Time-evolving block decimation (TEBD) applied to ultracold gases in optical lattices

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Outline:

1. Time-evolving block decimation (TEBD)

2. Cold atom systems and motivation of this work

3. Coherent quantum phase slips:
   Quantitative comparison with instanton techniques
   Danshita and Polkovnikov, PRB 82, 094304 (2010)

4. Superflow decay via quantum phase slips:
   Testing a scaling formula
   Danshita and Polkovnikov, PRA 85, 023638 (2012)

5. Conclusions

1.1. What we can do with TEBD/tDMRG

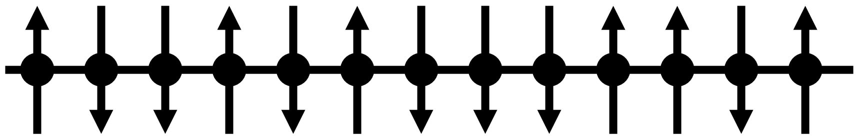
Vidal, PRL (2003); PRL (2004) / White and Feiguin, PRL (2004)

$$|\Psi(t)\rangle = \exp(-i\hat{H}t/\hbar)|\Psi_0\rangle$$

One can exactly compute the time-evolution of the many-body wave function in a 1D quantum lattice system (open boundary is favored).

Eg. Ising model with transverse magnetic field: $$\hat{H} = J\sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + h\sum_j \hat{\sigma}_j^x$$

A system of n spins



An arbitrary state: $$|\Psi\rangle = \sum_{i_1,i_2,i_3,\ldots,i_n=0}^{1} c_{i_1,i_2,i_3,\ldots,i_n}|i_1,i_2,i_3,\ldots,i_n\rangle$$

2^n states are needed to span the entire Hilbert space.

We need an efficient way to describe the many-body wave function and the time propagation operator.

Matrix product state

Suzuki-Trotter decomposition

1.2. Matrix product state (MPS) representation

An arbitrary state: $$|\Psi\rangle = \sum_{i_1,i_2,i_3,\ldots,i_n=0}^{1} c_{i_1,i_2,i_3,\ldots,i_n} |i_1, i_2, i_3, \ldots, i_n\rangle$$

Matrix product decomposition

$$c_{i_1 i_2 \ldots i_n} = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{n-1}=1}^{\chi} \Gamma^{[1]i_1}_{\alpha_1} \lambda^{[1]}_{\alpha_1} \Gamma^{[2]i_2}_{\alpha_1\alpha_2} \lambda^{[2]}_{\alpha_2} \Gamma^{[3]i_3}_{\alpha_2\alpha_3} \lambda^{[3]}_{\alpha_3} \cdots \lambda^{[n-2]}_{\alpha_{n-2}} \Gamma^{[n-1]i_{n-1}}_{\alpha_{n-2}\alpha_{n-1}} \lambda^{[n-1]}_{\alpha_{n-1}} \Gamma^{[n]i_L}_{\alpha_{n-1}}.$$

Γ: $d\times\chi\times\chi$-tensor, λ: χ-vector

λ^2 is the eigenvalue of the reduced density matrix.

Total number of the whole elements of this MPS : $n\times\chi^2\times d$

In general, to describe an arbitrary state, one has to take $\chi \sim d^{n/2}$

However, for the ground state and low-lying excited states, taking a finite χ gives sufficiently accurate results.

The size of MPS increases only linearly with n.

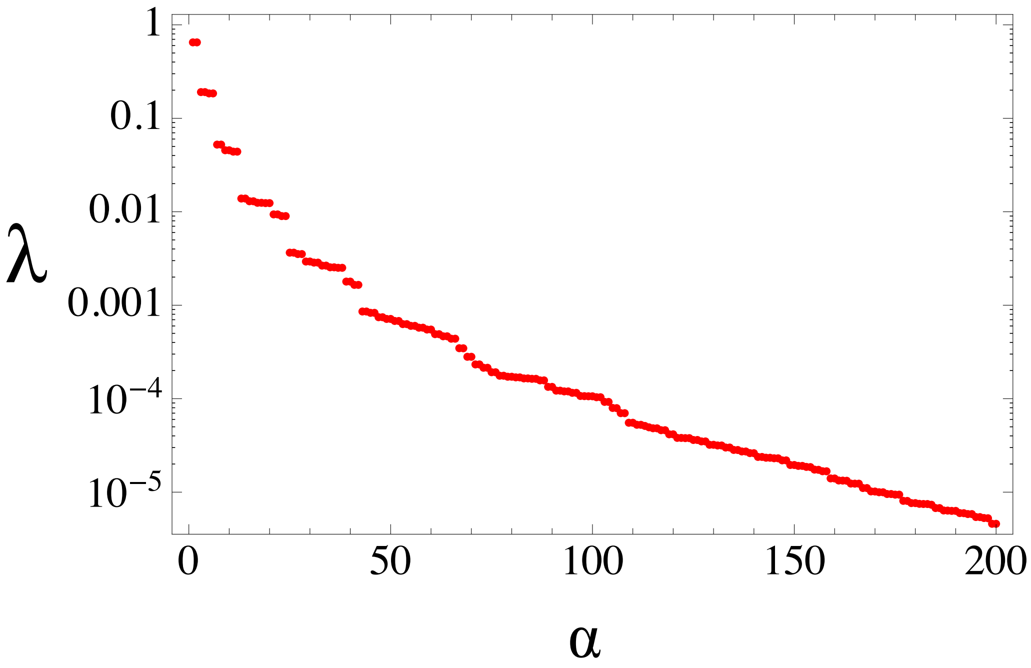
Observation ①: For the ground state,

$$\lambda_{\alpha}^{[l]} : \exp(-K\alpha), \quad K > 0$$

Observation ②: For lowly-excited states,

$$\lambda_{\alpha}^{[l]}(t) : \exp(-K(t)\alpha), \quad K(t) > 0$$

This requirement can be held only in 1D !!



Example: the ground state of the Bose-Hubbard model with U/J = 100, n=400, N=200, l = 200.

Taking a finite χ can give an accurate description of the many-body wave function.

1.3. Time propagation

$$|\Psi(t)\rangle = \exp(-i\hat{H}t/\hbar)|\Psi_0\rangle$$

Nearest neighbor Hamiltonian: $\hat{H} = \sum_j \hat{K}_1^{[j]} + \sum_j \hat{K}_2^{[j,j+1]}$

One-site operator: $\hat{K}_1^{[j]}$ Two-site operator: $\hat{K}_2^{[j,j+1]}$

Separate the Hamiltonian into the “even” part and “odd” part

$$\hat{H} = \hat{H}_{\rm even} + \hat{H}_{\rm odd}$$

where $\hat{H}_{\rm even} \equiv \sum_{{\rm even}\, j} \hat{H}^{[j]} = \sum_{{\rm even}\, j} (\hat{K}_1^{[j]} + \hat{K}_2^{[j,j+1]})$

$$\hat{H}_{\rm odd} \equiv \sum_{{\rm odd}\, j} \hat{H}^{[j]} = \sum_{{\rm odd}\, j} (\hat{K}_1^{[j]} + \hat{K}_2^{[j,j+1]})$$

Suzuki-Trotter decomposition:

$$\exp\left[-i(\hat{H}_{\text{even}}+\hat{H}_{\text{odd}})t\right]=\left\{\exp\left[-i(\hat{H}_{\text{even}}+\hat{H}_{\text{odd}})\delta\right]\right\}^{t/\delta}$$

$$\simeq\left\{\exp(-i\hat{H}_{\text{even}}\delta/2)\exp(-i\hat{H}_{\text{odd}}\delta)\exp(-i\hat{H}_{\text{even}}\delta/2)+O(\delta^3)\right\}^{t/\delta}$$

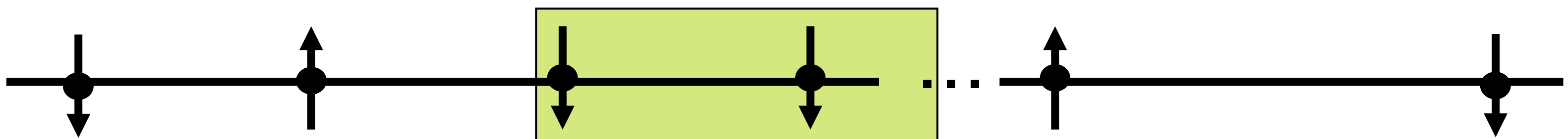
2 order Suzuki-Trotter decomposition

Furthermore, $\exp(-i\hat{H}_{\text{even}}\delta/2)=\prod_{\text{even } j}\exp(-i\hat{H}^{[j]}_{\text{even}}\delta/2)$

$$\exp(-i\hat{H}_{\text{odd}}\delta/2)=\prod_{\text{odd } j}\exp(-i\hat{H}^{[j]}_{\text{odd}}\delta/2)$$

Now the time propagation operator, whose dimension was originally $d^n\times d^n$, is decomposed to local two-site operators of $d^2\times d^2$.

