Title: Bosonic particle-correlated states

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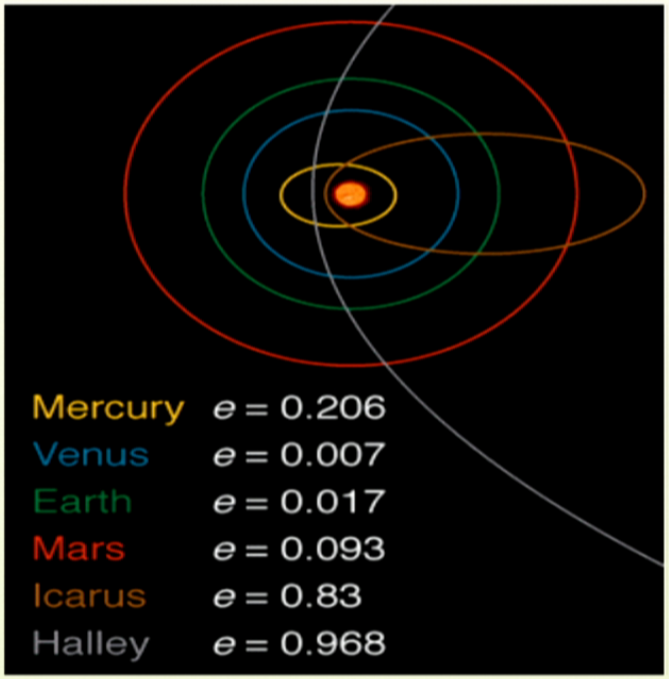
Abstract: Quantum many-body problems are notorious hard. This is partly because the Hilbert space becomes exponentially big with the particle number <var>N</var>. While exact solutions are often considered intractable, numerous approaches have been proposed using approximations. A common trait of these approaches is to use an ansatz such that the number of parameters either does not depend on <var>N</var> or is proportional to <var>N</var>, e.g., the matrix-product state for spin lattices, the BCS wave function for superconductivity, the Laughlin wave function for fractional quantum Hall effects, and the Gross-Pitaecskii theory for BECs. Among them the product ansatz for BECs has precisely predicted many useful properties of Bose gases at ultra-low temperature. As particle-particle correlation becomes important, however, it begins to fail. To capture the quantum correlations, we propose a new
 set of states, which constitute a natural generalization of the product-state ansatz. Our state of <var>N</var>=<var>d</var>×<var>n</var> identical particles is derived by symmetrizing the <var>n</var>-fold product of a <var>d</var>-particle quantum state. For fixed <var>d</var>, the parameter space of our state does not grow with <var>N</var>. Numerically, we show that our ansatz gives the right description for the ground state and time evolution of the two-site Bose-Hubbard model.

The Hilbert space increases exponentially.

The Hilbert space becomes exponentially BIG with the particle number N. As a consequence, one needs an exponentially large number of parameters merely to record an arbitrary state.

We need a good ansatz

Finding that an elliptical orbit fit the Mars data, Kepler concluded that all planets move in ellipses.



Circular orbit
Gross Pitaevskii ansatz

Elliptical orbit
Bosonic particle-correlated ansatz

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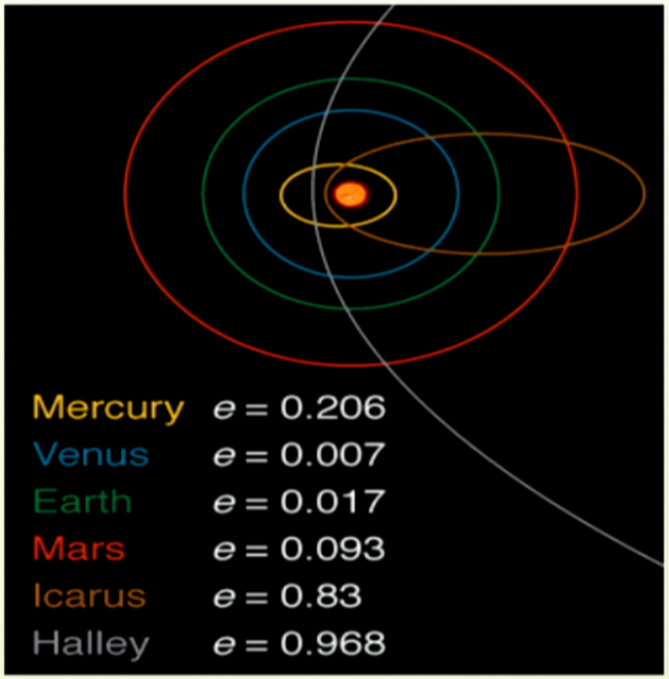

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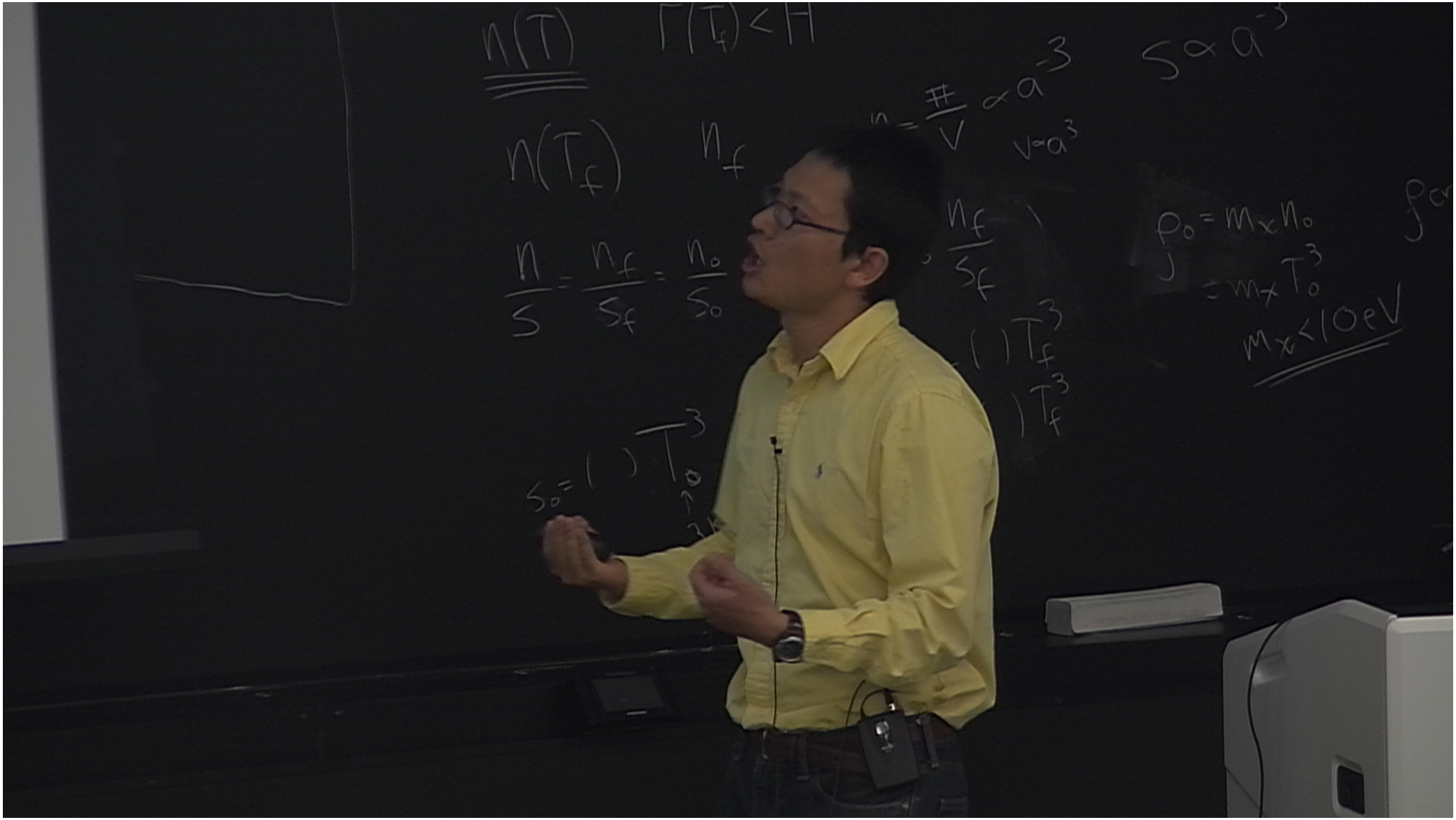
n(T)
Γ(T_f)<H
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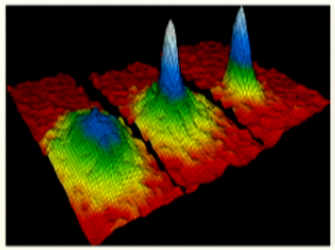
n_f
n/s = n_f/s_f = n_0/s_0
n = #/V ∝ a^-3
V∝a^3
s ∝ a^-3
n_f/s_f
ρ_0 = m_χ n_0
= m_χ T_0^3
m_χ < 10eV

