# ALGORITHMIC PERSPECTIVE ON STRONGLY CORRELATED SYSTEMS

Last Time: Eat a wave-function, return a property

Today: What wave-function?

    1. What is the class of wave-functions you might choose yours from?

    2. How do you choose your wave-function from this set?

**Q:** Can you do anything useful with this little chunk of Hilbert space?

**Q:** Can you even represent a quantum fluid?  A quantum solid?

Wave-functions for which you can build an efficient code.
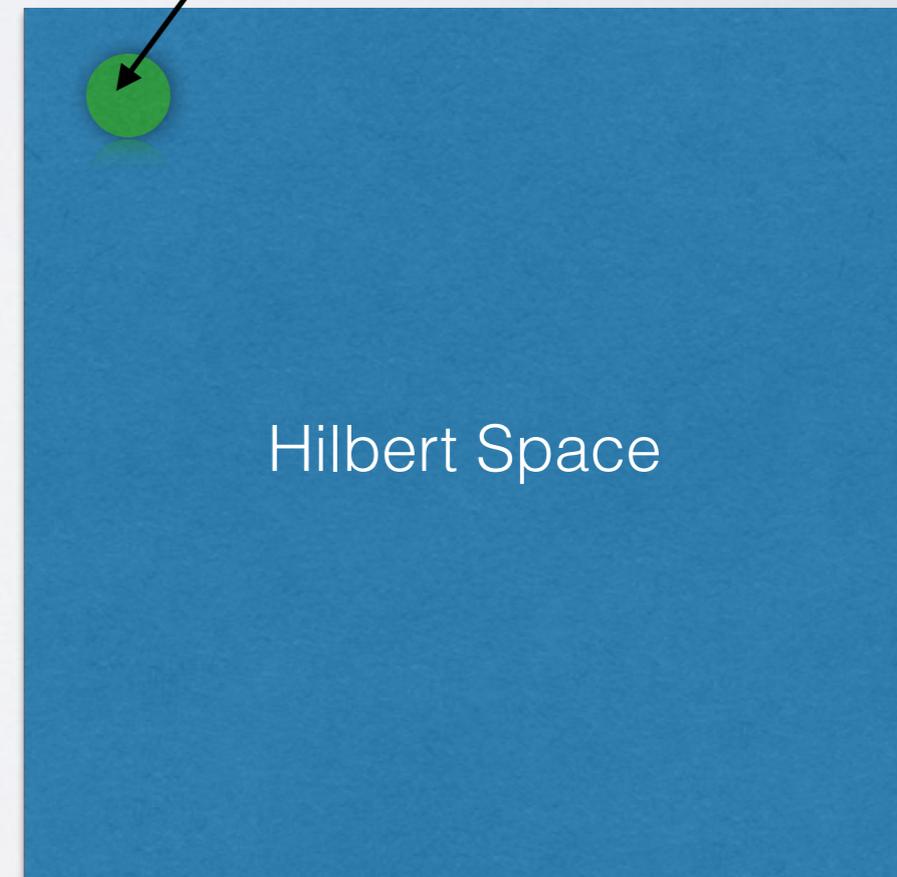
Hilbert Space

# A quantum fluid…

Want a wave-function such that the probability $|\Psi(R)|^2$ of particles being at position **R** makes it likely that the particles are distributed like a liquid (*consider first bosons*)

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Classical systems are liquids….
Classical systems are solids….

**Classical partition function:** $Z(R) = \int \exp[-\beta V(R)]$

The classical partition function tells us the particles are at position R with probability

$$P(R) \equiv \frac{\exp[-\beta V(R)]}{Z(R)}$$

Let us set $\Psi(R) \propto \exp\left[-\frac{\beta V(R)}{2}\right]$

Now we just need to choose a value of V(R) that classically gives a liquid at high temperature. *(almost anything … lennard-jones)*

Now we just need to choose a value of V(R) that classically gives a liquid at low temperature. *(almost anything … lennard-jones)*
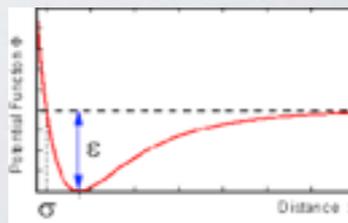
A quantum fluid (and solid) …

$$\Psi(R) \propto \exp\left[-\frac{\beta V(R)}{2}\right]$$

**liquid**                                                **solid**

$$\beta$$

**Q:** Does this wave-function have all the properties we want?

We essentially have all the "classical" stuff right. Let's consider the "quantum" stuff.

