# Numerical Approaches

## to some many-body problems

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# Outline

- **Motivation**: many-body problems in condensed matter physics
- **Spin models for the cuprates**: variational wavefunction Monte Carlo
- **Time-evolution of Bose-Einstein condensates**: numerical integrations for interacting systems
- **Non-equilibrium quantum phenomena**: exact solutions in 1d

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| | |
|---|---|
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| • **1D bosons:** | **Gil Refael (CalTech)** |
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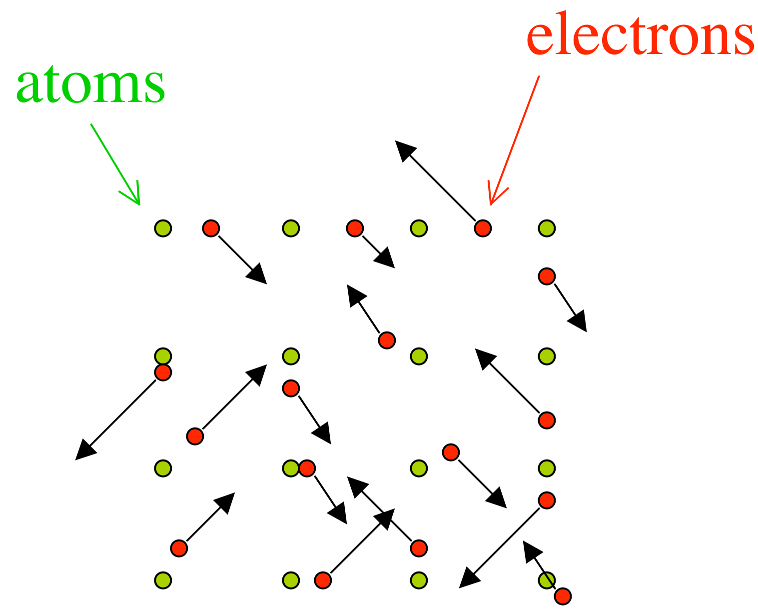
# The problem with condensed matter...

- known interactions:




$$V_{ion-e} = -\sum_{ion,e} \frac{Ze^2}{|\vec{r}_{ion} - \vec{r}_e|}$$

$$V_{e-e} = \sum_{<i,j>} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

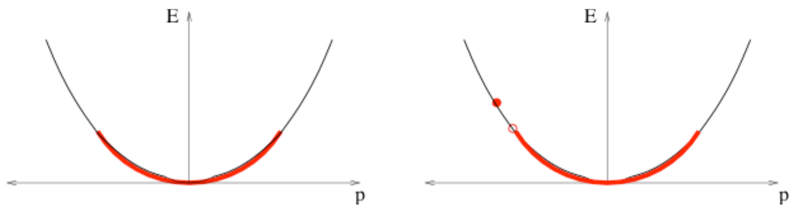
$\Rightarrow$ cannot be used to predict the phenomena for macroscopic systems!

# The problem with condensed matter...

## ⟹ low-energy effective models:

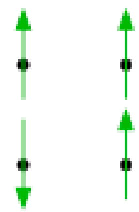
- **metals**: Fermi liquid theory

$$\hat{H} = \sum_k \epsilon_k c_k^\dagger c_k$$



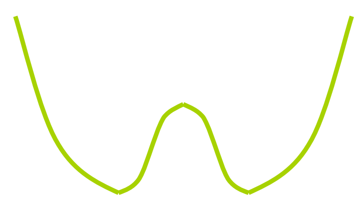

- **magnets**: spin models

$$\hat{H} = \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$



- **superfluids/superconductors**: order parameter models

$$\hat{H} = \int |\nabla\psi|^2 + r|\psi|^2 + u|\psi|^4$$



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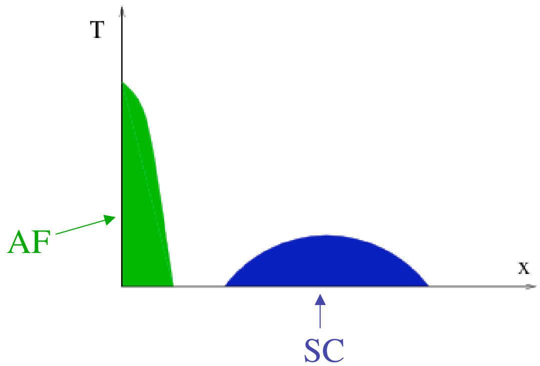
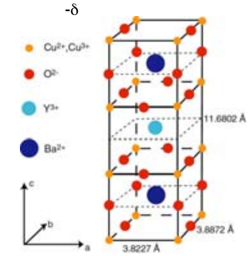
# The cuprate high $T_c$ superconductors



