The mathematics of dilute quantum gases

4. Bose-Einstein condensation and superfluidity

- Generalized Poincaré inequalities
- Bose-Einstein condensation for the homogeneous gas in the Gross-Pitaevskii limit
- Superfluidity in the Gross-Pitaevskii limit

We follow: Lieb, Seiringer, Solovej, Yngvason, "The mathematics of the Bose gas and its condensation", Chapters 4 and 5.

4.1. Bose-Einstein condensation (BEC), the Gross-Pitaevskii (GP) limit and the first main Theorem

We start by recalling some basic facts about BEC and we will be a little more precise at some points than in Chapter 2. In the last Chapter we have learned that the set of fermionic one-particle density matrices (1-pdms) is given by

Pauli principle, particle number

$$\{ \gamma \in \mathcal{B}(\mathcal{H}_1) \mid 0 \leq \gamma \leq 1, \ \mathrm{tr}\,\gamma = N \}, \qquad (1)$$

Set of bounded operators over the one-particle Hilbert space $\mathcal{H}_1$.

where N denotes the particle number. In case of Bosons we have the following statement (Lieb, Seiringer, "The stability of matter in quantum mechanics", Theorem 3.1).

Proposition: Let γ be a s.a., positive operator on $L^2(\mathbb{R}^3)$ with finite trace

$$\operatorname{tr}\gamma = N \tag{2}$$

and $N \in \mathbb{N}$, $N \geq 2$. Then there is a bosonic N-particle wave function Ψ such that γ is the 1-pdm of Ψ.

The reverse statement is also true. Since $\gamma \in \mathfrak{I}_1$ (trace class) and $\gamma \geq 0$, we know that it has an eigenfunction expansion of the form

$$\gamma = \sum_{\alpha=1}^{\infty} \gamma_\alpha \, |\Psi_\alpha\rangle\langle\Psi_\alpha| \tag{3}$$

with $0 \leq \gamma_\alpha \leq N$ because $\operatorname{tr}\gamma = \sum_{\alpha=1}^{\infty} \gamma_\alpha = N$. In a large particle number limit (as e.g. in the thermodynamic limit) we say that a sequence of wave functions shows BEC if it's 1-pdms γ_N obey

$$\liminf_{N\to\infty} \sup_{\|\Psi\|=1} \frac{\langle\Psi, \gamma_N \Psi\rangle}{N} > 0. \tag{4}$$

That is, the largest eigenvalue of γ_N grows proportionally to N (a macroscopic fraction of all particles do the same thing). Recall that for fermions $0 \leq \gamma_N \leq 1$ because of the Pauli principle. In a translation invariant system the eigenfunction related to the largest eigenvalue of γ_N is usually given by the constant function $1/L^{3/2}$ (we are in a box of side length L) and (4) is equivalent to

$$\frac{1}{L^3} \int_{[0,L]^6} \gamma_N(x,y)\, d(x,y) \geq cN \qquad (5)$$

for all large N, with $c>0$ depending only on the density $N/L^3 = \rho$. Proving (5) in the thermodynamic limit remains an open problem for almost 100 years.

In a certain limit, however, one can prove (5). This limit is called the Gross-Pitaevskii (GP) limit and it is relevant for the description of modern experiments with cold Bose gases. It can be viewed as a <u>combined</u>

thermodynamic and low-density limit. More precisely one takes the limit

$$N \to \infty,\ L \to \infty \text{ with } \rho = \frac{N}{L^3} \text{ fixed and } \frac{Na}{L} \text{ fixed.} \qquad (6)$$

$$\boxed{(*)\ \frac{Na}{L} = \frac{Na}{(N/\rho)^{1/3}} = \frac{N^{2/3}a}{\rho^{-1/3}} = \text{const} \Rightarrow a \sim \rho^{1/3} N^{-2/3}}$$

That is, as we take the thermodynamic limit we also let the scattering length go to zero.(*) The physical picture is the following: If we first take the thermodynamic limit and afterwards the low density limit we assume that we have to sets of parameters, namely $\{N, L\}$ and $\{\rho, a\}$. While N and L are large (we let them go to $+\infty$ first), ρ and a are comparable. This descripes purely macroscopic systems with e.g. $N \sim 10^{23}$ particles. In the GP regime there is only one limit, which means that all parameters remain comparable. $\frac{Na}{L} < +\infty$ in the GP limit, while it equals $+\infty$ in the thermodynamic limit. Since experiments are carried out with $10^3 - 10^6$ particles the GP limit is appropriate for their description.

In the following we will prove BEC for a Bose gas in a box with periodic or Neumann boundary conditions in the GP limit. Strictly speaking, to model experiments with trapped quantum gases one would need to consider Dirichlet boundary conditions. In the GP limit the boundary conditions can be seen in the energy and the condensate wave function would not be a constant if Dirichlet boundary conditions are considered. Also this case can be treated, but for the sake of mathematical simplicity we stick to periodic or Neumann boundary conditions, where the condensate wave function (eigenfunction of the largest eigenvalue of γ_N) is a constant.

