark 4.1 below.

We introduce again the rescaled $\widehat\rho_\gamma$ as in (2.22) and also

$$\widehat v(\mathbf{x}) = \gamma^{2/(s+2)}\, v\left(\gamma^{1/(s+2)}\mathbf{x}\right). \tag{4.1}$$

Note that the scattering length of $\widehat v$ is $\widehat a = a\,\gamma^{-1/(s+2)}$. Using $V \geq \mu^{\rm TF}(\gamma) - 8\pi\gamma\rho_\gamma^{\rm TF}$ and (2.7) we see that

$$\begin{aligned} E^{\rm QM}(N,a) \quad &\geq \quad E^{\rm TF}(N,\gamma/N) + 4\pi N\gamma^{s/(s+2)}\int \widehat\rho_\gamma^2 + \gamma^{-2/(s+2)}Q \\ &\qquad -8\pi N\gamma^{s/(s+2)}\|\widehat\rho_\gamma - \tilde\rho_{1,1}^{\rm TF}\|_\infty, \end{aligned} \tag{4.2}$$

with

$$Q = \inf_{\int|\Psi|^2=1} \sum_i \int \left(|\nabla_i\Psi|^2 + \sum_{j<i}\widehat v(\mathbf{x}_i - \mathbf{x}_j)|\Psi|^2 - 8\pi\gamma\tilde\rho_{1,1}^{\rm TF}(\mathbf{x}_i)|\Psi|^2\right). \tag{4.3}$$

Dividing space into boxes α of side length L with Neumann boundary conditions we get

$$Q \geq \sum_\alpha E^{\rm hom}(n_\alpha, L) - 8\pi\gamma\rho_{\alpha,\max}n_\alpha, \tag{4.4}$$

where $\rho_{\alpha,\max}$ denotes the maximal value of $\tilde\rho^{\rm TF}_{1,1}$ in the box α, and $E^{\rm hom}(n,L)$ is the energy of a homogeneous gas of n bosons in a box of side length L and Neumann boundary conditions. We can forget about the boxes where $\rho_{\alpha,\max}=0$, because the energy of particles in these boxes is positive.

We now want to use the lower bound on $E^{\rm hom}$ given in [2], namely

$$E^{\rm hom}(n,L)\geq 4\pi\frac{n^2}{L^2}\frac{1}{|\ln(\widehat{a}^2n/L^2)|}\left(1-C|\ln(\widehat{a}^2n/L^2)|^{-1/5}\right). \tag{4.5}$$

This bound holds for $n>(\text{const.})|\ln(\widehat{a}^2n/L^2)|^{1/5}$ and small enough $\widehat{a}^2n/L^2$. Now if the minimum in (4.4) is taken in some box α for some value n_α, we have

$$E^{\rm hom}(n_\alpha+1,L)-E^{\rm hom}(n_\alpha,L)\geq 8\pi\gamma\rho_{\alpha,\max}. \tag{4.6}$$

By a computation analogous to the upper bound (see [1]) one shows that

$$\begin{aligned}&E^{\rm hom}(n+1,L)-E^{\rm hom}(n,L)\\ &\leq 8\pi\frac{n}{L^2}\frac{1}{|\ln(\widehat{a}^2n/L^2)|}\left(1+O\left(|\ln(\widehat{a}^2n/L^2)|^{-1}\right)\right).\end{aligned} \tag{4.7}$$