Product ansatz for BECs



A Bose-Einstein condensate (BEC) is a state of matter of a dilute gas of weakly interacting bosons cooled to temperatures very close to absolute zero.

A large fraction of the bosons occupy the lowest quantum state, and quantum effects become apparent on a macroscopic scale.

$$\rho^{(1)}(\mathbf{x}\,|\,\mathbf{x}') = \frac{1}{N}\left\langle \psi^\dagger(\mathbf{x}')\,\psi(\mathbf{x})\right\rangle$$

$$= \lambda_0\,\psi_0(\mathbf{x})\psi_0^*(\mathbf{x}') + \sum_{j=1}^{\infty}\lambda_j\,\psi_j(\mathbf{x})\psi_j^*(\mathbf{x}')$$

Penrose-Onsager criterion: $\lambda_0 \approx 1$.

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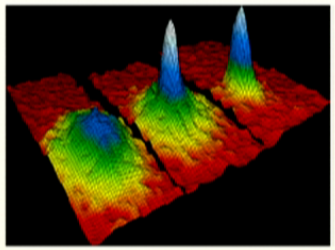

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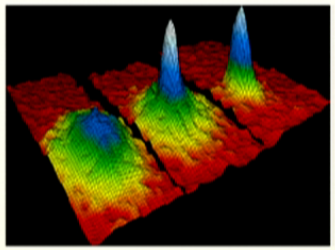

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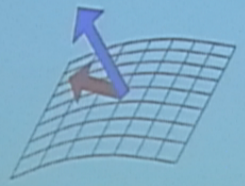
Product ansatz for BECs

When particle correlations are low, the product ansatz may be a good approximation for BECs,

$$\langle \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \,|\, \Psi_{\mathrm{GP}} \rangle = \psi_0(\mathbf{x}_1)\psi_0(\mathbf{x}_2)\cdots\psi_0(\mathbf{x}_N) \,.$$

The dynamical equation of the product ansatz can be derived by:

- Evolve the state for an infinitesimal time dt.
- Project the evolved state back to the product manifold.



$$\mathcal{H}|\Psi_{\mathrm{GP}}\rangle$$
$$i\hbar|\dot{\Psi}_{\mathrm{GP}}\rangle$$

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Product ansatz for BECs

The Gross-Pitaevskii equation:

$$i\hbar\,\dot{\psi}_0(\mathbf{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x},t) + gN|\psi_0(\mathbf{x},t)|^2\right)\psi_0(\mathbf{x},t)\ .$$

The error to the state vector is **not small** at all

$$\mathrm{Err}\big[|\,\Psi_{\mathrm{GP}}\,\rangle\big] \equiv \mathcal{H}\,|\,\Psi_{\mathrm{GP}}\,\rangle - i\hbar\,|\,\dot{\Psi}_{\mathrm{GP}}\,\rangle \sim 1\ .$$

But the error to the reduced density matrices (RDMs) are small

$$\mathrm{Err}\big[\rho^{(1)}\big] = 0\ , \qquad \mathrm{Err}\big[\rho^{(2)}\big] \sim 1/N\ ,$$

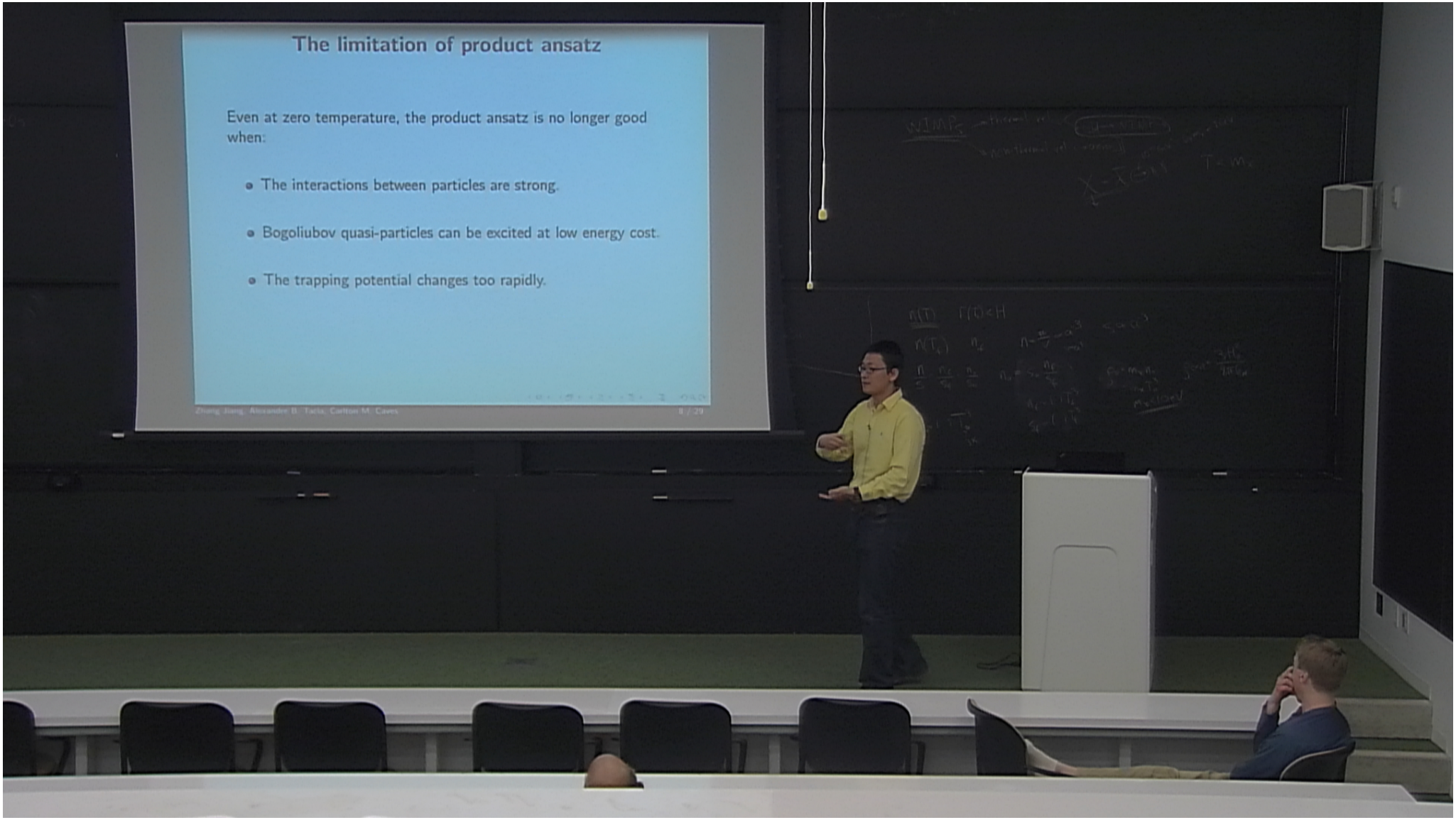
where,

$$\rho^{(1)}(\mathbf{x}\,|\,\mathbf{x}') = \frac{1}{N}\left\langle\psi^\dagger(\mathbf{x}')\,\psi(\mathbf{x})\right\rangle\ ,$$

$$\rho^{(2)}(\mathbf{x}_1,\mathbf{x}_2\,|\,\mathbf{x}_1',\mathbf{x}_2') = \frac{1}{N(N-1)}\left\langle\psi^\dagger(\mathbf{x}_1')\psi^\dagger(\mathbf{x}_2')\,\psi(\mathbf{x}_2)\psi(\mathbf{x}_1)\right\rangle\ .$$