One of the main theorems we are going to prove in this Chapter reads:

<u>Theorem 1 (BEC in GP limit):</u> Assume that, as $N \to \infty$, $\varrho = \frac{N}{L^3}$ and $g = \frac{Na}{L}$ stay fixed, and impose either periodic or Neumann boundary conditions for

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le i < j \le N} v(x_i - x_j) \qquad (7)$$

acting on $L^2_s([0,L]^{3N})$. Then

$$\lim_{N\to\infty} \frac{1}{N} \frac{1}{L^3} \int_{[0,L]^6} \gamma_N(x,y)\, d(x,y) = 1, \qquad (8)$$

where γ_N denotes the 1-pdm of the ground state wave function Ψ_N of H_N.

<u>Remark:</u> By scaling, the limit in Theorem 1 is equivalent to considering a Bose gas in a fixed box of side length $L=1$, and keeping Na fixed as $N \to \infty$, i.e., $a \sim \frac{1}{N}$. The ground state energy of the system is then, asymptotically as $N \to \infty$, given by $N \times 4\pi N a$ (Compare with

the result on finite boxes in Chapter 2.), and Theorem 1 implies that the 1-pdm γ_N of the ground state wave function converges, after division by N, to the projection onto the constant function. An analogous result holds true for inhomogeneous systems (Dirichlet BC's, Gases in other traps <-> replace $-\Delta$ by e.g. $-\Delta + x^2$).

One main ingredient in the proof of Theorem 1 is a generalized Poincaré inequality. Since it is of independent mathematical interest we state it here.

<u>Lemma 1 (Generalized Poincaré inequality)</u>: Let $K \subset \mathbb{R}^3$ be a cube of side length L, and define the average of a function $f \in L^1(K)$ by

$$\langle f \rangle_K = \frac{1}{L^3} \int_K f(x)\, dx. \tag{9}$$

Then there exists a constant C such that for all measurable sets $\Omega \subset K$ and all $f \in H^1(K)$ the inequality

$$\int_K |f(x) - \langle f \rangle_K|^2 dx \leq C \left(L^2 \int_\Omega |\nabla f(x)|^2 dx + |\Omega^c|^{2/3} \int_K |\nabla f(x)|^2 dx \right) \quad (10)$$

holds. Here $\Omega^c = K \setminus \Omega$, and $|\cdot|$ denotes Lebesgue measure of a set.

4.2 Proof of Theorem 1

We start with the proof of Lemma 1.

Proof of Lemma 1: Using the Poincaré inequality in the version on page 43 in Chapter 3 with the choice $g(x) = \frac{1}{L^3}$, we infer that there exists a constant $C>0$ such that

$$\| f - \langle f \rangle_K \|^2_{L^2(K)} \leq \frac{1}{2} C \, \| \nabla f \|^2_{L^{6/5}(K)} \tag{11}$$

$$\leq C \left(\|\nabla f\|^2_{L^{6/5}(\Omega)} + \|\nabla f\|^2_{L^{6/5}(\Omega^c)} \right).$$

An application of Hölder's inequality yields

$$\|\nabla f\|_{L^{6/5}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} \, |\Omega|^{1/3}, \tag{12}$$

and analogously with Ω replaced by Ω^c. When we estimate $|\Omega| \leq |K| = L^3$ in (12), this proves (10). $\blacksquare$

The proof of Theorem 1 has two main ingredients. One is localization of the energy that is stated in Lemma 2 below. This lemma is a refinement of the energy estimates for the Bose gas in Chapter 2 and says essentially that the kinetic energy of the ground state wave function is concentrated in a subset of configuration space where at least one pair of particles is close together and whose volume tends to zero as $a \to 0$. The other is the generalized Poincaré inequality, Lemma 1, from which one deduces that the 1-pdm of the ground state wavefunction is approximately constant if the kinetic energy is localized in a small set.

Lemma 2 (Localization of energy): Let Λ be a box of side length L. For all symmetric, normalized wave functions $\Psi(x_1 \ldots x_N)$ with periodic boundary conditions on Λ, and for

$N \geq Y^{1/17}$ with $Y = 4\pi\rho a^3/3$,

$$\frac{1}{N}\langle \Psi, H_N \Psi\rangle \geq \left(1 - \text{const.}\, Y^{1/17}\right) \tag{13}$$
$$\times \left(4\pi\rho a + \int_{K^{N-1}} \left[\int_{\Omega_X} \left| \nabla_{x_1} \Psi(x_1, X) \right|^2 dx_1 \right] dX \right),$$

where $X = (x_2 \ldots x_N)$, $dX = \prod_{j=2}^{N} dx_j$, and

$$\Omega_X = \left\{ x_1 \in K \;\middle|\; \min_{j \geq 2} |x_1 - x_j| \geq R \right\} \tag{14}$$

with $R = a Y^{-5/17}$.