For example, we want a boring solid not a supersolid. What do we have?

$$\lim_{|r_1 - r_1'| \to \infty} \rho_1(r_1, r_1') = 0 \quad \text{(implies no supersolid)}$$

$$\rho_1(r_1, r_1') = \int dr_2 dr_3 ... dr_n \, \underline{\Psi(r_1, r_2 ... r_n)} \, \Psi^*(r_1', r_2 ... r_n)$$

**choose probable spot R**

**Is the configuration where one particle
is moved far away also probable?**

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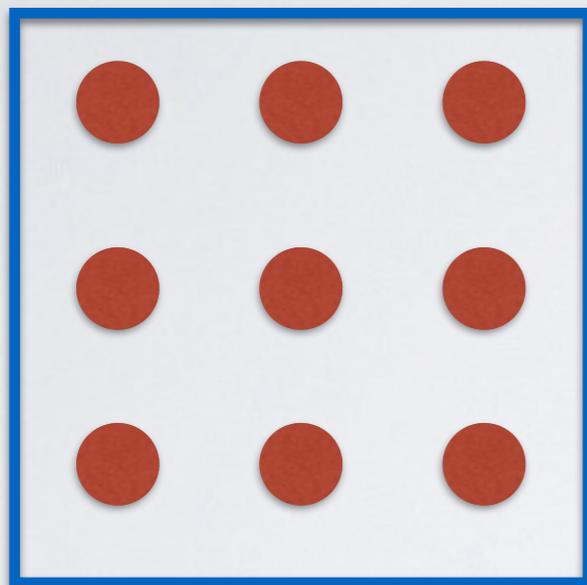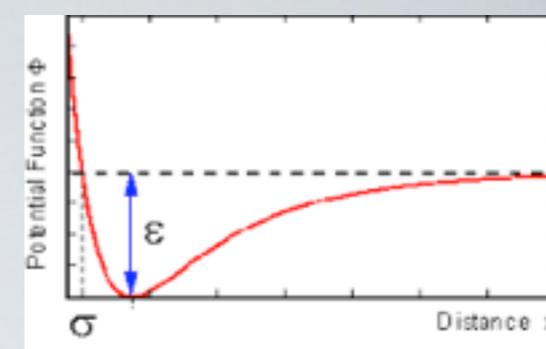


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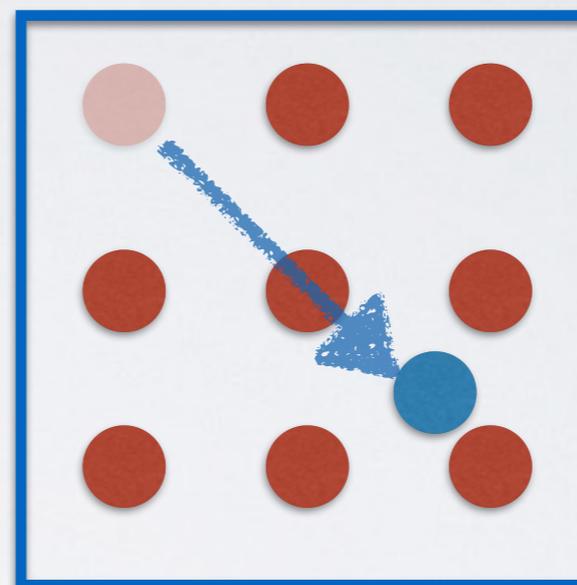
**Is the configuration where one particle is moved far away also probable?**

$$\Psi(R) \propto \exp\left[-\frac{\beta V(R)}{2}\right]$$

**This new configuration is less probable then the original one but not arbitrarily so and it doesn't get worse as I move far away.**