The lessons we learned

- Physically, the lower-order RDMs are most important.
- Good approximations do not necessarily mean small errors to the entire wavefunction.
- One crucial thing can be exploited is: $\mathcal{H}$ only includes up to 2-particle interactions.
- The errors to higher-order RDMs only weakly affect lower-order RDMs.


The limitation of product ansatz
Even at zero temperature, the product ansatz is no longer good when:
The interactions between particles are strong.
Bogoliubov quasi-particles can be excited at low energy cost.
The trapping potential changes too rapidly.
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Two-body interactions

Many quantum systems can be modeled by up to two-body interactions.

$$\mathcal{H}_{\mathrm{BEC}} = \int \psi^{\dagger}(\mathbf{x})\Big(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})\Big)\psi(\mathbf{x})\, d\mathbf{x}+\frac{g}{2}\int [\psi^{\dagger}(\mathbf{x})]^2\,\psi^2(\mathbf{x})\, d\mathbf{x}$$

$$\mathcal{H}_{\mathrm{Heisenberg}} = -J\sum_{j=1}^{N-1}\vec{\sigma}_j\cdot\vec{\sigma}_{j+1} - h\sum_{j=1}^{N}\sigma_j^{(z)}$$

$$\mathcal{H}_{\mathrm{QHE}} = \sum_j\Big\{\big|\, i\hbar\nabla_j + eA_j/c\,\big|^2 + V(z_j)\Big\} + \sum_{k>j}\frac{e^2}{|z_j - z_k|}$$

To solve many-body problems, two-body correlations need to be effectively represented.

Two-boson states

Any two-boson state can be written as:

$$|\,\Phi\,\rangle = \frac{1}{\sqrt{2}} \sum_{j,k=1}^{s} \Lambda_{jk}\, b_k^\dagger b_j^\dagger \,|\,\mathrm{vac}\,\rangle\,, \quad \Lambda_{jk} = \Lambda_{kj}\ .$$

Symmetric matrices can be diagonalized with unitary matrices,

$$\left(U \Lambda\, U^T\right)_{jk} = \delta_{jk} \sqrt{\lambda_j}\ .$$

We get the Schmidt form by changing the basis,

$$\boxed{|\,\Phi\,\rangle = \frac{1}{\sqrt{2}} \sum_{j=1}^{s} \sqrt{\lambda_j}\, a_j^{\dagger\,2} \,|\,\mathrm{vac}\,\rangle\ ,}$$

where $a_j^\dagger = \sum_k U_{kj}^* b_k^\dagger$.

The pair-correlated states

We can use the two-boson state to construct a state of $N = 2n$ bosons,

$$|\,\Psi_{\rm PCS}\,\rangle = \frac{1}{\sqrt{\mathsf{N}_{\vec{\lambda},n}}}\,(\mathcal{A}^\dagger)^n\,|\,{\rm vac}\,\rangle\,, \qquad \mathcal{A}^\dagger = \sum_{j=1}^{s}\sqrt{\lambda_j}\,a_j^{\dagger\,2}\,.$$

The state has the following wavefunction form,

$$\langle\,\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\,|\,\Psi_{\rm PCS}\,\rangle \propto \mathcal{P}_S\Big(\,\Phi(\mathbf{x}_1,\mathbf{x}_2)\,\Phi(\mathbf{x}_3,\mathbf{x}_4)\cdots\Phi(\mathbf{x}_{N-1},\mathbf{x}_N)\,\Big)\,,$$

where $\mathcal{P}_S$ is the projection operator onto the symmetric subspace.

The correlations in the two-particle state $|\,\Phi\,\rangle$ then "spread" to any two particles of the many-boson system.