Operation on two neighboring sites:



$$\sum_{\alpha_1,\cdots,\alpha_{n-1}}\Gamma^{[1]j_1}_{\alpha_1}\lambda^{[1]}_{\alpha_1}\Gamma^{[2]j_2}_{\alpha_1\alpha_2}\lambda^{[2]}_{\alpha_2}\Gamma^{[3]j_3}_{\alpha_2\alpha_3}\lambda^{[3]}_{\alpha_3}\Gamma^{[4]j_4}_{\alpha_2\alpha_3}\cdots\Gamma^{[n-1]j_{n-1}}_{\alpha_{n-2}\alpha_{n-1}}\lambda^{[n-1]}_{\alpha_{n-1}}\Gamma^{[n]j_n}_{\alpha_{n-1}}$$

$$U^{i_3i_4}_{i'_3i'_4}$$

Two site operation:

In a procedure without use of MPS, $\tilde{c}_{i_1 \cdots i_l i_{l+1} \cdots i_n} = \sum_{i'_l, i'_{l+1}} U^{i_l i_{l+1}}_{i'_l i'_{l+1}} c_{i_1 \cdots i'_l i'_{l+1} \cdots i_n}$

In the MPS description,

① Form a 4-rank tensor: $\Theta^{i_l i_{l+1}}_{\alpha_{l-1}\alpha_{l+1}} = \sum_{\alpha_l=1}^{\chi} \lambda^{[l-1]}_{\alpha_{l-1}} \Gamma^{[l]i_l}_{\alpha_{l-1}\alpha_l} \lambda^{[l]}_{\alpha_l} \Gamma^{[l+1]i_{l+1}}_{\alpha_l \alpha_{l+1}} \lambda^{[l+1]}_{\alpha_{l+1}}$

② Apply the operator: $\tilde{\Theta}^{i_l i_{l+1}}_{\alpha_{l-1}\alpha_{l+1}} = \sum_{i'_l, i'_{l+1}} U^{i_l, i_{l+1}}_{i'_l, i'_{l+1}} \Theta^{i'_l i'_{l+1}}_{\alpha_{l-1}\alpha_{l+1}}$

③ Form the reduced density matrix: $\rho^{[L] i_l \alpha_{l-1}}_{i'_l \alpha'_{l-1}} = \sum_{i_{l+1} \alpha_{l+1}} \tilde{\Theta}^{i_l i_{l+1}}_{\alpha_{l-1}\alpha_{l+1}} (\tilde{\Theta}^{i'_l i_{l+1}}_{\alpha'_{l-1}\alpha_{l+1}})^*$

$$\rho^{[R] i_{l+1} \alpha_{l+1}}_{i'_{l+1} \alpha'_{l+1}} = \sum_{i_l \alpha_{l-1}} \tilde{\Theta}^{i_l i_{l+1}}_{\alpha_{l-1}\alpha_{l+1}} (\tilde{\Theta}^{i_l i'_{l+1}}_{\alpha_{l-1}\alpha'_{l+1}})^*$$

④ Singular value decomposition: $\rho^{[L]} \longrightarrow \tilde{\Gamma}^{[l]}, \tilde{\lambda}^{[l]} \qquad \rho^{[R]} \longrightarrow \tilde{\Gamma}^{[l+1]}$

$$\tilde{\Theta}^{i_l i_{l+1}}_{\alpha_{l-1}\alpha_{l+1}} = \sum_{\alpha_l=1}^{\chi \times d} \lambda^{[l-1]}_{\alpha_{l-1}} \tilde{\Gamma}^{[l]i_l}_{\alpha_{l-1}\alpha_l} \tilde{\lambda}^{[l]}_{\alpha_l} \tilde{\Gamma}^{[l+1]i_{l+1}}_{\alpha_l \alpha_{l+1}} \lambda^{[l+1]}_{\alpha_{l+1}}$$

⑤ Truncation: $\chi \times d \longrightarrow \chi$ **Density matrix renormalization!!**

What we wanted to do:

① For a given Hamiltonian, calculate the ground state.

Imaginary time propagation:

$$|\Psi_{\rm g}\rangle = \lim_{\tau\to\infty} \frac{\exp(-H\tau)|\Phi_{\rm prd}\rangle}{||\exp(-H\tau)|\Phi_{\rm prd}\rangle||}$$

$$\text{where } |\Phi_{\rm prd}\rangle = \prod_{l=1}^{n} |\psi_l\rangle$$

Note:
This is not the most efficient way to obtain the ground state.

② For a given initial state and a given Hamiltonian, calculate the time evolution.

$$|\Psi(t)\rangle = \exp(-iHt)|\Psi_{\rm g}\rangle$$

For TEBD extended to periodic boundary condition, see Danshita and Naidon, PRA 79, 043601 (2009)

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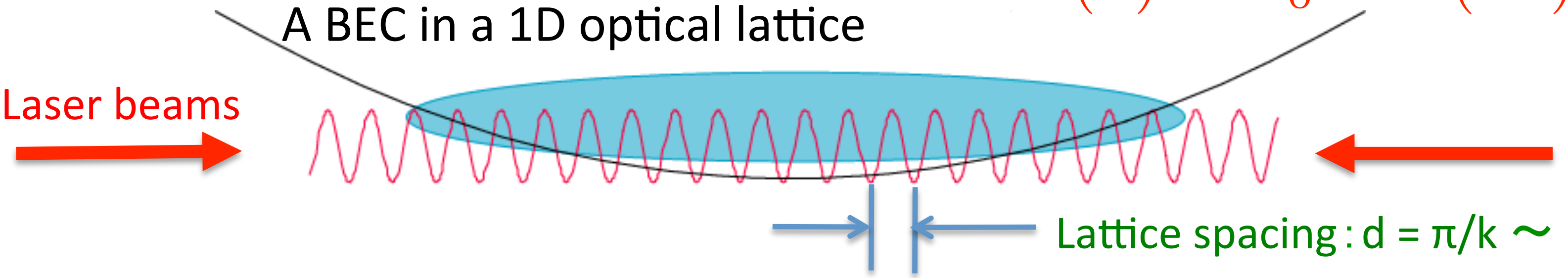
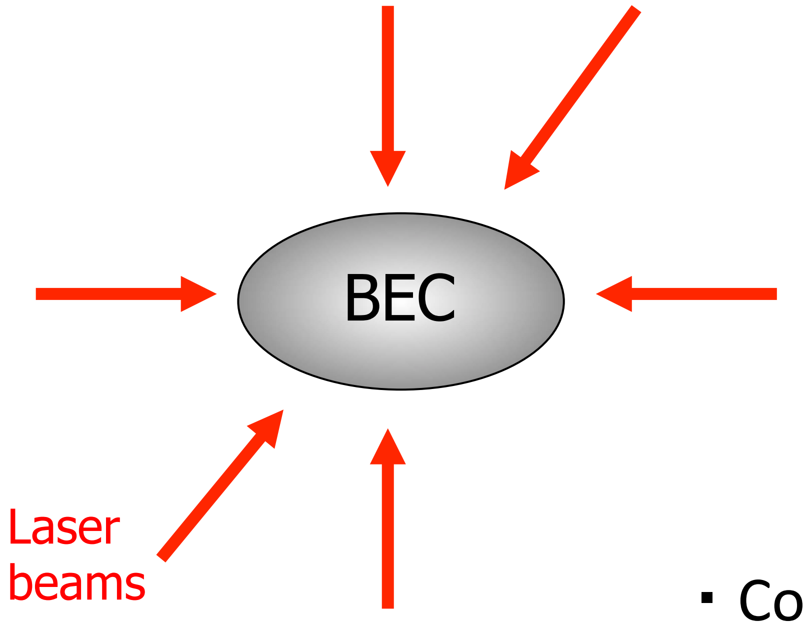
2.1. What is an optical lattice ?