Using Lemma (2.4) and the asymptotics of $\mu^{\rm TF}$ (Remark 2.1) we see that

$$\frac{\widehat{a}^2n}{L^2}\leq\frac{\widehat{a}^2N}{L^2}=N^{s/(s+2)}\left(\frac{N}{\gamma}\right)^{2/(s+2)}\frac{a^2}{L^2}\leq a^2\bar\rho\frac{C}{L^2}\left(\frac{N}{\gamma}\right)^{2/(s+2)}, \tag{4.8}$$

for some constant C, so (4.7) reads

$$\begin{aligned}&E^{\rm hom}(n+1,L)-E^{\rm hom}(n,L)\\ &\leq 8\pi\frac{n}{L^2}\frac{1}{|\ln(a^2\bar\rho)|}\left(1+O\left(\frac{1+|\ln((\gamma/N)^{2/(s+2)}L^2/C)|}{|\ln(a^2\bar\rho)|}\right)\right).\end{aligned} \tag{4.9}$$

So if L is fixed, our minimizing n_α is at least $\sim\rho_{\alpha,\max}L^2N$. If N is large enough and $a^2\bar\rho$ is small enough, we can thus use (4.5) in (4.4) to get

$$Q\geq\sum_\alpha 4\pi\left(\frac{n_\alpha^2}{L^2}\frac{1}{|\ln\left(\frac{\widehat{a}^2n_\alpha}{L^2}\right)|}\left(1-\frac{C}{|\ln\left(\frac{\widehat{a}^2N}{L^2}\right)|^{1/5}}\right)-2\frac{N\rho_{\alpha,\max}}{|\ln(a^2\bar\rho)|}\right). \tag{4.10}$$

Lemma 4.1. *For $0<x,b<1$ we have*

$$\frac{x^2}{|\ln x|}-2\frac{b}{|\ln b|}x\geq-\frac{b^2}{|\ln b|}\left(1+\frac{1}{(2|\ln b|)^2}\right). \tag{4.11}$$

Proof. Since $\ln x \geq -\frac{1}{de}x^{-d}$ for all $d > 0$ we have

$$\frac{x^2}{b^2}\frac{|\ln b|}{|\ln x|} - 2\frac{x}{b} \geq \frac{|\ln b|}{b^2} edx^{2+d} - \frac{2x}{b} \geq c(d)(b^d ed|\ln b|)^{-1/(1+d)} \tag{4.12}$$

with

$$c(d) = 2^{(2+d)/(1+d)}\left(\frac{1}{(2+d)^{(2+d)/(1+d)}} - \frac{1}{(2+d)^{1/(1+d)}}\right) \geq -1 - \frac{1}{4}d^2. \tag{4.13}$$

Choosing $d = 1/|\ln b|$ gives the desired result. □

Note that the Lemma above implies for $k \geq 1$

$$\frac{x^2}{|\ln x|} - 2\frac{b}{|\ln b|}xk \geq -\frac{b^2}{|\ln b|}\left(1 + \frac{1}{(2|\ln b|)^2}\right)k^2. \tag{4.14}$$

Applying this with $x = \widehat{a}^2 n_\alpha / L^2$ and $b = N\widehat{a}^2 \rho_{\alpha,\max}$ we get the bound

$$\begin{aligned} Q \;&\geq -4\pi N\gamma \sum_\alpha \rho_{\alpha,\max}^2 L^2 \\ &\times \left[\left(1 + \frac{1}{4|\ln(\widehat{a}^2 N\rho_{\alpha,\max})|^2}\right)\frac{|\ln(\widehat{a}^2 N\rho_{\alpha,\max})|}{|\ln(a^2\bar{\rho})|}\left(1 - \frac{C}{|\ln\left(\frac{\widehat{a}^2 N}{L^2}\right)|^{1/5}}\right)^{-1}\right] \end{aligned} \tag{4.15}$$

for (4.10). To estimate the error terms, note that as in (4.8)

$$\widehat{a}^2 N \sim a^2\bar{\rho}\left(\frac{N}{\gamma}\right)^{2/(s+2)}, \tag{4.16}$$