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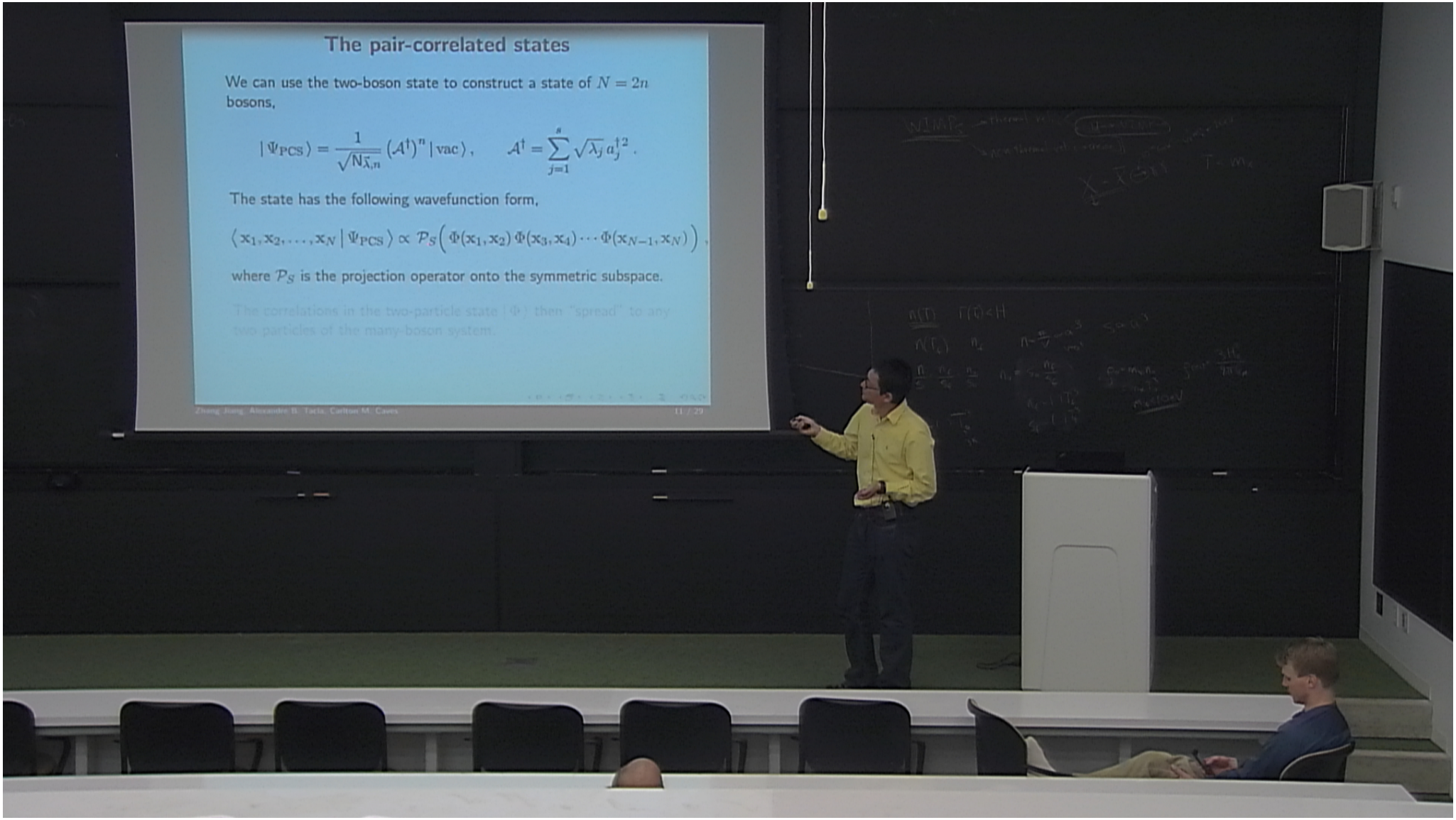
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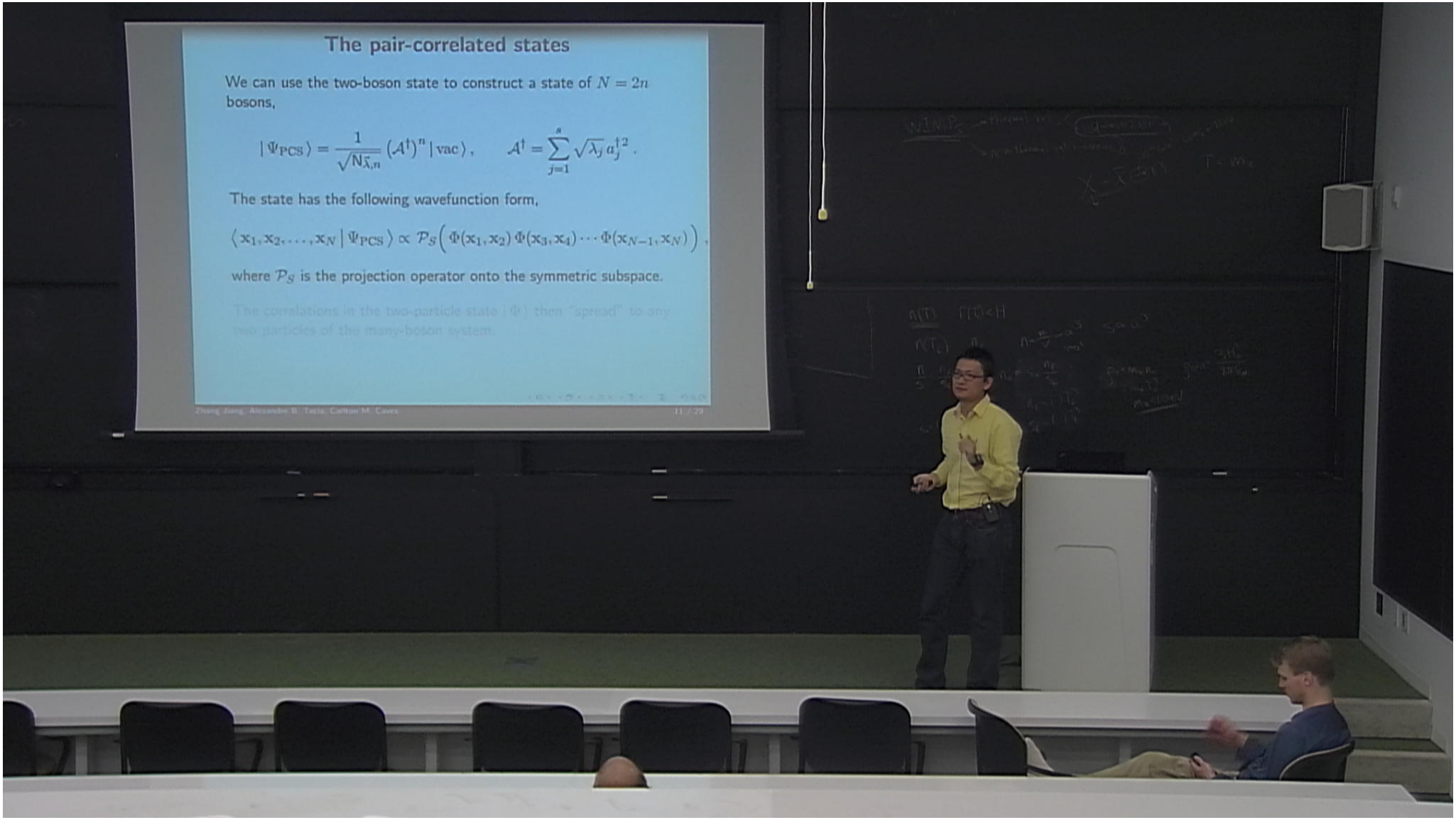
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The normalization factor $\mathsf{N}_{\vec{\lambda},n}$

$$\mathsf{N}_{\vec{\lambda},n} = \left\langle \mathrm{vac} \left| \mathcal{A}^n \mathcal{A}^{\dagger\, n} \right| \mathrm{vac} \right\rangle , \qquad \mathcal{A}^\dagger = \sum_{j=1}^{s} \sqrt{\lambda_j}\, a_j^{\dagger\, 2} .$$

Why we care about an "irrelevant" C-number?

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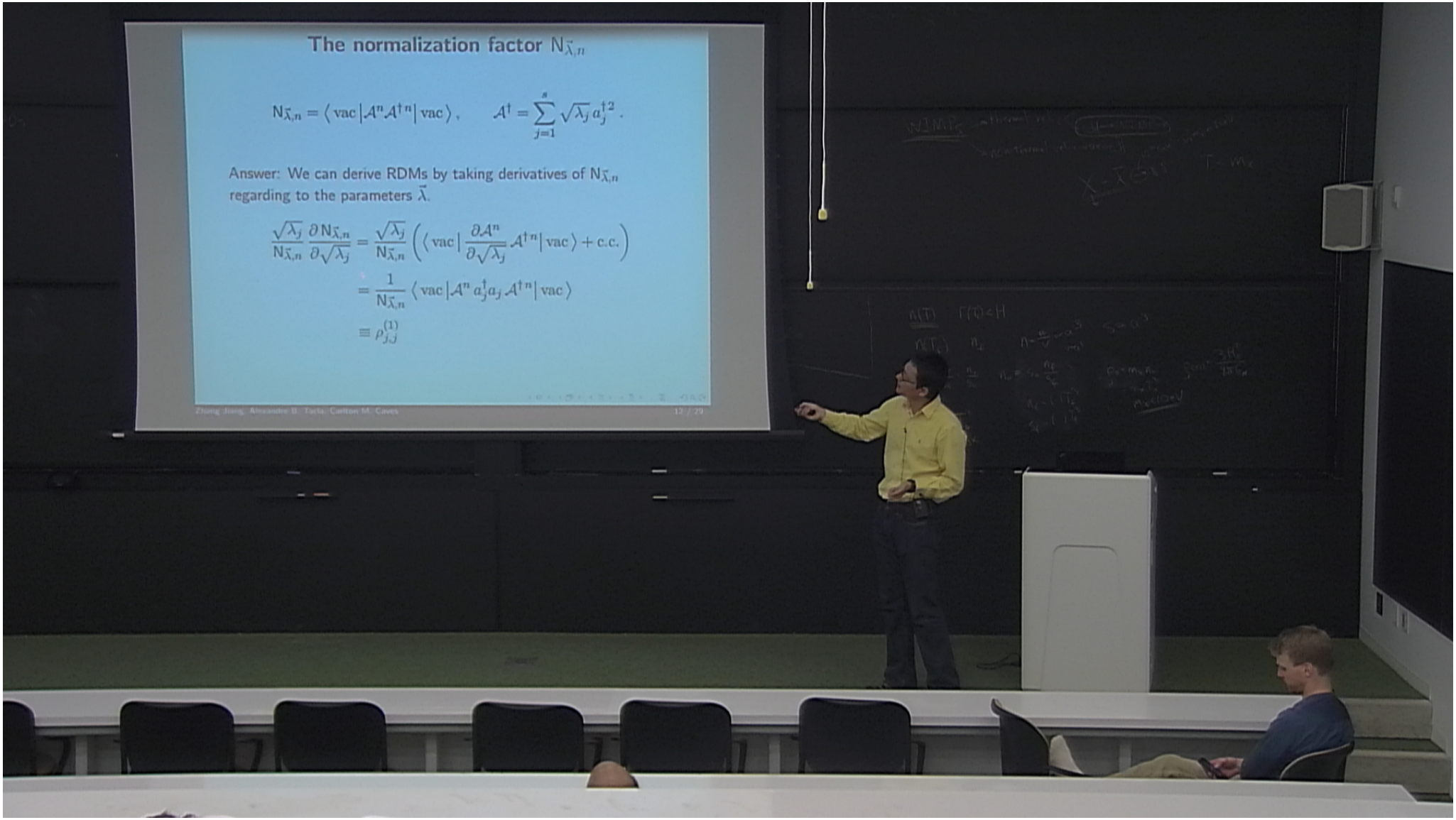
Answer: We can derive RDMs by taking derivatives of $\mathsf{N}_{\vec{\lambda},n}$ regarding to the parameters $\vec{\lambda}$.