I. Bloch et al., RMP (2008)

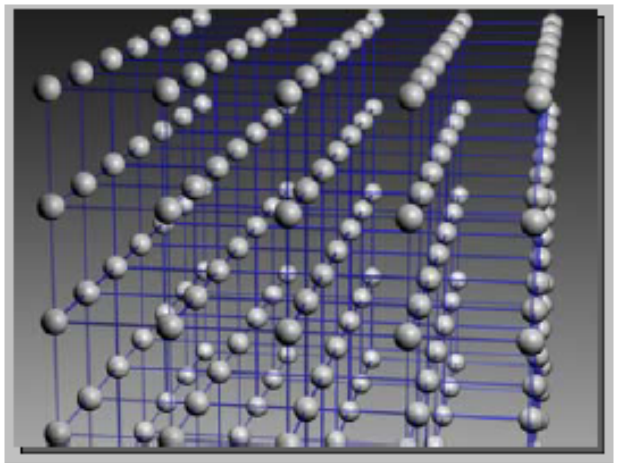
Interference of two counter-propagating laser beams → A periodic potential for atoms = An optical lattice

$$V(x) = V_0 \sin^2(kx)$$





A simple cubic lattice

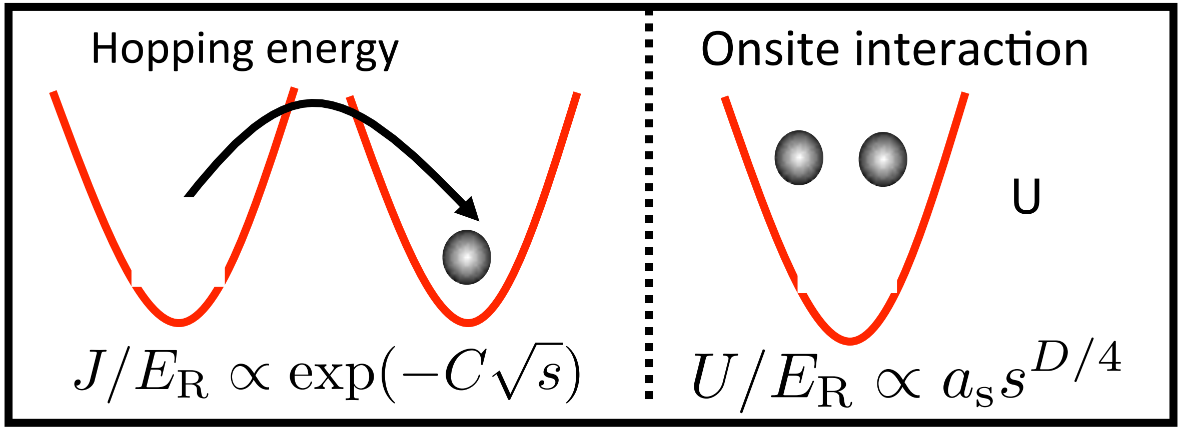


- Controllability
- Cleanness

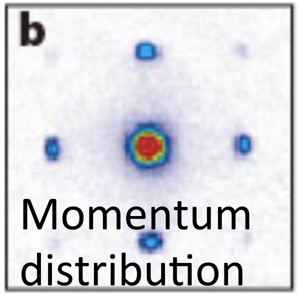
2.2. Bose-Hubbard model

$$\hat{H} = -J \sum_{\langle j,l \rangle} \hat{b}_j^\dagger \hat{b}_l + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1)$$

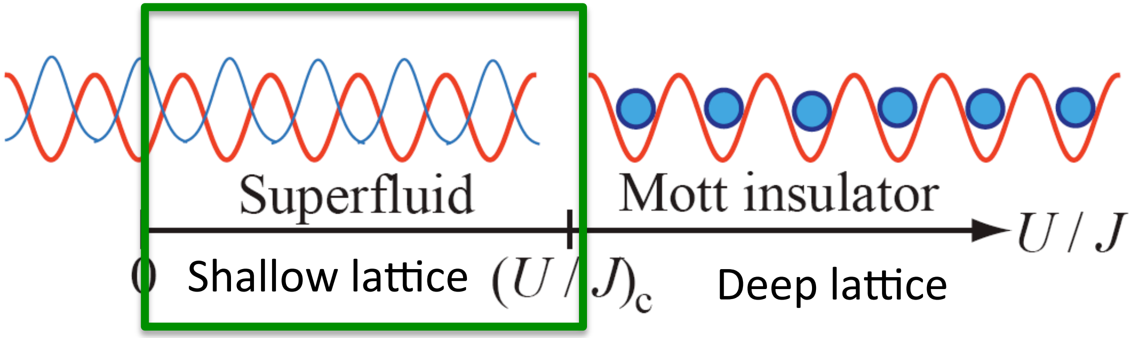
M. P. A. Fisher et al., PRB (1989)
D. Jaksch et al., PRL (1998)

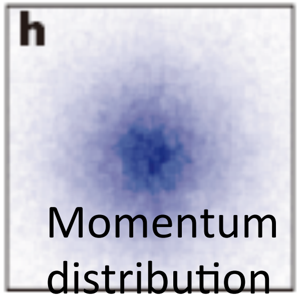


When the filling factor ν ≡ N/L is an integer, the SF to MI transition occurs with increasing U/J as demonstrated by Greiner et al., Nature (2002).



Momentum distribution at $V_0 = 3E_R$

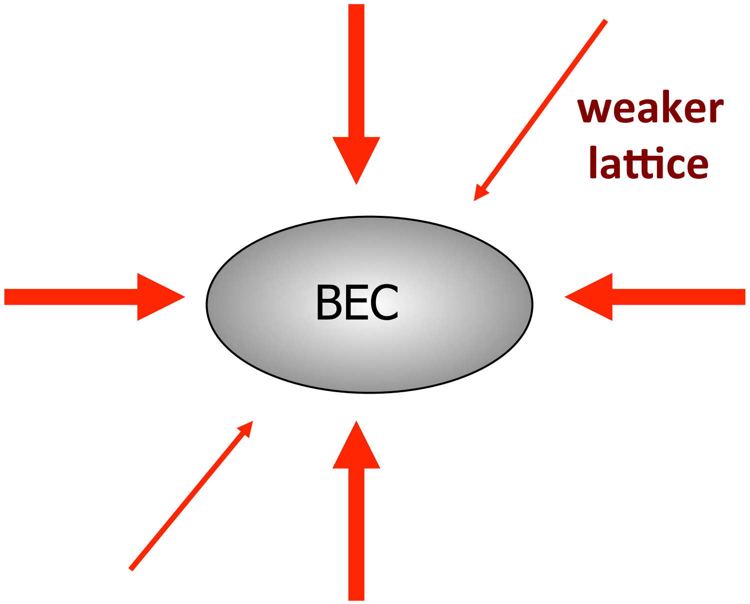




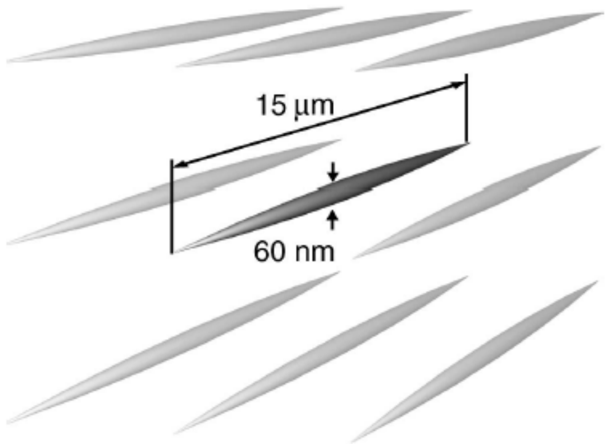
Momentum distribution at $V_0 = 20\ E_R$

We focus on the SF region up to the Mott transition in one dimension.