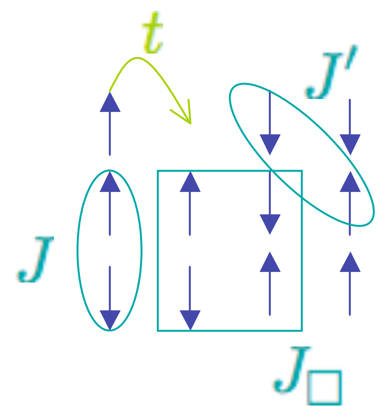

$YBa_2Cu_3O_{7-\delta}$



www.hut.fi/Units/AES/projects/prlaser/material.htm

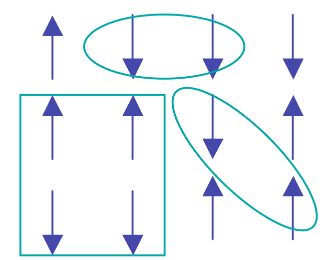
- **t-J model**

$$\hat{H} = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j + J' \sum_{<i',j'>} \vec{S}_{i'} \cdot \vec{S}_{j'} + J_{\square} \sum_{\square} P + P^{-1} + t \sum_{<i,j>} c_i^\dagger c_j + c_j^\dagger c_i$$




- **half-filling: Heisenberg models**

$$\hat{H} = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j + J' \sum_{<i',j'>} \vec{S}_{i'} \cdot \vec{S}_{j'} + J_{\square} \sum_{\square} P + P^{-1}$$



# Variational Wavefunction Monte Carlo

- Variational ground state:

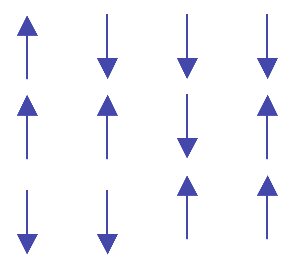
$$\langle \psi_{trial} | \hat{H} | \psi_{trial} \rangle \geq E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle$$

- **Problem**: calculating expectation values

$$|\psi_{trial}\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle \quad \text{with} \quad c_{\alpha} = \langle \alpha | \psi_{trial} \rangle$$

$\Rightarrow$ we would like to work with configurational states, $\{|\alpha\rangle\}$

$$|\alpha_1\rangle \; =$$



# Variational Wavefunction Monte Carlo

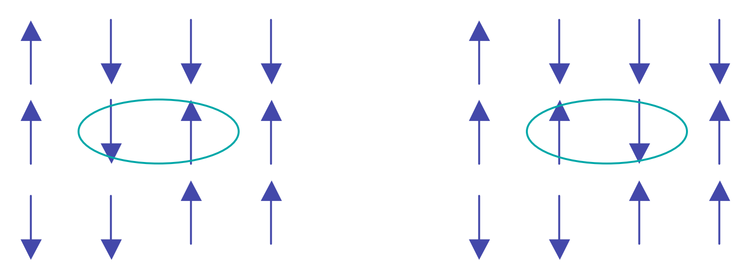
- (approximate) **Solution**: importance sampling

$$\langle \psi_{trial} | \hat{H} | \psi_{trial} \rangle = \sum_{\alpha} \overbrace{\langle \alpha | \hat{H} | \alpha \rangle}^{f(\alpha)} \overbrace{|c_\alpha|^2}^{\rho(\alpha)}$$