<u>Proof</u>: Since Ψ is symmetric, the l.h.s of (13) can be written as N times

$$\int_{K^{N-1}} \left[\int_K \left\{ \left|\nabla_{x_1}\Psi(x_1, X)\right|^2 + \frac{1}{2}\sum_{j\geq 2} v(x_1 - x_j)\left|\Psi(x_1, X)\right|^2 \right\} dX \right] dx_1. \tag{15}$$

Let us define

$$T = \int_{K^N} |\nabla_{x_1} \Psi(x_1, X)|^2 \, d(x_1, X), \tag{16}$$

$$T^{in} = \int_{K^{N-1}} \left[\int_{\Omega_X^c} |\nabla_{x_1} \Psi(x_1, X)|^2 dx_1 \right] dX, \tag{17}$$

$$T^{out} = \int_{K^{N-1}} \left[\int_{\Omega_X} |\nabla_{x_1} \Psi(x_1, X)|^2 dx_1 \right] dX, \tag{18}$$

and

$$\mathcal{J} = \frac{1}{2} \int_{K^{N-1}} \left[\int_{K} \sum_{j \geq 2} V(x_1 - x_2) \, |\Psi(x_1, X)|^2 dx_1 \right] dX. \tag{19}$$

Here $\Omega_X^c = \{ x_1 \in K \mid |x_1 - x_j| < R \text{ for some } j \geq 2 \}$ is (20)
the complement of Ω_X. The expression in (15) can be bounded as $(\varepsilon > 0, R > 0)$

$$\geq \varepsilon T + (1-\varepsilon)\left(T^{in} + \mathcal{J}\right) + (1-\varepsilon) T^{out} \tag{21}$$

To complete the proof we use several estimates from Chapter 2.

Using the notation of this Chapter, the relevant bounds are

$$\frac{E_0(N,L)}{N} \geq 4\pi a\rho \left(1 - \frac{1}{\rho \ell^3}\right) K(4\rho \ell^3, \ell), \tag{22}$$

(83), p. 38, Ch. 2

(85), p. 39, Ch. 2

$$K(4\rho\ell^3, \ell) \geq (1-\varepsilon)\left(1 - \frac{2R}{\ell}\right)^3 \left(1 - \text{const.}\,(a^3\rho)\,(\ell/a)^3\,(R/\ell)^3\right) \tag{23}$$

$$\times \left(1 - \frac{\ell^3}{R^3 - R_0^3}\,\frac{\text{const.}\; a^3\rho}{\varepsilon\,(a/\ell)^2 - \text{const.}\,(a^3\rho)\,(\ell/a)^3}\right),$$

$$\varepsilon \sim (a^3\rho)^\alpha, \quad a/\ell \sim (a^3\rho)^\beta, \quad (R^3 - R_0^3)/\ell^3 \sim (a^3\rho)^\gamma, \tag{24}$$

(86), p. 39, Ch. 2

$$\alpha = \frac{1}{17}, \quad \beta = \frac{6}{17}, \quad \gamma = \frac{3}{17}. \tag{25}$$

(87, p. 40, Ch. 2)

For $\varepsilon = Y^{\frac{1}{17}}$ and $R = a\,Y^{-5/17}$ (which follows from (24) and (25)) we thus obtain

$$\varepsilon T + (1-\varepsilon)\left(T^{in} + J\right) \geq \left(1 - \text{const.}\, Y^{\frac{1}{17}}\right) 4\pi a \rho \qquad (26)$$

as long as $N \geq Y^{-\frac{1}{17}}$. The main point here is that we only need the kinetic energy in a ball of radius R to prove the Dyson Lemma on p. 25 of Chapter 2 if $U(x)$ is chosen as in (64) on p. 28 in Chapter 2. In combination, (15), (21) and (26) prove (13).

$\blacksquare$

We are now prepared to give the proof of Theorem 1. Let Ψ be any symmetric wave function with $\langle \Psi, \Psi \rangle = 1$. From Lemma 1 we know that

$$\int_K \left| \Psi(x_1, X) - L^{-3} \int_K \Psi(x, X)\, dx \right|^2 dx_1 \qquad (27)$$

$$\leq C \left(L^2 \int_{\Omega_X} |\nabla_{x_1} \Psi(x_1, X)|^2 dx_1 + |\Omega_X^c|^{2/3} \int_K |\nabla_{x_1} \Psi(x_1, X)|^2 dx_1 \right),$$

and hence

$$\int_{K^{N-1}} \left[\int_K \left| \Psi(x_1,X) - L^{-3} \int_K \Psi(x,X)\,dx \right|^2 dx_1 \right] dX \tag{28}$$

$$\leq C \int_{K^{N-1}} \left(L^2 \int_{\Omega_X} |\nabla_{x_1} \Psi(x_1,X)|^2 dx_1 + L^2 Y^{4/51} \int_K |\nabla_{x_1} \Psi(x_1,X)|^2 dx_1 \right) dX,$$

with Ω_X defined in (14). To obtain (28) we used that

$$|\Omega_X^c| \leq \frac{4\pi}{3} N R^3 \overset{(24),(25)}{=} \text{const. } L^3 Y^{\frac{2}{17}}, \tag{29}$$

which follows from (14), (24) and (25). Using Lemma 2 and (28) we conclude that

$$\frac{1}{N} \langle \Psi, H_N \Psi \rangle \left(1 - \text{const. } Y^{\frac{1}{17}} \right)^{-1} \geq 4\pi a \rho \tag{30}$$

$$+ \frac{\text{const.}}{L^2} \int_{K^{N-1}} \left[\int_K \left| \Psi(x_1,X) - L^{-3} \int_K \Psi(x,X)\,dx \right|^2 dx_1 \right] dX$$

$$- \text{const. } Y^{\frac{4}{51}} \underbrace{\int_K |\nabla_{x_1} \Psi(x_1,X)|^2 dx_1}_{= \frac{1}{N} \langle \Psi, \sum_{i=1}^N -\Delta_i \Psi \rangle}$$