2.3. 1D gases produced by optical lattices



A 2D array of 1D Bose gases
H. Moritz et al., PRL (2003)

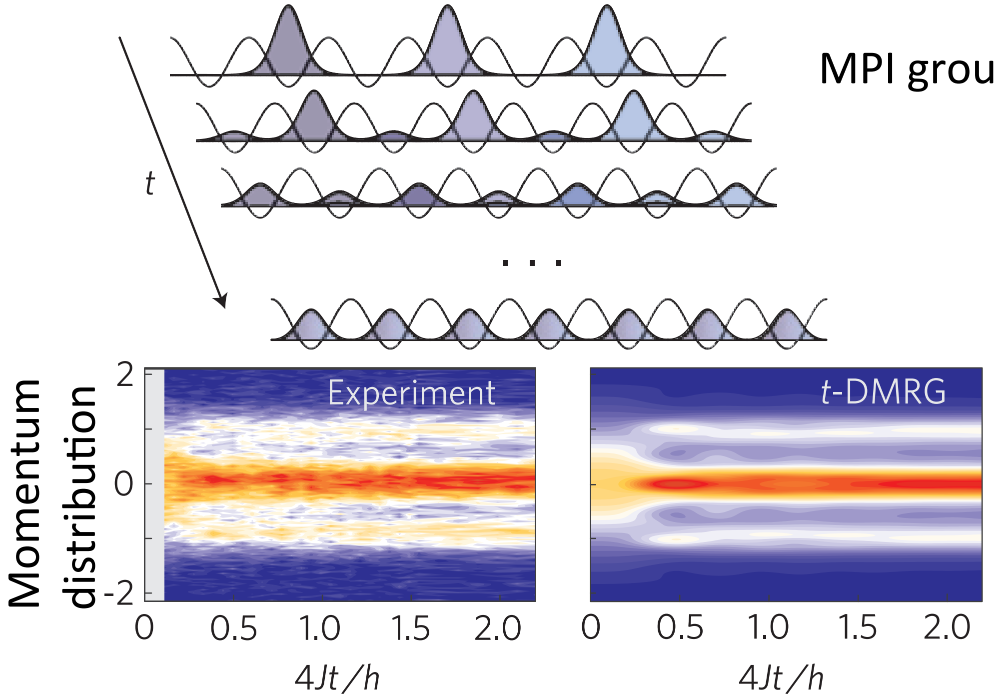


$$\hbar\omega_\perp \gg \mu,\ k_\mathrm{B}T$$

Advantages of one-dimensional systems:

- Stronger quantum fluctuations
- Reliable analytical and numerical methods are available
  e.g. Bosonization approach, Bethe ansatz,
  Density matrix renormalization group (DMRG)
  Quantum Monte Carlo (even for fermions)

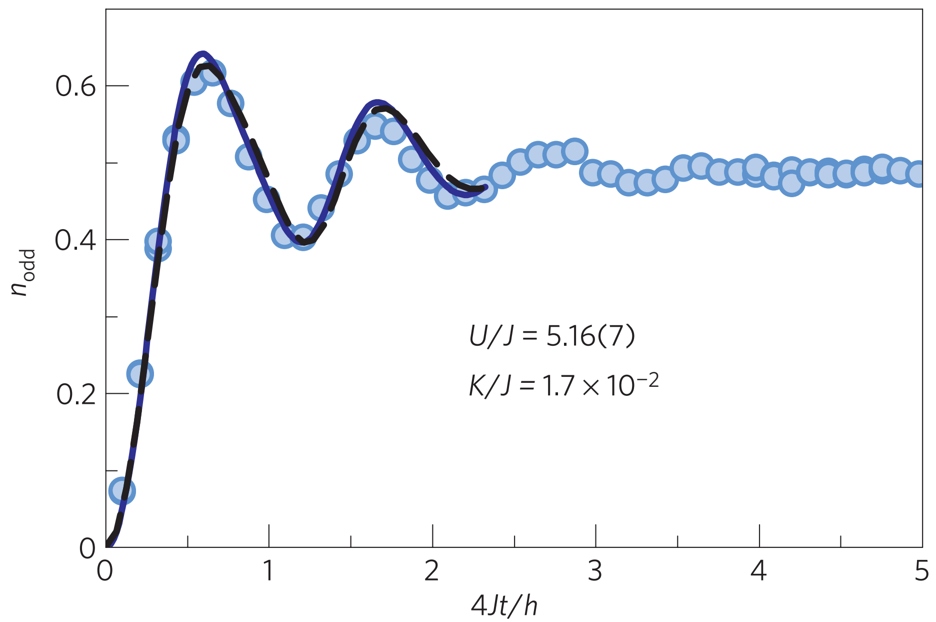
2.4. TEBD versus experiments



MPI group: I. Trotzky et al., Nat. Phys. 8, 325 (2012)

Quantitative comparison between TEBD and cold-atom experiment without free parameters !!!

TEBD agrees very well with the experiments.



Experiments can go further than TEBD …

Experiment

tDMRG (only nearest neighbor hopping)

tDMRG (upto next nearest hopping)

2.5. Applications of TEBD/tDMRG

- Dynamic correlation functions

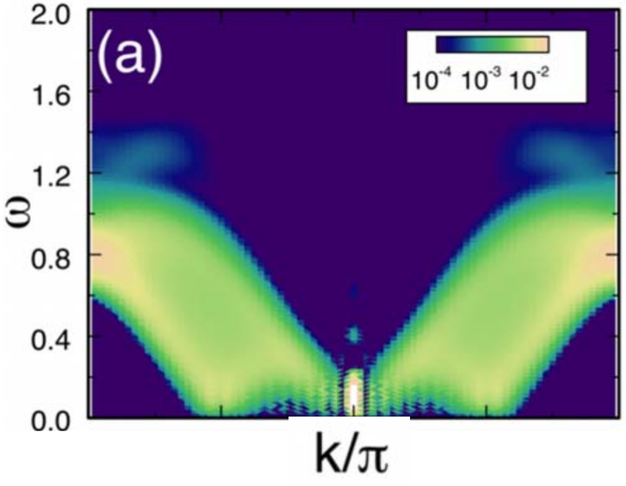
White and Affleck, PRB (2008)
Feiguin and Huse, PRB (2009) etc

$$G(x-x',t-t') = i\langle O(x',t')O^\dagger(x,t)\rangle$$

Fourier transform → Spectral weight

$$I(k,\omega) = \sum_n |\langle\psi_n|O_k|\psi_0\rangle|^2\delta(\omega - E_n + E_0)$$

e.g. Dynamic structure factor for the Hubbard model



- Non-equilibrium transport

Al-Hassanieh et al., PRB (2006); Feiguin et al., PRL (2008)
Heidrich-Meisner et al., EPJB (2009); Langer et al., PRB (2009);
Heidrich-Meisner et al., PRB (2009); Danshita and Clark, PRL (2009);
Montangero et al., PRA (2009) etc

