The Dilute, Cold Bose Gas

(Work with R. Seiringer, J-P. Solovej, J. Yngvason)

1. *The dilute repulsive Bose gas at low density (2D and 3D).* **(L, Yngvason)**

2. *Repulsive bosons in a trap (as used in recent experiments) and the 'Gross-Pitaevskii eqn.*

   (L, Seiringer, Yngvason)

3. *100%Bose-Einstein condensation in trapped gases.* **(L, Seiringer)**

4. *100% Superfluidity in trapped gases.*

   (L, Seiringer, Yngvason)

5. *One-dimensional physics in trapped gases.*

   (L, Seiringer, Yngvason)

6. *The Rotating Bose Gas*

   (L, Seiringer)

7. *Foldy's 'jellium' model of charged particles in a neutralizing background and Dyson's $N^{7/5}$ law* **(L, Solovej)**

3D DILUTE, REPULSIVE BOSE GAS

The Hamiltonian for a gas of N bosons of mass m and pair-potential $v(|\vec{x}_i - \vec{x}_j|)$, $\vec{x}_i \in R^3$:

$$H = -\mu \sum_{i=1}^{N} \Delta_i + \sum_{1 \leq i < j \leq N} v(|\vec{x}_i - \vec{x}_j|)$$

with $\mu = \hbar^2/2m$. These bosons are in a macroscopically large box of volume $V = L^3$ and $\rho \equiv N/V$ is the fixed density. 'Repulsive' means $v(|\vec{x}|) \geq 0$, $\forall \vec{x}$. Dilute means small ρ. For a 'trap' we add a confining potential $\sum_{i=1}^{N} V_{\mathrm{ext}}(\vec{x}_i)$.

The simplest question is the ground state energy (GSE) per particle

$$e_0(\rho) = E_0(N, V)/N.$$

In *1947* Bogolubov proposed the main features of the low density gas. To leading order in ρ, the energy was asserted to be

$$e_0(\rho) \approx \mu 4\pi \rho a \ , \tag{1}$$

where a is the *scattering length* of $v(|\vec{x}|)$.

Later, there were several alternative "derivations" of this but it was only in *1957* that Dyson found an *upper* bound like (1) for the *hard core* gas and a *lower* bound that was *14 times smaller!* That was the best lower bound until *1998!* There were *no other* bounds — which shows that bosons are much more complicated than fermions, i.e., boson correlations can be *subtle.*

Usually, upper bounds are easy to get, but bosons are so subtle that Dyson's *upper* bound needed a great deal of cleverness. Anyway, all we really needed, 40 years later, is a good lower bound, and that is our main concern here.

The basic problem is that when ρ is small the energy is also small. If (1) is true then the 'correlation' (or uncertainty principle) length, ℓ_c, is approximately $(\rho a)^{-1/2}$, while the average particle spacing is $\rho^{-1/3}$. Thus, in terms of the dimensionless number $Y = \rho a^3$ ($\approx 10^{-6}$ in many experiments)

$$\ell_c = (\rho a)^{-1/2} = (\rho a^3)^{-1/6} \rho^{-1/3} \gg \rho^{-1/3}.$$

For *fermions*, $\ell_c/\rho^{-1/3} \approx 1$, and there is no such problem .

On the other hand, if we use perturbation theory, starting from $\Psi(\vec{x}_i, \ldots, \vec{x}_N) \equiv \text{constant} = V^{-N/2}$, we would get

$$e_0(\rho) \approx \frac{1}{2}\rho \int v(\vec{x}) d^3\vec{x},$$

which is the wrong answer! [But $\frac{1}{2}\int v(\vec{x})d^3\vec{x}$ is the first perturbative (Born) approximation to $\mu 4\pi a$, and this led Landau/Bogolubov to guess that $\mu 4\pi\rho a$ is the correct answer.]

Next, we recall the definition of 'a', the *2-body scattering length*

$$-\mu\Delta\ \psi(r) + \frac{1}{2}v(r)\psi(r) = 0$$

$$\psi(r) = 1 - a/r \qquad \text{for } r > R_0$$

Note that a depends on μ, except for:

`HARD CORE:` $v(r) = \infty$ for $r < a$ and $= 0$ otherwise, $\psi(r) = \max(1 - a/r), 0.$

There are* <u>TWO</u> *regions:

1. <u>*Potential Energy Dominated*</u>: Large v (e.g., hard core). e_0 is <u>mostly kinetic</u> and a is independent of μ. We see this from $e_0 \approx \mu\rho a$, because $\mu\partial e_0/\partial\mu =$ (kinetic energy).

