Construction of Localized Wave Functions

and analysis of disordered Hubbard model parameters

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Outline

1. Motivation
   - Experiments on Disordered Optical Lattice
   - Existing Theory of Localized Basis Functions
2. Statistics
   - Probability distributions
3. Method
   - Matching density matrices
   - Convergence Test
4. Summary

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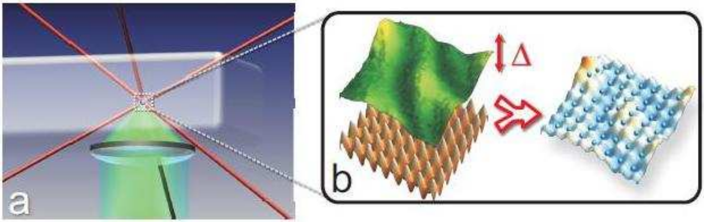
White *et al*. experiment of ^{87}Rb atoms

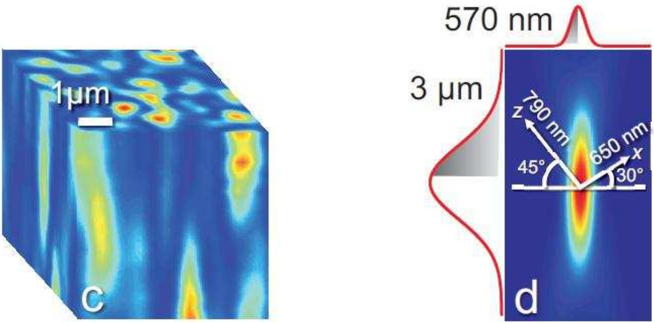
- Atoms trapped in cubic optical lattice: $a = 406$ nm

$$U_L(\mathbf{r}) = S_L \times \left[\cos\left(\frac{2\pi \mathbf{n}_1 \cdot \mathbf{r}}{a}\right) + \cos\left(\frac{2\pi \mathbf{n}_2 \cdot \mathbf{r}}{a}\right) + \cos\left(\frac{2\pi \mathbf{n}_3 \cdot \mathbf{r}}{a}\right)\right]$$



- RPL **102**, 055301 (2009)

- A speckle field produced by a lens and a diffuser



RPL **102**, 055301 (2009)

- Strength: $\langle U_D(\mathbf{r})\rangle = S_D$
- Spatial auto-correlation: $\Gamma(\mathbf{r}-\mathbf{r}') = \langle V_S(\mathbf{r})V_S(\mathbf{r}')\rangle$

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Mapping Continuum Hamiltonian to Second Quantized Form

- Continuum Hamiltonian

$$\mathcal{H}_N = \sum_{\alpha} \left[\frac{1}{2m} \mathbf{p}_\alpha^2 + U(\mathbf{r}_\alpha) \right] + \frac{1}{2} \sum_{\alpha<\beta} V(\mathbf{r}_\alpha - \mathbf{r}_\beta)$$

- Second quantized Hamiltonian

$$h = -\sum_{\langle ij \rangle} t_{ij} a_i^\dagger a_j + \sum_i \epsilon_i n_i$$

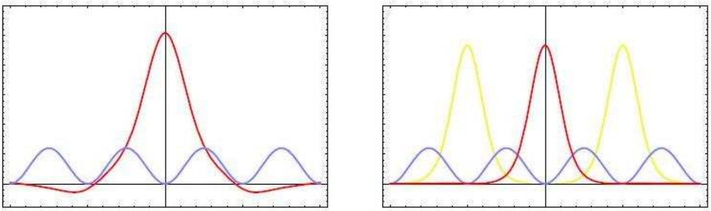
$$+\frac{1}{2} \sum_i u_i n_i (n_i - 1) + \frac{1}{2} \sum_{\langle ij \rangle} \tilde{u}_{ij} n_i n_j + \cdots\cdots$$

Maximally Localized Wannier Functions

- In a periodic potential

$$w_{ni}(\mathbf{r}) = w_n(\mathbf{r} - \mathbf{R}_i) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \psi_{n\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{R}_i}$$

- Maximally localized when purely real.