**You always have a supersolid with any wave-function with a short-range piece.**

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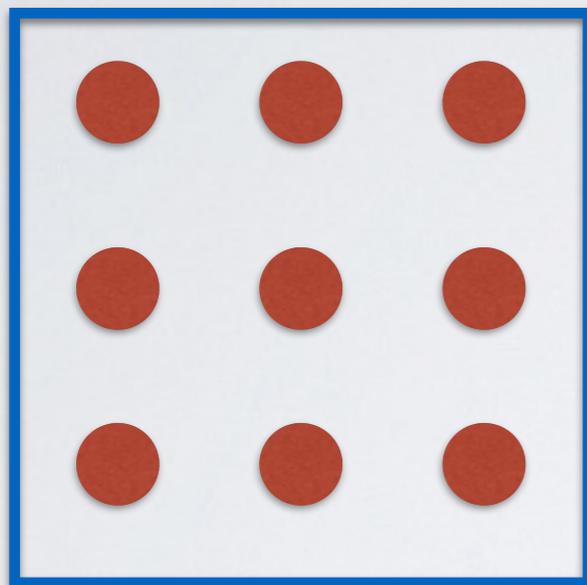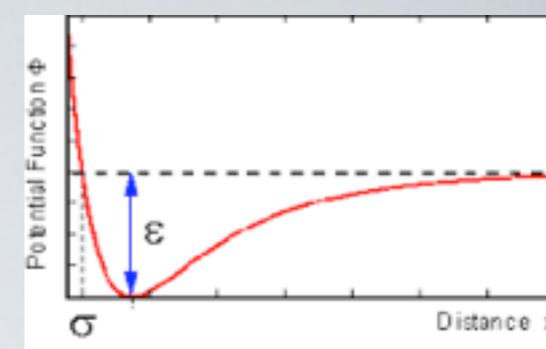
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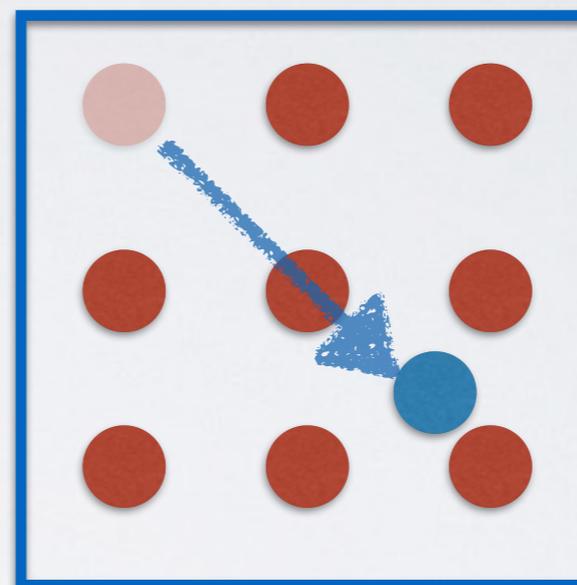
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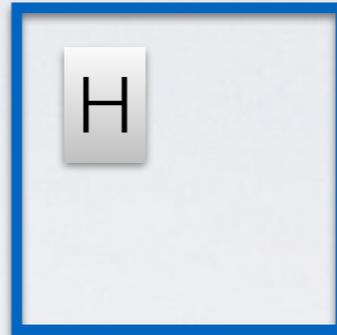
**What wave-function do I use for this system?**

