Variational study of impurity dynamics in 1D Bose lattice

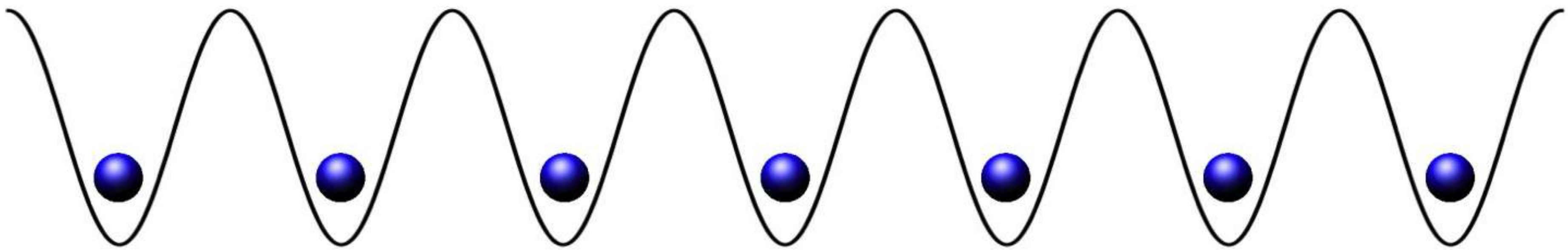
Shovan Dutta
09/18/2013

Ref: Shovan Dutta and Erich J. Mueller arXiv:1308.4876

Overview

- Bose-Hubbard model
- Experimental background
- Single impurity
  - Limiting behaviors
  - Variational wavefunction
  - Results
- Two impurities and bound states
- Summary & outlook

Bosons in optical lattice



- A good model: Bose-Hubbard Hamiltonian Jaksch et al PRL '98

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$

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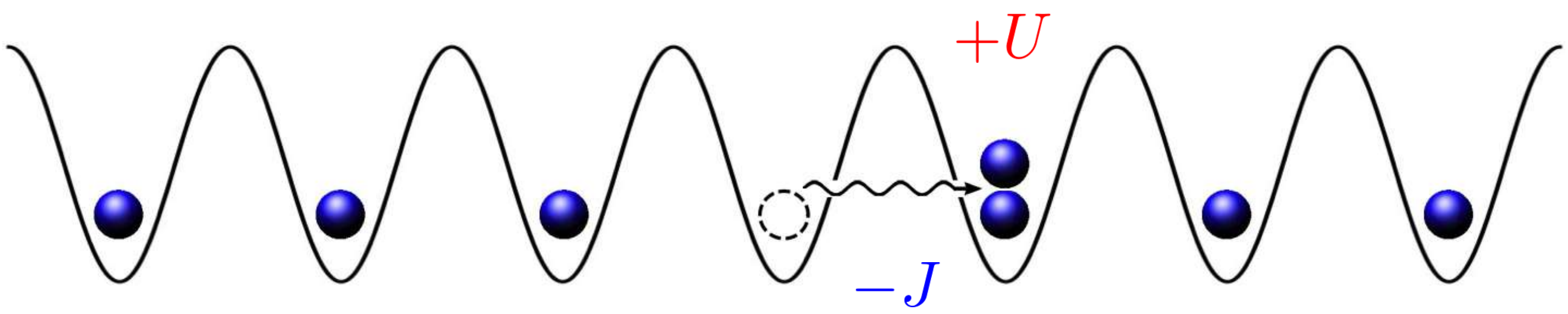

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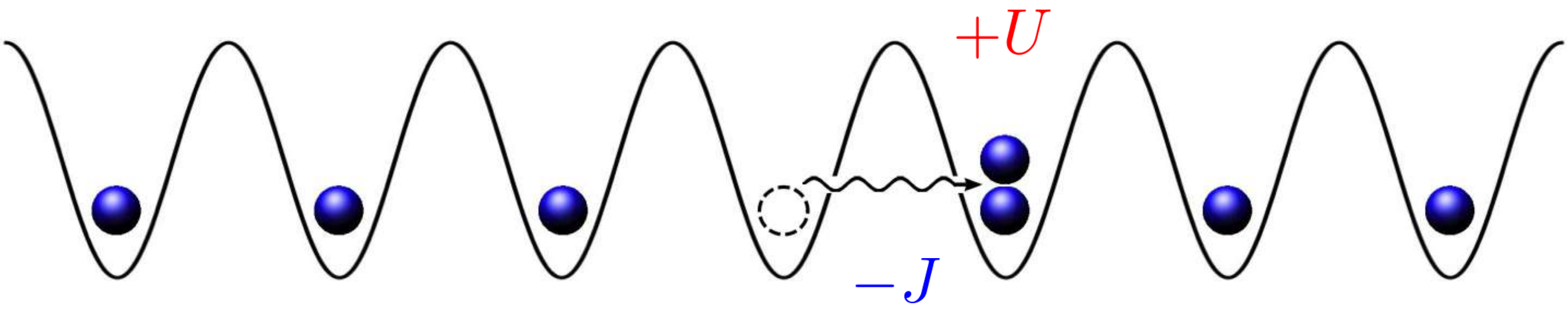

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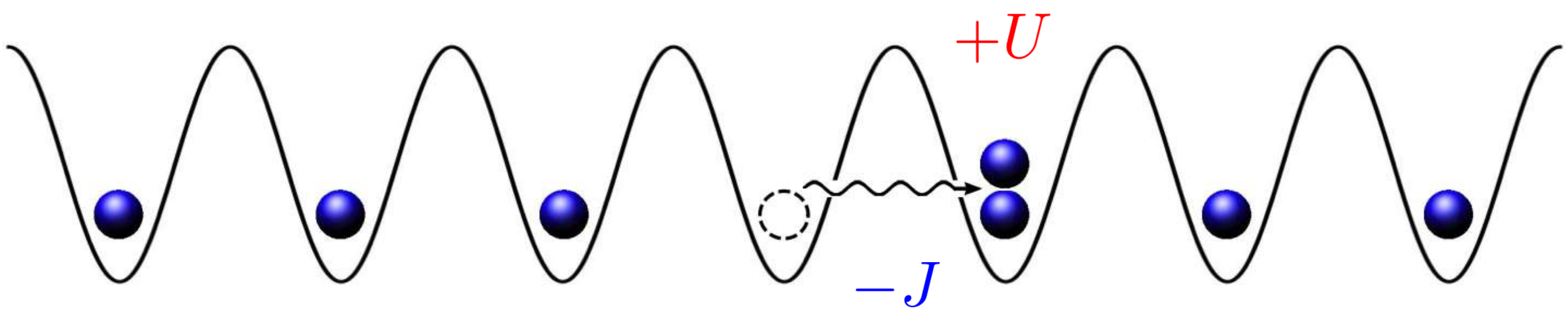

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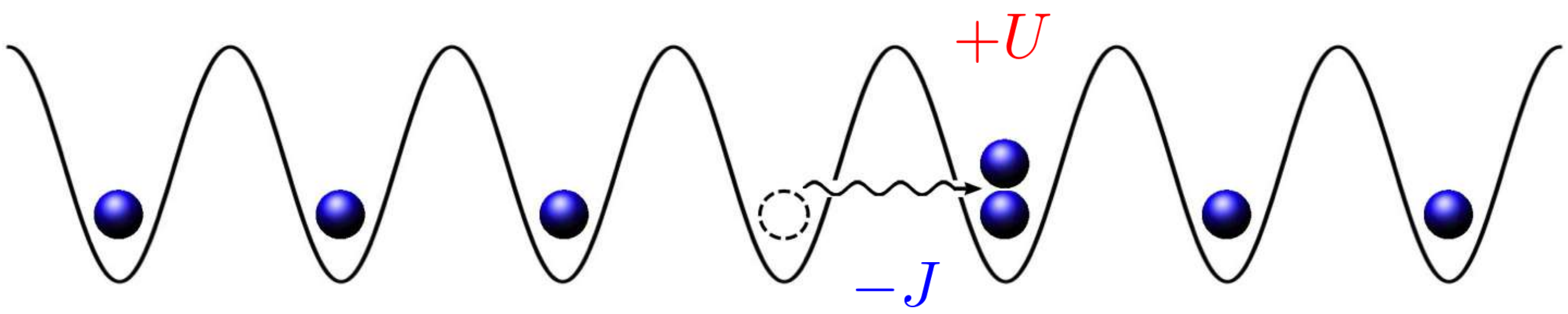

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- Condition: band gap $E_b \gg J,\ U,\ T.$ - satisfied in typical exp settings ($\lambda \sim 1\ \mu\mathrm{m},\ m \lesssim 100\ \mathrm{amu},\ T < 10^{-6}\ \mathrm{K}$).

Bosons in optical lattice

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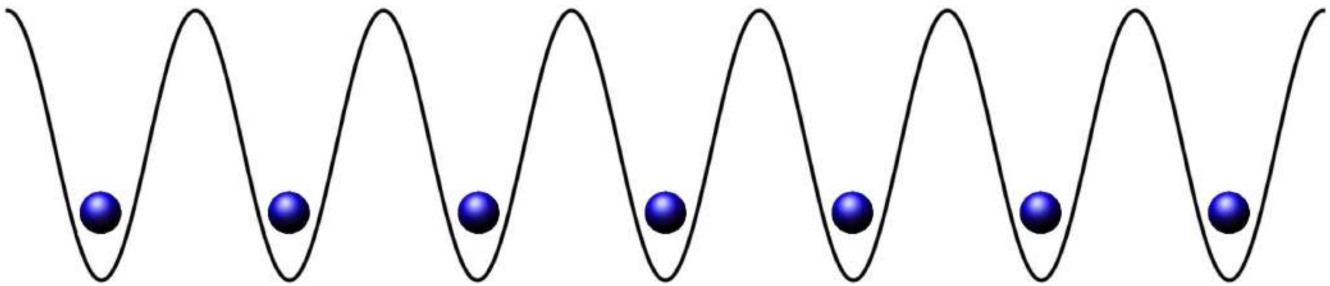
- $J/U \ll 1$: Mott Insulator



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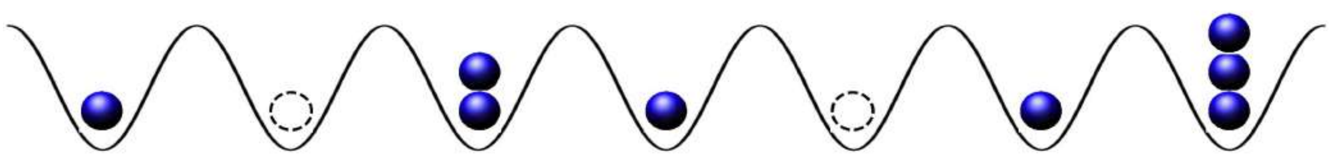

