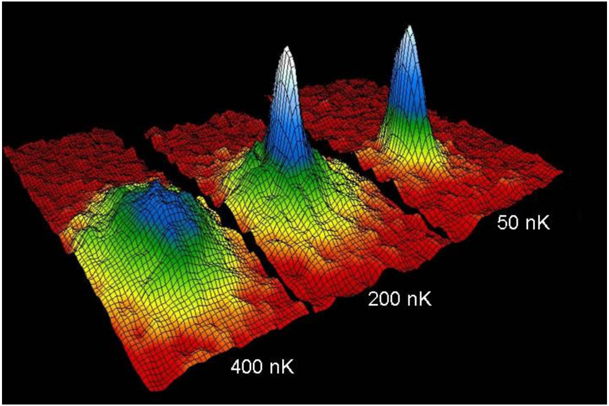
Bose-Einstein condensation and mean-field limits

Kay Kirkpatrick, UIUC

2016

Bose-Einstein condensation: from many quantum particles to a quantum "superparticle"



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Frontier Probability Days 2016

The big challenge: making physics rigorous

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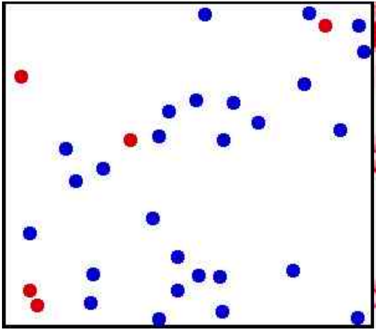
microscopic first principles $\rightsquigarrow$ zoom out $\rightsquigarrow$ MACROSCOPIC STATES



Courtesy Greg L and Digital Vision/Getty Images

1925: predicting Bose-Einstein condensation (BEC)

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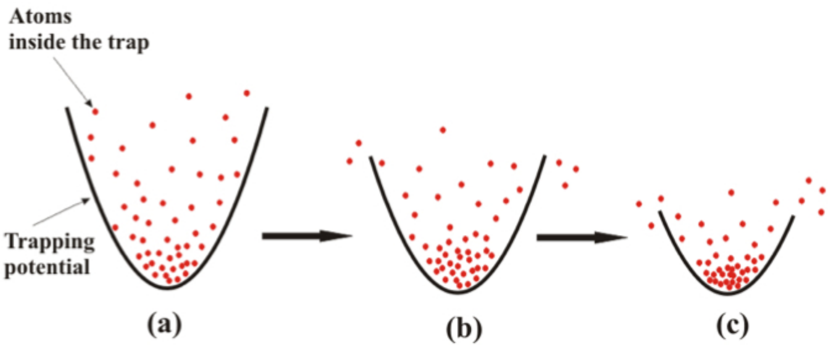
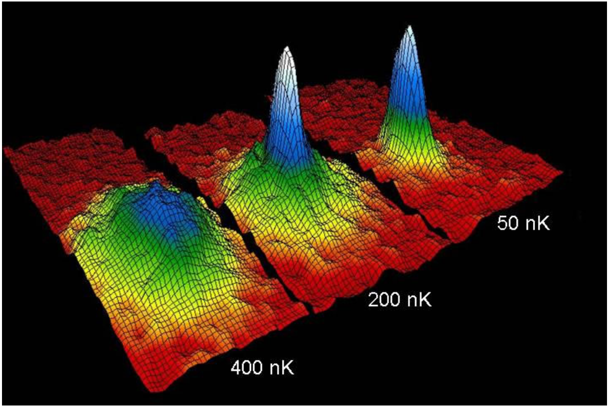
1995: Cornell-Wieman and Ketterle experiment



Courtesy U Michigan

After the trap was turned off

BEC stayed coherent like a single macroscopic quantum particle.