H

$\Psi_A$

E

H

$\Psi_A$

E

**Wave-functions I'm allowed to use**
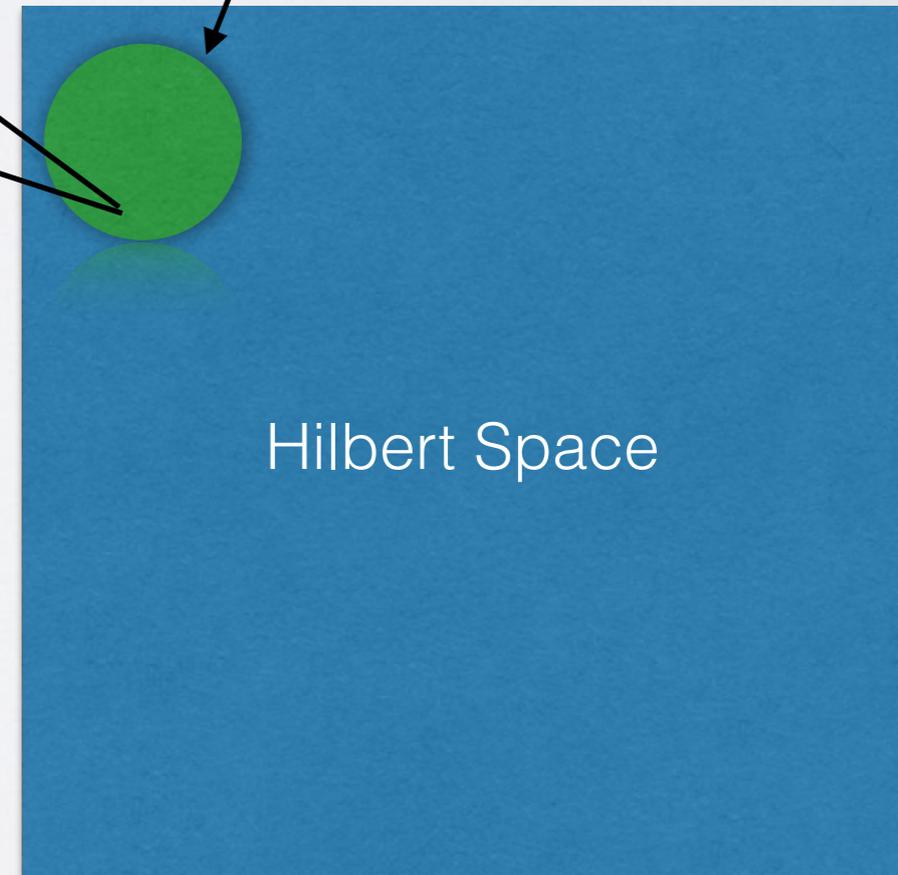
Hilbert Space

# Size extensivity

**What wave-function do I use for this system?** $\Psi_A \otimes \Psi_A$ | 2E

**But is this in my green circle?**

**If it is, then I'm size consistent. Otherwise, I am not.**

**Q:** **Is the set of wave-functions containing two-body potentials live in this class?**

H

H

$\Psi_A$

$\Psi_A$

E

E

**Wave-functions I'm allowed to use**
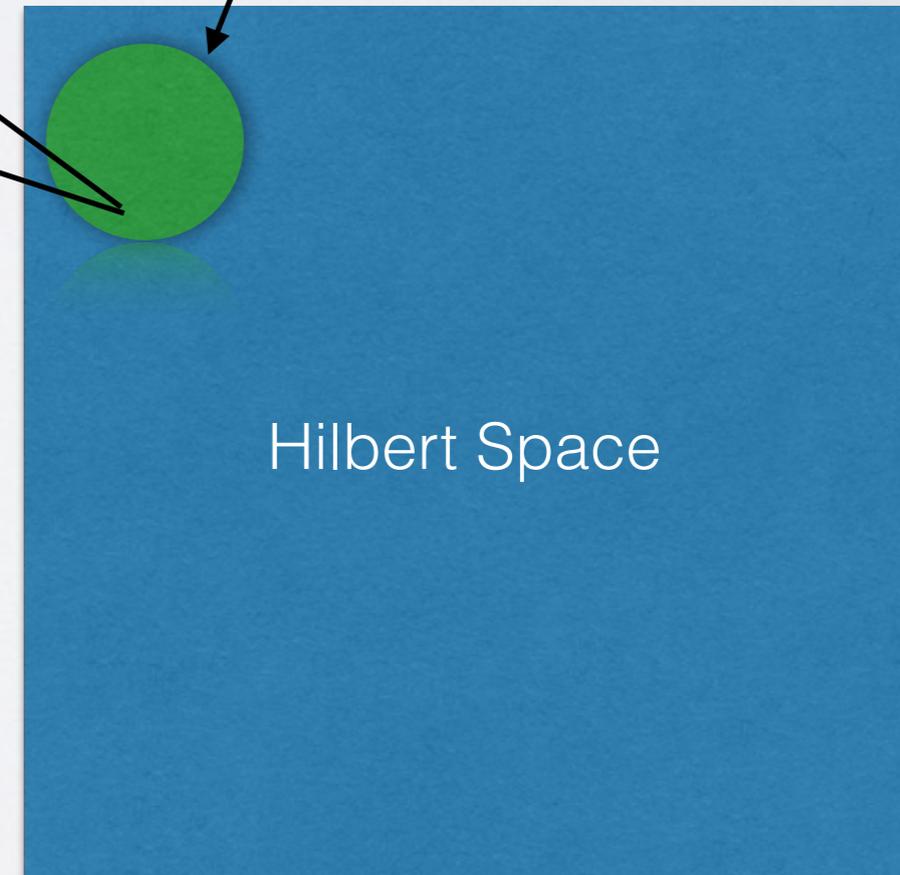
Hilbert Space

# Size extensivity



$\Psi_A$

H

E

$\Psi_A$

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E