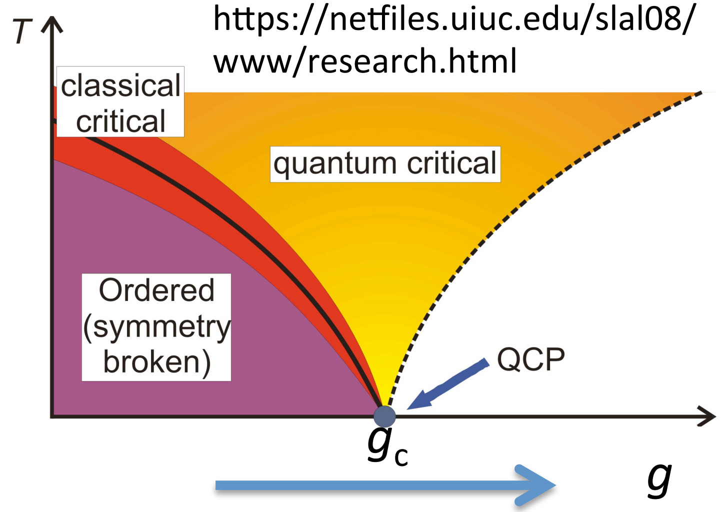
- Quench dynamics,
  especially across quantum critical points

Kollath et al., PRL (2007); Manmana et al., PRL (2007) etc

$$H(g_i < g_c) \rightarrow H(g_f > g_c)$$

quench !!

https://netfiles.uiuc.edu/slal08/www/research.html



and more!!

2.6. Macroscopic quantum tunneling (MQT)

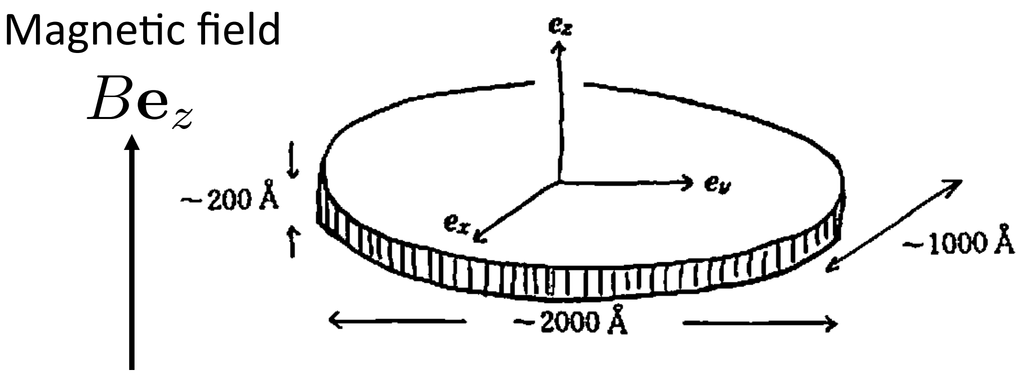
Tunneling of macroscopic (collective) variables

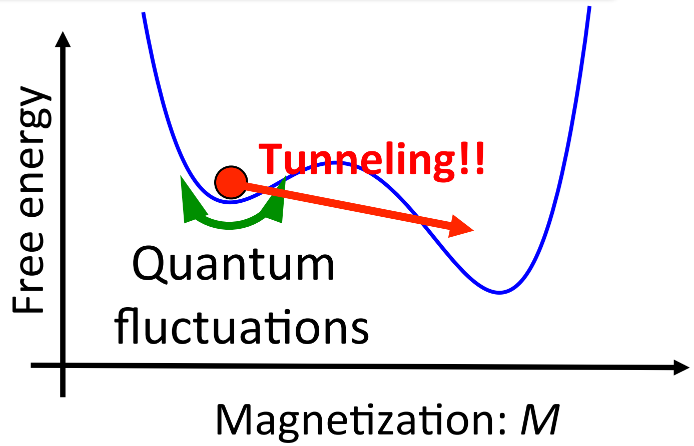
See e.g. a book by Takagi (2002)

Macroscopic quantum phenomenon of the second kind

Phenomenon	Macroscopic variable
Collapse of Bose condensates with attractive interactions	Radius of the condensate
Spin flip of single-domain ferromagnets	Magnetization
Phase separation of ^{3}He-^{4}He mixtures	Radius of a ^{3}He bubble
Superflow decay via phase slips	Superflow velocity

Sketch of a single-domain ferromagnet





2.7. Traditional method: Instanton technique

Coleman, PRD (1977);
Callan and Coleman, PRD (1977) ;
Polyakov, Nucl. Phys. B (1977)

In the semiclassical limit ($\hbar \ll s_I$),

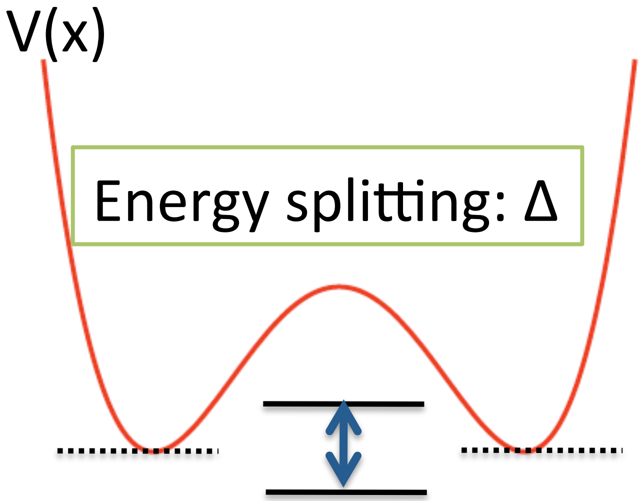
① For a coherent oscillation
in a symmetric double well

Energy splitting:

$$\Delta = 2\hbar A \sqrt{\frac{s_I}{2\pi\hbar}}[1 + O(\hbar)] \exp\left(-\frac{s_I}{\hbar}\right)$$

s_I : Instanton action

A : Coefficient from Gaussian fluctuations

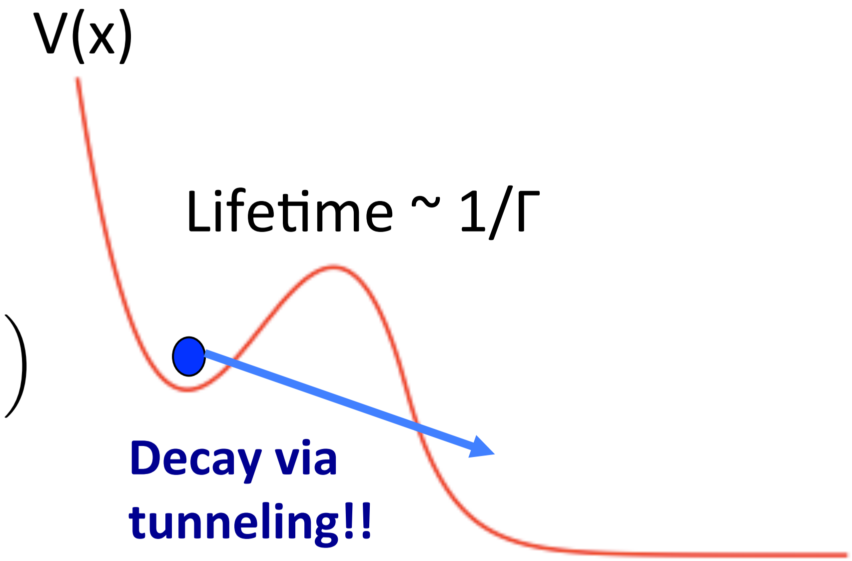


② For a decay of a metastable state
in a "bumpy" potential

Decay rate:

$$\Gamma = \hbar A \sqrt{\frac{s_B}{2\pi\hbar}}[1 + O(\hbar)] \exp\left(-\frac{s_B}{\hbar}\right)$$

s_B : Bounce action



Pros of TEBD/tDMRG over instanton

- More accurate
- Accessible to the region far away from the semi-classical limit
- Any observables can be calculated during real-time evolution

Cons

- Restricted to 1D systems
- Difficult to access the strictly semiclassical limit

2.8. Purposes of this work

We study the quantum nucleation of phase slips of the 1D Bose-Hubbard model in order to present the first application of TEBD to macroscopic quantum tunneling.