From the upper bound on p. 13 in Chapter 2 we know that

$$\frac{1}{N}\langle \Psi_0, H_N \Psi_0\rangle \leq 4\pi a\rho\left(1+\mathrm{const.}\,Y^{1/3}\right), \tag{31}$$

where Ψ_0 denotes the ground state wave function of H_N. The same is true for $\frac{1}{N}\langle \Psi_0, \sum_{i=1}^{N} -\Delta_i \Psi_0\rangle \leq \frac{1}{N}\langle \Psi_0, H_N\Psi_0\rangle$. In combination with (30), this implies

$$\begin{aligned}\frac{4\pi a\rho\left(1+\mathrm{const.}\,Y^{\frac{1}{3}}\right)}{\left(1-\mathrm{const.}\,Y^{\frac{1}{17}}\right)} &\geq \frac{1}{N}\langle \Psi_0, H_N\Psi_0\rangle \left(1-\mathrm{const.}\,Y^{\frac{1}{17}}\right)^{-1} \\ &\geq 4\pi a\rho - \mathrm{const.}\,Y^{\frac{4}{51}} a\rho \\ &+ \frac{\mathrm{const.}}{L^2}\int_{K^{N-1}}\left[\int_K \left|\Psi_0(x_1,X) - L^{-3}\int_K \Psi_0(x,X)\,dx\right|^2 dx_1\right] dX.\end{aligned} \tag{32}$$

We conclude that

$$\int_{K^{N-1}}\left[\int_K \left|\Psi_0(x_1,X) - L^{-3}\int_K \Psi_0(x,X)\,dx\right|^2 dx_1\right] dX \leq \mathrm{const.}\, L^2 a\rho\, Y^{\frac{1}{17}}. \tag{33}$$

In the GP limit we have

$$L^2 a\rho\, Y^{\frac{1}{17}} = L^2 a \underbrace{\rho}_{N/L^3} \left(4\pi \underbrace{\rho a^3}/8\right)^{\frac{1}{17}} \sim \left(\frac{1}{N^2}\right)^{1/17} = N^{-\frac{2}{17}} \tag{34}$$

$$\underbrace{a\rho L^2}_{\frac{Na}{L} = \text{const.}} \qquad \rho a^3 = \underbrace{\rho}_{N/L^3} \left(\frac{Na}{L}\right)^3 \frac{L^3}{N^3} = \frac{1}{N^2},$$

That is,

$$\int_{K^{N-1}} \left[\int_K \left| \Psi_0(x_1,X) - L^{-3} \int_K \Psi_0(x,X)\,dx \right|^2 dx_1 \right] dX \le \text{const.}\, N^{-\frac{2}{17}}. \tag{35}$$

The important point is that the r.h.s. goes to zero as $N \to \infty$.
It remains to note that the l.h.s. of (35) equals

$$\int_{K^N} |\Psi_0(x_1,X)|^2 dx_1 dX - 2\mathrm{Re}\left[\int_{K^{N-1}} \int_K \Psi_0(x_1,X)\,dx_1 \times \frac{1}{L^3} \int_K \overline{\Psi_0(x,X)}\,dx\,dX \right] \tag{36}$$

$$\frac{1}{L^3} \int_{K^{N-1}} \left| \int_K \Psi_0(x,X)\,dx \right|^2 dX$$

$$= 1 - \frac{1}{NL^3} \int_{K\times K} \gamma(x,x')\, d(x,x'),$$

where γ denotes the 1-pdm of Ψ_0. Accordingly,

$$0 \leq 1 - \frac{1}{NL^3} \int_{K\times K} \gamma(x,x')\, d(x,x') \leq \text{const.}\ N^{-\frac{2}{17}}, \tag{37}$$

that is, the ground state wave function Ψ_0 shows complete BEC. This proves Theorem 1.

4.3. Superfluidity and the second main Theorem

A fluid is called a superfluid if it flows without any resistance. If a superfluid is flowing for example in a ring shaped tube the velocity of the flow will never decrease. Such a behavior was first observed by Pyotr Kapitsa and John F. Allen and by Don Misener in 1937 in liquid Helium 4 at roughly 2.17 Kelvin. The fraction of the total density of particles that show superfluid behavior is called the superfluid fraction and their density is called the superfluid density.