$$\begin{aligned}
\frac{\sqrt{\lambda_j}}{\mathsf{N}_{\vec{\lambda},n}} \frac{\partial\, \mathsf{N}_{\vec{\lambda},n}}{\partial \sqrt{\lambda_j}} &= \frac{\sqrt{\lambda_j}}{\mathsf{N}_{\vec{\lambda},n}} \left(\left\langle \mathrm{vac} \right| \frac{\partial \mathcal{A}^n}{\partial \sqrt{\lambda_j}} \mathcal{A}^{\dagger\, n} \left| \mathrm{vac} \right\rangle + \mathrm{c.c.} \right) \\
&= \frac{1}{\mathsf{N}_{\vec{\lambda},n}} \left\langle \mathrm{vac} \left| \mathcal{A}^n\, a_j^\dagger a_j\, \mathcal{A}^{\dagger\, n} \right| \mathrm{vac} \right\rangle \\
&\equiv \rho_{j,j}^{(1)}
\end{aligned}$$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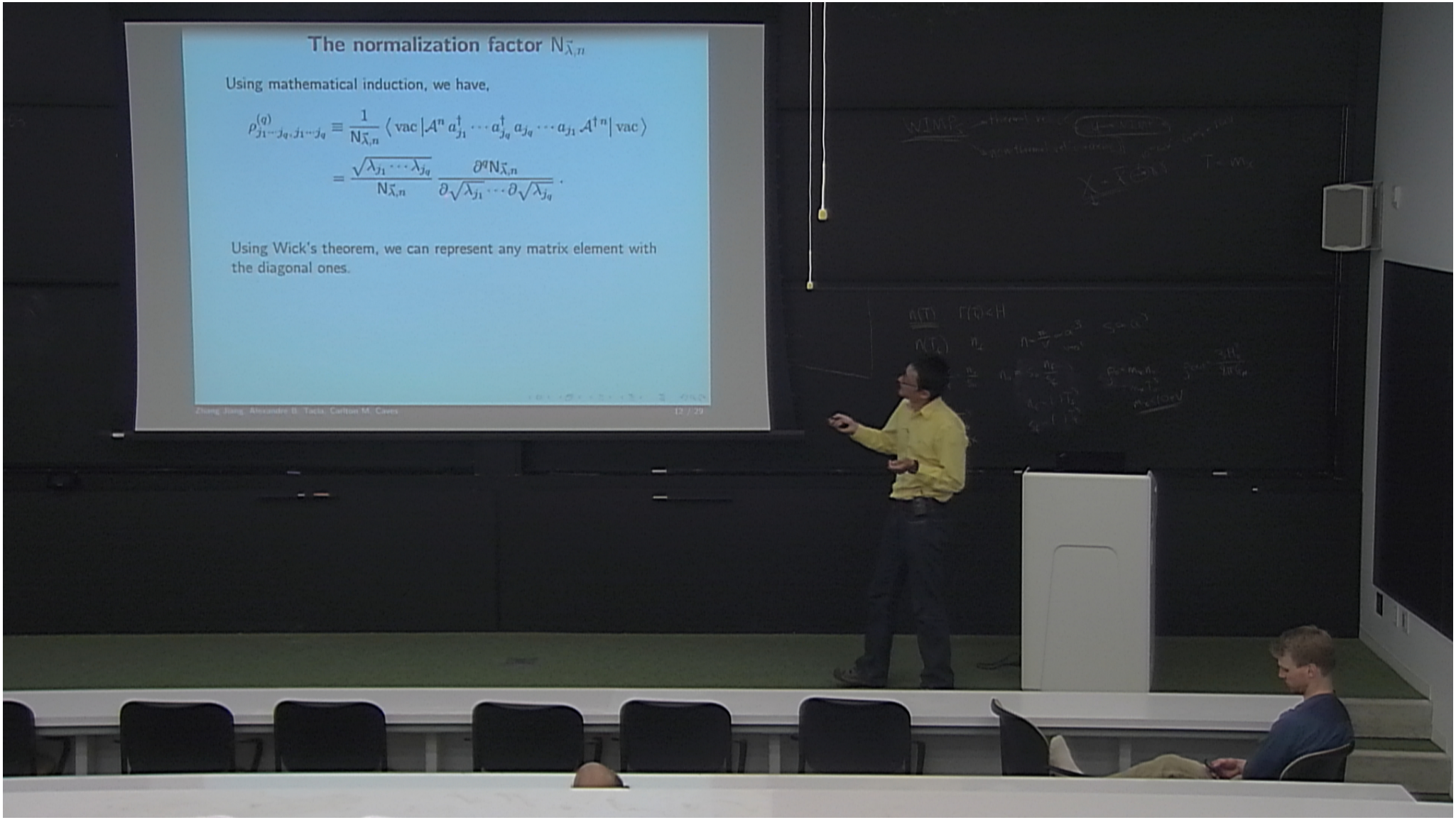
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$$\rho^{(q)}_{j_1\cdots j_q,j_1\cdots j_q} \equiv \frac{1}{\mathrm{N}_{\vec{\lambda},n}} \langle \mathrm{vac} | \mathcal{A}^n a^\dagger_{j_1} \cdots a^\dagger_{j_q} a_{j_q} \cdots a_{j_1} \mathcal{A}^{\dagger n} | \mathrm{vac} \rangle$$
$$= \frac{\sqrt{\lambda_{j_1} \cdots \lambda_{j_q}}}{\mathrm{N}_{\vec{\lambda},n}} \frac{\partial^q \mathrm{N}_{\vec{\lambda},n}}{\partial\sqrt{\lambda_{j_1}} \cdots \partial\sqrt{\lambda_{j_q}}}.$$
Using Wick's theorem, we can represent any matrix element with the diagonal ones.
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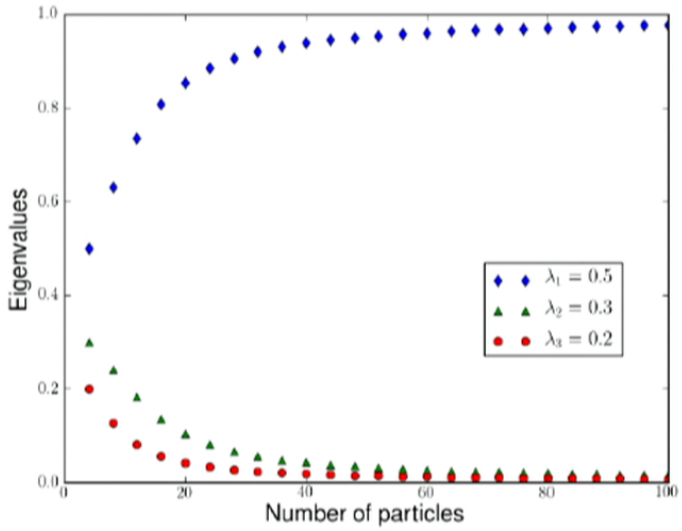
Using Wick's theorem, we can represent any matrix element with the diagonal ones.