Advantages of this system:

1. Nucleation rate can be calculated by the instanton method in the quantum rotor regime ($\nu \gg 1$)

2. The effective Planck's constant is well defined and can be tuned by the Bose-Hubbard parameters !!!

$$h_{\mathrm{e}} = \sqrt{U/(\nu J)}$$

U: onsite interaction, *J*: hopping

ν : atom number per site (filling factor)

3. Relevant to experiments of ultracold atomic gases

Note: Quantum nucleation of phase slips are originally suggested in the context of superconducting nanowires to explain supercurrent decay.
See, e.g., K. Yu. Arutyunov et al., Phys. Rep. (2008)

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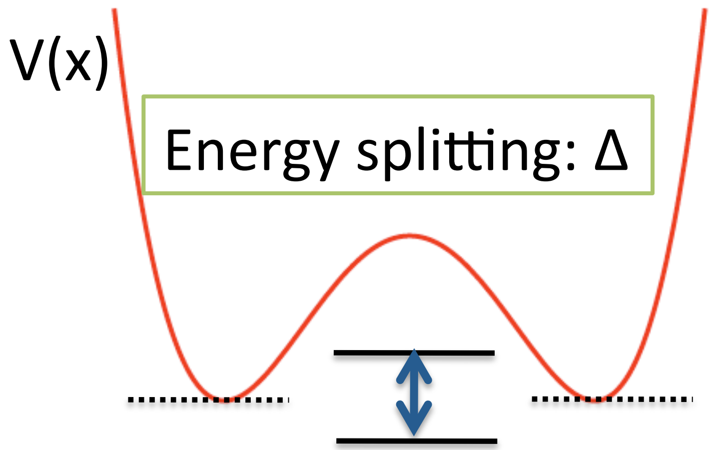


3.1. Overview of coherent phase slips

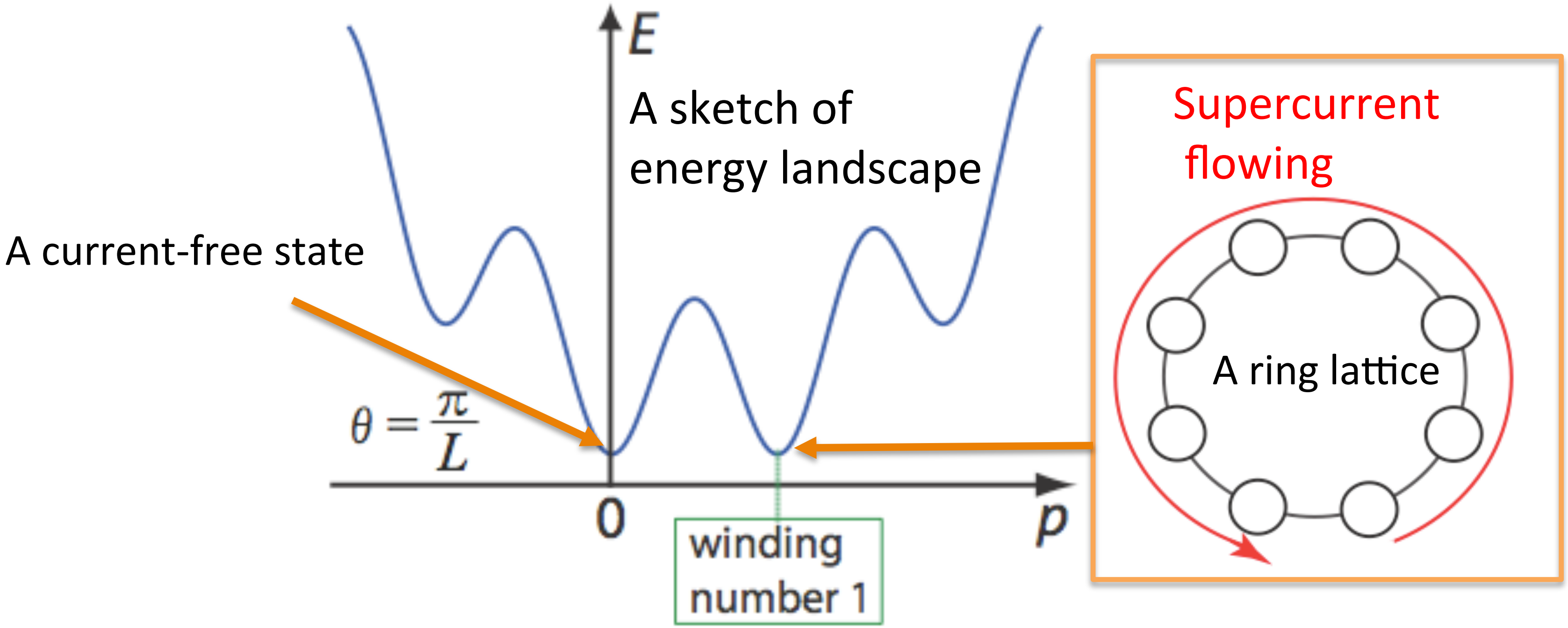
Bose-Hubbard model with a phase twist:

$$\hat{H} = -J \sum_{j=1}^{L} (e^{-i\theta} \hat{b}_j^\dagger \hat{b}_{j+1} + \text{h.c.}) + \frac{U}{2} \sum_{j=1}^{L} \hat{n}_j (\hat{n}_j - 1).$$

U : onsite interaction, J : hopping energy, θ : phase twist

L : number of lattice sites, N : total number of particles

The (quasi-)momentum is discretized: p=2π n/L



Our target is the tunneling between the states with winding number n=0 and n=1.

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Bose-Hubbard model with a phase twist:

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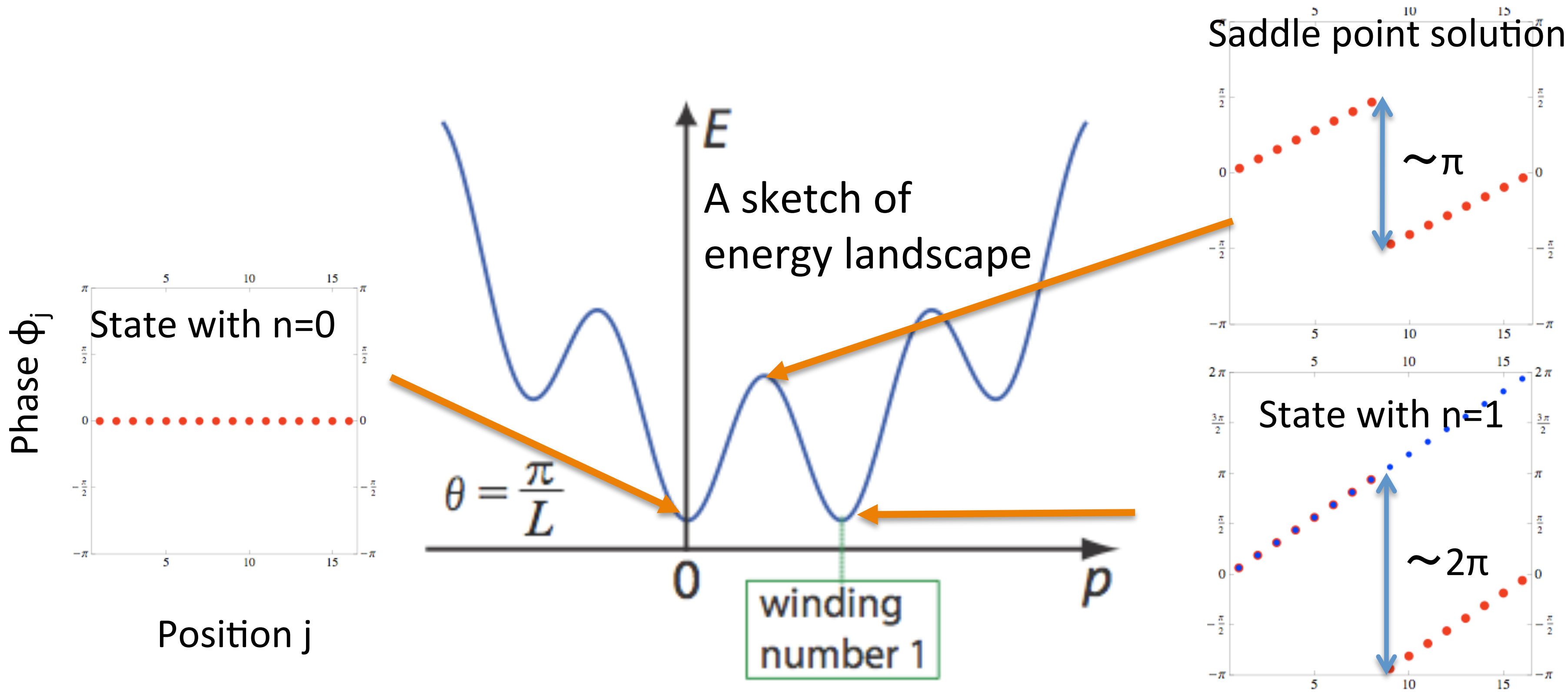