Disordered Lattice

- Construct an orthonormal subset of states
  - Wannier-like localized
  - Span the lowest energy manifold

$$\langle \mathbf{r} | w_i \rangle = w_i(\mathbf{r}), \quad i = 1, 2, ..., N$$

  - Orthogonality
  - Free of sign problem $t_{ij} \geq 0$
- Various kinds of generalizations
  - Perturbative approach (W.Kohn, ...)
  - Variational approach (N.Marzari, D.Vanderbilt, ...)
  - Envelope-function formalism (B. Foreman,...)
  - . . . . . .

Measure of Localization and Energy

- Hubbard Parameters
  - Onsite energy: $\epsilon_i = \int w_i^*(\mathbf{r})\hat{\mathcal{H}}_1 w_i(\mathbf{r}) d^3\mathbf{r}$
  - Hopping coefficient: $t_{ij} = -\int w_i^*(\mathbf{r})\hat{\mathcal{H}}_1 w_j(\mathbf{r}) d^3\mathbf{r}$
  - On-site interaction: $u_i = \frac{4\pi a_s \hbar^2}{m} \int |w_i(\mathbf{r})|^4 d^3\mathbf{r}$
  - Off-site interaction: $\tilde{u}_{ij} = \frac{4\pi a_s \hbar^2}{m} \int |w_i(\mathbf{r})|^2 |w_j(\mathbf{r})|^2 d^3\mathbf{r}$
- Short range model potential

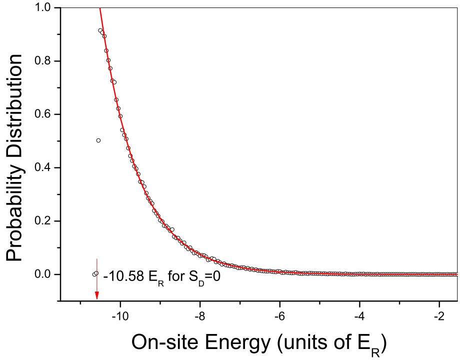
$$V(\mathbf{r}-\mathbf{r}') = \frac{4\pi a_s \hbar^2}{m}\delta\left(\mathbf{r}-\mathbf{r}'\right)$$

Parameter setting for statistics

- Depth of optical lattice: $S_L = 14\,E_R$
- Strength of random field: $S_D = 1\,E_R$
- 1000 samples of 6^3 sites lattice
- $a_s = 0.013\,a$

Outline

Probability distribution for on-site energy



- A steep onset at low energy
- A tail at high energy
- Fit to exponential

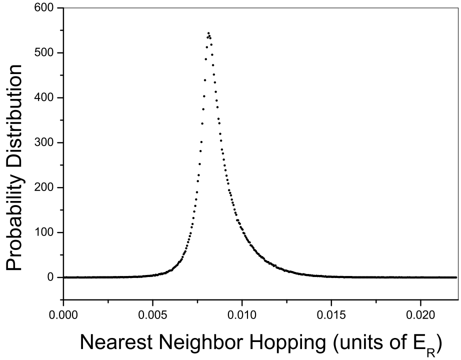
$$P(\varepsilon) \sim \exp\left(-\varepsilon/\Gamma\right)$$

where $\Gamma \approx 0.97 E_R$

- Correlation

$$\frac{\left\langle \varepsilon_i \varepsilon_j \right\rangle - \left\langle \varepsilon_i \right\rangle \left\langle \varepsilon_j \right\rangle}{\left\langle \varepsilon^2 \right\rangle - \left\langle \varepsilon \right\rangle^2} \approx 0.49$$