THERE IS NO PERTURBATION THEORY IN THIS REGION

2. <u>*Kinetic Energy Dominated*</u>: e_0 is <u>mostly potential</u>. $a \approx \mu^{-1}$. Thus, e_0 is independent of μ. Simple perturbation theory is valid.

The energy, e_0, cannot distinguish the 2 regions. Does Bose condensation distinguish them? No one really knows.

<u>THEOREM</u>: With $Y \equiv \rho a^3$ and $v(\vec{x}) \geq 0, \forall \vec{x}$,

$$\boxed{e_0(\rho) \geq \mu 4\pi\rho a\left(1 - 9Y^{1/17}\right)}$$

FOR THE FUTURE :

There are two obvious next steps.

$\boxed{A.}$ **Prove the next term in the low density expansion (Bogolubov, Huang-Lee-Yang)**

In particular, the leading corrections to (1) supposedly involves only $Y = \rho a^3$, namely $4\pi\mu\rho a\{\frac{128}{15\sqrt{\pi}}Y^{1/2}\}$.

$\boxed{B.}$ **Prove existence of Bose-Einstein condensation: the *largest eigenvalue* of the one-particle density matrix**

$$\gamma(\vec{x}, \vec{x}') = N \int \Psi(\vec{x}, \vec{x}_2, \ldots \vec{x}_N)\Psi(\vec{x}', \vec{x}_2, \ldots \vec{x}_N) \, d\vec{x}_2 \cdots d\vec{x}_N$$

is of order N.

Physical estimates of this quantity vary widely. It has, however, been proved for traps (100%) in place of the infinite, homogeneous box.

THE *2D* DILUTE, REPULSIVE BOSE GAS

A noteworthy feature of the 3D result is that the energy is

$$E_0 = 4\pi\mu a N\rho = (8\pi\mu a/V)\cdot N(N-1)/2,$$

i.e., E_0 is asymptotically just the energy of two particles in the big box times the number of pairs of particles. This "classical" fact is not trivial since it is NOT possible to think of the particles as "independent, except for occasional collisions". This "classical" result will surely not hold in 1D, but it might be expected to hold in 2D. ***It does not!***

The answer turns out to be:

$$e_0(\rho) = \frac{E_0}{N} \approx \frac{\mu 4\pi\rho}{|\ln(\rho a^2)|}.$$

This is MUCH LARGER than the energy per particle for two particles in a large box, namely

$$E_0(N = 2) \approx \frac{\mu 4\pi\rho}{|\ln(a^2/L^2)|}.$$

Oddly, the correct formula was realized, by Schick, only in 1971! and proved only recently.

THE GROSS–PITAEVSKII EQUATION

For a ‘trap’ we add a confining potential V, with $V(\vec{x}) \to \infty$ as $|\vec{x}| \to \infty$.

$$H = \sum_{i=1}^{N} -\mu\Delta_i + V(\vec{x}_i) + \sum_{1\le i<j\le N} v(|\vec{x}_i - \vec{x}_j|)$$

If $v = 0$, then

$$\Psi_0(\vec{x}_1, \dots, \vec{x}_N) = \textstyle\prod_{i=1}^{N} \Phi_0(\vec{x}_i)$$

with Φ_0= normalized ground state of $-\Delta + V(\vec{x})$ with eigenvalue $= \lambda$.

Associated with the quantum mechanical GSE problem is the GP energy functional

$$\mathcal{E}^{\mathrm{GP}}[\Phi] = \int_{R^3} \left(\mu|\nabla\Phi|^2 + V|\Phi|^2 + 4\pi\mu a|\Phi|^4\right) d^3\vec{x}$$

with the subsidiary condition

$$\int_{R^3} |\Phi|^2 = N$$

and corresponding energy

$$E^{\mathrm{GP}}(N) = \inf\{\mathcal{E}^{\mathrm{GP}}[\Phi] \ : \ \int |\Phi|^2 = N\} = \mathcal{E}^{\mathrm{GP}}[\Phi^{\mathrm{GP}}].$$

As before, a is the scattering length of v. It is not hard to prove that for every choice of the real number N there is a unique minimizer for Φ^{GP} for $\mathcal{E}^{\mathrm{GP}}$.