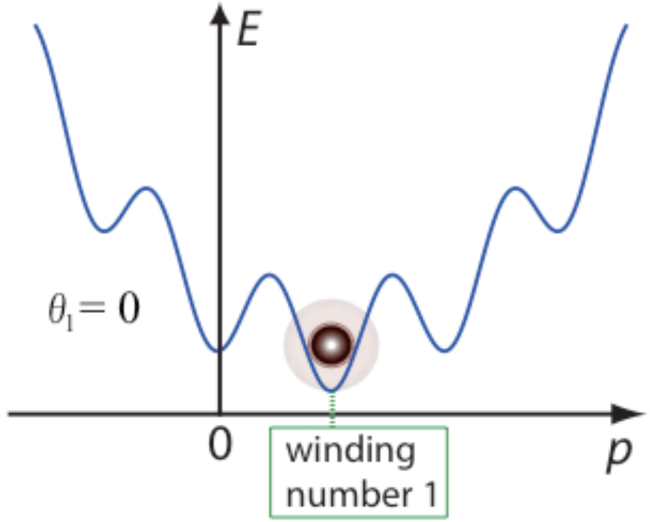
The phase-kink slips during the tunneling process

3.2. How to simulate the supercurrent dynamics

① Imaginary time evolution for $\theta = 2\pi/L$

↓

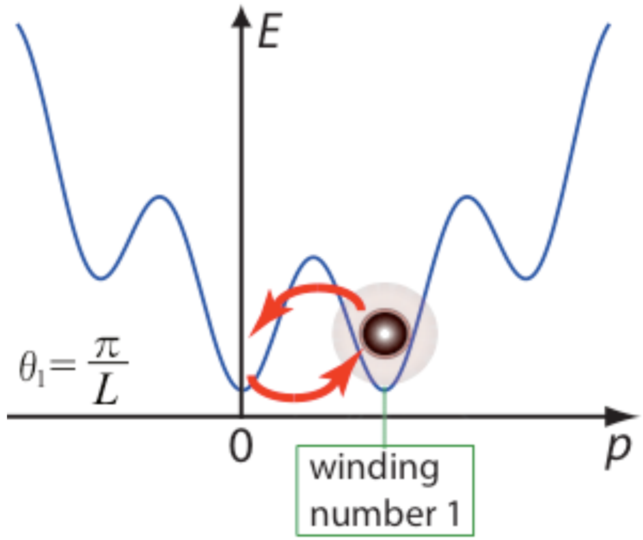
We obtain a state with n=1, $|\Phi_{n=1}\rangle$, where n is the winding number.



② Setting $\theta = \theta_1 = \pi/L$,

we calculate $e^{-iHt}|\Phi_{n=1}\rangle$

and necessary observables.



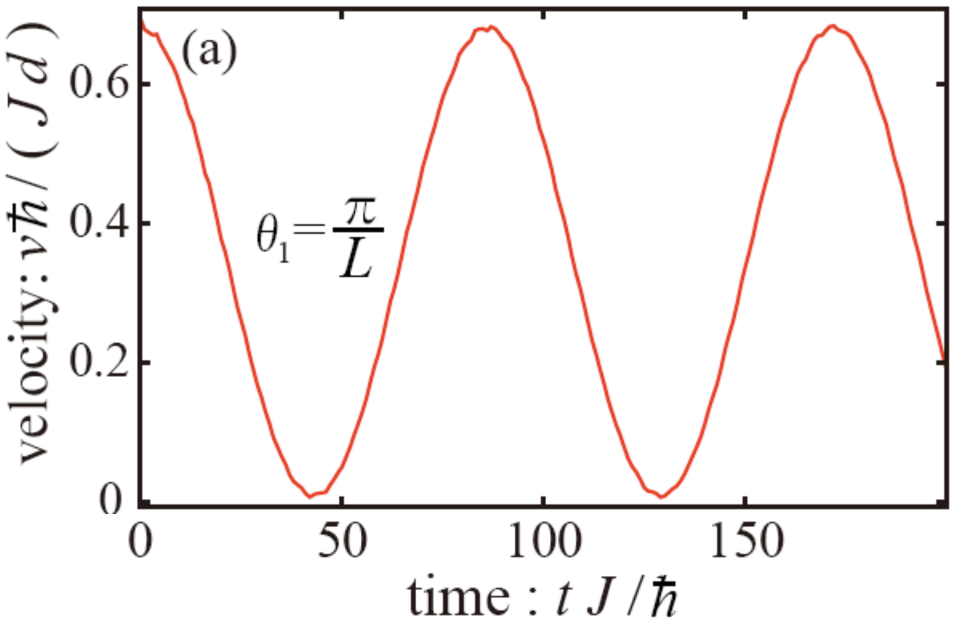
3.3. Time evolution of the flow velocity

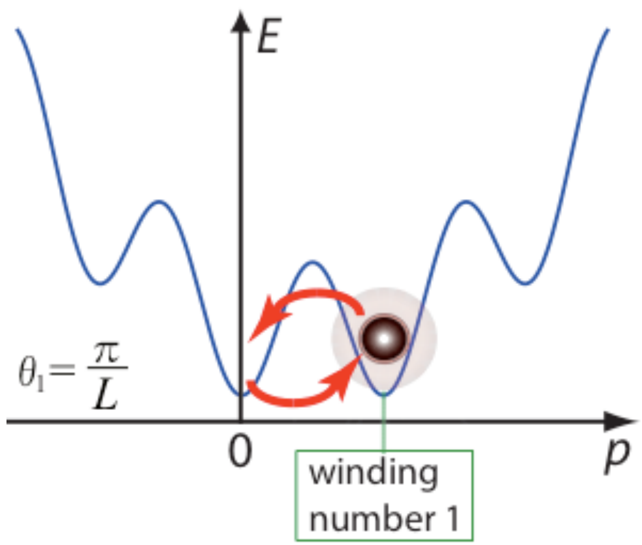
d: lattice spacing

U/J=2.5, (L=16, N=16)

Flow velocity: $v = \frac{Jd}{i\hbar N} \sum_j \langle \hat{b}_j^\dagger \hat{b}_{j+1} - h.c. \rangle$