Probability distribution for n.n. hopping coefficients

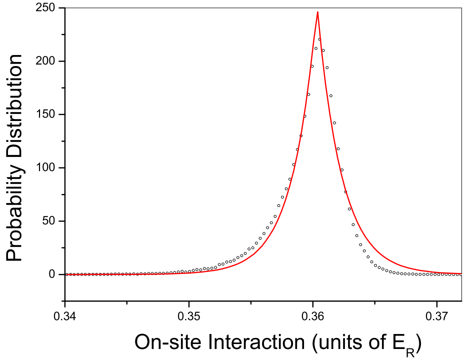


- Asymmetrically centered
- Only positive $t_{\langle ij \rangle}$ were found
- Relative width

$$\frac{\delta t}{\langle t \rangle} = 0.15$$

- Prokofev, Troyer, *et al.* arXiv:0909.4593

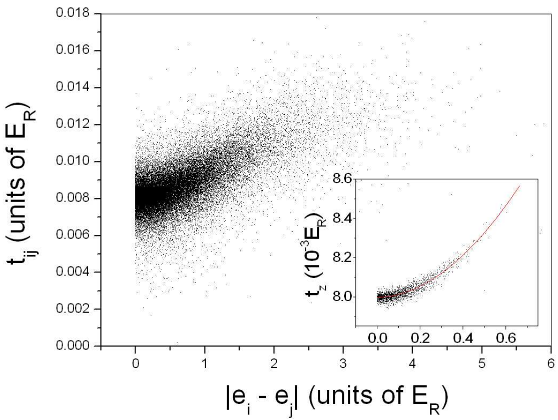
Probability distribution for on-site interaction



- Narrow peak
- Centered at $0.36E_R$
- Relative width

$$\frac{\delta u}{\langle u \rangle} = 0.01$$

Correlation between on-site energy and hopping



Outline

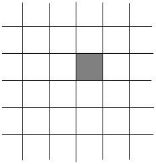
Continuum density matrix

- Unnormalized single particle density matrix

$$\rho\left(\mathbf{r},\mathbf{r}';\beta\right) = \langle \mathbf{r}|e^{-\beta\hat{\mathcal{H}}_1}|\mathbf{r}'\rangle.$$

- Choose a trial orthogonal set of localized basis

$$\begin{aligned} w_i(\mathbf{r};0) &= 1, \quad \text{inside Wigner Seitz cell} \\ &= 0, \quad \text{otherwise} \end{aligned}$$



Course-graining of continuum model

- Find h such that

$$\begin{aligned} S_{ij}(\beta) &= \langle w_i(0)|e^{-\beta\hat{\mathcal{H}}_1}|w_j(0)\rangle \\ &= e^{-\beta\hat{h}} \end{aligned}$$

- Formal solution

$$\hat{h} = \lim_{\beta\to\infty} -\frac{1}{\beta}\log\hat{S}\left(\beta\right)$$

Outline of procedure

- 1. Trial basis set

$$\begin{aligned} w_i(\mathbf{r};0) &= 1, \quad \text{inside Wigner Seitz cell} \\ &= 0, \quad \text{otherwise} \end{aligned}$$

- 2. Imaginary time evolution

$$|w_i(\tau)\rangle = e^{-\tau\hat{\mathcal{H}}_1}|w_i(0)\rangle, \quad i = 1, ..., N$$

- 3. Construct overlap matrix

$$\hat{S}(\tau) = \langle w_i(\tau)|w_j(\tau)\rangle$$

- 4. Löwdin orthogonalization

$$|w_i(\tau)\rangle \mapsto \hat{S}^{-1/2}(\tau)|w_i(\tau)\rangle$$

Zhou and Ceperley, *Phys. Rev. A.* **81** 013402 (2010)