The large N limit

In the large N limit, only the greatest Schmidt coefficients contribute to the lower-order RDMs.



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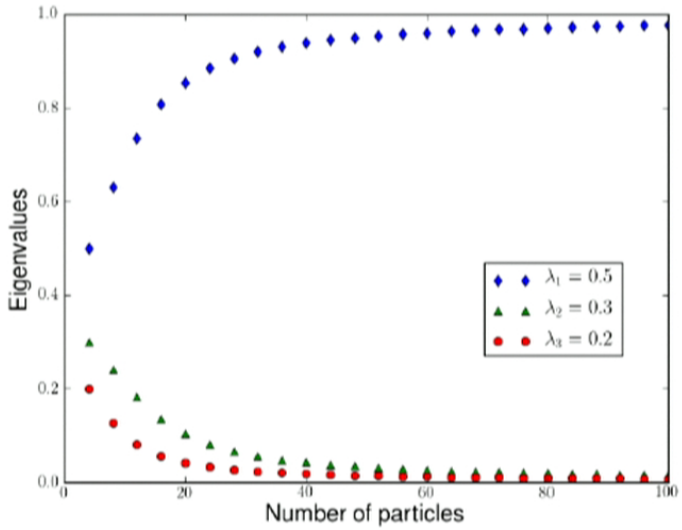

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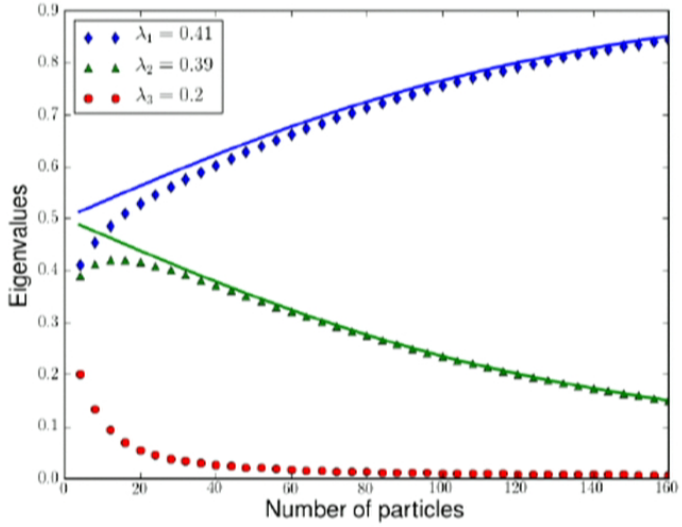
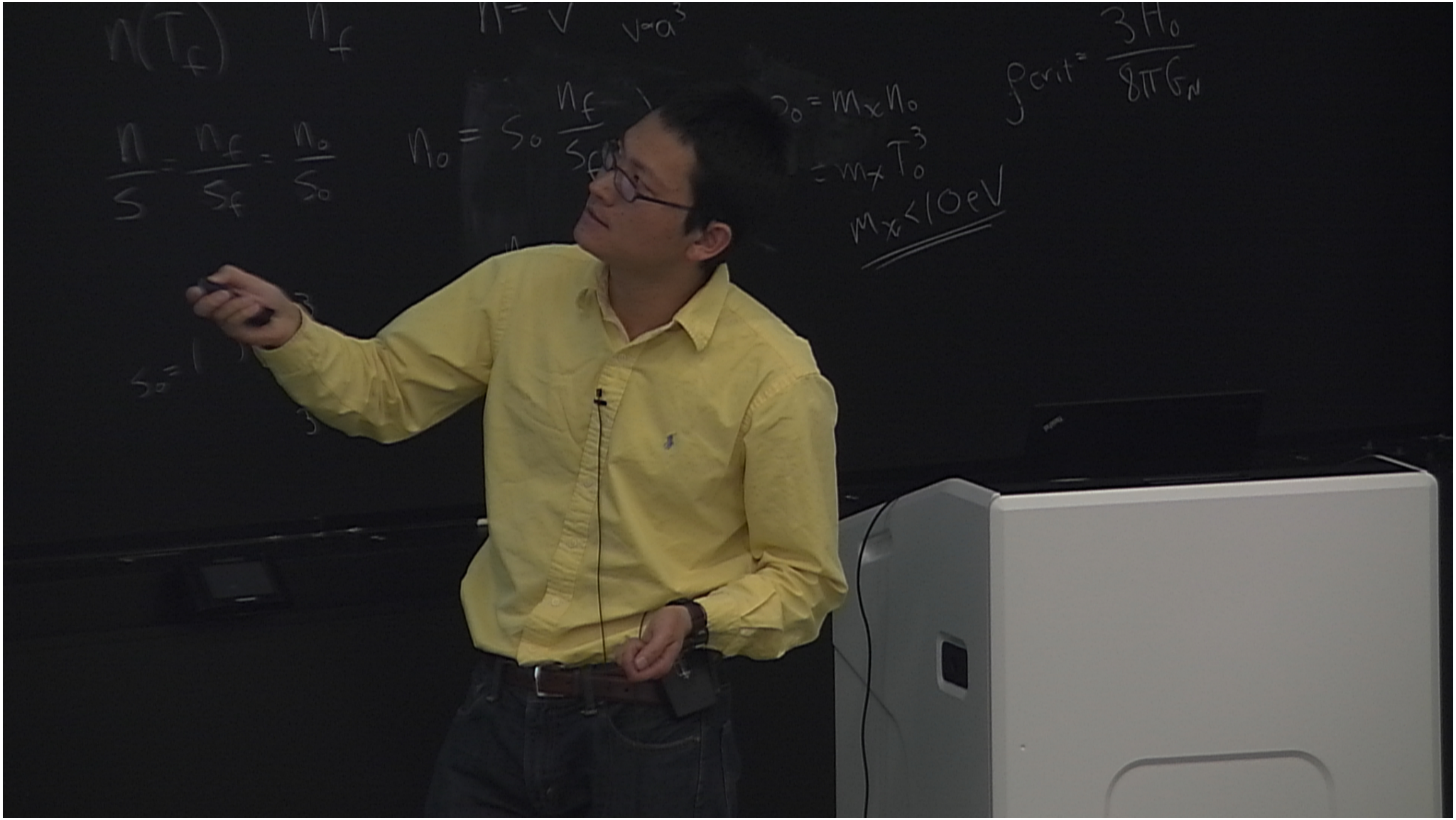


Without changing the RDMs, we only keep the greatest Schmidt coefficients, and renormalize them to unity.


$n(T_f)$
n_f
$n = \frac{N}{V}$
$V = a^3$
$\frac{n}{s} = \frac{n_f}{s_f} = \frac{n_0}{s_0}$
$n_0 = s_0 \frac{n_f}{s_f}$
$\rho_0 = m_\chi n_0$
$= m_\chi T_0^3$
$m_\chi < 10\,eV$
$\rho_{crit} = \frac{3H_0}{8\pi G_N}$

The large N limit

In the large N limit, the coefficients $\vec{\lambda}$ are almost degenerate,

$$\lambda_j \equiv \frac{1}{s}\left(1+\frac{\zeta_j}{n}\right).$$

The normalization factor reads

$$\mathsf{N}_{\vec{\lambda},n} \approx \frac{4^n n!}{2s^n \pi^{s/2}}\,\Gamma\Big(n+\frac{s}{2}\Big)\int_{|\vec{z}|=1}\exp\Big(\sum_{j=1}^{s}\zeta_j z_j^2\Big)\,d\Omega$$

where $d\Omega$ stands for the area element of the unit s-dimensional hypersurface, $|\vec{z}|=1$.