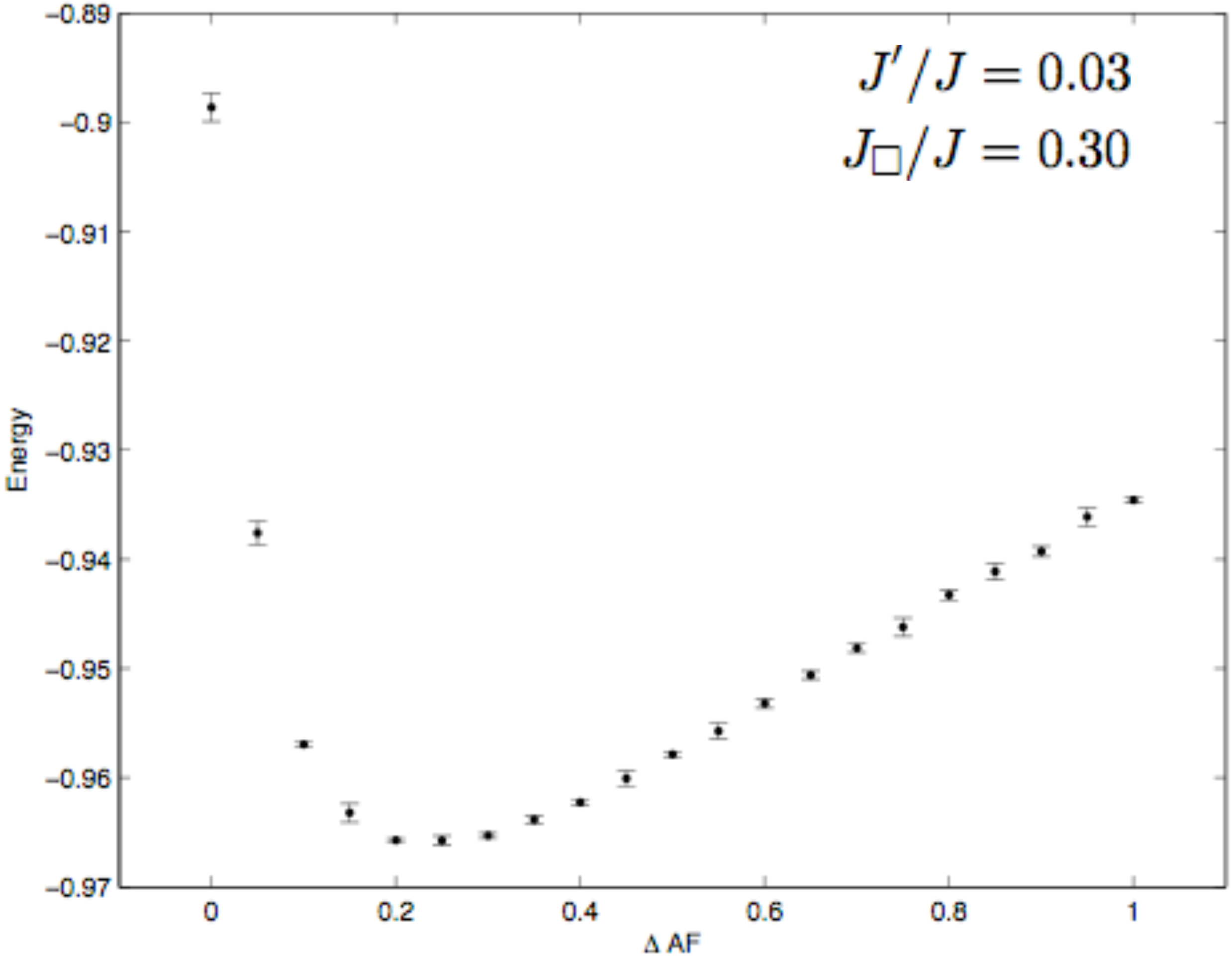
$$= \sum_{\alpha} f(\alpha) \rho(\alpha)$$