Momentum is concentrated after release at 50 nK. (Atomic Lab)

The mathematics of BEC

Gross and Pitaevskii, 1961: a good model of BEC is the cubic nonlinear Schrödinger equation (NLS):

$$i\partial_t \varphi = -\Delta\varphi + \mu|\varphi|^2\varphi$$

Fruitful NLS research: competition between two RHS terms

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Can we rigorously connect the physics and the math?

Yes!

Outline

microscopic first principles $\rightsquigarrow$ $\rightsquigarrow$ Macroscopic states

1. N bosons $\rightsquigarrow$ mean-field limit $\rightsquigarrow$ Hartree equation
2. N bosons $\rightsquigarrow$ localizing limit $\rightsquigarrow$ NLS
3. Quantum probability and CLT

A quantum “particle” is really a wavefunction

For each t, $\psi(x,t) \in L^2(\mathbb{R}^d)$ solves a Schrödinger equation

$$i\partial_t \psi = -\Delta\psi + V_{ext}(x)\psi$$

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- $-\Delta = -\sum_{i=1}^{d} \partial_{x^i x^i} \geq 0$
- external trapping potential V_{ext}
- solution $\psi(x,t) = e^{-iHt}\psi_0(x)$

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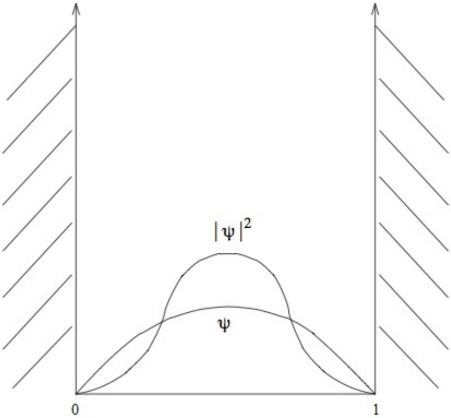
- $\int |\psi_0|^2 = 1 \implies |\psi(x,t)|^2$ is a probability density for all t.
  Exercise: why?

Particle in a box



$V_{ext} =$ "$\infty \cdot \mathbf{1}_{[0,1]^c}$" has ground state $\psi(x) = \sqrt{2}\sin(\pi x)$

The microscopic N-particle model

Wavefunction $\psi_N(\mathbf{x}, t) = \psi_N(x_1, ..., x_N, t) \in L^2(\mathbb{R}^{dN}) \; \forall t$
solves the N-body Schrödinger equation:

$$i\partial_t \psi_N = \sum_{j=1}^{N} -\Delta_{x_j} \psi_N + \sum_{i<j}^{N} U(x_i - x_j)\psi_N =: H_N \psi_N$$

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- pair interaction potential U
- solution $\psi_N(\mathbf{x}, t) = e^{-iH_N t}\psi_N^0(\mathbf{x})$
- joint density $|\psi_N(x_1, \ldots, x_N, t)|^2$

More assumptions

For N bosons, ψ_N is symmetric (particles are exchangeable):

$$\psi_N(x_{\sigma(1)}, ..., x_{\sigma(N)}, t) = \psi_N(x_1, ..., x_N, t) \text{ for } \sigma \in S_N.$$

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But interactions create correlations for $t > 0$.

Mean-field pair interaction $U = \frac{1}{N} V$

Weak: order $1/N$. Long distance: $V \in L^\infty(\mathbb{R}^3)$.

$$i\partial_t \psi_N = \sum_{j=1}^{N} -\Delta_{x_j} \psi_N + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)\psi_N.$$

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Spohn, 1980: If ψ_N is initially factorized and approximately factorized for all t, i.e., $\psi_N(\mathbf{x}, t) \simeq \prod_{j=1}^{N} \varphi(x_j, t)$, then $\psi_N \to \varphi$ in the sense of marginals, and φ solves the Hartree equation:

$$i\partial_t \varphi = -\Delta\varphi + (V * |\varphi|^2)\varphi.$$

Why do interactions become the nonlinearity?

$$i\partial_t \psi_N = \sum -\Delta_{x_j}\psi_N + \tfrac{1}{N}\sum\sum V(x_i - x_j)\psi_N$$

