The Boson system: An introduction. I.

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Applied PDE & Particle Systems RITs
15 September 2014

Quantum system evolution: Non-relativistic case

The state of an *N*-particle system is described by the *N*-body wavefunction, Ψ_N

$\text{(Linear) Schrödinger equation:}$

$$\hat{H}\Psi_N(t,\vec{x}_N) = i\partial_t\Psi_N(t,\vec{x}_N); \quad \Psi_N(t,\cdot) \in L^2(\mathbb{R}^{3N})$$

Many-body Hamiltonian: operator in N-particle Hilbert space

State vector in Hilbert space $|\Psi_N\rangle$

Of particular interest are systems of identical particles

Bosons:

N-body wave function must be symmetric under particle permutations:

$$\Psi_N(t, x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(N)}) = \Psi_N(t, x_1, x_2, \ldots, x_N)$$

permutations

A quantum state can be occupied by any number of Bosons

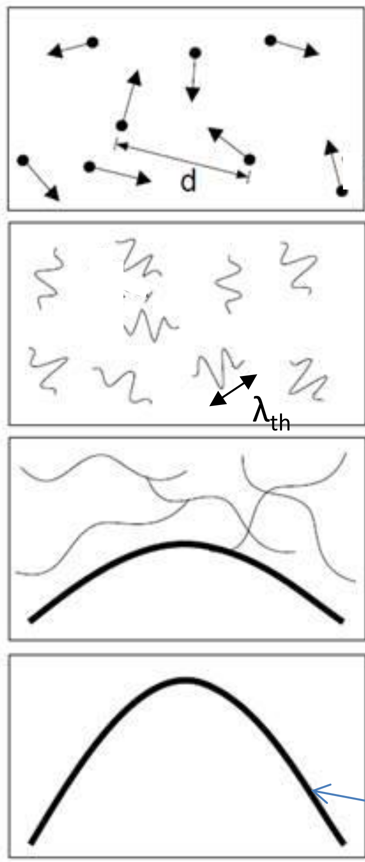
Fermions:

$$\Psi_N(t, x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(N)}) = \mathrm{sgn}(\pi)\, \Psi_N(t, x_1, x_2, \ldots, x_N)$$

-1 for odd permutations;
1 for even permutations

There are restrictions in occupancy of a quantum state by Fermions (``Pauli exclusion principle")

Basic schematic view of ideal Boson gas



High T:
"billiard balls"

Low T:
Evident wave-like behavior

$T \simeq T_c$: BEC onset
"Matter wave overlap"
$d \sim \lambda_{\rm th}$

$T << T_c$
$d \ll \lambda_{\rm th}$

Bose-Einstein condensate

[Schematic: Ketterle, 1999]

The **matter wave** can be described by single-particle **mean field**

The B and E of Bose-Einstein Condensation

- **BEC**: ***Macroscopic occupation of a 1-particle quantum state.***

- In 1924, Bose re-derived Planck's black-body radiation law by using certain partition of phase space of photons.
- Einstein [1924, 1925] applied Bose's method to gas of non-interacting *spinless* massive particles, **Bosons**.

BEC via density matrix

[Penrose, Onsager, 1957]

- Need an operator which, for an ideal gas, has eigenvalues equal to the (average) occupation numbers of 1-particle stationary quantum states.

- Define 1-particle (reduced) density operator $\hat{\gamma}$

$$\hat{\gamma} = N \ \mathrm{tr}_{2\ldots N}\,(\hat{\rho})\,; \qquad \hat{\rho} = |\Psi_N\rangle\langle\Psi_N| \text{ for pure state}$$

N-particle density op. (matrix)

- Configuration representation of 1-part. reduced density operator:

$$\gamma(x,y) = \langle x|\hat{\gamma}|y\rangle = N \lim_{|\ \ |\to\infty} \int_{\ \ N-1} \Psi_N(x,\vec{x}_{N-1})\Psi_N^*(y,\vec{x}_{N-1})\ d\vec{x}_{N-1};$$