We define the part in $\mathsf{N}_{\vec{\lambda},n}$ with $\vec{\lambda}$ dependence to be

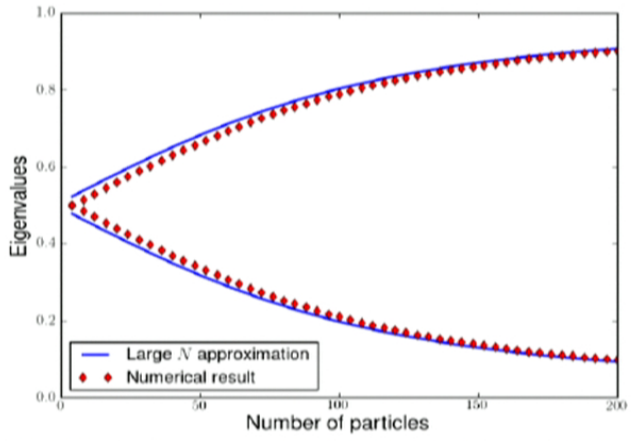
$$\Upsilon(\vec{\zeta}) \equiv \int_{|\vec{z}|=1}\exp\Big(\sum_{j=1}^{s}\zeta_j z_j^2\Big)\,d\Omega\,.$$

The $s = 2$ case

The $s = 2$ case can be solved explicitly,

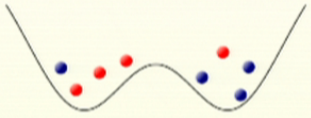
$$\Upsilon(\zeta_1, \zeta_2) = 2\pi \exp\left[\frac{1}{2}(\zeta_1 + \zeta_2)\right] I_0\left[\frac{1}{2}(\zeta_1 - \zeta_2)\right],$$

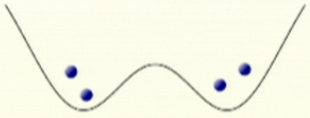
where I_j is the j-th order modified Bessel function.



Double-well trapping potential: ground states

As we raise the barrier in the middle of a double-well potential, the coherence between the two parts eventually breaks.





$$\left(a_0^\dagger\right)^N |\,\mathrm{vac}\,\rangle \qquad \left(a_{\mathrm{left}}^\dagger\right)^{N/2}\left(a_{\mathrm{right}}^\dagger\right)^{N/2} |\,\mathrm{vac}\,\rangle$$

$$\Downarrow \qquad\qquad \Downarrow$$

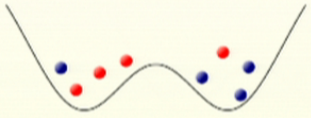
$$\left(a_0^{\dagger\,2}\right)^{N/2} |\,\mathrm{vac}\,\rangle \qquad \left(a_{\mathrm{left}}^\dagger\, a_{\mathrm{right}}^\dagger\right)^{N/2} |\,\mathrm{vac}\,\rangle$$

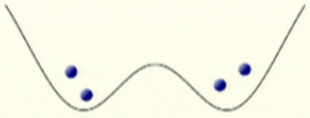
$$\Downarrow$$

$$\frac{1}{2^N}\left[\left(a_{\mathrm{left}}^\dagger + a_{\mathrm{right}}^\dagger\right)^2 + \left(ia_{\mathrm{left}}^\dagger - ia_{\mathrm{right}}^\dagger\right)^2\right]^{N/2} |\,\mathrm{vac}\,\rangle$$

Double-well trapping potential: ground states

As we raise the barrier in the middle of a double-well potential, the coherence between the two parts eventually breaks.





$$\left(a_0^\dagger\right)^N |\,\mathrm{vac}\,\rangle \qquad \left(a_{\mathrm{left}}^\dagger\right)^{N/2}\left(a_{\mathrm{right}}^\dagger\right)^{N/2} |\,\mathrm{vac}\,\rangle$$

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$$\Downarrow$$

$$\frac{1}{2^N}\left[\left(a_{\mathrm{left}}^\dagger + a_{\mathrm{right}}^\dagger\right)^2 + \left(ia_{\mathrm{left}}^\dagger - ia_{\mathrm{right}}^\dagger\right)^2\right]^{N/2} |\,\mathrm{vac}\,\rangle$$

2-site Bose-Hubbard model (ground state)

Continue to deviate from a single condensate: $\mathrm{tr}\left([\rho^{(1)}]^2\right) \approx 0.872$.

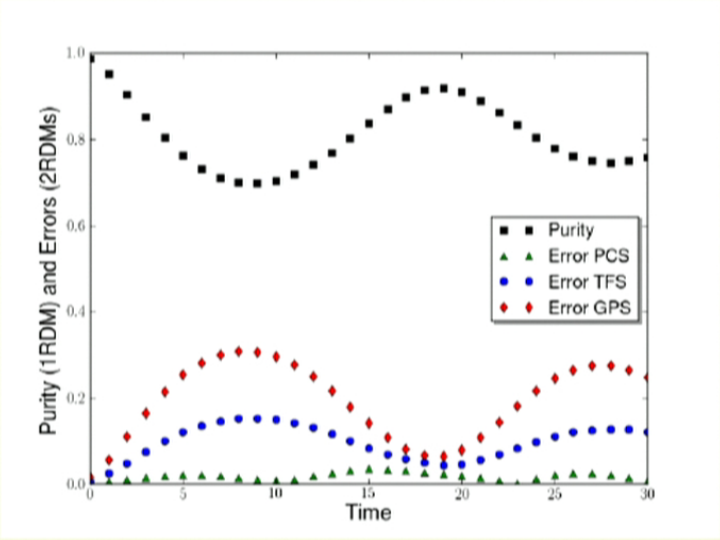
$$\rho^{(2)}_{\mathrm{BPCS}} \approx \begin{pmatrix} 0.876 & 0. & 0. & -0.055 \\ 0. & 0.055 & 0.055 & 0. \\ 0. & 0.055 & 0.055 & 0. \\ -0.055 & 0. & 0. & 0.015 \end{pmatrix}$$

$$\rho^{(2)}_{\mathrm{EXACT}} \approx \begin{pmatrix} 0.875 & 0. & 0. & -0.058 \\ 0. & 0.056 & 0.056 & 0. \\ 0. & 0.056 & 0.056 & 0. \\ -0.058 & 0. & 0. & 0.014 \end{pmatrix}$$

$$\rho^{(2)}_{\mathrm{TFS}} \approx \begin{pmatrix} 0.866 & 0. & 0. & 0. \\ 0. & 0.065 & 0.065 & 0. \\ 0. & 0.065 & 0.065 & 0. \\ 0. & 0. & 0. & 0.004 \end{pmatrix}$$

2-site Bose-Hubbard model (time evolution)

Initially, the bosons condensate to a single BEC. Then, we suddenly turn on strong interactions between the bosons.



The errors are the trace distances from the exact solution.