Particle 1 sees

$$\begin{aligned}\frac{1}{N}\sum_{j=2}^{N} V(x_1 - x_j) &\simeq \frac{1}{N}\sum_{j=2}^{N}\int V(x_1 - y)|\varphi(y)|^2 dy \\ &= \frac{N-1}{N}\int V(x_1 - y)|\varphi(y)|^2 dy \\ &\xrightarrow{N\to\infty} (V * |\varphi|^2)(x_1)\end{aligned}$$

Convergence $\psi_N \to \varphi$ in the sense of marginals means

$$\left\| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right\|_{Tr} \xrightarrow{N\to\infty} 0,$$

where $|\varphi\rangle\langle\varphi|(x_1, x_1') = \overline{\varphi}(x_1)\varphi(x_1')$ and

one-particle marginal density $\gamma_N^{(1)} := Tr_{N-1}|\psi_N\rangle\langle\psi_N|$ has kernel

$$\gamma_N^{(1)}(x_1; x_1', t) := \int \overline{\psi}_N(x_1, \mathbf{x}_{N-1}, t)\psi_N(x_1', \mathbf{x}_{N-1}, t) d\mathbf{x}_{N-1}.$$

Other mean-field limit theorems

Erdös and Yau, 2001: Convergence of marginals for Coulomb interaction, $V(\mathbf{x}) = 1/|\mathbf{x}|$, not assuming approximate factorization.

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$$\left\| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right\|_{Tr} \leq \frac{Ce^{Kt}}{N}.$$

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Preview of localizing interactions: $(V_N * |\varphi|^2)\varphi \to (\delta * |\varphi|^2)\varphi$
Erdös, Schlein, Yau, K., Staffilani, Chen, Pavlovic, Tzirakis...

Definition of BEC at zero temperature

Almost all particles are in the same one-particle state:

$\{\psi_N \in L^2_s(\mathbb{R}^{3N})\}_{N\in\mathbb{N}}$ exhibits **Bose-Einstein condensation** into one-particle quantum state $\varphi \in L^2(\mathbb{R}^3)$ iff

one-particle marginals converge in trace norm:

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Generalizes factorized: $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$ is BEC into φ.

BEC limit theorems with parameter $\beta \in (0,1]$

Now localized strong interactions: $N^{d\beta} V(N^{\beta}(\cdot)) \to b_0 \delta$.

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{N} N^{d\beta} V(N^{\beta}(x_i - x_j)).$$

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Theorems (Erdös-Schlein-Yau 2006-2008 $d = 3$
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Systems that are initially BEC remain condensed for all time, and the macroscopic evolution is the NLS:

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$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N}\sum_{i<j}^{N} N^{d\beta} V(N^{\beta}(x_i - x_j))$$

$$\begin{array}{lccccl} & & N\text{-body Schrod.} & & \\ \textit{micro}: & \psi_N^0 & \longrightarrow & \psi_N & \\ \text{init. BEC} & \downarrow & & \downarrow & \textbf{marg.} \\ \textit{MACRO}: & \varphi_0 & \longrightarrow & \varphi & \\ & & \textbf{NLS evolution} & & \end{array}$$

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A taste of quantum probability $(\mathcal{H}, \mathcal{P}, \varphi)$

Hilbert space $\mathcal{H}$, set of projections $\mathcal{P}$, and state φ.