Bosons in optical lattice

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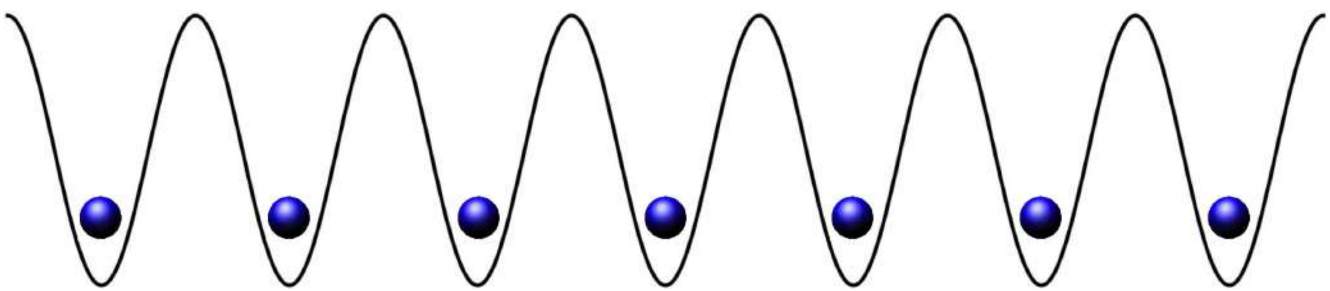

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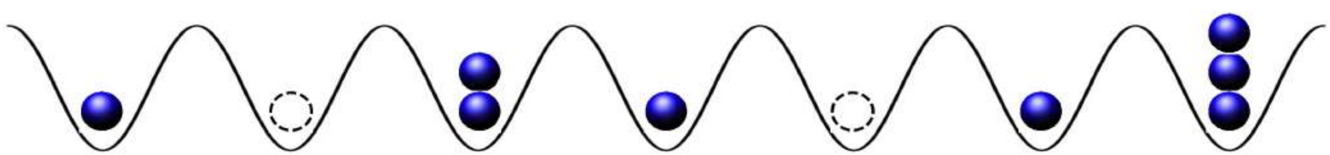

- Phase transition occurs at $J/U \approx 0.29$ (mean field theory gives 0.09).

Motivation

* Experiment by Bloch group on spin impurity: Nature Phys '13

$^{87}\mathrm{Rb}$

 $\equiv \uparrow \equiv |F=1, m_F=-1\rangle$

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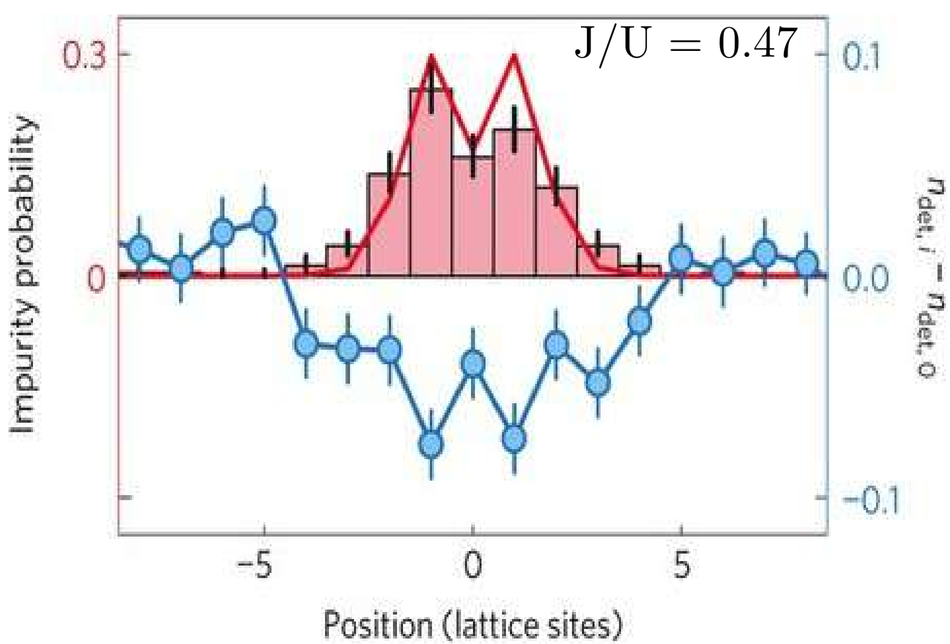
- Polaron-like dynamics



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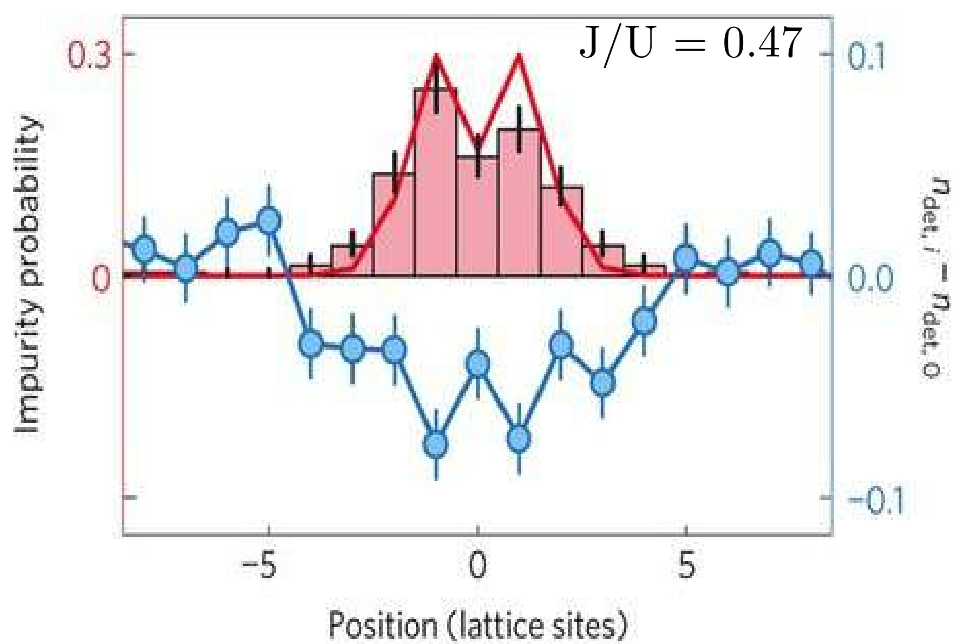
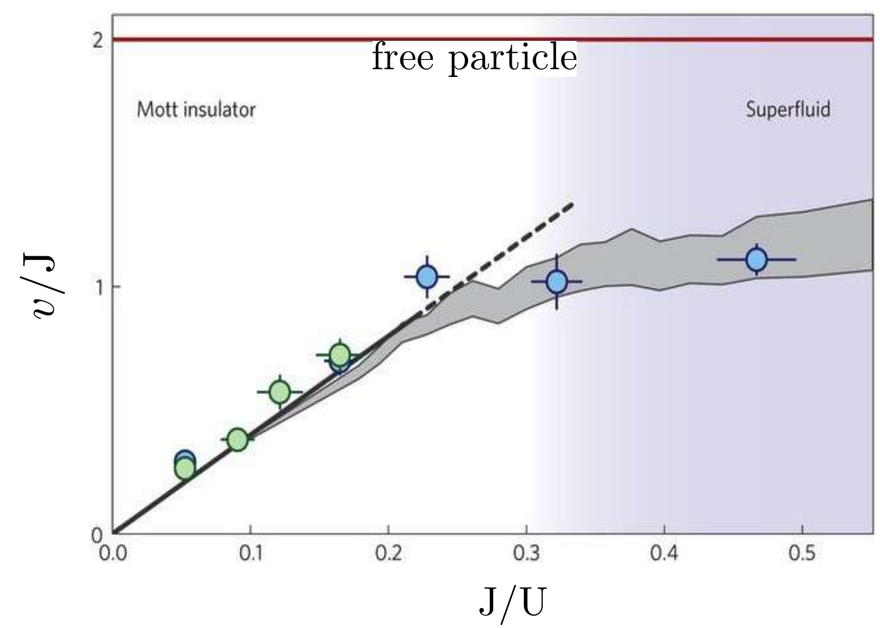
- Polaron-like dynamics & Renormalized impurity hopping





Model

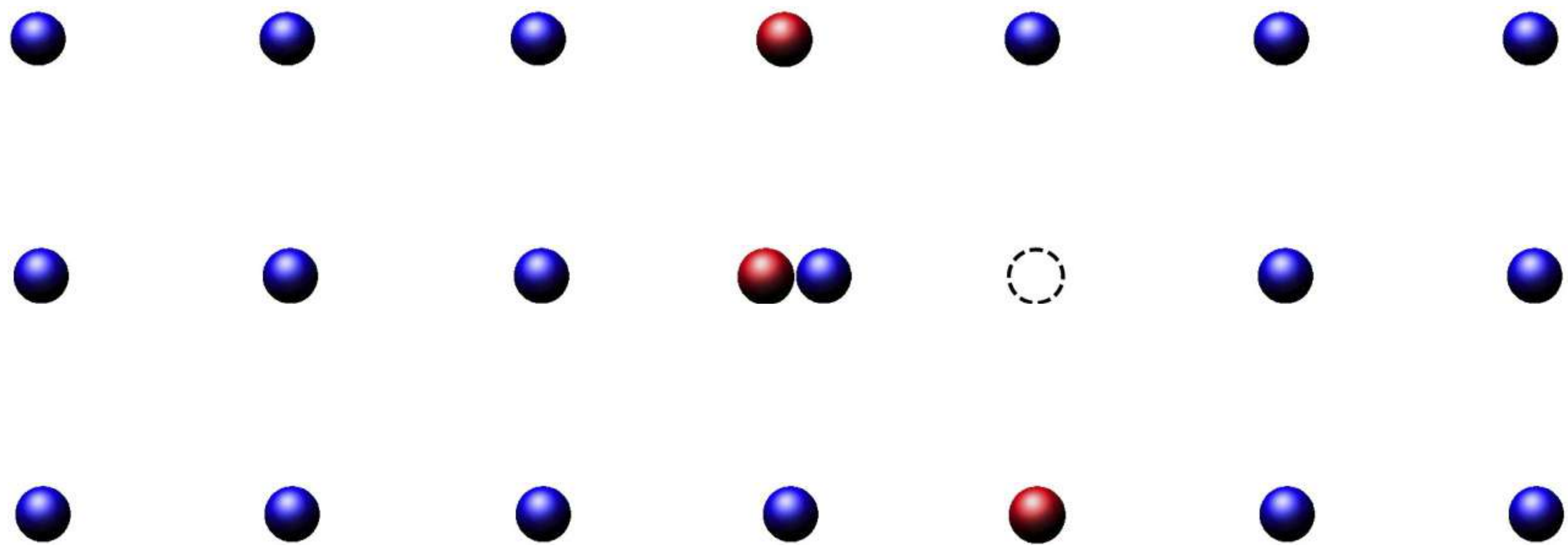
- Two-species Bose-Hubbard Hamiltonian:

$$\hat{H} = -J \sum_{\langle i,j \rangle, \sigma} \hat{b}^{\dagger}_{i,\sigma} \hat{b}_{j,\sigma} + \frac{U}{2} \sum_{i,\sigma,\sigma'} \hat{n}_{i,\sigma} \hat{n}_{i,\sigma'} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma}$$