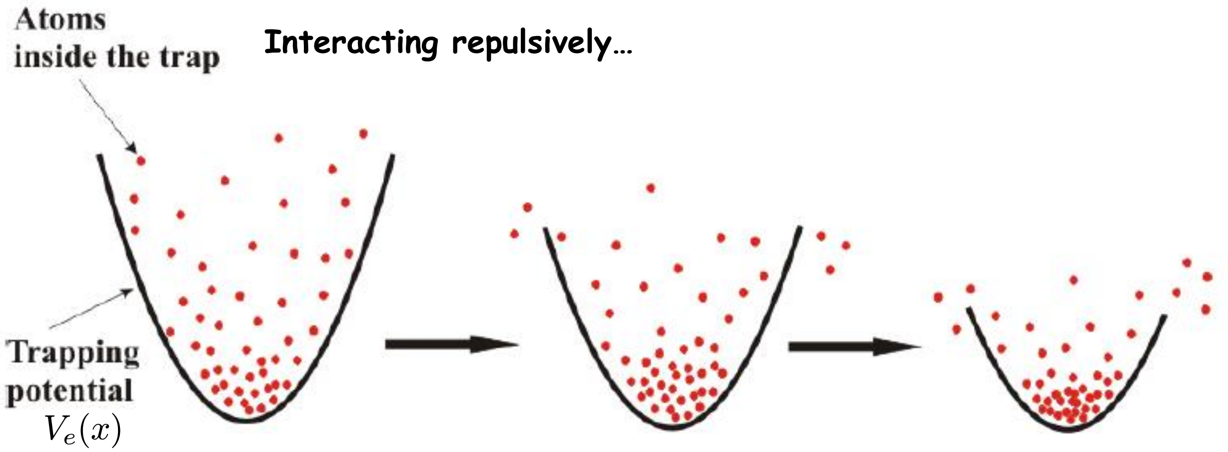
$$(x, y \in \mathbb{R}^3, \text{-} \ \subseteq \mathbb{R}^3) \qquad \vec{x}_{N-1} = (x_2,\ldots,x_N) \in \mathbb{R}^{3(N-1)}$$

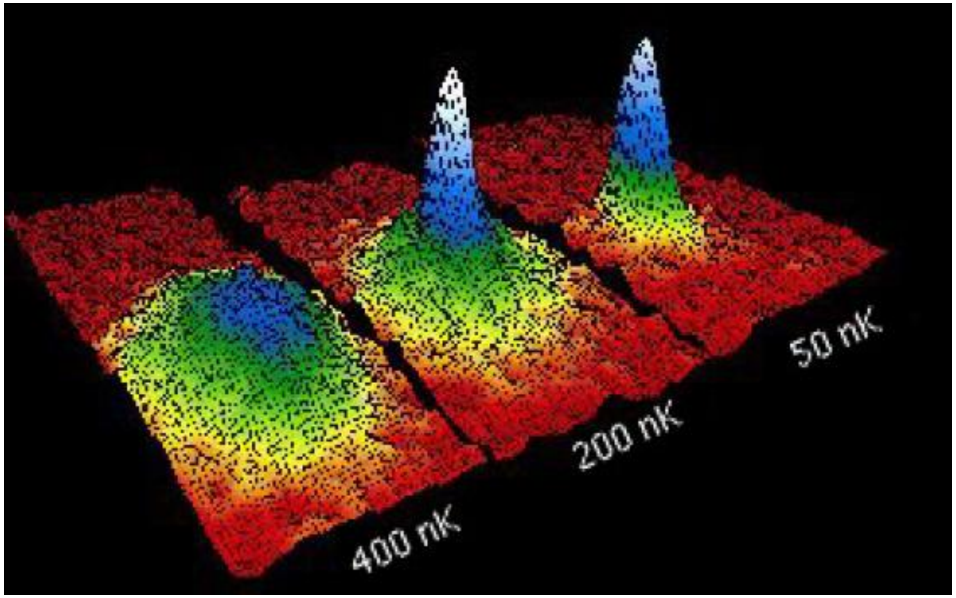
- Criterion for BEC in **ground state**: maximal eigenvalue of $\hat{\gamma}$ is $\mathcal{O}(N)$

Experiments in **trapped** dilute atomic gases

[(MIT) Ketterle group: Davis *et al*., 1995; (JILA) Cornell group: Anderson *et al*., 1995]

Interacting repulsively…





[Courtesy of MIT group]

Key Elements for theory:

- Weak particle interactions
- Macroscopic trap

Applications:

BEC still has limited throughput, and is primarily confined to lab settings; no commercial, large-scale use of it.

- Precision measurements (of acceleration, gravity gradients etc) based on atom interferometry.
- Emulation of complex condensed-matter systems, esp. their phase transitions, using optical lattices.
- Quantum information.
- Lithography: Creation of patterns on templates (far from industrial production as yet).