Quantum random variables (RVs)

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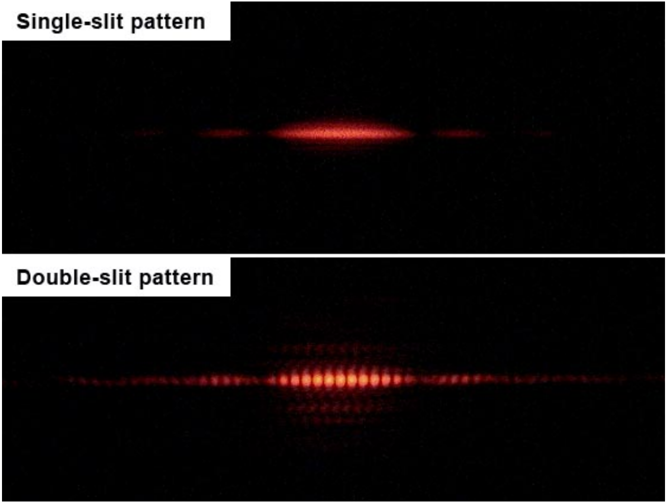
Quantum random variables (RVs) or observables: operators on $\mathcal{H}$.

The expectation of an observable A in a pure state is

$$\mathbb{E}_{\varphi}[A] := \langle \varphi | A\varphi \rangle = \int \varphi(x)\overline{A\varphi}(x)dx.$$

Position observable is $X(\varphi)(x) := x\varphi(x)$ with density $|\varphi|^2$.

Only some probability facts have quantum analogues



Courtesy of Jordgette

The BEC limit theorems imply quantum LLNs

If A is a one-particle observable and

$$A_j = 1 \otimes \cdots \otimes 1 \otimes A \otimes 1 \otimes \cdots \otimes 1,$$

then for each $\epsilon > 0$,

$$\limsup_{N\to\infty} \mathbb{P}_{\psi_N} \left\{ \left| \frac{1}{N} \sum_{j=1}^{N} A_j \right. \right.$$

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BEC can explode as a bosenova

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We need a control theory of BEC

- Central limit theorem for BEC (Ben Arous-K.-Schlein, 2013)

  Our quantum CLT has correlations coming from interactions

- Another noncommutative CLT for quantum groups (Brannan-K., 2015)

Our CLT for interacting quantum many-body systems

Theorem (Ben Arous, K., Schlein, 2013): Under suitable assumptions on the initial state ψ_N^0, φ_0, A, and V, then for $t \in \mathbb{R}$

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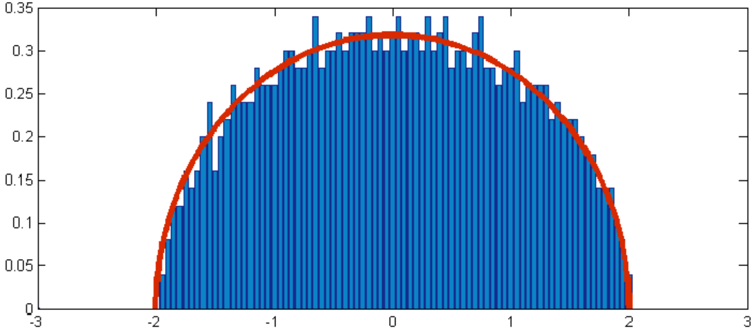
σ_t^2 has $\varphi_0 \rightsquigarrow \varphi_t$.... and twisted by the Bogoliubov transform.

We've made part of the physics of BEC rigorous and ...

- Other mean-field models: my PhD students Leslie Ross (physics) and Tayyab Nawaz (math)
- Quantum group models of freely independent RVs with Michael Brannan (now at Texas A&M)

In free probability, semicircle distribution is 'normal'



1955 Wigner modeled heavy-atom spectra by eigenvalue statistics of random matrices

Banica-Collins '07, Brannan '13: Rescaled generators from quantum group $O_N^+ := C^*(u_{ij} : U = [u_{ij}] \text{ unitary}, U = \overline{U})$ are asymptotically free semicircular:

$$\{\sqrt{N} u_{ij}\}_{1 \leq i,j \leq N} \xrightarrow{N \to \infty} \mathbf{S} = \{s_{ij}\}_{1 \leq i,j \leq N}.$$

Semicircular means $s_{ij} = s_{ij}^*$ and Haar mixed moments are

$$\phi(s_{i(1)j} s_{i(2)j} \dots s_{i(k)j}) = \#\{\pi \in NC_2(k) : ker\ i \geq \pi\}.$$