- Interaction and tunneling spin-independent – a good approximation for $^{87}\mathrm{Rb}$.
- Lets see the limiting behaviors…

J<<U: Mott Insulator

- Impurity can spread by 2nd order tunneling:



Effective tunneling = J^2/U

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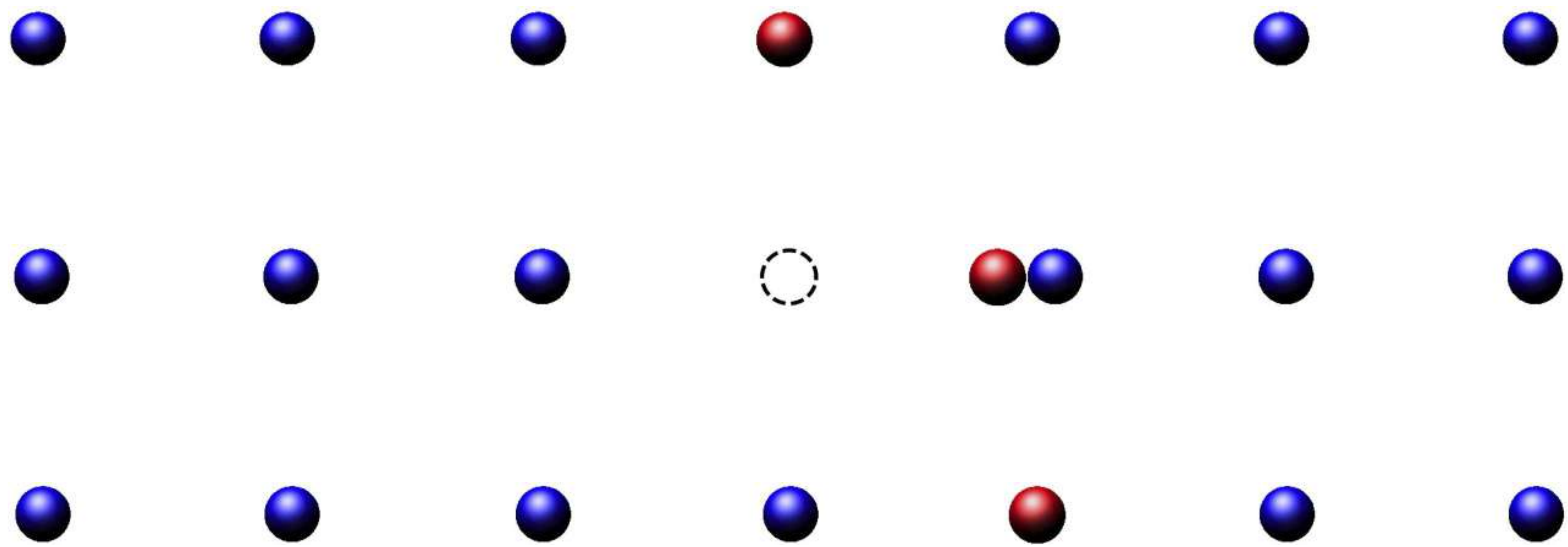

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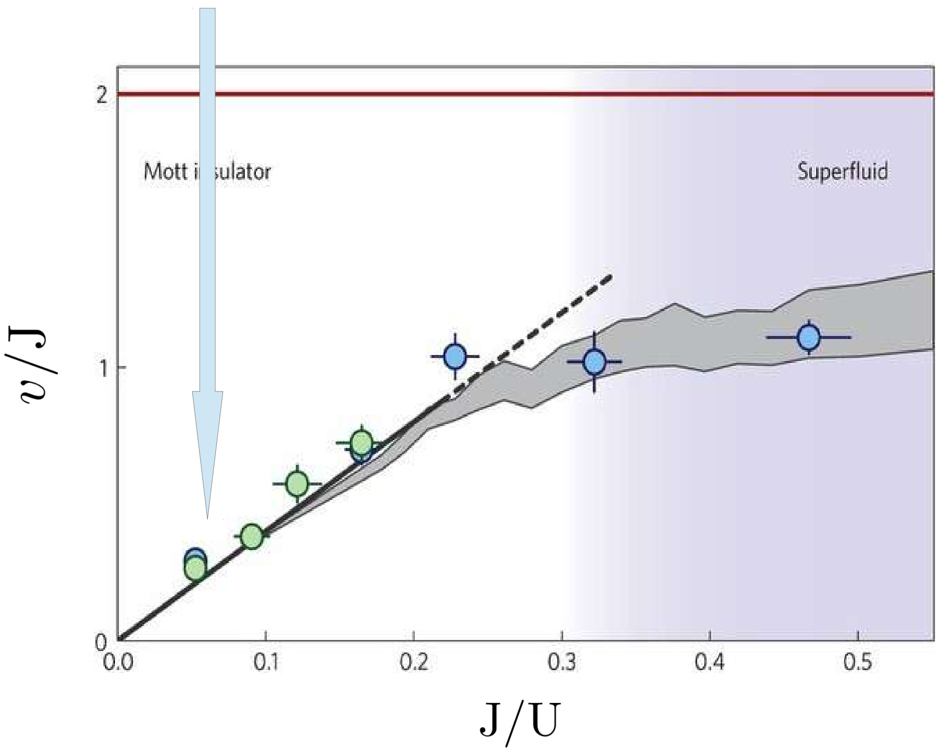


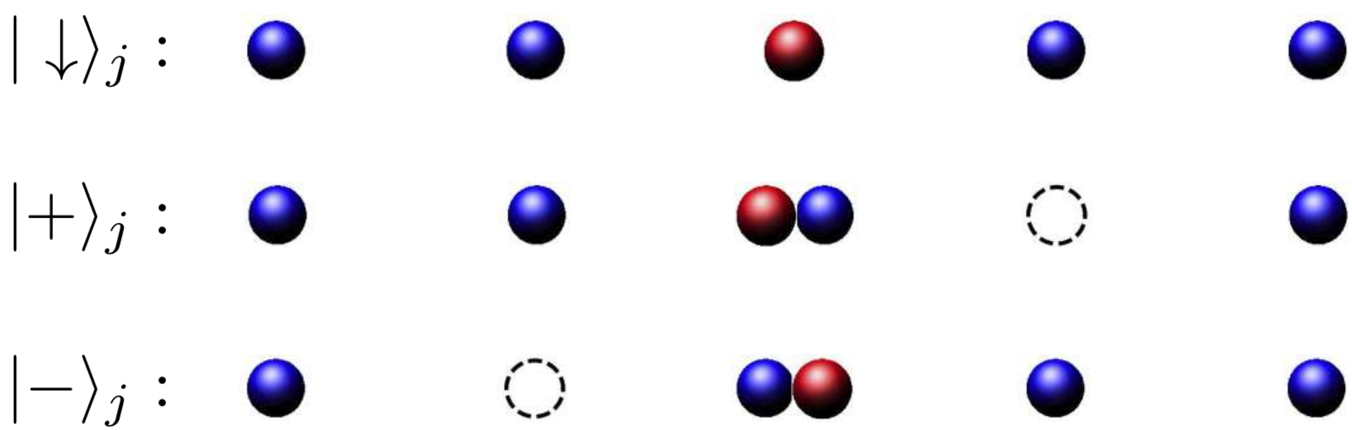
J<<U: Mott Insulator

- 2nd order perturbation theory gives

$$\varepsilon_{\mathrm{Mott}}(k) = \varepsilon_{\mathrm{Mott}}(0) + \frac{4J^2}{U}(1 - \cos k)$$

corresponding to

$$|k_{\mathrm{Mott}}\rangle = \sum_j e^{ikj}\left[|\downarrow\rangle_j \;+\; \frac{J}{U}\left\{(1+e^{ik})\,|+\rangle_j \;+\; (1+e^{-ik})\,|-\rangle_j\right\}\right]$$



U<<J: Deep Superfluid

- Bogoliubov approximation: take quadratic fluctuations about the ground state using $\hat{b}_{0,\uparrow/\downarrow} = \sqrt{N^{\uparrow/\downarrow}}$.
- Diagonalize via Bogoliubov transformation.