Dynamical equation for the PCS ansatz

Remember the PCS ansatz has the form:

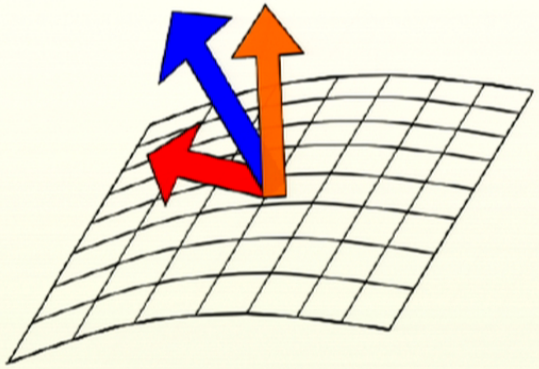
$$|\,\Psi_{\rm PCS}(t)\,\rangle = \frac{1}{\sqrt{\mathsf{N}_{\vec{\lambda},n}}}\,[\mathcal{A}^\dagger(t)]^n\,|\,{\rm vac}\,\rangle\,, \qquad \mathcal{A}(t) = \sum_{j=1}^{s}\sqrt{\lambda_j(t)}\,\left[a_j^\dagger(t)\right]^2\,,$$

where $a_j^\dagger(t)$ corresponds to the orbital $\psi_j(t)$,

$$a_j^\dagger(t) = \int \psi^\dagger(\mathbf{x})\psi_j(\mathbf{x},t)\,d\mathbf{x}\,, \quad j = 1,2,\ldots,s\,.$$

We need a set of coupled equations to determine the dynamics of both $\lambda_j(t)$ and $\psi_j(\mathbf{x},t)$.

Dynamical equation for the PCS ansatz



$$\mathcal{H}\,|\,\Psi_{\mathrm{PCS}}\,\rangle$$

$$i\hbar\,|\,\dot{\Psi}_{\mathrm{PCS}}\,\rangle$$

$$|\,\tilde{\Psi}_{\mathrm{PCS}}\,\rangle = \mathcal{H}\,|\,\Psi_{\mathrm{PCS}}\,\rangle - i\hbar\,|\,\dot{\Psi}_{\mathrm{PCS}}\,\rangle$$

The error is perpendicular to any infinitesimal variation:

$$\langle\,\delta\Psi_{\mathrm{PCS}}\,|\,\tilde{\Psi}_{\mathrm{PCS}}\,\rangle = 0\,, \quad \forall\,\delta\Psi_{\mathrm{PCS}}\,.$$

An equivalent way to write the above equation is:

$$0 = \langle\,\mathrm{vac}\,|\,\mathcal{A}^{n-1}\,a_j a_k\,|\,\tilde{\Psi}_{\mathrm{PCS}}\,\rangle\,, \quad \forall\,j,k \in \{1,2,\ldots,+\infty\}\,.$$

The single-particle RDM is unchanged by the projection.

Determining $\Psi_{\rm PCS}$ from $\rho^{(1)}$

The PCS ansatz state,

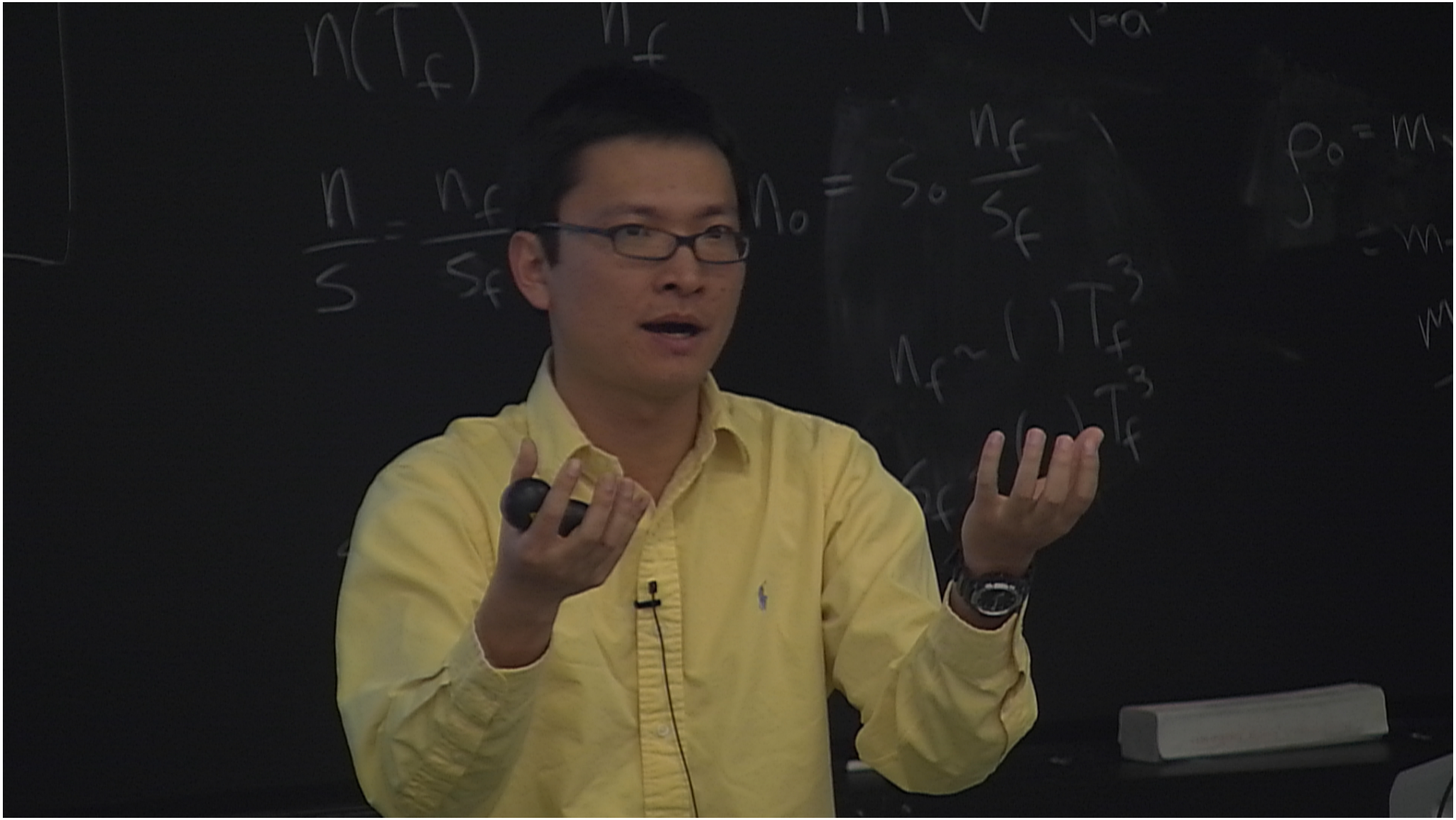
$$|\,\Psi_{\rm PCS}(t)\,\rangle = \frac{1}{\sqrt{\mathsf{N}_{\vec{\lambda},n}}}\,[\mathcal{A}^\dagger(t)]^n\,|\,{\rm vac}\,\rangle$$

is determined by the single-particle RDM,

$$\rho^{(1)}(\mathbf{x}\,|\,\mathbf{x}'\,;\,t) = \frac{1}{N}\,\langle\,\Psi_{\rm PCS}(t)\,|\psi^\dagger(\mathbf{x}')\psi(\mathbf{x})|\,\Psi_{\rm PCS}(t)\,\rangle\ .$$

One strategy to derive time evolution of the PCS ansatz is to evolve $\rho^{(1)}$ and then update $|\,\Psi_{\rm PCS}\,\rangle$ using the evolved $\rho^{(1)}$.

$$\boxed{\rho^{(1)}(t) \overset{\mathcal{H}}{\Longrightarrow} \rho^{(1)}(t+dt) \overset{\text{update}}{\Longrightarrow} |\,\Psi_{\rm PCS}(t+dt)\,\rangle}$$


$n(T_f)$
n_f
$V=a^3$
$\frac{n}{s} = \frac{n_f}{s_f}$
$n_0 = s_0 \frac{n_f}{s_f}$
$\rho_0 = m$
$n_f \sim ( ) T_f^3$
$( ) T_f^3$