RELATION OF $\mathcal{E}^{\mathrm{GP}}$ AND E_0:

If $v = 0$ then clearly $\Phi^{\mathrm{GP}} = \sqrt{N}\ \Phi_0$, and then $\mathcal{E}^{\mathrm{GP}} = N\lambda = E_0$. In the other extreme, if $V(\vec{x}) = 0$ for $\vec{x}$ inside a large box of volume L^3 and $V(\vec{x}) = \infty$ otherwise, then we take $\Phi^{\mathrm{GP}} \approx \sqrt{N/L^3}$ and we get $E^{\mathrm{GP}}(N) = 4\pi\mu a N^2/L^3 =$ previous, homogeneous E_0 in the low density regime. (In this case, the gradient term in $\mathcal{E}^{\mathrm{GP}}[\Phi]$ plays no role.)

In general, we expect that $\mathcal{E}^{\mathrm{GP}} = E_0$ in a suitable limit. This limit has to be chosen so that *all three* terms in $E^{\mathrm{GP}}[\Phi]$ make a contribution. It turns out that fixing Na is the right thing to do (and this is quite good experimentally since N is about 1 to 1000 times $1/a$).

THEOREM*: *if Na is fixed,

$$\lim_{N\to\infty} \frac{E^{\mathrm{QM}}(N,a)}{E^{\mathrm{GP}}(N,a)} = 1$$

(If $Na \to \infty$ as $N \to \infty$, but $\langle\rho\rangle_{av} a^3 \to 0$, then simply omit the $\int |\nabla\Phi|^2$ term in $\mathcal{E}^{\mathrm{GP}}$; this dull theory is mis-called 'Thomas-Fermi theory' and is often used by lazy people even if $Na \not\to \infty$.)

Moreover, the GP density is a limit of the QM density:

$$\lim_{N\to\infty} \frac{1}{N} \rho^{\mathrm{QM}}_{N,a}(\vec{x}) = \left|\Phi^{\mathrm{GP}}_{1,Na}(\vec{x})\right|^2$$

if Na is fixed. (Convergence in weak L^1-sense.)

BOSE EINSTEIN CONDENSATION IN THE GP LIMIT

Almost all theoretical interpretations of the trap experiments take BEC for granted. Moreover, it is assumed that the condensation is 100% into the solution Φ^{GP} of the GP equation, i.e., in the GP limit

THEOREM

$$\lim_{N\to\infty}\frac{1}{N}\gamma(\vec{x},\vec{x}')=\Phi^{\mathrm{GP}}(\vec{x})\Phi^{\mathrm{GP}}(\vec{x}')$$

if Na is fixed (convergence in trace class norm).

This has now been *proved* and is the first proof of BEC in a physically realistic, continuum (as distinct from lattice) model!

COROLLARY.

$$\lim_{N\to\infty} \frac{1}{N}\widehat{\rho}(\vec{k}) = |\widehat{\Phi}^{\mathrm{GP}}(\vec{k})|^2 \ ,$$

strongly in $L^1(\mathrm{R}^3)$, where

$$\widehat{\rho}(\vec{k}) = \int \gamma(\vec{x}, \vec{x}')\, \exp[i\vec{k}\cdot(\vec{x}-\vec{x}')] d\vec{x} d\vec{x}'$$

denotes the one-particle momentum density of the GS Ψ.

Note that the results are independent of v! I.e., in the limit of a dilute gas only the scattering length matters!

SUPERFLUIDITY IN THE GP LIMIT

Consider a finite cylinder based on an annulus in R^2. Replace ∇ in the kinetic energy of N bosons by $\nabla + i\varphi A(\vec{x})$ for some vector potential A in the θ-direction, and ask for the response of the system.

For $|\varphi|$ small enough there is a unique, radial minimizer Φ^{GP} of the GP functional. It is real and we have, in this case,

THEOREM.

$$\lim_{N\to\infty} \frac{E_0(N,a,\varphi)}{N} = E^{\mathrm{GP}}(Na,\varphi)$$

and

$$\lim_{N\to\infty} \frac{1}{N}\gamma(\vec{x},\vec{x}') = \Phi^{\mathrm{GP}}(\vec{x})\Phi^{\mathrm{GP}}(\vec{x}')$$

in the limit $N \to \infty$, Na and φ fixed.