$$\approx \sum_{MC} f(\alpha_{MC})$$

with $\mathcal{P}_{\alpha \to \alpha'} = \dfrac{\rho(\alpha')}{\rho(\alpha)}$

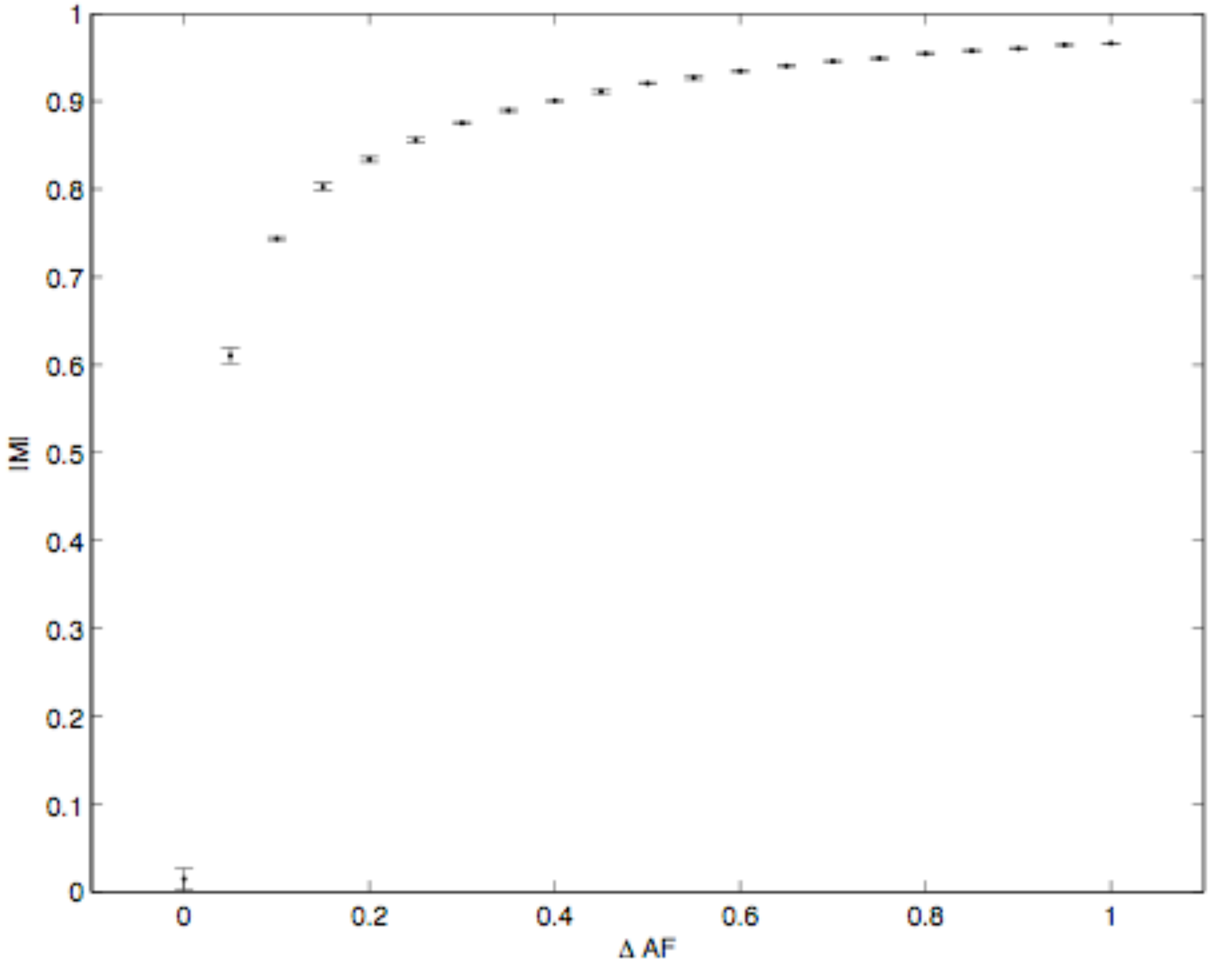


# Results: best AF wavefunction




XinXin Du '06, Senior Honors Thesis, WC

# Results: best AF wavefunction




XinXin Du ‘06, ibid.

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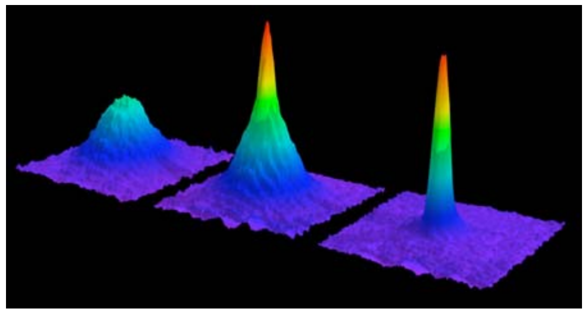
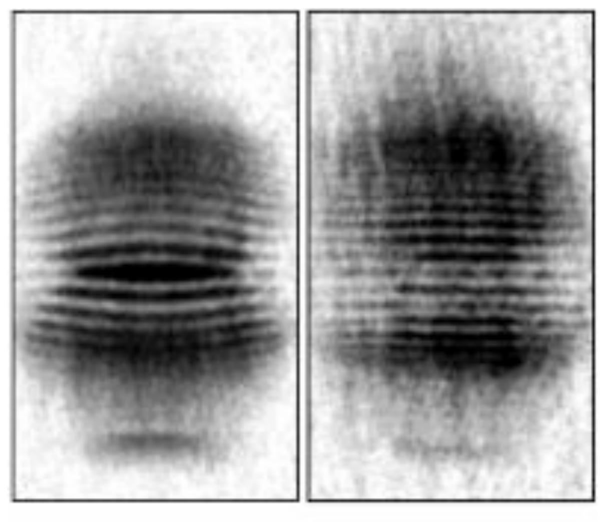
# Bose-Einstein Condensation

- dilute gas in harmonic trap
- *T*~ nK



Ketterle et al. '95

- Condensate wavefunction, $\psi$
- Release from trap and expansion, $\psi(\vec{r}, t)$
- Interferrence experiment:



Ketterle et al. '97

# Bose-Einstein Condensation

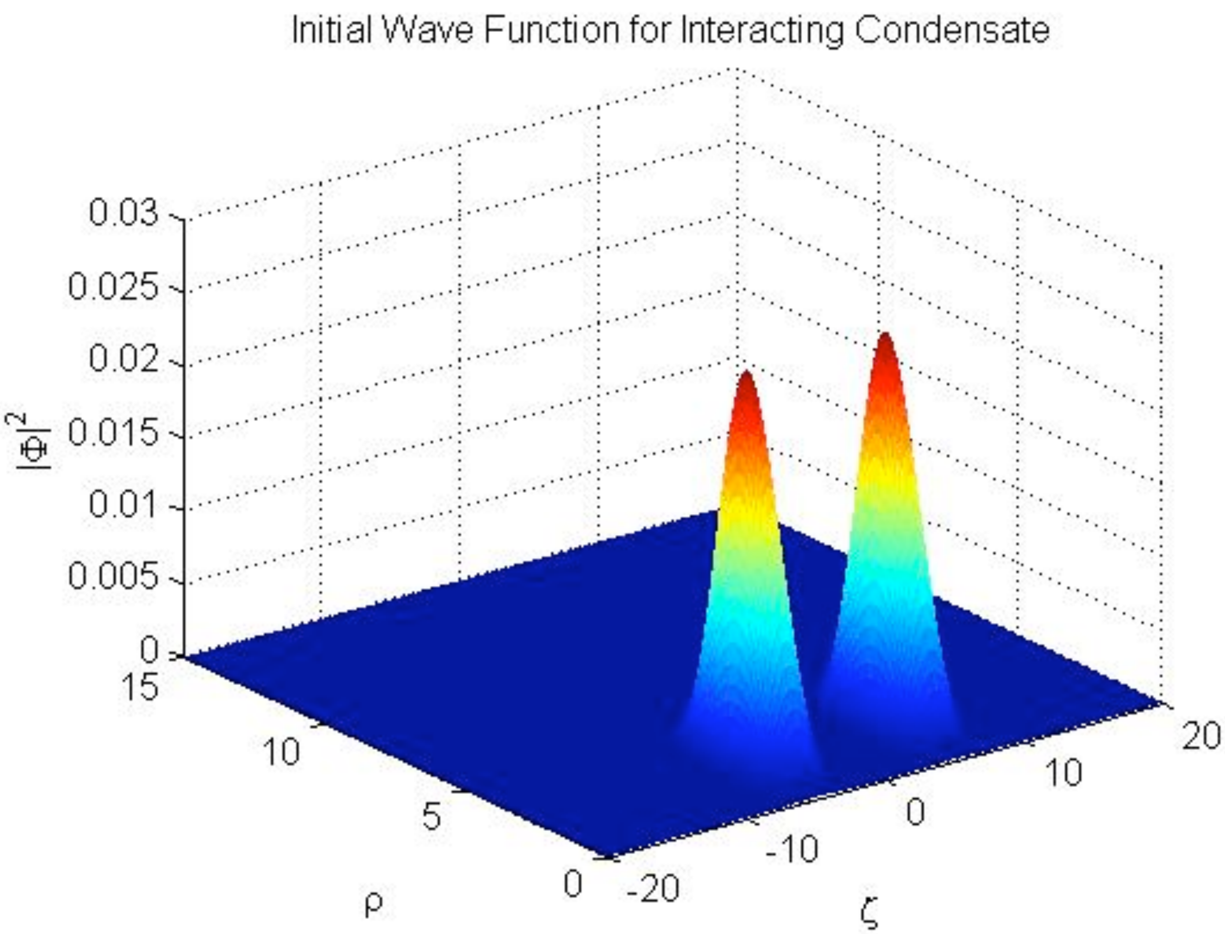
- Interacting BEC: Gross-Pitaevskii equation

$$i\frac{d\psi}{dt} = -\frac{1}{2m}\nabla^2\psi + V(\vec{r})\psi + g|\psi|^2\psi$$

- Two issues:
  1. Initial (ground state) with interactions
  2. Time evolution (expansion) with interactions

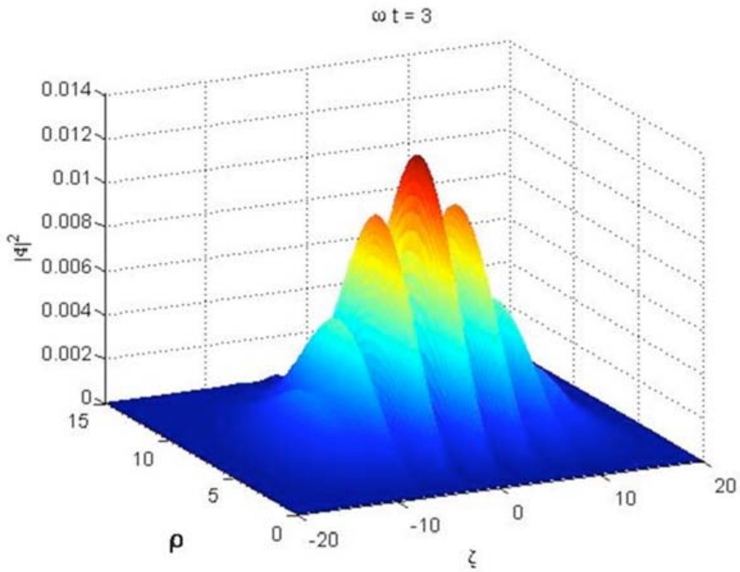
⇒ Recent work: Chiofalo et al. 2000
Cerimele et al. 2000