**To answer this sort of question, let's consider charge fluctuation.**

**Q: Can I have the correct energy if a fixed number of bosons doesn't stay in each box?**

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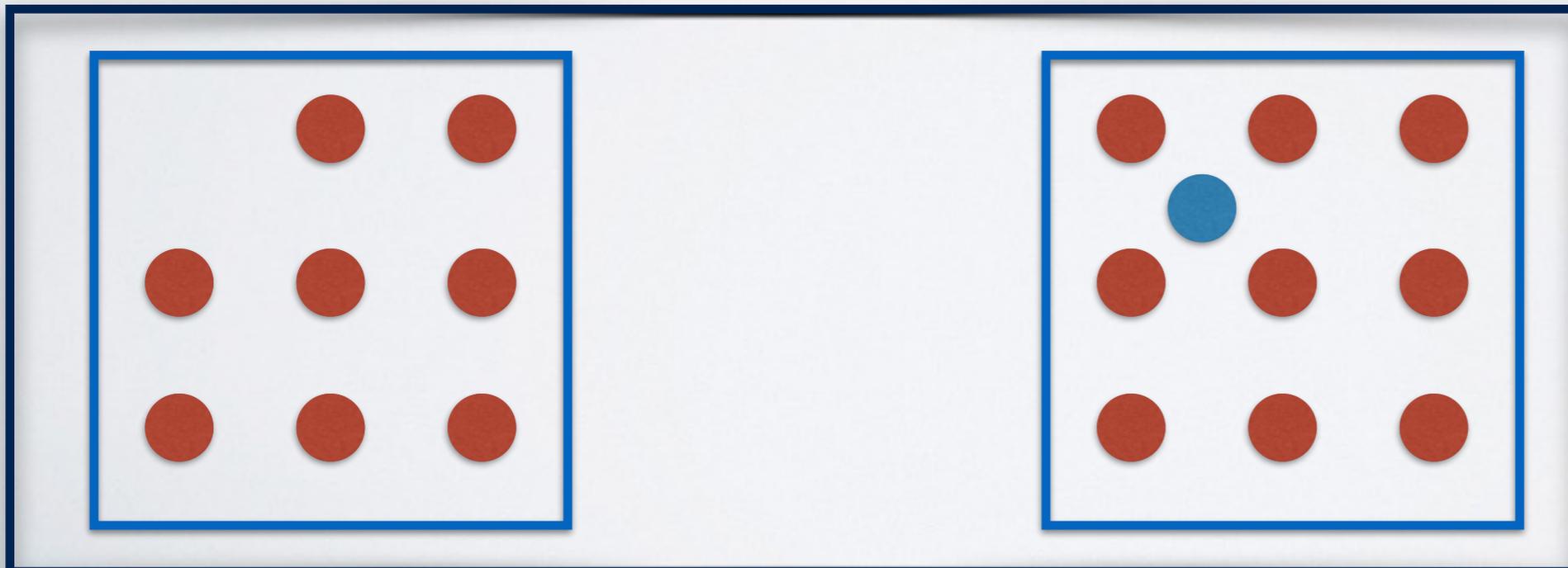
$$\Psi(R) \propto \exp\left[-\frac{\beta V(R)}{2}\right]$$

**This can be partially fixed by just forbidding double occupancy (*a bit of a hack*)**

# The upshot

By modeling a wave-function after the classical partition function, we can generate a wide set of "classical" phases via quantum wave functions: solids, liquids, etc. But such wave-functions get the "quantum mechanics" wrong.  In particular, we aways have

- superflow

- failure to be size extensive

These has all been with Bosons.    Let's start again with fermions.