The above example can also be turned around. If a superfluid is flowing in a ring shaped tube without resistance, then a superfluid at rest would show no response when we start to slowly move (rotate) the tube (there is no friction). Motivated by these two examples

The superfluid fraction is often defined in the following way: Let E_0 denote the ground state energy of the system in the rest frame and E_0' the ground state energy of the system in the moving frame, when a velocity field v is imposed e.g. by moving walls of a container. Then for small v

$$\frac{E_0'}{N} = \frac{E_0}{N} + \left(\frac{\rho_s}{\rho}\right)\frac{1}{2}mv^2 + O(|v|^4), \tag{38}$$

where N is the particle number and m the particle mass. For a detailed motivation of (38) see P.C. Hohenberg, P.C. Martin, "Microscopic theory of Superfluid Helium, Ann. Phys. (NY) 34, 291 (1965). ← If you cannot access the reference please contact me.

Remark: It is important here that the error term (38) holds uniformly for large N, i.e., that the error term $O(|v|^4)$ can be bounded independently of N. For fixed N and a finite box, (38) with $\rho_s/\rho = 1$ always holds for a Bose gas with an arbitrary interaction if v is small enough because of the discreteness of the energy spectrum.

It is important to note that there are other definitions of the superfluid density that may lead to different results.

We will not go into more details here because it is not clear that there is one definition that is apropriate for all purposes.

As an example we mention that definition (8P) implies that the ideal Bose gas Bose gas is a perfect superfluid ($\rho_s = \rho$), whereas the definition of Landau in terms of a linear dispersion relation of elementary excitations would indicate otherwise (google Landau criterion for Superfluidity or consult Landau, Lifschitz, "Statistical Physics, Part II" if you are not familiar with this). The main result we will prove in this section shows that according to (8P), the ground state of a three-dimensional Bose gas in the GP limit is a perfect superfluid ($\rho_s = \rho$).

One of the unresolved issues in the theory of superfluidity is its relation to BEC. It has been argued that in general neither condition is necessary for the other, but in the case we consider here, i.e. the GP limit of a 3d gas, we show that 100% BEC into the constant function prevails even if an external velocity field is imposed.

A simple example illustrating the fact that BEC is not necessary for superfluidity is the 1d hard-core Bose gas. This system is well known to be superfluid in its ground state in the sense of (38) but it shows no BEC.

To avoid the mathematical complications of a ring shaped tube we consider a Bose gas in a box with side length L and boundary conditions instead. Imposing an external velocity field $v = (0, 0, \pm|v|)$ means that the momentum operator $p = -i\nabla$ is replaced by $p - mv$. In our previous discussion we always assumed that the kinetic energy is given by p^2, that is, $m = \frac{1}{2}$ $\left(E_{kin} = \frac{p^2}{2m}\right)$, and we will do the same here. The Hamiltonian of the system thus reads

$$H_N' = \sum_{j=1}^{N} \nabla_{j,\varphi}^2 + \sum_{1 \leq i < j \leq N} v_N(x_i - x_j) \qquad (39)$$

with $\nabla_{j,\varphi} = \nabla_j + i(0, 0, \varphi/L)$ and $\varphi = \frac{\pm|v|L}{2}$. For Ψ_0 the ground state of H_N', let γ_N be its 1-pdm. The second main result of this Chapter is the following statement.

Theorem 2 (Superfluidity and BEC of homogeneous gas):

For $|\varphi| \leq \pi$ we have

$$\lim_{N\to\infty} \frac{E_0(N,a,\varphi)}{N} = \lim_{N\to\infty} \inf_{\|\Psi\|=1} \langle \Psi, H_N^\varphi \Psi \rangle = 4\pi a\rho + \frac{1}{2}\frac{\varphi^2}{L^2} \qquad (40)$$

in the GP limit $N\to\infty$ with Na/L and L fixed. Here $\rho = \frac{N}{L^3}$, so $a\rho$ is fixed too. In the same limit, for $|\varphi| < \pi$,

$$\lim_{N\to\infty} \frac{1}{N}\gamma_N(x,x') = \frac{1}{L^3} \qquad (41)$$

in trace class norm, i.e., $\lim_{N\to\infty} \mathrm{tr}\left[\left| \gamma_N/N - |L^{-3/2}\rangle\langle L^{-3/2}| \right| \right] = 0.$

Remark 1: As discussed in Section 4.1, the scattering length a behaves as $a \sim \frac{1}{N}$ if L is fixed.

Remark 2: By the definition of ρ_s in (38) and the definition of φ on p. 21, (40) shows that $\rho_s = \rho$, i.e. there is 100% superfluidity. For $\varphi = 0$, (40) follows from the results of

Chapter 2 (Eq. (8)), while (41) for $\varphi = 0$ is the BEC result from Theorem 1.