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- Diagonalize via Bogoliubov transformation.

$$\hat{H} = E_0 + \sum_{p \neq 0} (\varepsilon_c(p)\ \hat{c}_p^\dagger \hat{c}_p + \varepsilon_0(p)\ \hat{d}_p^\dagger \hat{d}_p)$$

$$\varepsilon_0(p) = 2J\ (1 - \cos p)$$

$$\varepsilon_c(p) = \sqrt{(\varepsilon_0(p))^2 + 2\ \varepsilon_0(p)\ U\ (n^\uparrow + n^\downarrow)}$$

$$\hat{b}_{p,\uparrow/\downarrow} = \sqrt{n^{\uparrow/\downarrow}}\ (u_p \hat{c}_p + v_p \hat{c}_{-p}^\dagger) \mp \sqrt{n^{\downarrow/\uparrow}}\ \hat{d}_p$$

$$u_p, v_p = \frac{1}{2}\left[\sqrt{\varepsilon_0(p)/\varepsilon_c(p)} \pm \sqrt{\varepsilon_c(p)/\varepsilon_0(p)}\right]$$

U<<J: Deep Superfluid

- When $n^{\downarrow} \to 0$ and $n^{\uparrow} \to 1$, $\langle \hat{b}^{\dagger}_{j,\uparrow} \hat{b}_{j,\uparrow} \hat{b}^{\dagger}_{0,\downarrow} \hat{b}_{0,\downarrow} \rangle = n^{\downarrow}\, n^{\uparrow}_{j}$.

$$\begin{array}{cccccccccccccccccc} & & -M & & & & -j & & -1 & 0 & 1 & & j & & & & M & \\ \cdots & \uparrow & \downarrow & \uparrow & \cdots & \cdots & \uparrow & \cdots & \uparrow & \downarrow & \uparrow & \cdots & \uparrow & \cdots & \cdots & \uparrow & \downarrow & \uparrow \cdots \end{array}$$

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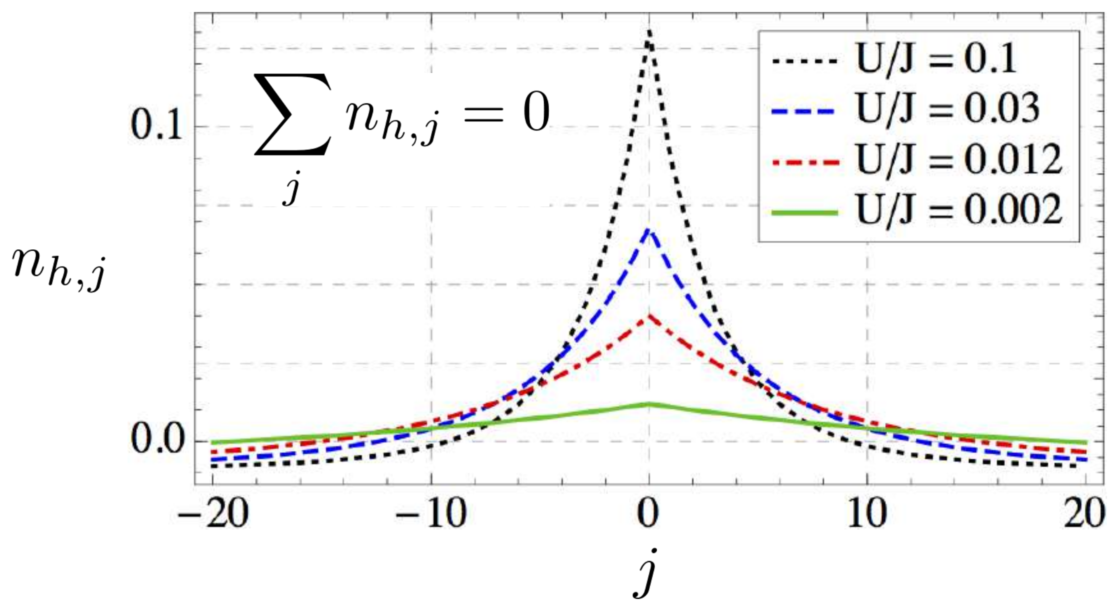
$$\Longrightarrow \; n_{h,j} \equiv 1 - n^{\uparrow}_{j} = \frac{1}{\mathcal{N}} \sum_{p \neq 0} \left(1 - \frac{1}{\sqrt{1 + \frac{U/J}{1 - \cos p}}} \right) \cos pj$$



Variational Wavefunction

☆

$$|j\rangle = \sum_i \left(f_i \, \hat{b}_{i+j,\uparrow} \hat{b}^\dagger_{j,\downarrow} |MF\rangle \right) + A \, \hat{b}^\dagger_{j,\downarrow} |MF\rangle$$

Variational parameters

$$|MF\rangle = \prod_l \sum_n \beta_n |n\rangle_l$$ (Gutzwiller mean-field ground state)

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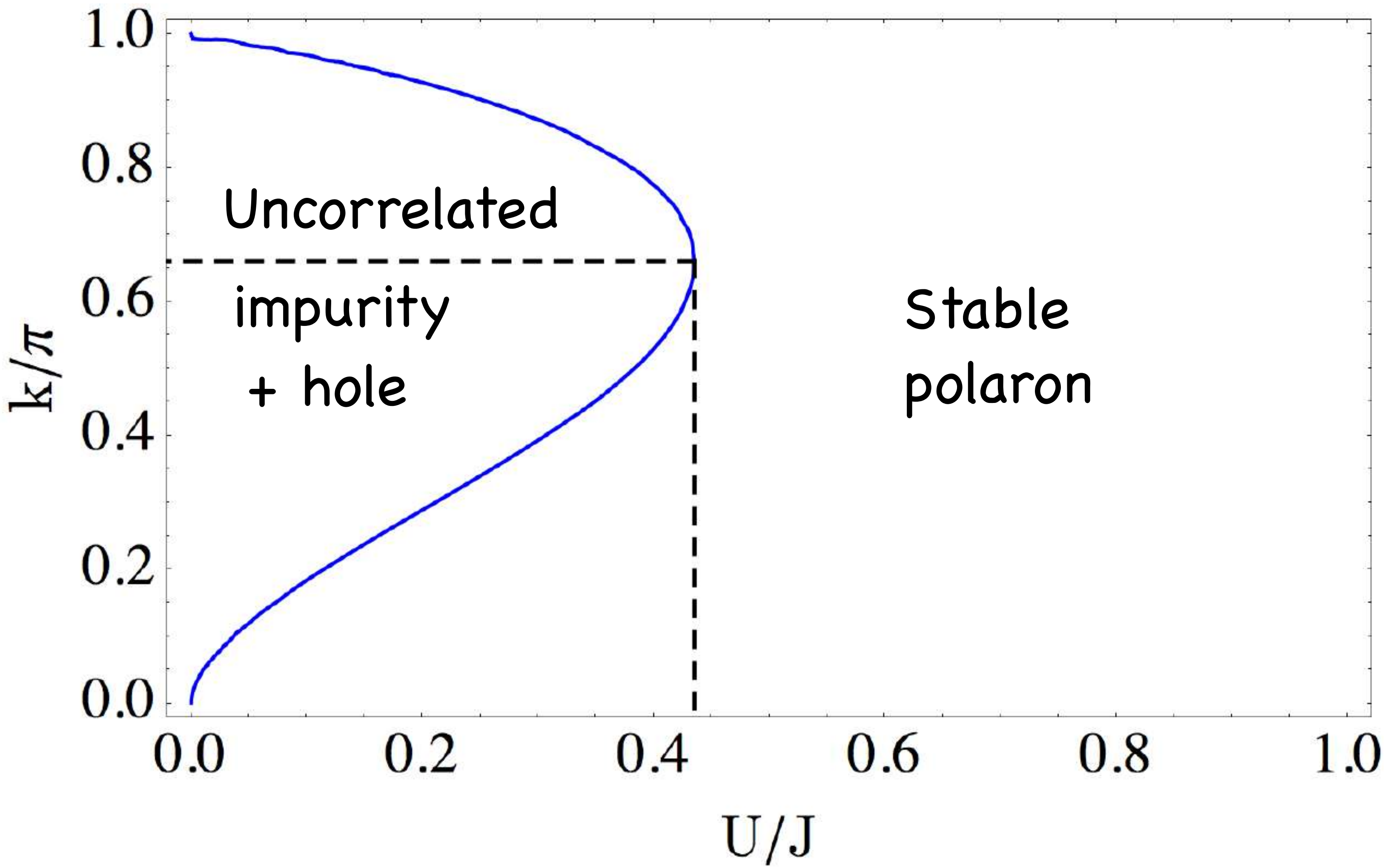
- Expect: i) Mott: $f_{\pm 1} \simeq (J/U)(1 + e^{\pm ik}) f_0$