Theorem (Brannan, K. 2016): Deformed quantum groups with $F \in GL(N, \mathbb{C})$, defined by

$$O_F^+ := C^*(u_{ij} : U = [u_{ij}] \text{ unitary and } U = F\overline{U}F^{-1})$$

have an action on Free Araki-Woods factors (type III_λ)

$$\Gamma := \Gamma(\mathbb{R}^n, V_t)'' := \{\ell(\xi) + \ell(\xi)^* : \xi \in H_{\mathbb{R}}\}.''$$

And $\exists \, \{F(n)\}_{n \geq 1}$ s.t. rescaled generators are asymptotically free and generalized circular:

$$\{\|F(n)\|_2 u_{ij}\}_{ij} \xrightarrow{N \to \infty} \mathbf{C}.$$

We create a quantum Weingarten-type calculus.

How does physics work?

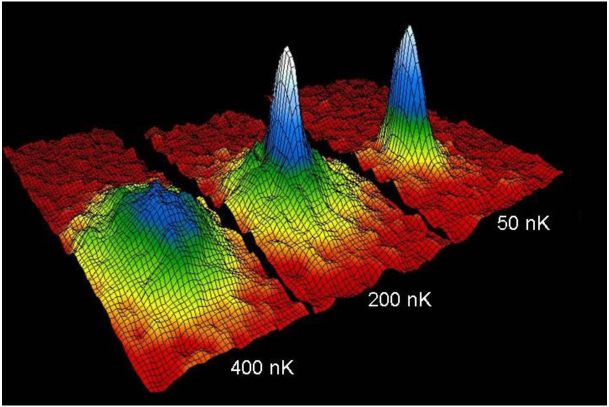
Physics

$\downarrow \qquad \uparrow$

Probability, PDE

Thanks

NSF DMS-1106770, OISE-0730136, CAREER DMS-1254791



arXiv:0808.0505 (AJM), 1009.5737 (CPAM), 1111.6999 (CMP), 1505.05137(PJM)

Our novelty is the bosonic Bogoliubov transform

$$\Theta_{t,s} : (\varphi(\cdot, t), \overline{\varphi}(\cdot, t)) \mapsto (\varphi(\cdot, s), \overline{\varphi}(\cdot, s))$$

written

$$\Theta_{t,0} = \begin{pmatrix} U_t & JV_tJ \\ V_t & JU_tJ \end{pmatrix},$$

Here $Jf = \overline{f}$ and U_t, V_t are certain linear maps...

The correct variance is our guess twisted by $\Theta_{t,0}$:

$$\sigma_t^2 = ||U_tA\varphi_t + JV_tA\varphi_t||^2 - |\langle\varphi_t|U_tA\varphi_t + JV_tA\varphi_t\rangle|^2.$$

Proof: moments of $\mathcal{A}_t = \frac{1}{\sqrt{N}} \sum (A_j - \mathbb{E}_{\varphi_t} A) = \frac{1}{\sqrt{N}} \sum \widetilde{A} j$ go to the normal moments

$$\mathbb{E}_{\psi_N} \left(\frac{1}{\sqrt{N}} \sum_{j=1}^{N} (A_j - \mathbb{E}_{\varphi_t} A) \right)^2 = Tr\, \gamma_N^{(1)} \widetilde{A}^2 + N Tr\, \gamma_N^{(2)} (\widetilde{A} \otimes \widetilde{A})$$

First term: $\|\widetilde{A}\varphi_t\|^2$, same as i.i.d. cancels part of second term.

Remainder of second term gives the Bogoliubov-twisted variance.

The higher moments: Bounds on moments of observables w.r.t. full fluctuation dynamics around the mean-field approximation and the limiting dynamics given by the Bogoliubov transform.