(a Galilea transformation)

<u>Remark 3:</u> By a unitary gauge transformation,

$$(U\Psi)(x_1 \ldots x_N) = e^{i\varphi\left(\sum_{i=1}^{N}\left(\frac{x_i}{L}\right)_3\right)} \Psi(x_1 \ldots x_N), \tag{42}$$

last component of the vector (x_i/L)

the passage from

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le i < j \le N} V(x_i - x_j) \tag{43}$$

to H_N'

is equivalent to replacing periodic boundary conditions in a box of side length L by the twisted boundary conditions

$$\Psi(x_1 + (0,0,L), x_2 \ldots x_N) = e^{i\varphi} \Psi(x_1, x_2, \ldots x_N) \tag{44}$$

in the direction of the velocity field (and the same for the other coordinates), while retaining the original Hamiltonian H_N in (43). This explains also why it is no restriction to consider only $-\pi \le \varphi \le \pi$ in the Theorem (E_0 is 2π periodic in φ).

Remark 4: The reason for the restriction $|\varphi|<\pi$ in the second part of the Theorem is that for $|\varphi|=\pi$ there are two ground states of the operator $\left(\nabla+i\left(0,0,\varphi/L\right)\right)^2$ with periodic boundary conditions. All we can say in this case is that there is a subsequence of γ_N that converges to a density matrix of rank ≤ 2, whose range is spanned by the two condensate functions related to the two ground states.

Remark 5: Eq. (41) implies BEC in the sense of (4). This follows because the trace norm dominates the operator norm, i.e., $\|A\| \leq \|A\|_1$, and hence

$$\left\|\gamma_N/N - |L^{-3/2}\rangle\langle L^{-3/2}|\right\|_1 \geq \left\|\gamma_N/N - |L^{-3/2}\rangle\langle L^{-3/2}|\right\| \geq \left|\,\|\gamma_N/N\| - \underbrace{1}_{\|\,|L^{-3/2}\rangle\langle L^{-3/2}|\,\|=1}\right|.$$

Accordingly, the largest eigenvalue of γ_N/N, which equals $\|\gamma_N/N\|$ converges to 1 as $N\to\infty$.

As in the proof of Theorem 1 a generalized Poincaré inequality also plays a crucial role in the proof of Theorem 2. In the version that we need here, the Laplacian is replaced by ∇_φ^2 with $\nabla_\varphi = \nabla + i\left(0,0,\varphi/L\right)$ and reads:

Lemma 3 (Generalized Poincaré inequality with a vector potential):

For any $|\varphi|<\pi$ there are constants $c, C>0$ such that for all subsets $\Omega\subset K=[0,L]^3$ and all functions $f\in H^1(K)$ with periodic boundary conditions on K the following estimate holds:

$$\|\nabla_\varphi f\|^2_{L^2(\Omega)} \geq \frac{\varphi^2}{L^2}\|f\|^2_{L^2(K)} + \frac{c}{L^2}\|f-\langle f\rangle_K\|^2_{L^2(K)} \qquad (45)$$

$$- C\left(\|\nabla_\varphi f\|^2_{L^2(K)} + \frac{1}{L^2}\|f\|^2_{L^2(K)}\right)\left(\frac{|\Omega^c|}{L^3}\right)^{1/2}.$$

Here $|\Omega^c|$ is the volume of $\Omega^c = K\setminus\Omega$, the complement of Ω in K.

Remark: The proof of Lemma 3 requires more analysis than the one of Lemma 2 and will not be carried out here. It can be found in the book mentioned on the cover page of this Chapter in Chapter 4, see Lemma 4.2.

4.4. Proof of Theorem 2

As in the proof of Theorem 1 we need a localization Lemma for the energy. In the case with a vector potential it reads:

Lemma 4 (Localization of energy): Let K be a box of side length L. For all symmetric, normalized wave functions $\Psi(x_1 \ldots x_N)$ with periodic boundary conditions on K, and for

$N \geq Y^{1/17}$ with $Y = 4\pi\rho a^3/3$,

$$\frac{1}{N}\langle \Psi, H_N' \Psi\rangle \geq \left(1 - \text{const.}\, Y^{1/17}\right) \tag{46}$$
$$\times \left(4\pi\rho a + \int_{K^{N-1}} \left[\int_{\Omega_X} \left| \nabla_{x_1,\varphi} \Psi(x_1, X) \right|^2 dx_1 \right] dX \right),$$

where $X = (x_2 \ldots x_N)$, $dX = \prod_{j=2}^{N} dx_j$, Ω_X defined in (14) and with $R = a Y^{-5/17}$.

The proof is almost the same than the one of Lemma 2 except for the fact that now

$$\int_{K^{N-1}}\left(\int_{K}\Big[|\nabla_{x_1,\varphi}\Psi(x_1,X)|^2+\frac{1}{2}\sum_{j\geq 2}v(x_1-x_j)|\Psi(x_1,X)|^2\Big]dx_1\right)dX$$

$$\geq \varepsilon T+(1-\varepsilon)\left(T^{in}+J\right)+(1-\varepsilon)T_{\varphi}^{out} \qquad (47)$$

with

$$T=\int_{K^N}\left|\nabla_{x_1}|\Psi(x_1,X)|\right|^2 d(x_1,X), \qquad (48)$$

$$T^{in}=\int_{K^{N-1}}\Big[\int_{\Omega_X^c}\left|\nabla_{x_1}|\Psi(x_1,X)|\right|^2 dx_1\Big]dX \qquad (49)$$

and

$$T^{out}=\int_{K^{N-1}}\Big[\int_{\Omega_X}|\nabla_{x_1,\varphi}\Psi(x_1,X)|^2 dx_1\Big]dX. \qquad (50)$$