# A more realistic view of (the fiction) of Hilbert Space

$\Psi_6 \quad \Psi_N$

**List of Codes**

for i=1:20  println("${i}") end

asdfdscwe;fkja;khvasdfefff

zxcvqqefposd;lknaccdsa

return exp[-beta * dot(r1,r2) ]

**?**
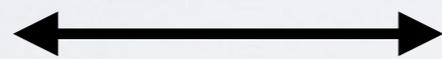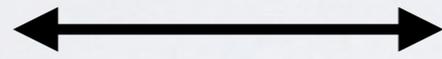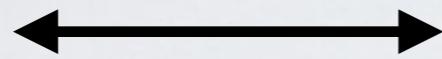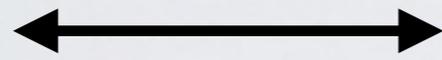
**List of Wavefunctions**

$\Psi_1$

$\Psi_2$

$\Psi_3$

$\Psi_4$

$\Psi_5$

$\vdots$

$\Psi_N$

**Wave-functions for which you can build an inefficient code.**

*(also, wave-functions you can write a PRL about)*

**Wave-functions for which you can build an efficient code.**

Hilbert Space
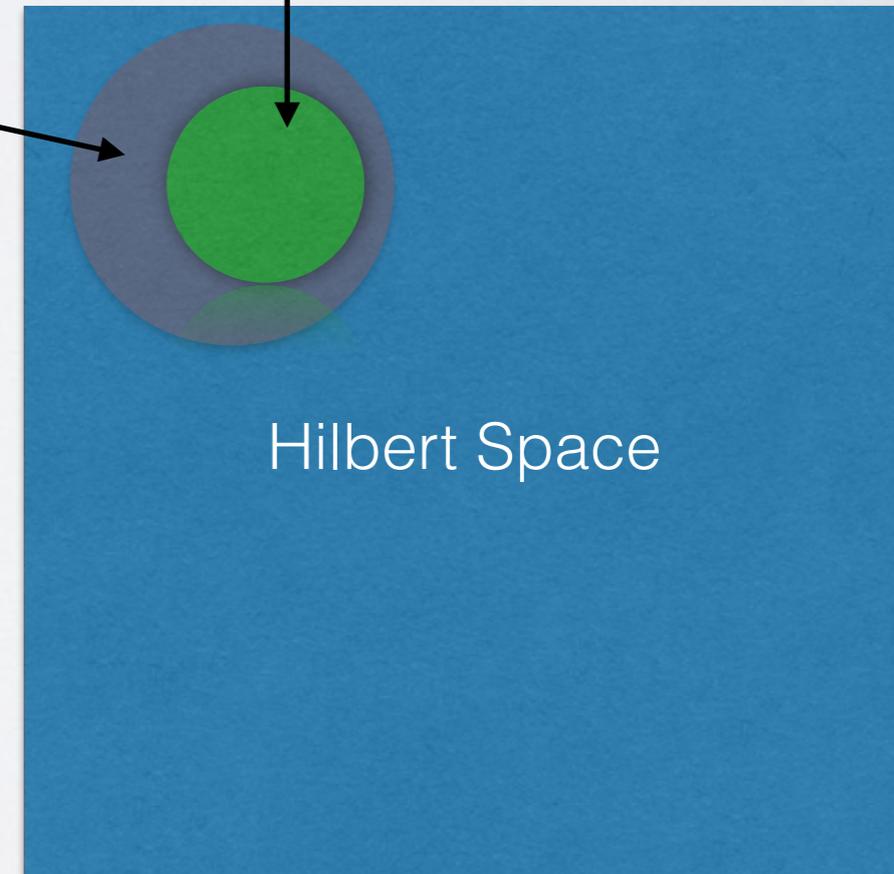
# Fermions

**Q:** What is the difference between bosons and fermions?

Bosons commute with the symmetry operator S

Fermions commute with the anti-symmetrization operator A

$$H = -t \sum_{ij\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}$$

**free fermions**

We can solve this exactly. The ground state of this Hamiltonian is a product of Slater Determinants (one for spin up and one for spin down)

$$\Psi(R) = \det M_{\uparrow}[R] \det M_{\downarrow}[R]$$
$$M_{ij}[R] = \phi_i(r_j)$$

3-dimensional function

Good starting point (aside: why didn't we do use this as our starting point for fermions?)