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Program

New Challenges in PDE: Deterministic Dynamics and Randomness in High and Infinite Dimensional Systems

August 17, 2015 to December 18, 2015

Organizers

Kay Kirkpatrick (University of Illinois at Urbana-Champaign), Yvan Martel (École Polytechnique), Jonathan Mattingly (Duke University), Andrea Nahmod (University of Massachusetts, Amherst), Pierre Raphael (Universite de Nice Sophia-Antipolis), Luc Rey-Bellet (University of Massachusetts, Amherst), LEAD Gigliola Staffilani (Massachusetts Institute of Technology), Daniel Tataru (University of California, Berkeley)

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- N bosons $\rightsquigarrow$ localizing limit $\rightsquigarrow$ NLS
- Moving to quantum probability

BEC limit theorems with parameter $\beta \in (0, 1]$

Now localized strong interactions: $N^{d\beta} V(N^{\beta}(\cdot)) \to b_0 \delta$.

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Coagulation and Smoluchowski eqn: Hammond and Rezakhanlou.

Our CLT for interacting quantum many-body systems

Theorem (Ben Arous, K., Schlein, 2013): If the initial state is factorized $\psi_N^0 = \varphi_0^{\otimes N}$ with normalized $\varphi_0 \in H^1(\mathbb{R}^3)$, and A is compact self-adjoint on $L^2(\mathbb{R}^3)$, and $V \leq 1/|\cdot|$, then for $t \in \mathbb{R}$

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Distribution of $\mathcal{A}_t$ from $\psi_N = \psi_{N,t}$.

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The obvious variance is correct at $t = 0$ only (i.i.d.):

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Our CLT for interacting quantum many-body systems

Theorem (Ben Arous, K., Schlein, 2013): If the initial state is factorized $\psi_N^0 = \varphi_0^{\otimes N}$ with normalized $\varphi_0 \in H^1(\mathbb{R}^3)$, and A is compact self-adjoint on $L^2(\mathbb{R}^3)$, and $V \leq 1/|\cdot|$, then for $t \in \mathbb{R}$

$$\mathcal{A}_t := \frac{1}{\sqrt{N}} \sum_{j=1}^{N} (A_j - \mathbb{E}_{\varphi_t} A) \xrightarrow{\text{distrib. as } N \to \infty} \mathcal{N}(0, \sigma_t^2).$$

Distribution of $\mathcal{A}_t$ from $\psi_N = \psi_{N,t}$.

The obvious variance is correct at $t = 0$ only (i.i.d.):

$$\sigma_0^2 = \mathbb{E}_{\varphi_0}[A^2] - (\mathbb{E}_{\varphi_0} A)^2 = ||A\varphi_0||^2 - \langle \varphi_0 | A \varphi_0 \rangle^2.$$

The variance σ_t^2 is more subtle than replacing φ_0 by φ_t.

Proof: first moment of $\mathcal{A}_t = \frac{1}{\sqrt{N}} \sum (A_j - \mathbb{E}_{\varphi_t} A)$

First moment goes to the normal thing:

$$|\mathbb{E}_{\psi_N} \mathcal{A}_t| = \left| \frac{1}{\sqrt{N}} \sum_{j=1}^{N} Tr\, A(\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|) \right|$$

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$$\leq \frac{||A||}{\sqrt{N}} \sum_{j=1}^{N} Tr \left| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right|$$

$$\lesssim \frac{||A||}{\sqrt{N}} \frac{Ne^{Kt}}{N} \to 0.$$

The bosonic Fock space

Fock space:
$$\mathcal{F} = \bigoplus_{n\geq 0} L^2_s(\mathbb{R}^{3n}, dx_1 \dots dx_n)$$

Inner product:
$$\langle \Psi, \Phi \rangle = \overline{\psi^{(0)}}\varphi^{(0)} + \sum_{n\geq 1} \langle \psi^{(n)}, \varphi^{(n)} \rangle \,.$$

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Number-of-particles operator: $\mathcal{N}\{\psi^{(n)}\}_{n \geq 0} = \{n\psi^{(n)}\}_{n \geq 0}$, eigenvectors $\{0, \dots, 0, \psi^{(m)}, 0, \dots\}$.