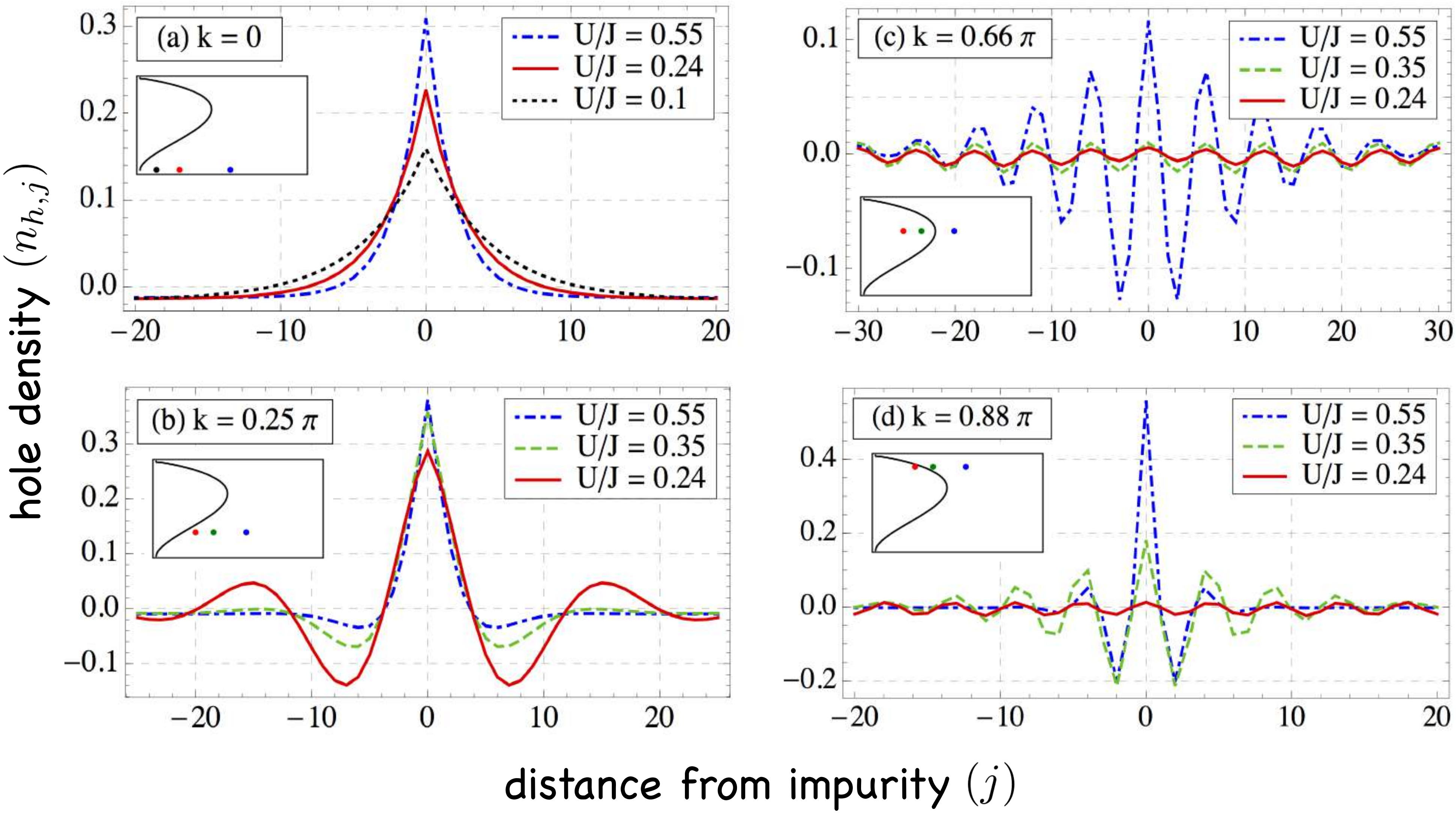
  ii) Deep superfluid: $f_i \simeq f_j$

Main Result



Polaron observed in experiment at $U/J \approx 2.13$

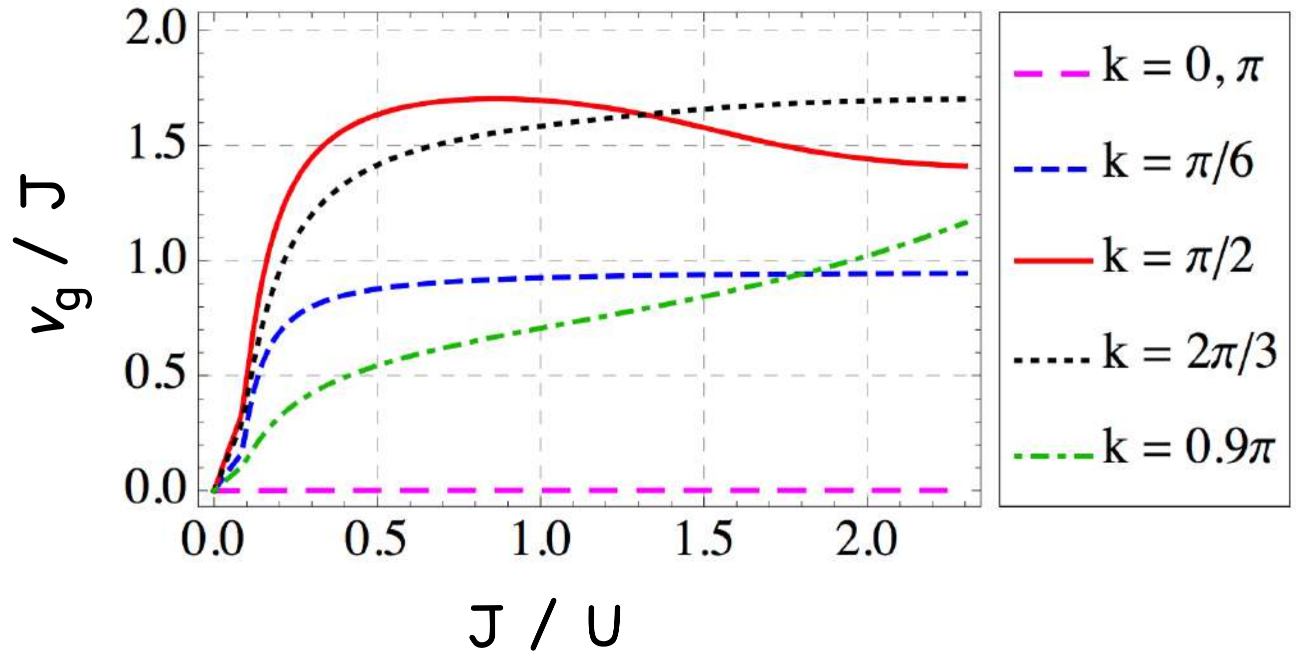
Main Result



hole density $(n_{h,j})$
(a) k = 0
U/J = 0.55
U/J = 0.24
U/J = 0.1
(c) k = 0.66 π
U/J = 0.55
U/J = 0.35
U/J = 0.24
(b) k = 0.25 π
U/J = 0.55
U/J = 0.35
U/J = 0.24
(d) k = 0.88 π
U/J = 0.55
U/J = 0.35
U/J = 0.24
distance from impurity (j)

Polaron

- Polaron size is larger for smaller U/J
- Moving polaron is bigger (max around k = 0.66 π)
- Bath density oscillates with λ ≈ 4π/k



Impurity spreading

- Localized impurity: $|\psi(0)\rangle = \hat{b}_{0,\uparrow}\hat{b}^{\dagger}_{0,\downarrow}|MF\rangle$

$$|\psi(t)\rangle = \sum_k \langle k|\psi(0)\rangle \; |k\rangle \; e^{-iE_{\mathrm{var}}(k)t}$$

- Impurity distribution: $P_{\mathrm{J/U}}(j,t) = \langle\psi(t)|\hat{b}^{\dagger}_{j,\downarrow}\hat{b}_{j,\downarrow}|\psi(t)\rangle$

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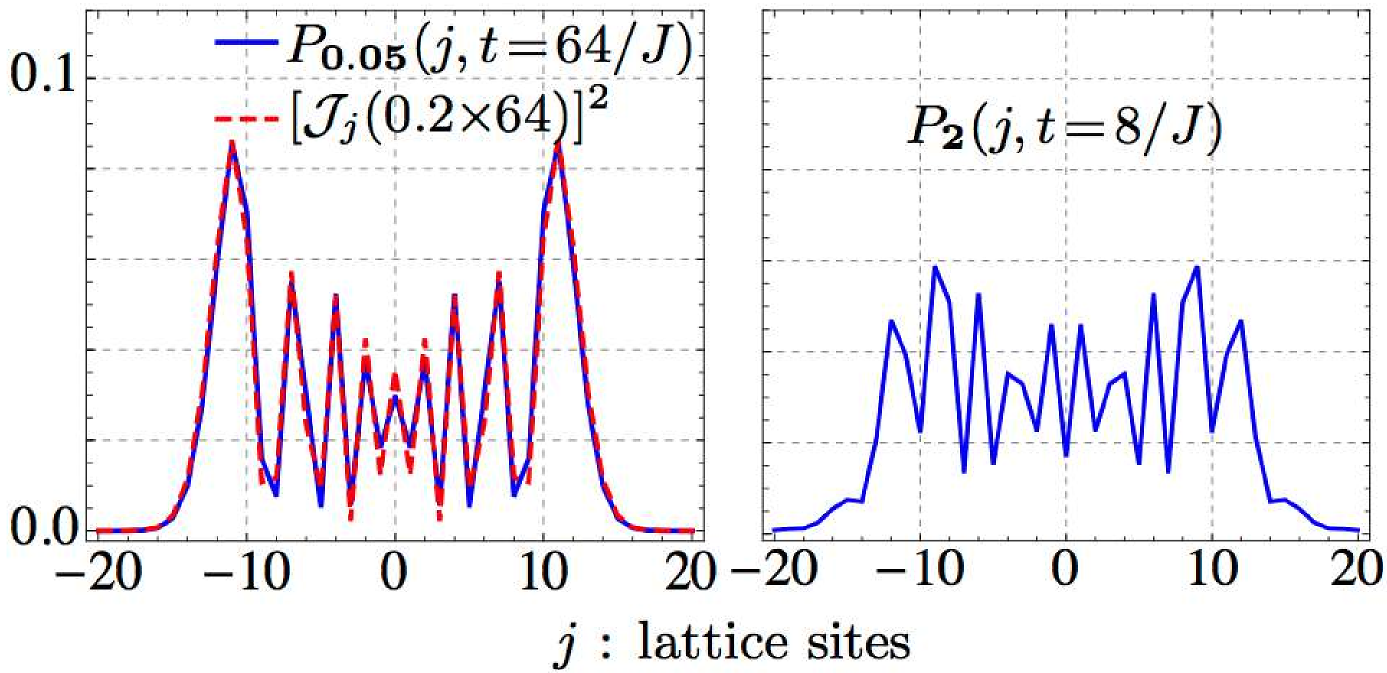