so $|\ln(\widehat{a}^2 N)| = |\ln(a^2\bar{\rho})| + O(\ln|\ln(a^2\bar{\rho})|)$ for small $a^2\bar{\rho}$. Using $\|\widehat{\rho}_\gamma - \tilde{\rho}_{1,1}^{\mathrm{TF}}\|_\infty \to 0$ (Theorem 2.1 (iii)) and $\int \widehat{\rho}_\gamma^2 \to \int (\tilde{\rho}_{1,1}^{\mathrm{TF}})^2$ as $\gamma \to \infty$ (which follows from the uniform convergence and boundedness of the supports) we get

$$\liminf_{N\to\infty} \frac{E^{\mathrm{QM}}(N,a)}{E^{\mathrm{TF}}(N, 1/|\ln(a^2\bar{\rho})|)} \geq 1 - (\mathrm{const.})\left(\sum_\alpha \rho_{\alpha,\max}^2 L^2 - \int (\tilde{\rho}_{1,1}^{\mathrm{TF}})^2\right). \tag{4.17}$$

Since this holds for all choices of the boxes α with arbitrary small side length L, and by the assumptions on V $\tilde{\rho}_{1,1}^{\mathrm{TF}}$ is continuous and has compact support, we can conclude

$$\liminf_{N\to\infty} \frac{E^{\mathrm{QM}}(N,a)}{E^{\mathrm{TF}}(N, 1/|\ln(a^2\bar{\rho})|)} \geq 1 \tag{4.18}$$

in the limit $N \to \infty$, $a^2\bar{\rho} \to 0$ and $N/|\ln(a^2\bar{\rho})| \to \infty$.

Remark 4.1 (The GP case). In the derivation of the lower bound we have assumed that $\gamma \to \infty$ with N, i.e. $N \gg |\ln(a^2\bar{\rho})|$, which seems natural because otherwise the scattering length would have to decrease exponentially with N. However, for fixed γ one can use the methods of [1] (with slight modifications: One uses the 2D bounds on the homogeneous gas and Lemma (4.1)) to compute a lower bound in terms of the GP energy. The result is

$$\liminf_{N\to\infty} \frac{E^{\rm QM}(N,a)}{E^{\rm GP}(N, 1/|\ln(a^2\bar{\rho})|)} \geq 1 \tag{4.19}$$

in the limit $N \to \infty$, $a^2\bar{\rho} \to 0$ with $\gamma = N/|\ln(a^2\bar{\rho})|$ fixed.

5 The limit theorems

We have now all the estimates needed for Theorems 1.1–1.4. The upper bound (3.8) and the lower bound (4.19) prove Theorem 1.1. The energy limit Theorem 1.3 for the TF case follows from (3.8), Theorem 2.1 (i) and (4.18).

The convergence of the energies implies the convergence of the densities in the usual way by variation of the external potential. Replacing $V(\mathbf{x})$ by $V(\mathbf{x}) + \delta\gamma^{s/(s+2)}Y(\gamma^{-1/(s+2)}\mathbf{x})$ for some positive $Y \in C_0^\infty$ and redoing the upper and lower bounds we see that Theorem 1.3 and Theorem 2.1 (i) hold with W replaced by $W + \delta Y$. Differentiating with respect to δ at $\delta = 0$ yields

$$\lim_{N\to\infty} \frac{\gamma^{2/(s+2)}}{N} \rho^{\rm QM}_{N,a}(\gamma^{1/(s+2)}\mathbf{x}) = \tilde{\rho}^{\rm TF}_{1,1}(\mathbf{x}) \tag{5.1}$$

in the sense of distributions. Since the functions all have norm 1, we can conclude that there is even weak L^1-convergence.

Remark 5.1 (The 3D case). In [1] the analogues of Theorems 1.1 and 1.2 were shown for the three-dimensional Bose gas. Using the methods developed here one can extend these results to analogues of Theorems 1.3 and 1.4. In 3D the coupling constant is $g = a$, so $\gamma = Na$. Moreover, the relevant mean 3D density is $\bar{\rho}_\gamma \sim N(Na)^{-3/(s+3)}$.

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