Hamiltonian:
$$\mathcal{H}^{(m)}_N = \sum_{j=1}^{m} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{m} V(x_i - x_j) \,.$$

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Then $e^{-i\mathcal{H}_N t}\{0, \dots, 0, \psi_N, 0, \dots\} = \{0, \dots, 0, e^{-iH_N t}\psi_N, 0, \dots\}$.

Advantage: Particle number not fixed.

Creation and annihilation operators

$$\left(a^*(f)\psi\right)^{(n)}(x_1,\ldots,x_n) = \frac{1}{\sqrt{n}}\sum_{j=1}^{n} f(x_j)\psi^{(n-1)}(x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_n)$$

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Operator-valued distributions a_x, a_x^*:

$$a(f) = \int dx \overline{f(x)} a_x, \qquad \text{and} \qquad a^*(f) = \int dx\, f(x)\, a_x^*\,.$$

Hamiltonian (commutes w/ particle number op. $\mathcal{N} = \int dx\, a_x^* a_x$):

$$\mathcal{H}_N = \int dx\, \nabla_x a_x^*\, \nabla_x a_x + \frac{1}{2N}\int dxdy\, V(x-y) a_x^* a_y^* a_y a_x\,.$$

Replacement for product states

Product state with N particles all in state φ:

$$\{0, \dots, 0, \varphi^{\otimes N}, 0, \dots\} = \frac{(a^*(\varphi))^N}{\sqrt{N!}} \Omega \, .$$

Here the vacuum vector is $\Omega = \{1, 0, 0, \dots\}$.

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Weyl operator $W(\varphi) = e^{(a^*(\varphi) - a(\varphi))}$ to make a coherent state, with all particles all in state φ:

$$W(\varphi)\Omega = e^{-\|\varphi\|^2/2} \sum_{j=0} \frac{a^*(\varphi)^j}{j!}\Omega = e^{-\|\varphi\|^2/2}\{1, \varphi, \frac{\varphi^{\otimes 2}}{\sqrt{2!}}, \ldots, \frac{\varphi^{\otimes j}}{\sqrt{j!}}, \ldots\}\,.$$

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With respect to this coherent state, $\mathcal{N}$ is a Poisson($\|\varphi\|^2$) RV.

The fluctuation dynamics

Around the mean-field approximation $W(\sqrt{N}\varphi_t)\Omega$, fluctuations

$$\mathcal{U}_N(t;s) = W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}_N(t-s)}W(\sqrt{N}\varphi_s),$$

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with generator

$$\begin{aligned}\mathcal{L}_N(t) = &\int dx\, \nabla_x a_x^* \nabla_x a_x + \int dx\, (V * |\varphi_t|^2)(x) a_x^* a_x \\ &+ \frac{1}{2}\int dxdy\, V(x-y)\, \left(\varphi_t(x)\varphi_t(y)a_x^* a_y^* + \overline{\varphi}_t(x)\overline{\varphi}_t(y)a_x a_y\right) \\ &+ \int dxdy\, V(x-y)\, \varphi_t(x)\overline{\varphi}_t(y) a_x^* a_y + o(1) \\ = &\,\mathcal{L}_\infty(t) + o(1).\end{aligned}$$

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& + \frac{1}{2}\int dxdy\, V(x-y)\, \left(\varphi_t(x)\varphi_t(y)a_x^*a_y^* + \overline{\varphi}_t(x)\overline{\varphi}_t(y)a_x a_y\right) \\
& + \int dxdy\, V(x-y)\, \varphi_t(x)\overline{\varphi}_t(y)a_x^* a_y + o(1) \\
= & \, \mathcal{L}_\infty(t) + o(1).
\end{aligned}$$

Limiting dynamics $\mathcal{U}_\infty(t,s)$ has generator $\mathcal{L}_\infty(t)$ and is described by the Bogoliubov transformation.