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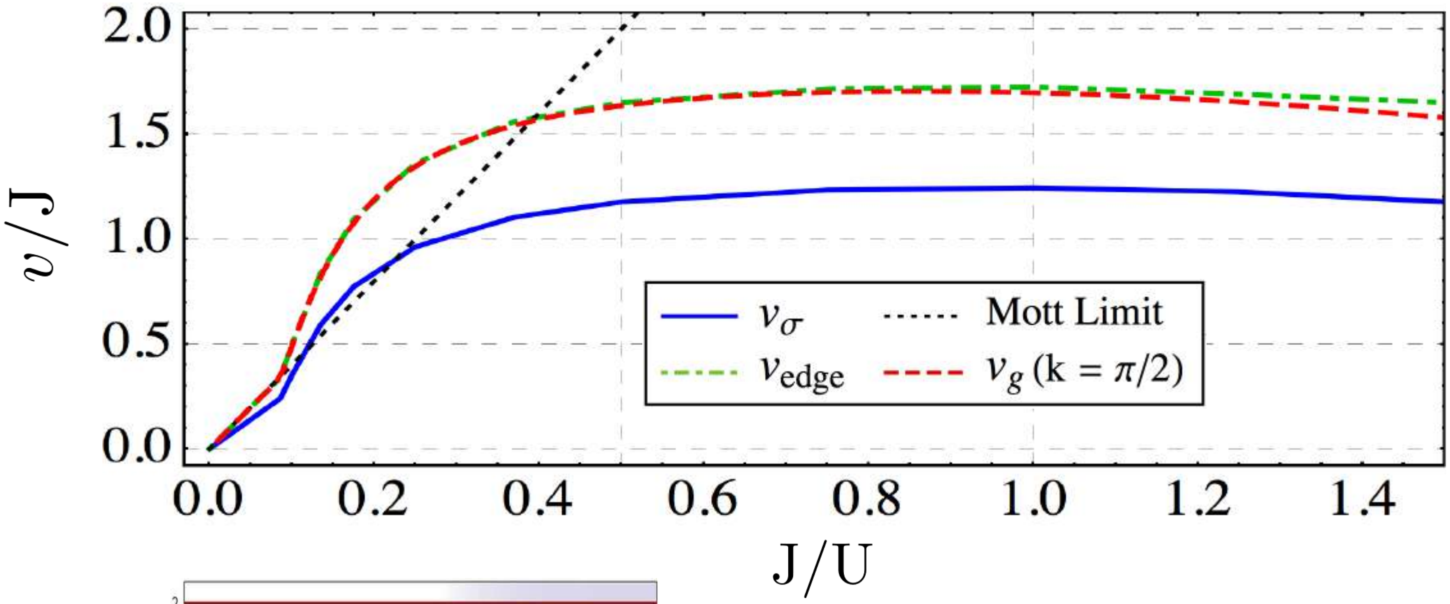
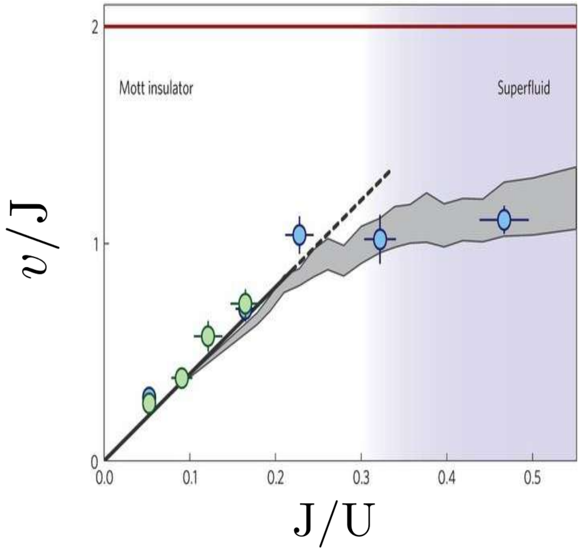
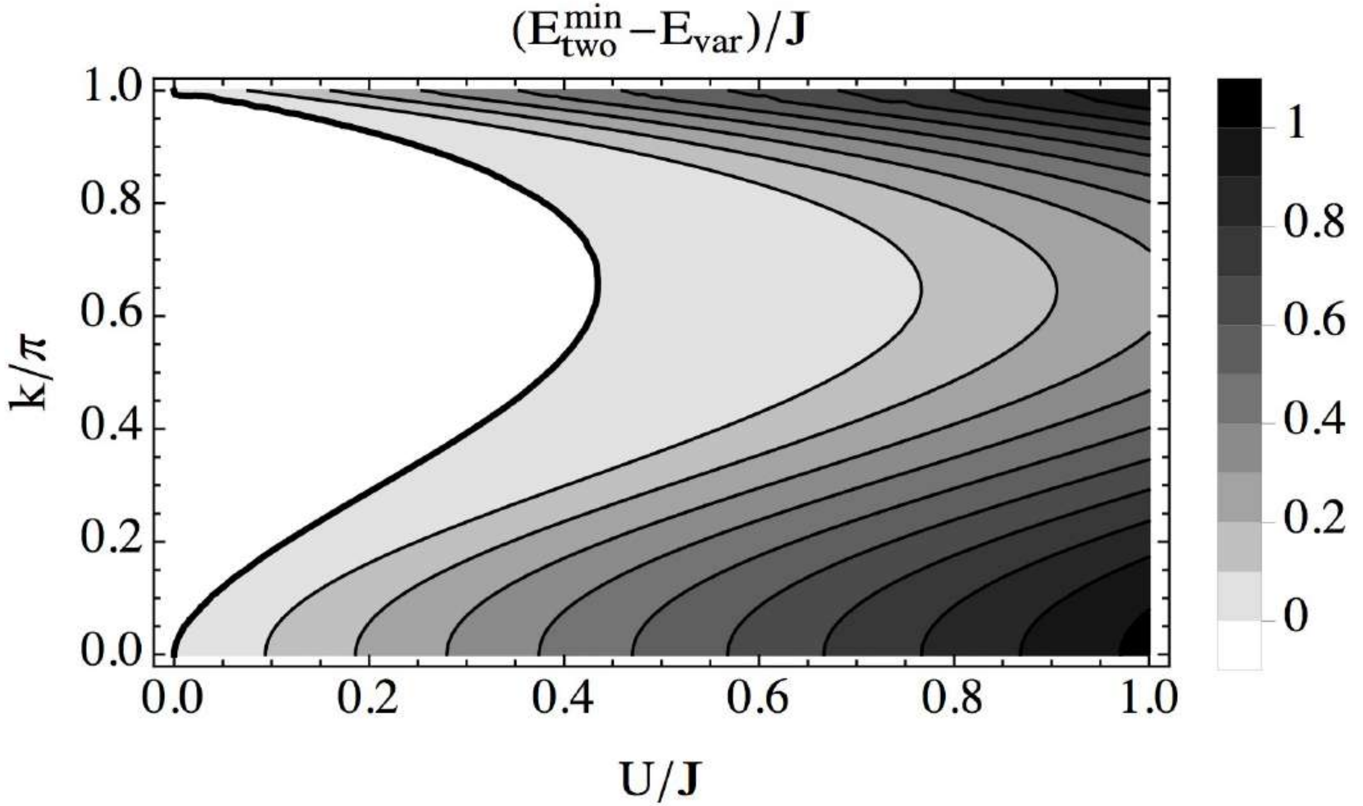




Uncorrelated impurity & hole

- Consider the wavefunction $|k;p\rangle = \hat{b}_{p,\uparrow}\hat{b}^{\dagger}_{p-k,\downarrow}|MF\rangle$ having energy $E_{two}(k,p)$.



Polaron instability

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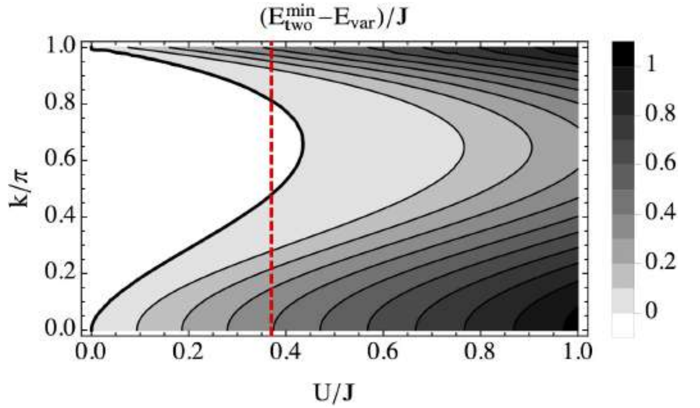