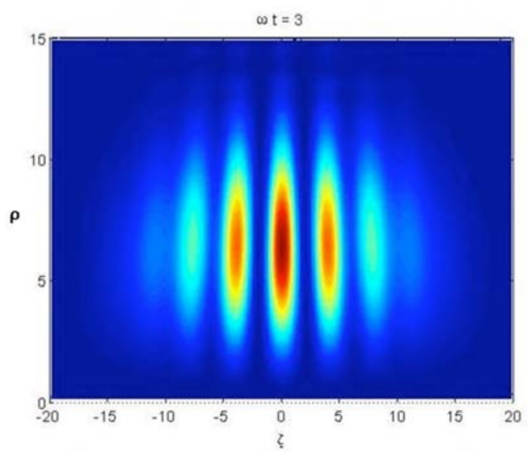
# Results: ground state for 2 BECs

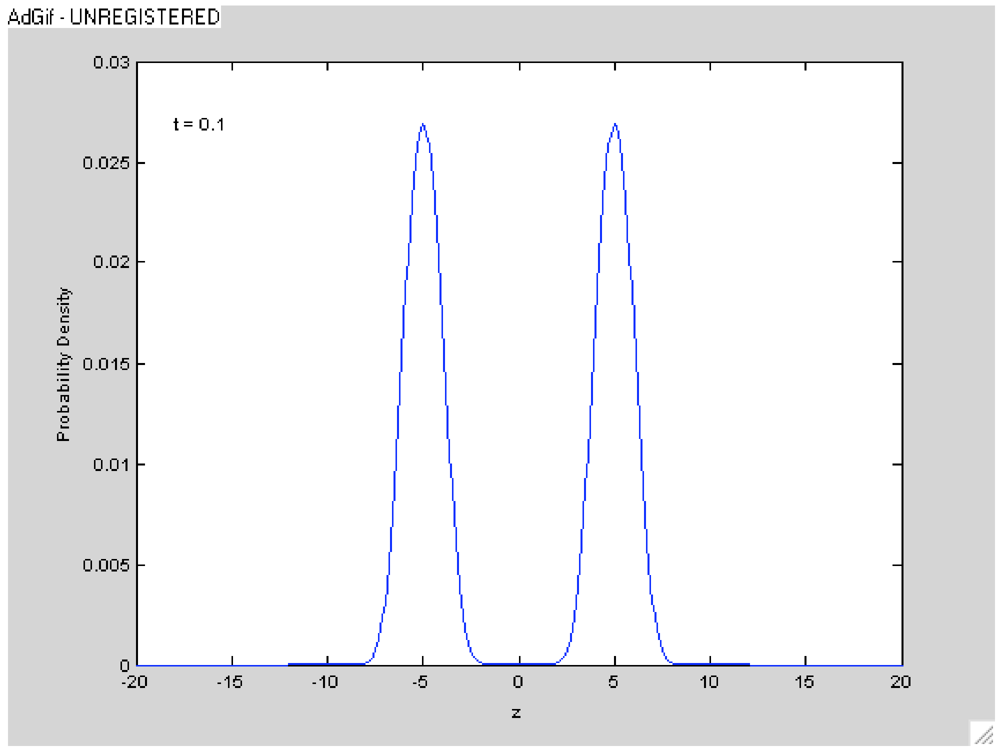



Merideth Frey '07, Senior Honors Thesis, WC

# Results: time evolution and interferrence

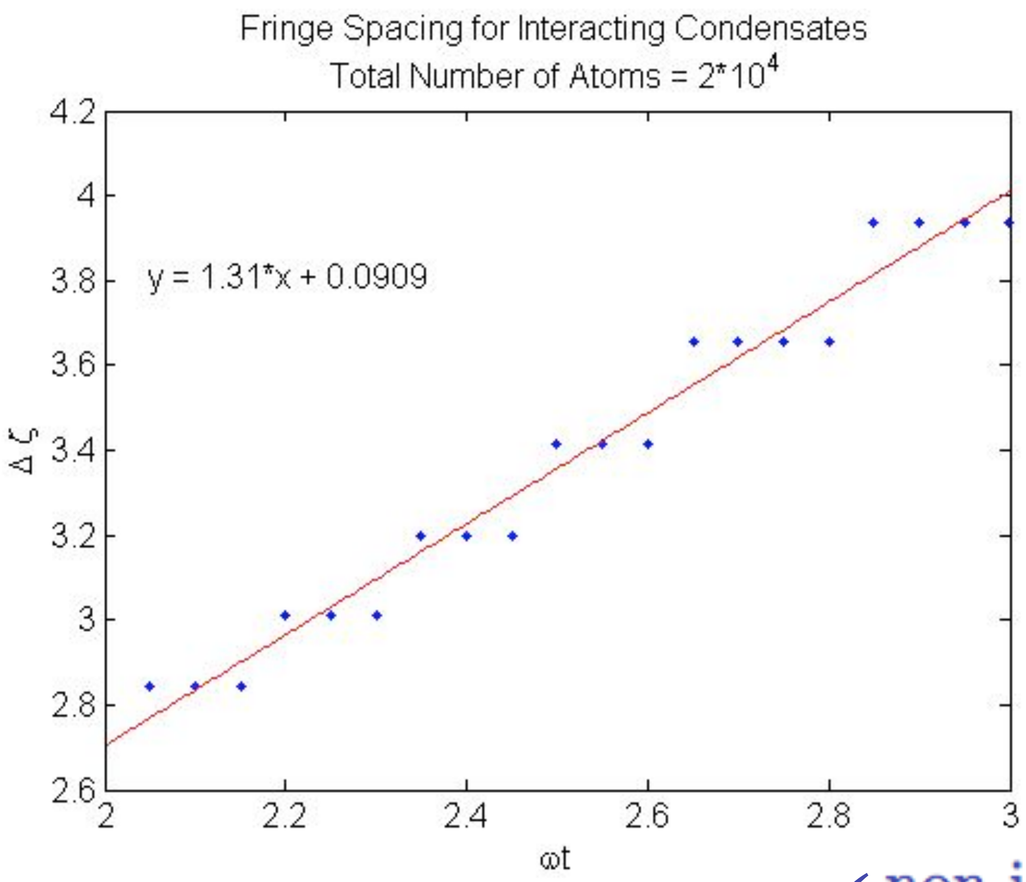



Merideth Frey ‘07, ibid

# Results: fringe spacing




Merideth Frey '07, ibid