Aside:  Why not start with free bosons

$$H = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma}$$

**free bosons**

$$\Psi(R) = \text{per } M_\uparrow[R]\text{per } M_\downarrow[R]$$   **x Not efficient**

$$M_{ij}[R] = \phi_i(r_j)$$

3-dimensional function

# Back to fermions: Interactions

$$H = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

We need a set of wave-functions for these Hamiltonians.
Let's start by using the set of all slater-determinants.

$$\Psi(R) = \det M_\uparrow[R] \det M_\downarrow[R]$$
$$M_{ij}[R] = \phi_i(r_j)$$

<span style="color:red">3-dimensional function</span>

**(This is Hartree Fock)**

**Q:** Am I size-consistent?

# Size consistency for Slater-Determinants

**System A**
**Energy: Ea**

**System B**
**Energy: Eb**

**System A and B together**

**Energy: Ea + Eb**
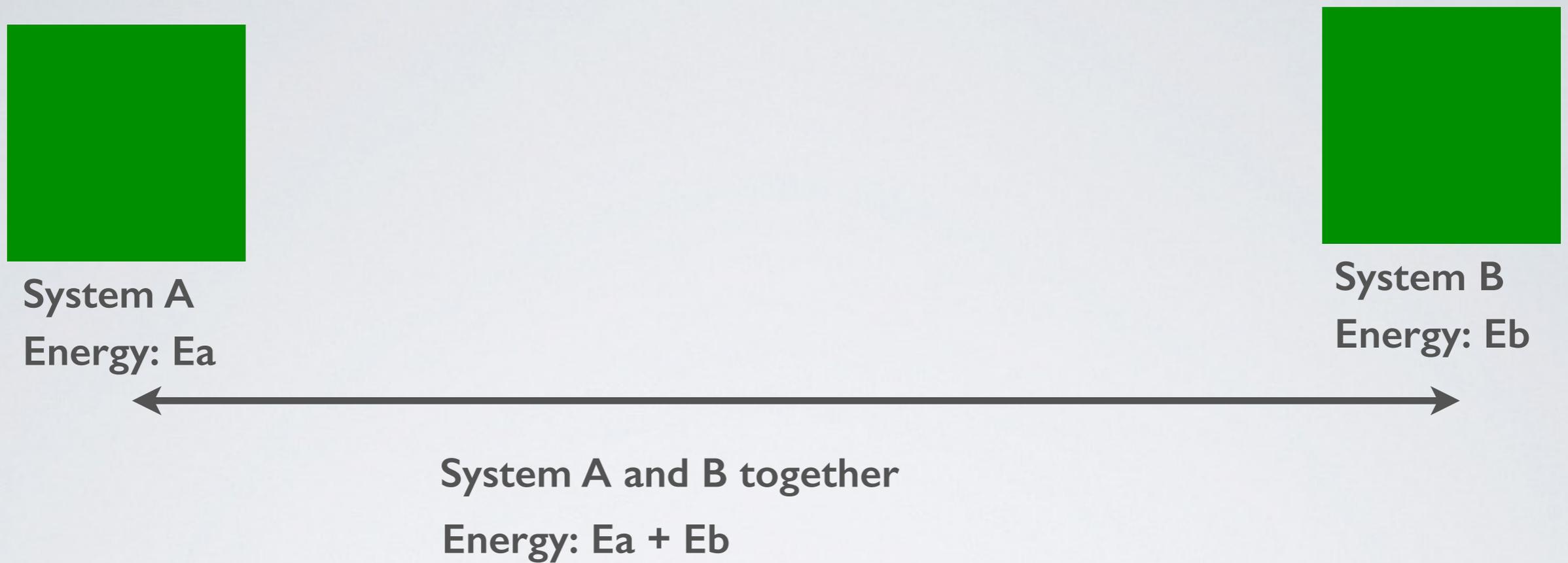
**Single slater determinant is size-consistent**

single particle orbitals for A
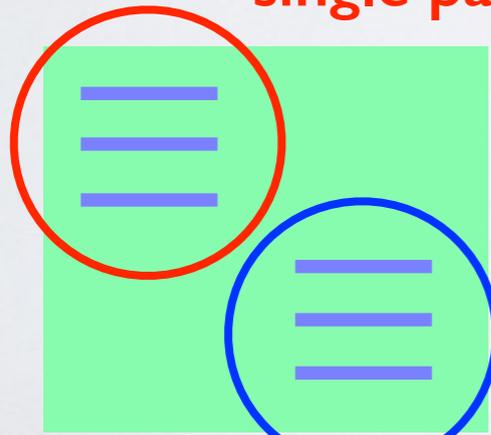
single particle orbitals for B

# Beyond Hartree Fock

- Quantum Chemistry:

   **Multi-determinants**

   **Coupled Cluster**

- Slater-Jastrow++

- Tensor Networks

# Beyond Hartree Fock

- Quantum Chemistry:

  **Multi-determinants**

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# The right physics... beyond free-fermions:

$$H = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

**Q:** **What's missing from** $\quad \Psi(R) = \det M_\uparrow[R] \det M_\downarrow[R]$

**A:** **Correlation: Need to keep electrons apart!**

$$\Psi(R) = \det M[R] \exp[-u(|r_i - r_j|)]$$

keep electrons apart

Further beyond free-fermions:

$$\Psi(R) = \det M[R] \exp[-U(R)]$$