A multiple-scale perspective of **weakly interacting trapped** gas undergoing BEC

Length scales:

Scattering length

Mean interparticle distance

Correlation length due to short-range repulsions

Thermal De Broglie wavelength

Size of (macroscopic) trap

$$a \ll d \ll \lambda_{\mathrm{cor}} \ll \lambda_{\mathrm{th}} \lesssim \lambda_{\mathrm{trap}}$$

diluteness ($a \ll d$)

Many-body Boson evolution

Evolution on N Bosons with repulsive interactions:

Square integrable, symmetric

$$\hat{H}_N \Psi_N(t,\vec{x}) = i\partial_t \Psi_N(t,\vec{x}); \quad \Psi_N(t,\cdot) \in L^2_s(\mathbb{R}^{3N})$$

many-body Schrödinger eq.

$$\hat{H}_N = \sum_{j=1}^{N} [-\Delta_j + V_e(x_j)] + \sum_{\substack{j,l=1\\ j<l}}^{N} \mathcal{V}(x_j, x_l) \qquad (\hbar = 2m = 1)$$

PDE Hamiltonian

Short-ranged, repulsive, symmetric; usually $\mathcal{V} = V(x_j - x_l)$

No exact solutions of form $\Phi(t,x_1)\Phi(t,x_2)\dots\Phi(t,x_N) = \prod_{j=1}^{N} \Phi(t,x_j)$

Bound state:

$$\Psi_N(t,\vec{x}) = e^{-itE_N}\Psi_N(\vec{x})$$

Ground state: E_N is lowest

Why is BEC interesting in applied math (today)?

High-dimensional PDE !
Impractical for predictions

$$\hat{H}_N \Psi_N(t,\vec{x}) = i\partial_t \Psi_N(t,\vec{x}); \quad \Psi_N(t,\cdot) \in L^2_s(\mathbb{R}^{3N})$$

$$\hat{H}_N = \sum_{j=1}^{N} [-\Delta_j + V_e(x_j)] + \sum_{j<l} \mathcal{V}(x_j, x_l) \qquad (\hbar = 2m = 1)$$

- What macroscopic description, **mean field limit**, emerges, and in what sense, in **lower dimensions** as *N*→∞ ?

Nonlinear Schrodinger-type eq in **3D**: Gross [1961], Pitaevskii [1961], and Wu [1961]

- What corrections exist beyond this limit for **large but finite** *N*, in a controllable ``PDE sense''?

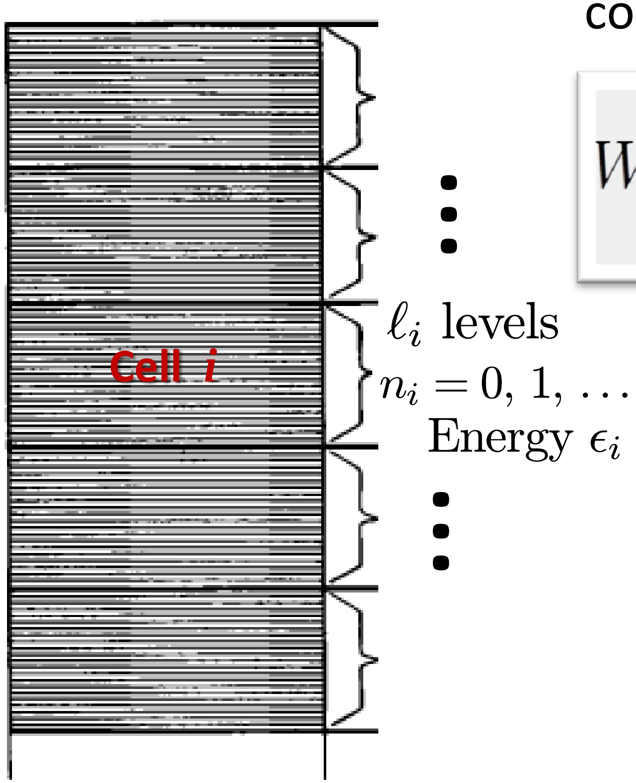
A taste of BEC in non-interacting Boson gas

[Bose, 1924, Einstein, 1924, 1925]

Digression: Bose statistics (ideal Bose gas, N particles)

[K. Huang, *Statistical Mechanics*]

Partitioning of free-particle states



Total energy: E

Number of states of the system corresponding to set of occupation numbers $\{n_i\}_{i=1,2,\ldots}$.

$$W\{n_1, n_2, \ldots\} = \prod_i w_i$$

Number of ways to arrange n_i particles in ℓ_i levels

To find average occupation numbers, $\bar{n}_i$:

Maximize entropy $S = k_B \log W\{n_i\}$

under the constraints

$$\sum_i n_i = N, \quad \sum_i n_i \epsilon_i = E$$

$$\Rightarrow \bar{n}_i = \frac{1}{z^{-1} e^{\epsilon_i/(k_B T)} - 1}$$

Lagrange Multiplier; Fugacity z

N non-interacting Bosons (in periodic box of volume L^3)

Lowest energy is 0

$$\sum_{k\neq 0} \bar{n}_k/N \to \text{integral}$$

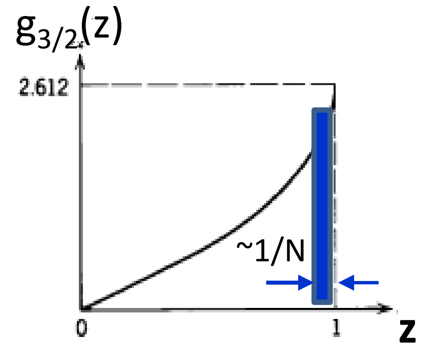
Single out 0-th momentum contribution!

$$N = \sum_k \bar{n}_k \;\Rightarrow\; 1 = \underbrace{\left(\frac{N}{L^3}\right)}_{\mathcal{O}(1)}^{-1} \underbrace{\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}}_{\lambda^{-3}} g_{3/2}(z) + \frac{1}{N}\underbrace{\frac{z}{1-z}}_{\bar{n}_0}$$

Ave. occupation numbers over momenta k, from Bose statistics

$$g_{3/2}(z) = \frac{4}{\sqrt{\pi}}\int_0^\infty dx\, \frac{x^2}{z^{-1}e^{x^2}-1}$$

$$z = e^{\mu/(k_BT)},\ \mu < 0$$



Condition of condensation (N: large):

Finite fraction of particles at 0 momentum:

$$\boxed{\frac{\bar{n}_0}{N} = \mathcal{O}(1)} \quad \Longleftarrow \quad \frac{N}{L^3} - \lambda^{-3} g_{3/2}(1) > 0,\ \text{or } 0 < T < T_c$$

$$T = T_c: \quad \frac{N}{L^3} = \lambda^{-3} g_{3/2}(1)$$

No condensation: $\dfrac{\bar{n}_0}{N} = o(1)$

Weakly interacting Boson gas

[Bogoliubov, 1947; Lee, Huang, Yang, 1957; Wu, 1961]

Weakly interacting Bosons in periodic box, T=0: Statics

[Bogoliubov, 1947; Lee, Huang, Yang, 1957]

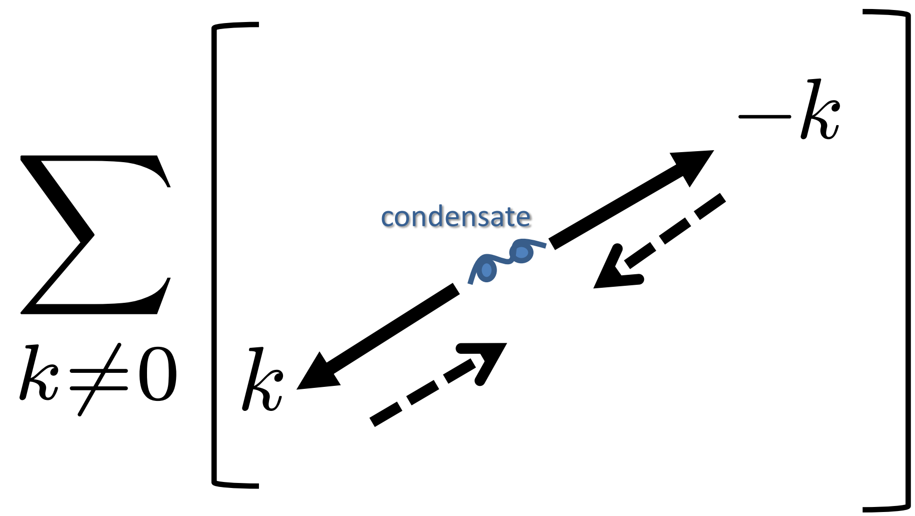
Macroscopic single-particle quantum state (condensate): Zero-momentum eigenstate.

Fact:

A small fraction of particles leak out from the condensate to other states.