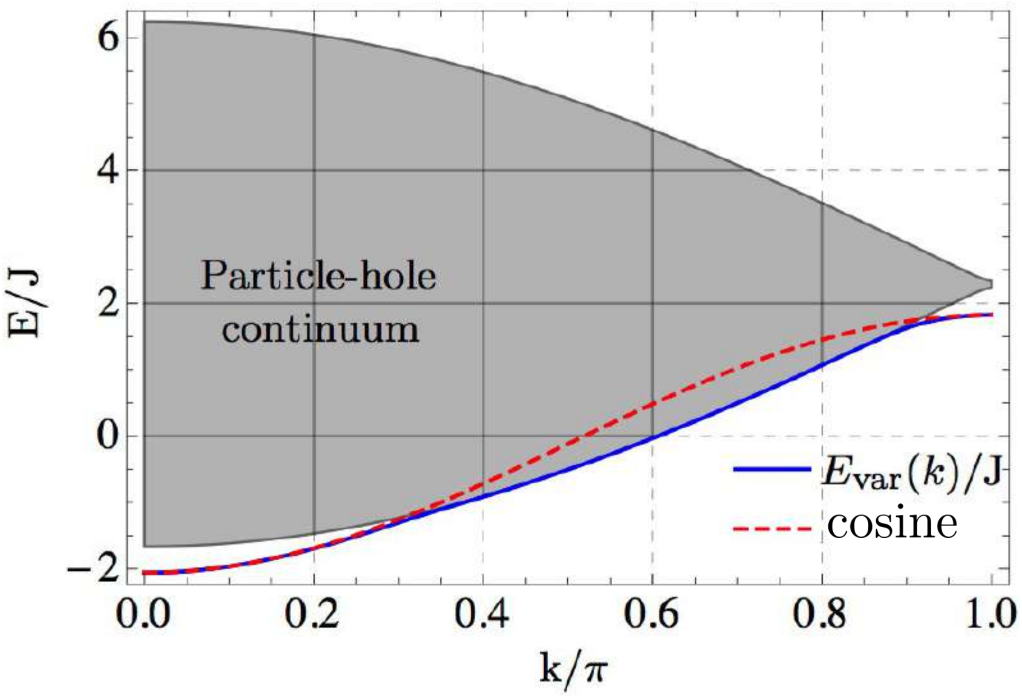

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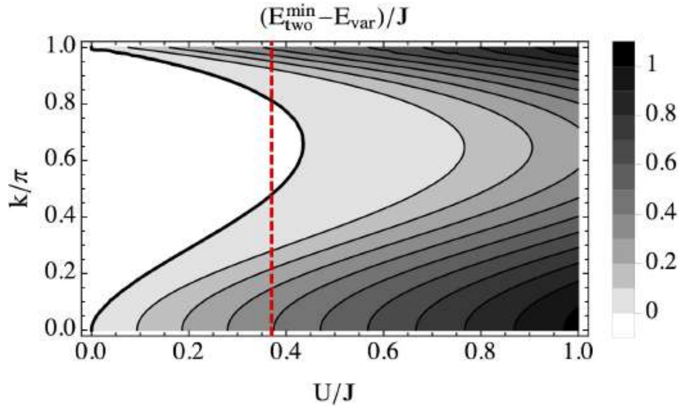
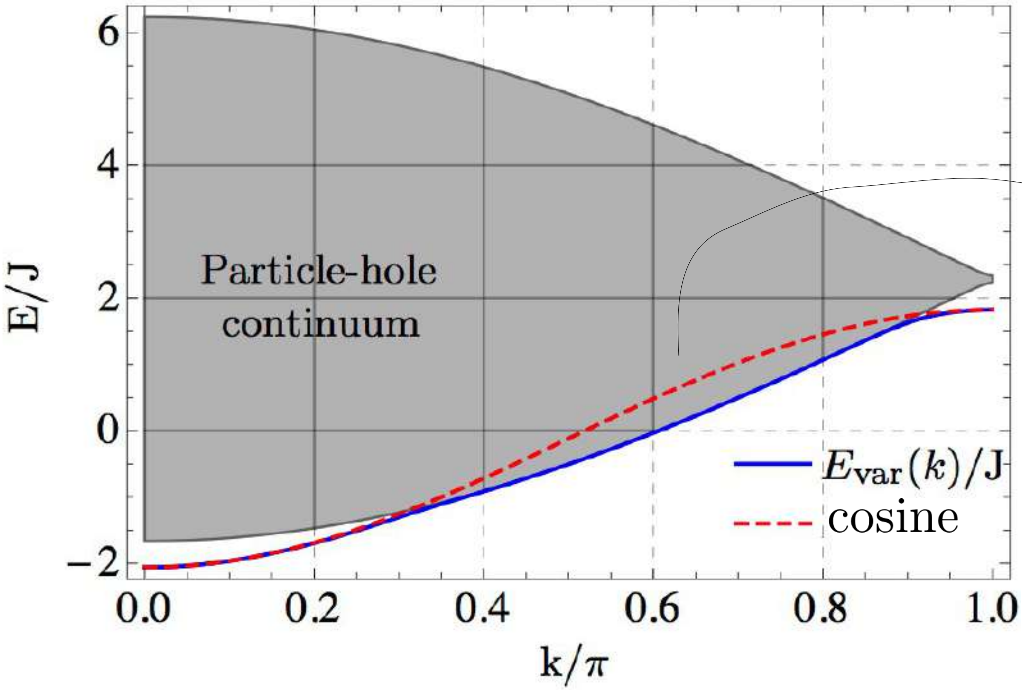
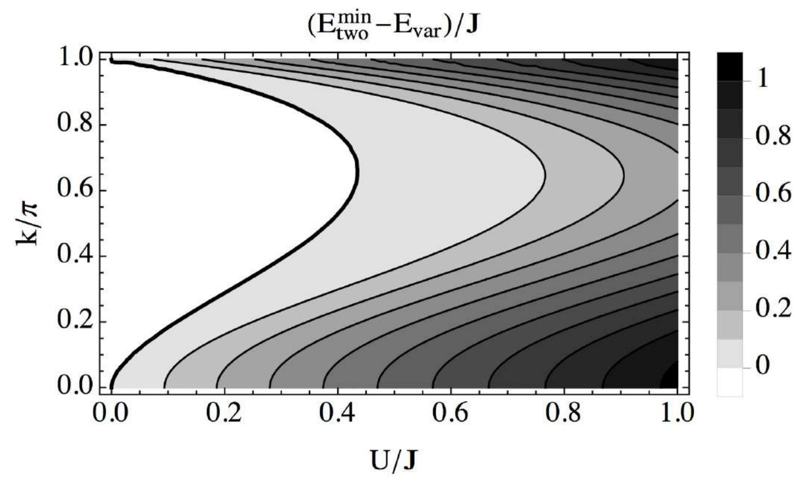


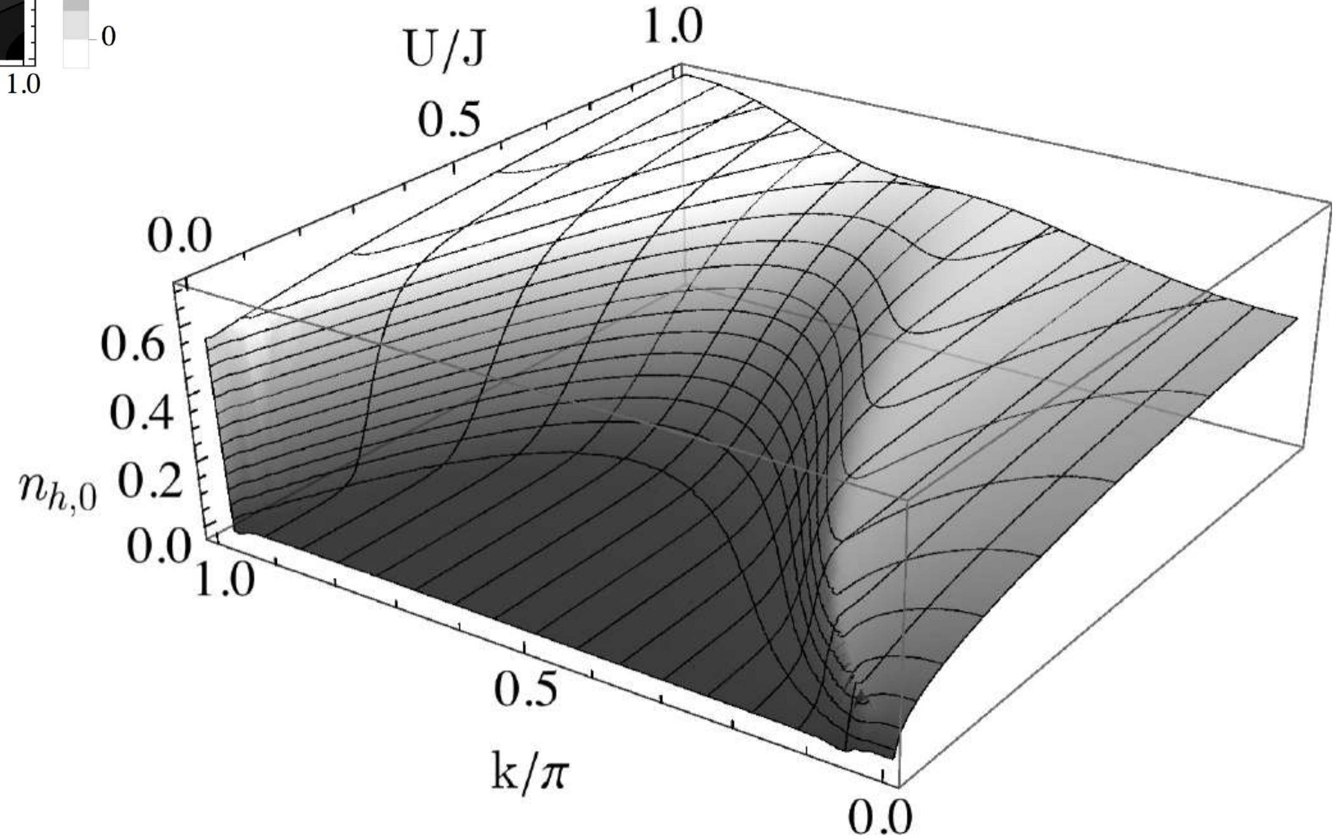


Polaron unstable due to Landau damping

Probing the crossover



Drastic fall of hole density at impurity site



Two impurities and bipolarons

Q. Can we get bound states of two polarons?

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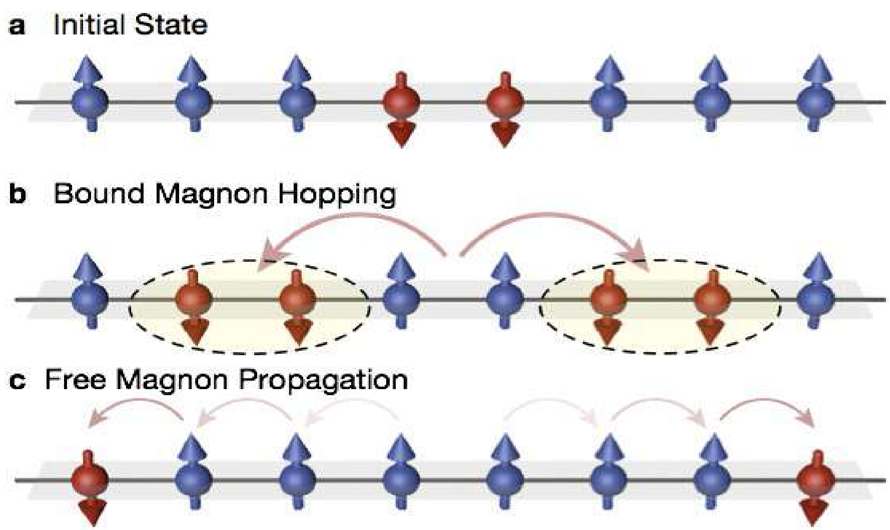
- Fukuhara et al observed two-magnon bound states in Mott insulating phase arXiv:1305.6598



- Do such bound states (bipolarons) exist in superfluid?

Two impurities and bipolarons

- Variational wavefunction (for k = 0):

$$|\psi\rangle = \sum_{d\geq 0,\, j} \left[A(d) + \sum_{l} g(d,l)\ \hat{b}_{j+l,\uparrow} \right] \hat{b}^{\dagger}_{j,\downarrow} \hat{b}^{\dagger}_{j+d,\downarrow} |MF\rangle$$

Variational parameters

Two impurities and bipolarons

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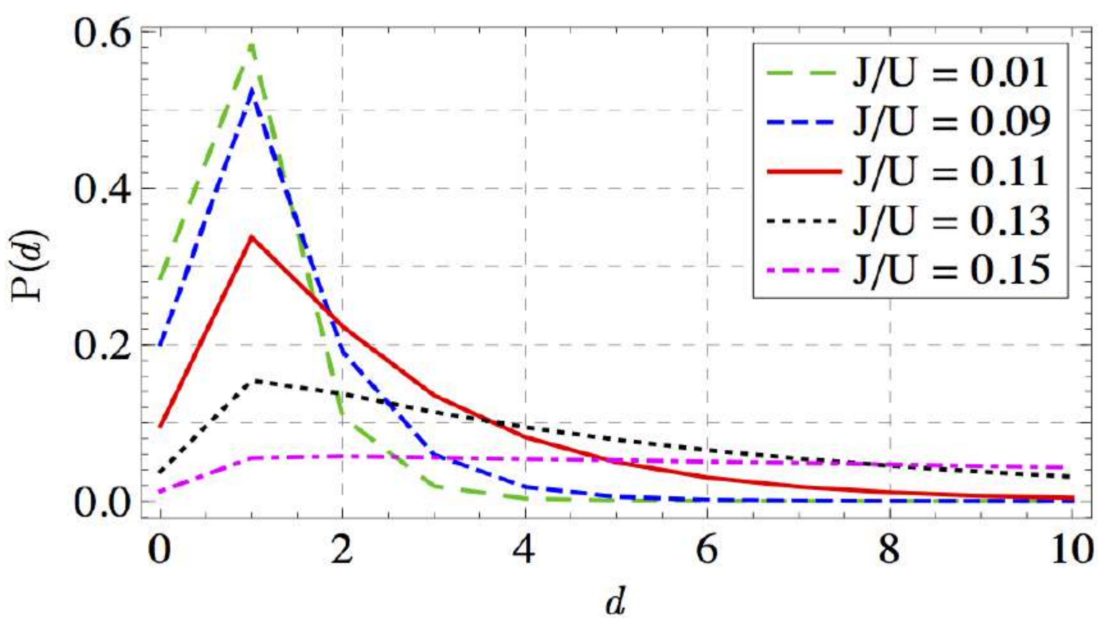
- Separation probability $P(d) = \sum_{j} \langle \psi | \hat{b}^{\dagger}_{j+d,\downarrow} \hat{b}^{\dagger}_{j,\downarrow} \hat{b}_{j,\downarrow} \hat{b}_{j+d,\downarrow} |\psi\rangle$