Note that we have $\nabla_{x_1}|\Psi(x_1,X)|$ instead of $\nabla_{x_1}\Psi(x_1,X)$ in (48) and (49). Eq. (47) follows from the diamagnetic inequality, which in our case reads:

<u>Diamagnetic inequality</u>: Let $A : \mathbb{R}^3 \to \mathbb{R}^3$ be in $L^2(K)$ and let $f \in L^2(K)$ be such that $(\partial_j + iA_j)f \in L^2(K)$ for $j = 1,2,3$. Then $|f| \in H^1(K)$ and the diamagnetic inequality,

$$\big|\nabla |f(x)|\big| \leq \big|(\nabla + iA)f(x)\big|, \tag{51}$$

holds pointwise for almost every $x \in K$.

For a proof see Lieb, Loss, "Analysis", Theorem 7.21.

The name of the diamagnetic inequality stems from the fact that it can be used to show that an external magnetic field always raises the ground state energy of a quantum particle.

The rest of the proof of Lemma 4 goes as the proof of Lemma 2. The only additional piece of information we need is that the ground state ψ_0 of H_N satisfies

$\Psi(x_1 \ldots x_N) = |\Psi(x_1 \ldots x_N)|$, that is, the kinetic energy in (48) and (48) is as useful for the lower bound of the ground state energy as the one where $\nabla_{x_1}|\Psi(x_1,X)|$ is replaced by $\nabla_{x_1}\Psi(x_1,X)$.

$\blacksquare$

We combine the localization Lemma 4 as in the proof of Theorem 1 with the generalized Poincaré inequality, that is, Lemma 3. Let Ψ be a symmetric functions with $\langle \Psi,\Psi\rangle = 1$. We have (Poincaré inequality)

$$\|\nabla_{x_1,\varphi}\Psi(x_1,X)\|^2_{L^2(\Omega_X, dx_1)} \geq \frac{\varphi^2}{L^2}\|\Psi(x_1,X)\|^2_{L^2(K,dx_1)} \tag{52}$$

$$+ \frac{c}{L^2}\left\| \Psi(x_1,X) - \frac{1}{L^3}\int_K \Psi(x,X)\,dx \right\|^2_{L^2(K,dx_1)}$$

$$- C\left(\|\nabla_{x_1,\varphi}\Psi(x_1,X)\|^2_{L^2(K,dx_1)} + \frac{1}{L^2}\|\Psi(x_1,X)\|^2_{L^2(K)} \right) \times \left(\frac{|\Omega_X^c|}{L^3}\right)^{1/2}.$$

With the localization Lemma and (51) we see that

$$\frac{1}{N}\langle \Psi, H_N' \Psi\rangle \geq \left(1 - \text{const.}\, Y^{1/17}\right) \tag{53}$$
$$\times \Bigg(4\pi \rho a + \frac{\varphi^2}{L^2}$$
$$+ \frac{c}{L^2}\int_{K^{N-1}}\int_K \left| \Psi(x_1, X) - \frac{1}{L^3}\int_K \Psi(x, X)\,dx \right|^2 dx_1\, dX$$
$$- C\left(\langle \Psi, \sum_{i=1}^N -\nabla_{x_i,\varphi}^2 \Psi\rangle + \frac{1}{L^2}\right) \underbrace{\left(\frac{|\Omega_X^c|}{L^3}\right)^{1/2}}_{\underset{(29)}{\leq}\ \text{const.}\, Y^{\frac{1}{17}}} \Bigg).$$

As in the proof of Theorem 1, we need also need an upper bound to the ground state energy. Using the ground state Ψ_0 as a trial function, we check that

$$E_0(N,a,\varphi) \leq \langle \Psi_0, H_N' \Psi_0\rangle = E_0(N,a,0) + N\frac{\varphi^2}{N^2}, \tag{54}$$

because $\langle \Psi_0, \nabla_i \Psi_0 \rangle = 0$. The last statement follows from (a) the fact that the lowest eigenvalue of H_N is simple (see p. 26 of the introduction) and (b) the fact that $[H_N, P_N] = 0$ with P_N denoting the reflection at the mid-point of the box (in case of $[-L/2, L/2]^3$ this would be $x=0$).

In combination with the upper bound from Chapter 2 this implies

$$E_0(N,a,\varphi) \leq 4\pi a N\rho\left(1+\text{const.}\, Y^{1/3}\right) + N\frac{\varphi^2}{L^2}. \quad (55)$$

Since $V \geq 0$ we also have

$$\left\langle \Psi_0', \sum_{i=1}^{N} -\nabla_{x_i,\varphi}^2 \Psi_0' \right\rangle \leq 4\pi a N\rho\left(1+\text{const.}\, Y^{1/3}\right) + N\frac{\varphi^2}{L^2}, \quad (56)$$

where Ψ_0' denotes the ground state wave function of H_N'.