THE ROTATING BOSE GAS

Experiments on rotating traps display the interesting phenomenon of *VORTICES*. At first the gas does not rotate, but at a critical rotation rate the gas acquires angular momentum, which is localized in vortices. As the speed increases more vortices are formed and they display interesting patterns; rotational symmetry is broken! As observed, each off-axis vortex has angular momentum

$$\boxed{\hbar.}$$

***Without rotation* the absolute GS of the Hamiltonian is the *same* as the bosonic GS. This well known fact plays a key role in our earlier proofs. But, as Seiringer showed, the bosonic GS is *not* the absolute GS with rapid rotation. The existence of symmetry breaking vortices is thus a true manifestation of Bose-Einstein statistics!**

Is the GP equation correct in the rapidly rotating case? The answer was not obvious for quite some time, but the correctness of GP has recently been proved. Again, there is 100% BEC. The proof is quite different from the previous one; coherent states play an important technical role.

The GP equation with rotation deserves to be studied more rigorously to clarify the multi-vortex solutions. With rotation frequency $\vec{\Omega}$ it is

$$\frac{-\hbar^2}{2m}\Delta\Phi + i\hbar\nabla\cdot(\vec{\Omega}\wedge\vec{x})\Phi + V\Phi + 8\pi a|\Phi|^2\Phi = \lambda\Phi$$

and $\int|\Phi(x)|^2 dx = N$ as before.

Let Γ be the set of all limit points of 1pdm of approximate ground states:

$$\Gamma = \left\{ \gamma \,:\, \exists \text{ sequence } \gamma_N,\ \lim_{N\to\infty} \frac{1}{N} \mathrm{Tr}\, H_N \gamma_N = E^{\mathrm{GP}}(Na),\ \ \lim_{N\to\infty} \frac{1}{N}\ \gamma_N^{(1)} = \gamma \right\}.$$

Compactness implies that $\mathrm{Tr}\,\gamma = 1$ for all $\gamma \in \Gamma$.

(i) Γ is a compact and convex subset of the set of all trace class operators.

(ii) Let $\Gamma_{\mathrm{ext}} \subset \Gamma$ denote the set of extreme points in Γ.

We have $\Gamma_{\mathrm{ext}} = \{ |\phi\rangle\langle\phi| \,:\, \mathcal{E}^{\mathrm{GP}}[\phi] = E^{\mathrm{GP}}(Na) \}$.

(iii) For each $\gamma \in \Gamma$, there is a positive (regular Borel) measure $d\mu_\gamma$, supported in Γ_{ext}, with $\int_{\Gamma_{\mathrm{ext}}} d\mu_\gamma(\phi) = 1$, such that (in weak sense)

$$\gamma = \int_{\Gamma_{\mathrm{ext}}} d\mu_\gamma(\phi)\, |\phi\rangle\langle\phi|\,.$$

$\mathcal{FROM\ THREE\text{–}D\ \ TO\ \ ONE\text{–}D}$

Four decades ago Liniger and I found the ground state and elementary excitations of the 1D bose gas with $\delta-$function interaction. Just for fun! Now this system can be produced in elongated 3D traps! The 1D Hamiltonian with coupling constant $g \geq 0$ is

$$H = \sum_{j=1}^{N} -\partial_j^2 + g \sum_{1\leq i<j\leq N} \delta(z_i - z_j)$$

with GSE in the thermodynamic limit given by $N\,\overline{\rho}^{\,2}\ e(g/\overline{\rho})$, where $\overline{\rho} = N/L$

Let r be the cross-sectional radius and L the length of the trap. This is produced by an appropriate potential $V(x, y, z)$. One might think that in order to get 1D behavior one needs $r \sim a$. ***NOT SO!!***

It is only necessary that the transverse energy gap $\gg$ the longitudinal energy, i.e., $\sim r^{-2} \gg e(g/\overline{\rho})$ with $g \sim ar^{-2}$.

$\boxed{\textit{This is truly quantum-mechanical!}}$

The particles then behave as 'planes' that can move through each other with a 1D δ−function interaction.

There are 5 different parameter regions that occur, but it suffices to say that the LL energy is the leading non-trivial energy when $g/\overline{\rho} \sim a(r^2\,\overline{\rho})^{-1} > 0$ in the limit. This agrees with experiments.