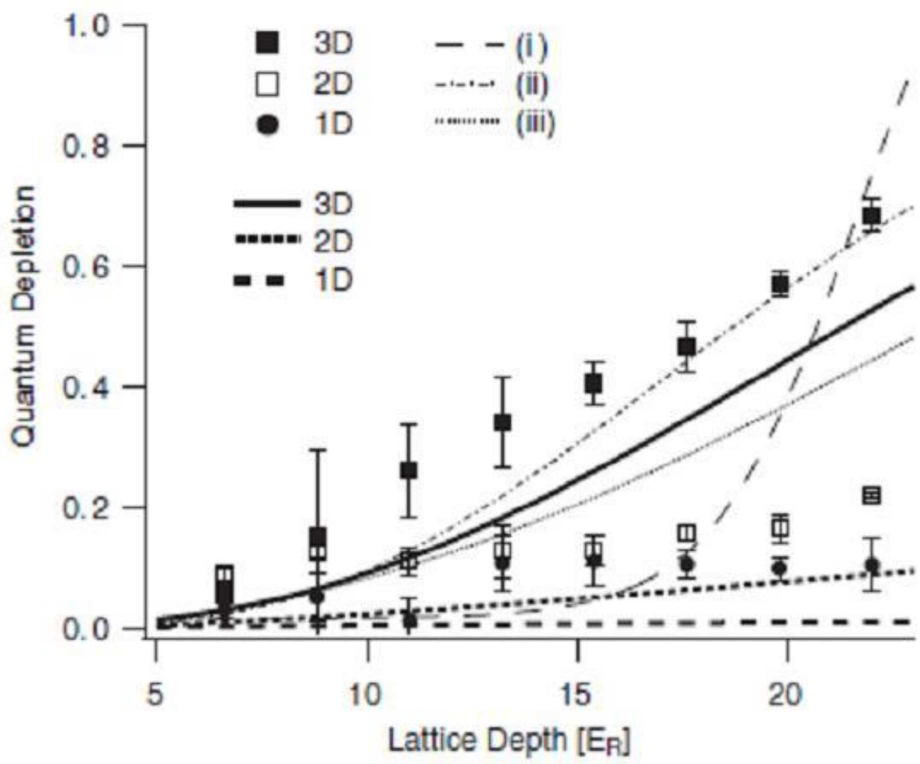
Emerging concept: Particles are primarily scattered from zero momentum to pairs of opposite momenta and vice versa.

Pair excitation hypothesis



What is the ground state energy?

Fraction of atoms escaping the macroscopic state: Observation of **quantum depletion** [Xu et al., 2006]



Digression: Second quantization: Bosonic Fock space $\mathbb{F}$

$$\mathbb{F} = \mathbb{C} \oplus \bigoplus_{n\geq 1} \left(L^2(\mathbb{R}^3)\right)^{sn}$$

- Elements of $\mathbb{F}$ (space with indefinite number of Bosons):

$Z = \{Z^{(n)}\}_{n\geq 0}$ where $Z^{(0)}$: complex number, $Z^{(n)} \in L^2_s(\mathbb{R}^{3n})$. Inner product: $\langle Z, \Psi\rangle_{\mathbb{F}} = \sum_{n\geq 0} \int_{\mathbb{R}^{3n}} Z^{(n)}(x) {\Psi^{(n)}}^*(x) \mathrm{d}x$.

- Annihilation & creation operators for 1-part. state Φ are $a_\Phi, a^*_\Phi : \mathbb{F} \to \mathbb{F}$. (adjoint)

$$(a^*_\Phi Z)^{(n)}(\vec{x}_n) = n^{-1/2} \sum_{j=1}^{n} \Phi(x_j) Z^{(n-1)}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n) \ ,$$

$$(a_\Phi Z)^{(n)}(\vec{x}_n) = \sqrt{n+1} \int_{\mathbb{R}^3} \mathrm{d}x_0 \, \Phi^*(x_0) Z^{(n+1)}(x_0, \vec{x}_n) \ , \ \vec{x}_n := (x_1, \ldots, x_n)$$

Commutation relation: $[a_\Phi, a^*_\Phi] = a_\Phi a^*_\Phi - a^*_\Phi a_\Phi = \|\Phi\|^2_{L^2}$.

- Periodic bc's: Momentum creation and annihilation operators:

a^*_k and a_k, for $\Phi(x) = (1/\sqrt{|\text{-}\ |}) e^{ik\cdot x}$.

$$[a_k, a^*_{k'}] = \delta_{k,k'}$$

- Vacuum (no particles): $|\text{vac}\rangle = \{c, 0, 0, \ldots\}$. $\quad a_\Phi|\text{vac}\rangle = 0$, $a^*_\Phi|\text{vac}\rangle = |\Phi\rangle$

Digression: Second quantization (cont.)