Using (53) with the choice $\Psi = \Psi_0'$, (55) and (56) we check that

$$\frac{4\pi a \rho\left(1+\text{const.}\, Y^{1/3}\right)+\frac{\varphi^2}{L^2}}{\left(1-\text{const.}\, Y^{\frac{1}{17}}\right)} \geqslant \frac{1}{N}\langle \Psi_0', H_N' \Psi_0' \rangle \left(1-\text{const.}\, Y^{\frac{1}{17}}\right)^{-1}$$

$$\geqslant 4\pi\rho a+\frac{\varphi^2}{L^2}-\text{const.}\left(\rho a+\frac{1}{L^2}\right)Y^{\frac{1}{17}} \tag{57}$$

$$+\frac{c}{L^2}\int_{K^{N-1}}\int_{K}\left|\Psi_0'(x_1,X)-\frac{1}{L^3}\int_K \Psi_0'(x,X)dx\right|^2 dx_1\, dX$$

holds for any $|\varphi|<\pi$. When we drop the last term on the r.h.s. of (57) for a lower bound we have thus shown that

$$4\pi\rho a\left(1+\text{const.}\, Y^{1/3}\right)+\frac{\varphi^2}{L^2} \geqslant E_0(N,a,\varphi) \tag{58}$$

$$\geqslant \left(4\pi\rho a+\frac{\varphi^2}{L^2}\right)\left(1-\text{const.}\, Y^{\frac{1}{17}}\right),$$

which proves (40) in this case (the upper bound also holds for $|\varphi|=\pi$ but for the lower bound we used Lemma 3, which requires $|\varphi|<\pi$). To extend the result to $|\varphi|=\pi$, we use continuity. More precisely, $E_0(N,a,\varphi)/N - \varphi^2/L^2$ is a concave function of φ, and therefore stays concave in the $N\to\infty$ limit. Accordingly, the limit is a continuous function of φ and, after having taken the limit $N\to\infty$ in Eq. (58), we can take the limit $\varphi\to\tilde{\varphi}$ with $|\tilde{\varphi}|=\pi$ to prove (40) also in this case. It remains to prove (41).

To that end, we note that (56) implies

$$\int_{K^{N-1}}\left[\int_K \left|\Psi_0^{\varphi}(x_1,X) - L^{-3}\int_K \Psi_0^{\varphi}(x,X)\,dx\right|^2 dx_1\right] dX \tag{59}$$
$$\leq \text{const.}\, L^2 a\rho\, Y^{\frac{1}{17}} = \text{const.}\, N^{-\frac{2}{17}}.$$

Using (36) we thus find

$$0 \leq 1 - \frac{1}{NL^3}\int_{K\times K} \gamma_N(x,x')\,d(x,x') \leq \text{const.}\, N^{-\frac{2}{17}}, \tag{60}$$

where γ_N denotes the 1-pdm of the ground state wave function of H_N'. It remains to show that (60) implies

$$\lim_{N\to\infty} \operatorname{tr}\Big[\big| \gamma_N/N - |L^{-3/2}\rangle\langle L^{-3/2}| \big| \Big] = 0, \qquad (61)$$

where $|L^{-3/2}\rangle\langle L^{-3/2}|$ denotes the projection onto the constant function, i.e.

$$\Big(|L^{-3/2}\rangle\langle L^{-3/2}|\Psi\Big)(x) = \frac{1}{L^3}\int_K \Psi(y)\,dy. \qquad (62)$$

First we note that (60) implies

$$\langle L^{-3/2}, \gamma_N/N\, L^{-3/2}\rangle \xrightarrow{N\to\infty} 1. \qquad (63)$$

We also know that

$$\operatorname{tr}\gamma_N/N = 1 \qquad (64)$$

for all $N \geq 1$. Eqs. (63) and (64) imply that

$$\lim_{N\to\infty} \langle \varphi, \gamma_N/N\, \Psi\rangle = \langle \varphi, |L^{-3/2}\rangle\langle L^{-3/2}|\Psi\rangle \qquad (65)$$

for all $\varphi, \Psi \in L^2(K)$ (Check this!). The convergence in (65) is called convergence in the weak operator topology. Eq. (61) now follows from the following general statement:

<u>Lemma 5:</u> Suppose that $A_n \to A$, $|A_n| \to |A|$, and $|A_n^*| \to |A|$ in the weak operator topology, and that $\|A_n\|_1 \to \|A\|_1$. Then $\|A_n - A\|_1 \to 0$.

<u>Proof:</u> See B. Simon, "Trace ideals and their application", Cambridge University Press (1979), Theorem 2.20. (2nd. Ed.)

In our case $\gamma_N/N = |\gamma_N/N| = |\gamma_N^*/N|$ and the same for $|L^{-3/2}\rangle\langle L^{-3/2}|$. Note also that $\mathrm{tr}\left[|L^{-3/2}\rangle\langle L^{-3/2}|\right] = 1$ because the operator is a rank one projection. In combination, Lemma 5, (64) and (65) therefore prove (61). This finishes the proof of Theorem 2.