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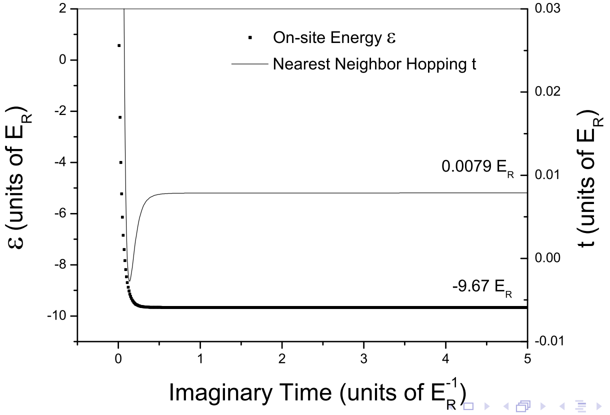
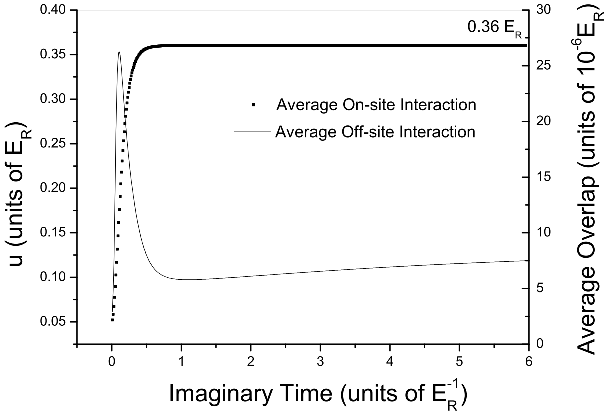
$$h_{ij}(\beta) = \langle \tilde{w}_i(\beta/2)|\hat{\mathcal{H}}_1|\tilde{w}_j(\beta/2)\rangle$$

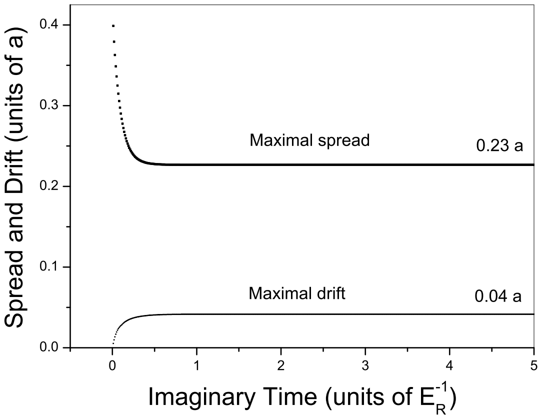


Hubbard Parameters: $S_L = 14\,E_R$, $S_D = 1\,E_R$

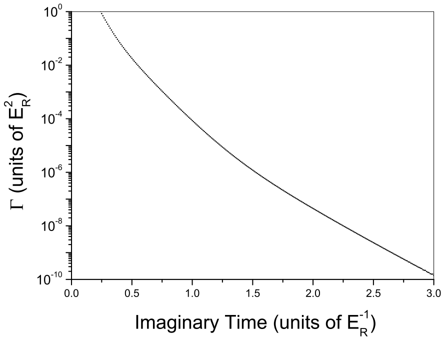
^{87}Rb: $a_s = 5.29$ nm $= 0.013\,a$



Spatial Spread and Drift: $S_L = 14$, $S_D = 1$



Energy convergence rate: $S_L = 14$, $S_D = 1$



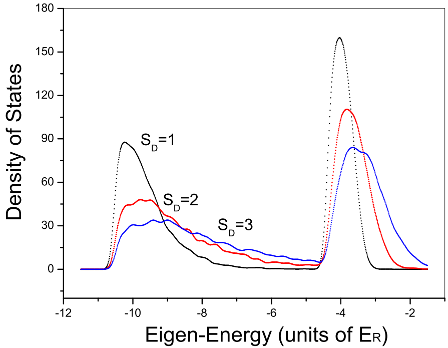
- Convergence rate:

$$\Gamma = \frac{1}{N}\sum_i \left|\frac{d}{d\tau}E^{(i)}_{\texttt{lattice}}\right|$$

- Recall the assumption

$$\lim_{\beta\to\infty}\left(\frac{d\hat{h}}{d\beta}\right) = 0$$

Density of states



- First band broadened
- $S_D < 2$, gap persists
- $S_D \geq 2$, fail to converge

Summary and Outlook

- Summary
  - Coarse-grained effective lattice Hamiltonian
  - Wannier-like basis spanning the lowest energy manifold
  - Imaginary time projection and Löwdin orthogonalization
  - Correlated disorder
- Outlook
  - More than one basis functions per site at strong disorder
  - Evaluate Hubbard U beyond perturbation theory
  - QMC calculation using the parameterized Hubbard model