The use of Fock-space language enables convenient notation (and not only).

Example: The Bosonic wave function with n_1 atoms at state Φ_1 ,…, n_M atoms at Φ_M (where these states are orthogonal) is represented by the vector (living in Fock space):

$$\prod_{j=1}^{M} \frac{(a^*_{\Phi_j})^{n_j}}{\sqrt{n_j!}} |\text{vac}\rangle = (0, 0, \ldots, Z^{(n_1+n_2+\ldots+n_M)}, 0, \ldots)$$

Digression: Second quantization (cont.)

The algebra for many Bosons is facilitated through replacing operators in a Hilbert space of a fixed number of atoms with operators in the Fock space; in particular,

$$\hat{H}_n \text{ replaced by } \mathcal{H}$$

$\hat{H}_n$: Op. in Hilbert space with *n* particles

$\mathcal{H}$: Op. in Fock space, with indefinite number of particles

Interpretation:

$$\mathcal{H}\left(c, Z^{(1)}, \ldots, Z^{(n)}, \ldots\right) = \left(0, \hat{H}_1 Z^{(1)}, \ldots, \hat{H}_n Z^{(n)}, \ldots\right)$$

$\mathcal{H}$: Operator In Fock space

$\left(c, Z^{(1)}, \ldots, Z^{(n)}, \ldots\right)$: vector in Fock space

$Z^{(n)}$: *n*-particle wavefunction

$\hat{H}_n$: *n*-particle operator

Projection to the ``N-particle sector'', *n=N*, forms a constraint

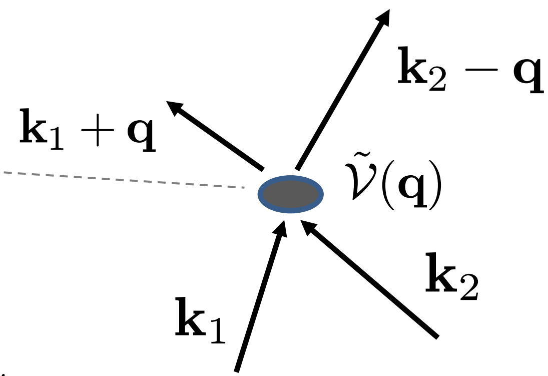
$$\text{Number operator for Bosons at momentum } k: \; \mathcal{N}_k = a_k^* a_k$$

Weakly interacting Bosons in a periodic box Ω, T=0: Statics

[Bogoliubov, 1947; Lee, Huang, Yang, 1957]

PDE Hamiltonian:

$$\hat{H}_N = \sum_{j=1}^{N}(-\Delta_j) + \frac{1}{2}\sum_{\substack{j,l=1 \\ j\neq l}}^{N} \mathcal{V}(x_j - x_l) \qquad (\hbar = 2m = 1)$$



This is replaced by Hamiltonian in Fock space:

$$\mathcal{H} = \sum_k k^2 \, a_k^* a_k + \frac{1}{2|\text{-}|} \sum_{k_1,k_2,q} a^*_{k_1+q} a^*_{k_2-q} \, \tilde{\mathcal{V}}(q) \, a_{k_1} a_{k_2}$$

$a_k^* a_k$: Operator for number of Bosons at mom. k; $|\text{-}|$: volume

$$\tilde{\mathcal{V}}(q) = \int \mathcal{V}(x)\, e^{-iq\cdot x}\, dx$$

In a dilute gas, the actual form of $\mathcal{V}$ is not important. What matters is an effective potential that reproduces the correct low-energy behavior in the far field.

Lee, Huang, and Yang set: $$\mathcal{V}(x_i - x_j) \to \mathcal{V}' = 8\pi a \delta(x_i - x_j)\frac{\partial}{\partial r_{ij}} r_{ij}, \qquad r_{ij} = |x_i - x_j|$$

a: *Low-energy* scattering length

Fermi pseudopotential

Length a comes from solving: $$-\Delta w + (1/2)\mathcal{V}(x) w = 0, \qquad \lim_{|x|\to\infty} w = 1$$

In particular, $$w(x) \sim 1 - \frac{a}{|x|} \quad \text{as } |x| \to \infty$$

Definition of a

[Blatt, Weiskopf, 1952]

To be continued….