$$\Psi(R) = \det M[R] \exp\left[-\sum_{i,j} u_2(r_i, r_j) - \sum_{i,j,k} u_3(r_i, r_j, r_k) + ...\right]$$

arbitrary (bosonic) correlation

We can write a wave-function as
  (fermion piece) * (boson piece)

At interparticle coalescence points, potential diverges:

Electron-nucleus $\quad -\dfrac{Z}{r_{i\alpha}}$

Electron-electron $\quad \dfrac{1}{r_{ij}}$

Local energy $\quad \boxed{\dfrac{\mathcal{H}\Psi}{\Psi} = -\dfrac{1}{2}\sum_i \dfrac{\nabla_i^2 \Psi}{\Psi} + V}$ must be <u>finite</u>

$\Rightarrow$ Kinetic energy must have opposite divergence

$\Rightarrow$ $\Psi$ must satisfy <u>Kato's cusp conditions</u>:

$$\boxed{\left.\dfrac{\partial\hat{\Psi}}{\partial r_{ij}}\right|_{r_{ij}=0} = \mu_{ij}q_i\,q_j\Psi(r_{ij}=0)}$$

for two particles of masses $m_i$, $m_j$ and charges $q_i$, $q_j$

Note: all other interparticle distances are $> 0$,

$\hat{\Psi}$ is a spherical average, and $\mu_{ij} = \dfrac{m_i\,m_j}{m_i + m_j}$

**Cusp conditions: example**

Consider $r_{ij} \to 0$ and all other particles well separated

The local energy close to $r = r_{ij} = 0$ is:

$$-\frac{1}{2\mu_{ij}} \frac{\nabla^2 \Psi}{\Psi} + V(r) = \text{finite}$$

Assume $\boxed{\Psi(r = r_{ij} = 0) \neq 0}$

$$-\frac{1}{2\mu_{ij}} \frac{\Psi''}{\Psi} - \frac{1}{\mu_{ij}} \frac{1}{r} \frac{\Psi'}{\Psi} + V(r) = \text{finite}$$

The condition for $E_L$ to be finite at $r = 0$ is

$$\frac{\Psi'}{\Psi} = \mu_{ij} \, r \, V(r)$$

- Electron-nucleus: $V = -\dfrac{Z}{r}, \mu = 1 \Rightarrow \boxed{\left.\dfrac{\Psi'}{\Psi}\right|_{r=0} = -Z}$

- Electron-electron: $V = \dfrac{1}{r}, \quad \mu = \tfrac{1}{2} \Rightarrow \boxed{\left.\dfrac{\Psi'}{\Psi}\right|_{r=0} = 1/2}$