(non-interacting wavefunction: $\Delta \propto t$)

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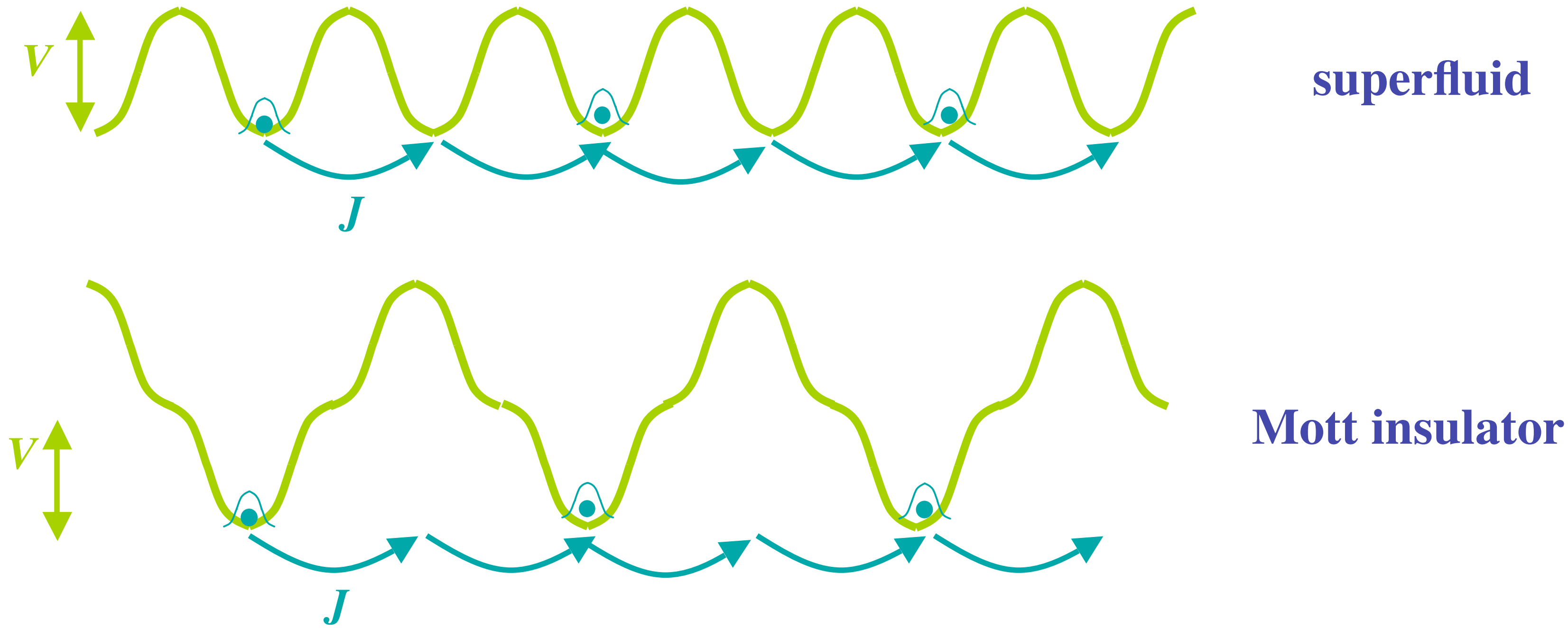
# 1d lattice bosons at half filling




- bosons in 1d, **tunable**, lattice potential
- bosons in **hardcore** limit

(makes system exactly solvable -- corresponds to T-G gas)