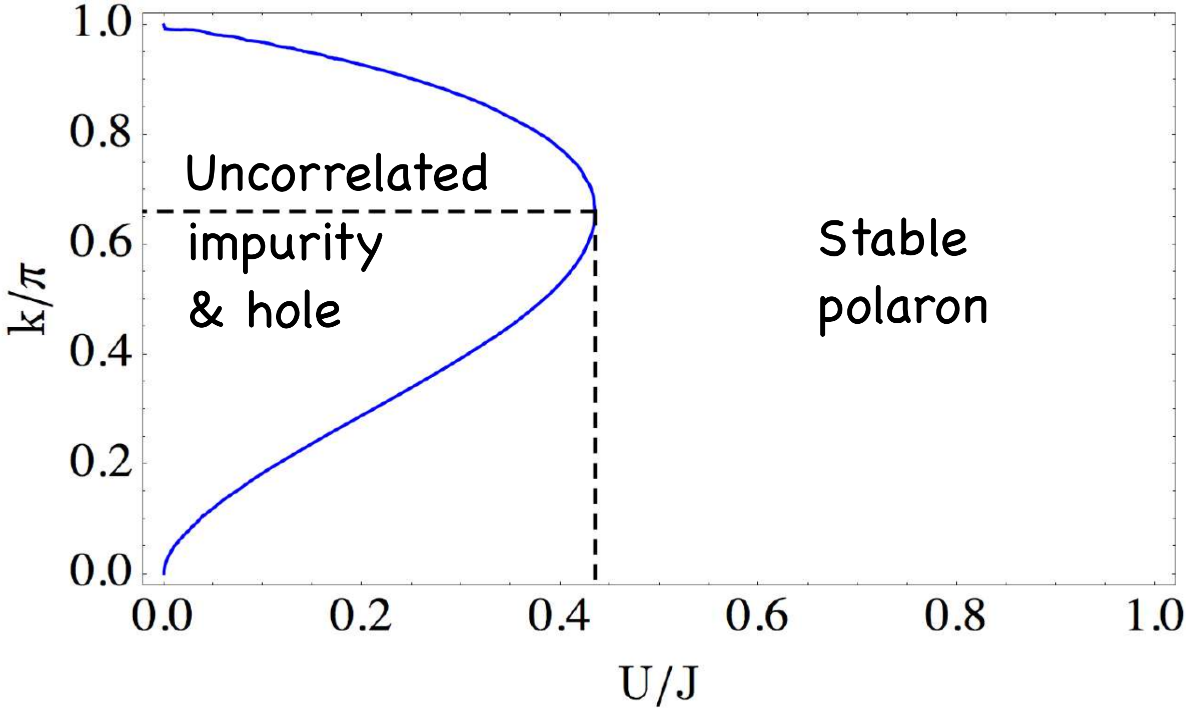
- Polarons bound for $\mathrm{J/U} \lesssim 0.15$
- Phase transition occurs at J/U ≈ 0.09

Two impurities and bipolarons

- We get 4 regions with increasing J/U:
  - i) MI with stable polarons and bipolarons
  - ii) SF with stable polarons and bipolarons
  - iii) SF with stable polarons but no bipolaron
  - iv) SF with stable polarons only in a narrow k range

Summary & Outlook

- We have studied spin impurities in 1D Bose lattice through a simple variational ansatz
- Single impurity:



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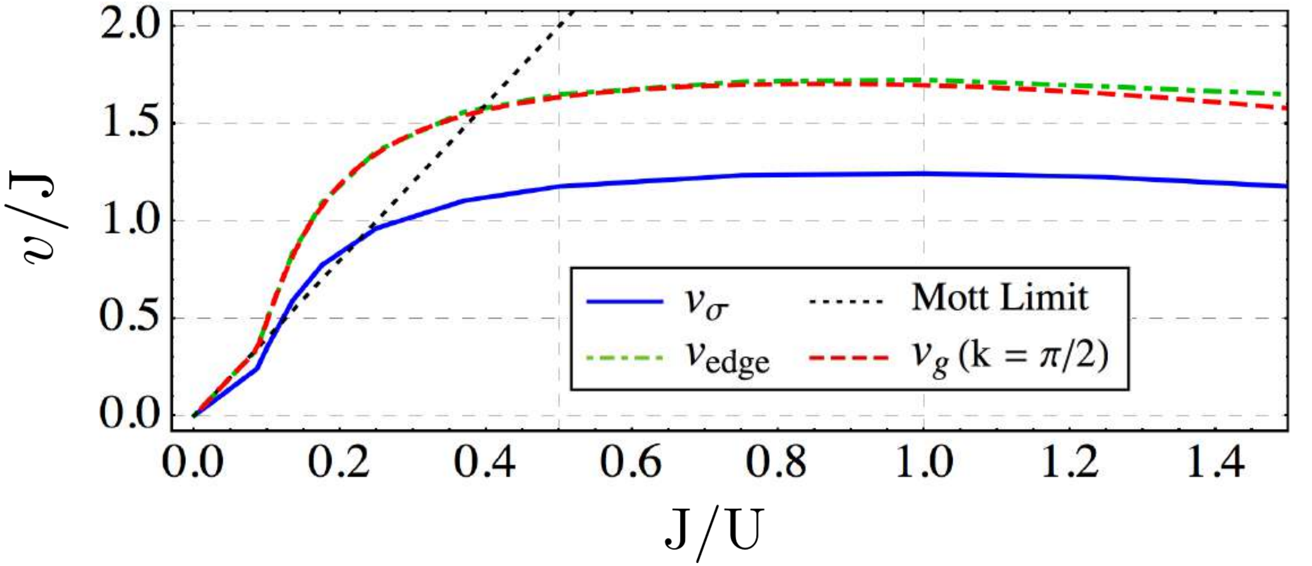
- Single impurity:
  - polaron size max for k ≈ 0.66 π and larger for smaller U/J
  - impurity hopping flattens off inside superfluid



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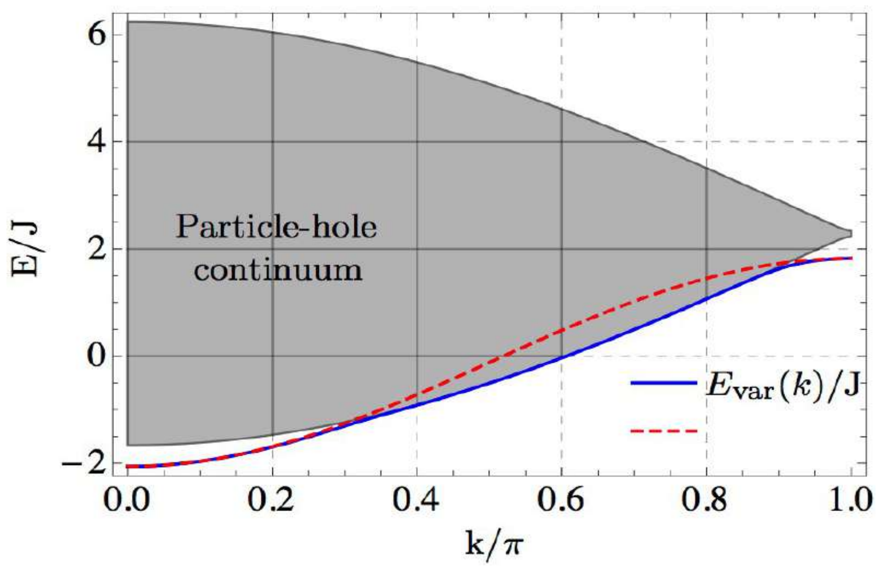
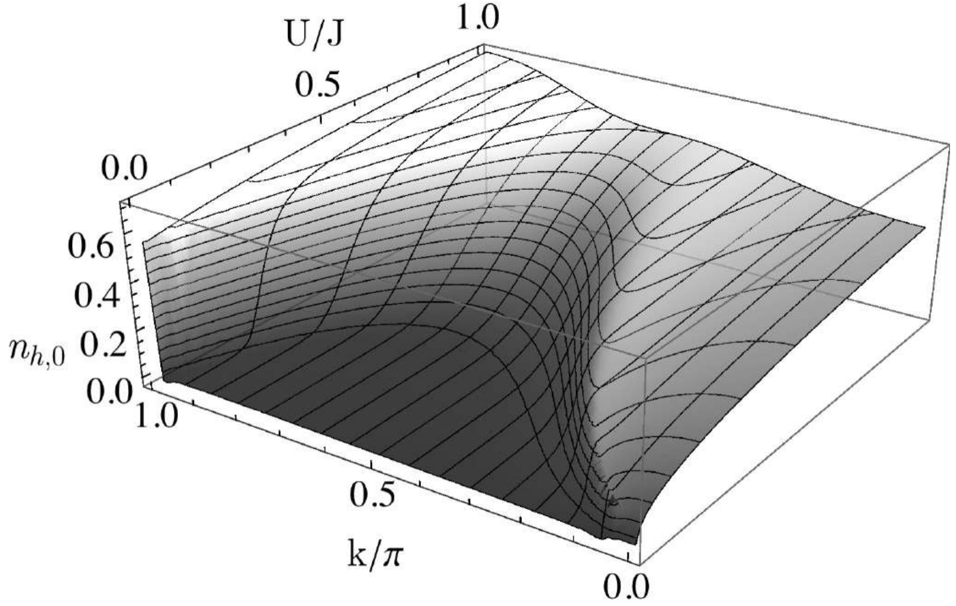
- Single impurity:

polaron becomes unstable at weaker interactions



crossover can be probed experimentally



Summary & Outlook

- We have studied spin impurities in 1D Bose lattice through a simple variational ansatz
- Two impurities:
  - stable bipolarons exist for strong interactions (both in MI & SF)
  - future experiments can test this
- Q: i) What changes at different filling and higher D?

  ii) Effects of disorder?

  iii) Is the kink in impurity speed real?

Shovan Dutta and Erich J. Mueller, arXiv:1308.4876