THE CHARGED BOSE GAS

The setting now changes abruptly. Instead of particles interacting with a short-range potential $v(\vec{x}_i - \vec{x}_j)$ they interact via the Coulomb potential

$$v(|\vec{x}_i - \vec{x}_j|) = |\vec{x}_i - \vec{x}_j|^{-1}$$

(in 3 dimensions). There are N particles in a large box of volume L^3 as before, with $\rho = N/L^3$. This is the $\boxed{\textit{One-Component Gas.}}$

To offset the huge Coulomb repulsion (which would drive the particles to the walls of the box) we add a uniform negative background of precisely the same charge, namely density ρ. Our Hamiltonian is thus

$$H = -\mu \sum_{i=1}^{N} \Delta_i + V(\vec{x}_i) + \sum_{1 \le i < j \le N} v(|\vec{x}_i - \vec{x}_j|) + C$$

with $\quad V(\vec{x}) = -\rho \int_{BOX} |\vec{x} - \vec{y}|^{-1} d^3y \quad$ and $\quad C = \frac{1}{2}\rho \int_{BOX} V(\vec{x}) d^3x$.

Despite the fact that the Coulomb potential is positive definite, each particle interacts only with others and not with itself. Thus, E_0 can be (and is) negative (just take Ψ ≈const). This time, *large* ρ is the regime in which one expects Bogolubov's theory to be correct, at least approximately.

Another way in which this problem is different from the previous one is that *perturbation theory is correct to leading order*. If one computes $(\Psi, H\Psi)$ with Ψ ≈const, one gets the right answer, namely 0. It is the next order in $1/\rho$ that is interesting, and this is *entirely* due to correlations.

In 1961 Foldy calculated this correlation energy according to the prescription of Bogolubov's 1947 theory. That theory was not exact for the dilute Bose gas, as we have seen, even to leading order. We are now looking at *second* order, which should be even worse. Nevertheless, there was good physical intuition that this calculation should be asymptotically *exact*. *It is!* (Lieb-Solovej lower-bound in 2001 and Solovej upper-bound in 2004 (math-ph/0406014))

The Bogolubov theory states that the main contribution to the energy comes from pairing of particles into momenta $\vec{k}, -\vec{k}$ and is the bosonic analogue of the BCS theory of superconductivity which came a decade later. I.e., Ψ_0 is a sum of products of germs of the form $\exp\{i\vec{k}\cdot(\vec{x}_i - \vec{x}_j)\}$.

Foldy's energy, based on Boglubov's ansatz, has now been proved. His calculation yields an upper bound. The lower bound is the hard part, and Solovej and I do this using the decomposition into 'Neumann boxes'. But unlike the short range case, many complicated gymnastics are needed to control the long range $|\vec{x}|^{-1}$ Coulomb potential.

__*THEOREM*__**:** ***For large ρ***

$$E_0/N = e_0(\rho) \sim -I_0\rho^{1/4}$$

with $I_0 = 0.803\,(2\pi/3\mu)$.

In 1988 Conlon, L, and Yau got the $\rho^{1/4}$ law as a lower bound, but with the wrong constant.

For the $\boxed{\textit{Two-Component Gas}}$ we just have two kinds of bosons (charges ± 1) and *no charged background and no box.* N particles total.

Dyson showed that the 2-component gas energy was at least as negative as $-CN^{7/5}$ and this was proved later by Conlon, L, Yau (but with an incorrect C). He conjectured that the large N limit of the energy is obtained by minimizing the 'mean-field' density functional

$$\mu \int_{R^3} |\nabla \sqrt{\rho}|^2 - I_0 \int_{R^3} \rho^{5/4} \qquad **$$

with $\int \rho = 1$. Defining $\Phi(x) = N^{-4/5}\sqrt{\rho(N^{-1/5}x)}$ with $\int \Phi^2 = 1$, this functional becomes

$$N^{7/5}\left(\mu \int_{R^3} |\nabla \Phi|^2 - I_0 \int_{R^3} \Phi^{5/2}\right),$$

which leads to

$$-2\mu\Delta\Phi(x) - \frac{5}{2} I_0 \ \Phi(x)^{3/2} + \gamma\Phi(x) = 0,$$

where γ is a chemical potential. This was proved in 2003 by L and Solovej as a lower bound. Note that ** has I_0, not $2I_0$ or $\frac{1}{2}I_0$. Solovej proved the upper bound in 2004 (math-ph/0406014).