# time-evolution after quick change

- initial state: ground state of

$$H_0 = -J \sum_{<i,j>} \left( b_i^\dagger b_j + h.c. \right)$$

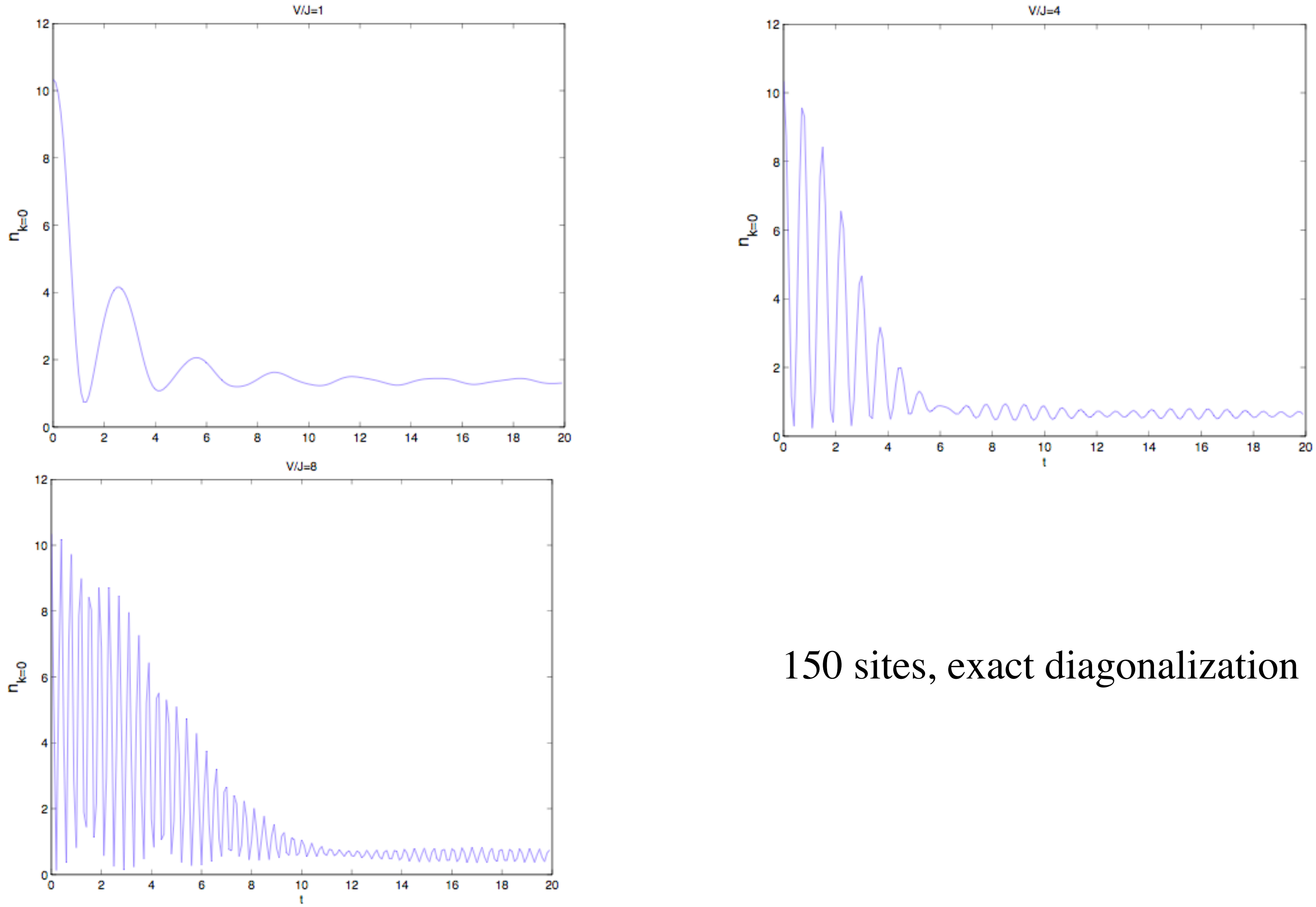
- time evolution after superlattice applied

$$H_1 = -J \sum_{<i,j>} \left( b_i^\dagger b_j + h.c. \right) + V \sum_i (-1)^i b_i^\dagger b_i$$

- superfluid correlations: occupation of $k = 0$ state

$$< n_{k=0} >_t$$

# Results: for various *V/J*




150 sites, exact diagonalization

# Conclusions

- computational approaches to many-body problems in condensed matter physics are accessible to undergrads

→ **modeling cuprates**: variational wavefunction Monte Carlo on fermion wavefunctions

→ **time-evolution of Bose-Einstein condensates**: new numerical integrations for interacting systems

→ **Non-equilibrium quantum phenomena**: exact diagonalization of 1d systems