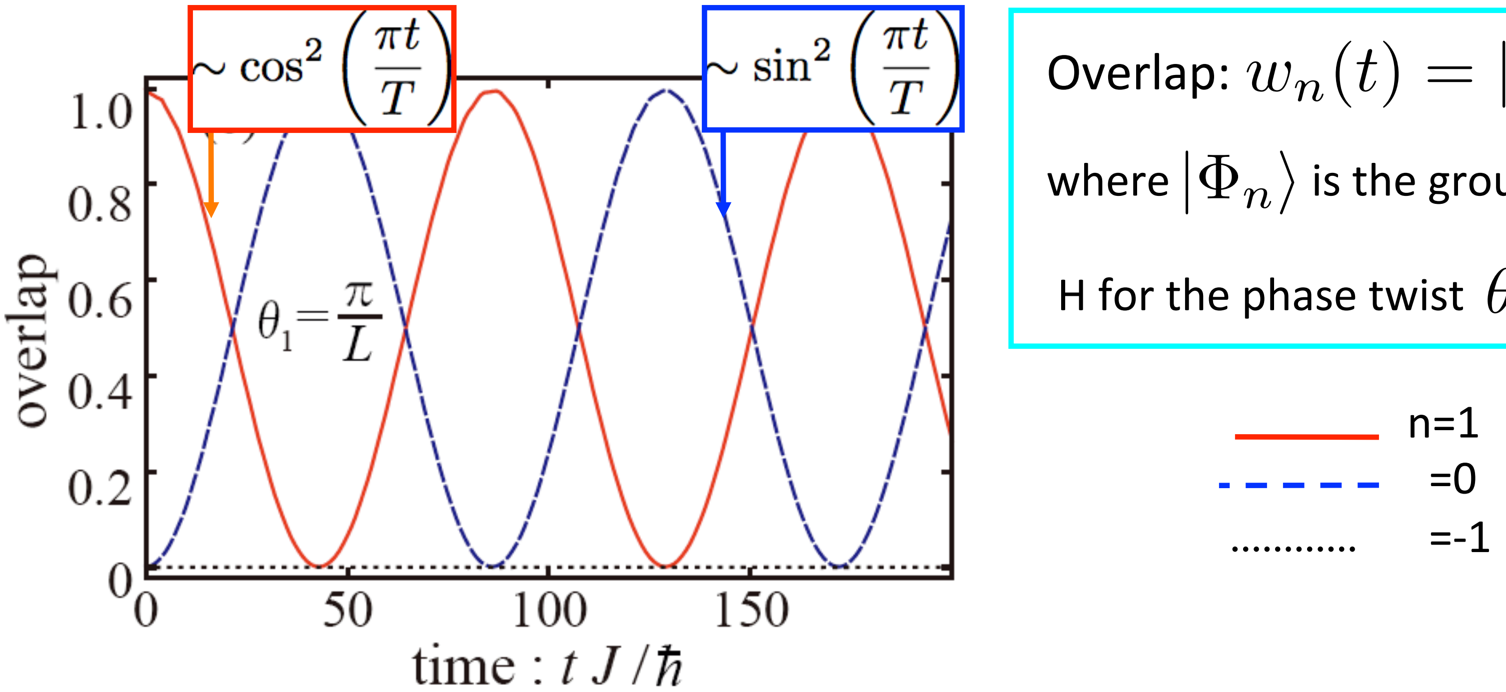
$|\Phi_0\rangle$ and $|\Phi_1\rangle$ are degenerate.





Coherent oscillation between the velocity v(t=0) and 0 !

3.4. Overlaps and momentum occupations



Overlap: $w_n(t) = |\langle \Phi_n | \Psi(t) \rangle|^2$

where $|\Phi_n\rangle$ is the ground state of

H for the phase twist $\theta = 2\pi n / L$

The wave function is approximately described by a cat state,

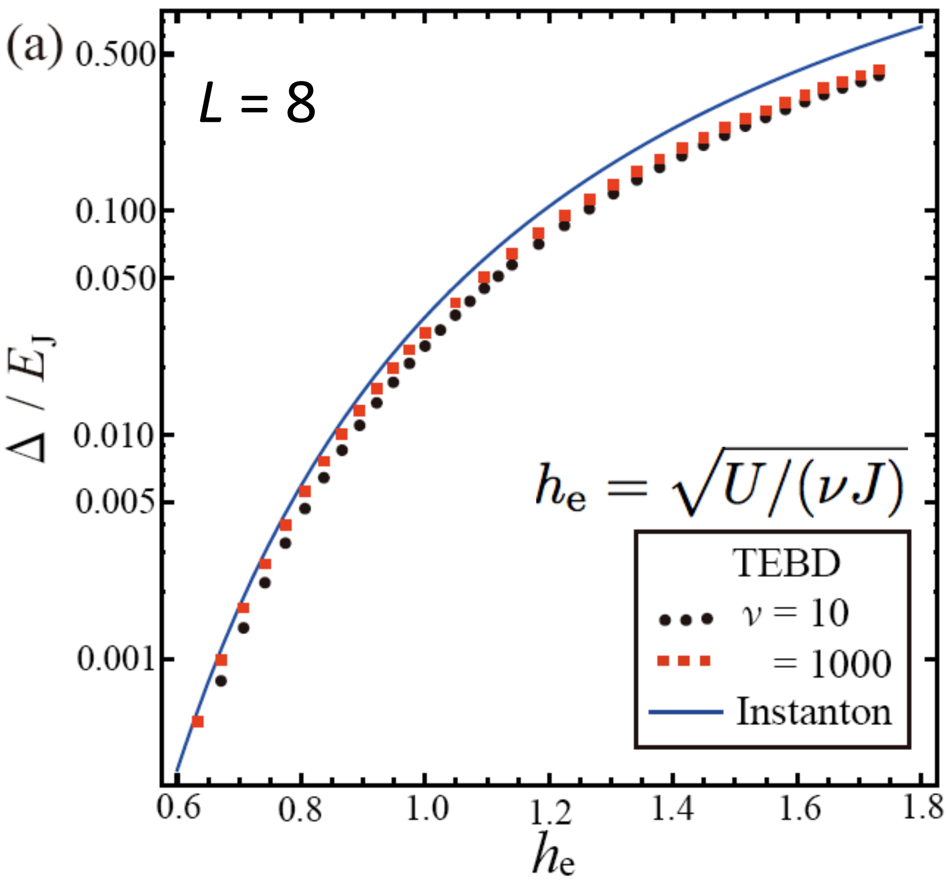
$$|\Psi(t)\rangle \simeq \cos\left(\frac{\pi t}{T}\right)|\Phi_1\rangle + i \sin\left(\frac{\pi t}{T}\right)|\Phi_0\rangle$$

The coherent oscillation is due to **MQT**!

T : period of the oscillation

Energy splitting: $\Delta = \dfrac{2\pi\hbar}{T}$

3.5. Comparison between instanton and TEBD

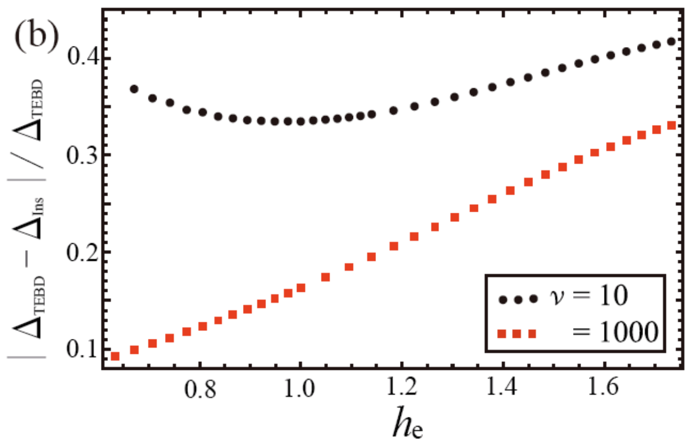


Instanton energy splitting for ν>>1:

$$\frac{\Delta_{\rm Ins}}{E_{\rm J}} = 2LA\sqrt{\frac{\tilde{s}_I}{2\pi h_{\rm e}}}\exp\left(-\frac{\tilde{s}_I}{h_{\rm e}}\right)$$

For *L*=8, $\tilde{s}_I = 7.363,\ \ A = 3.06$

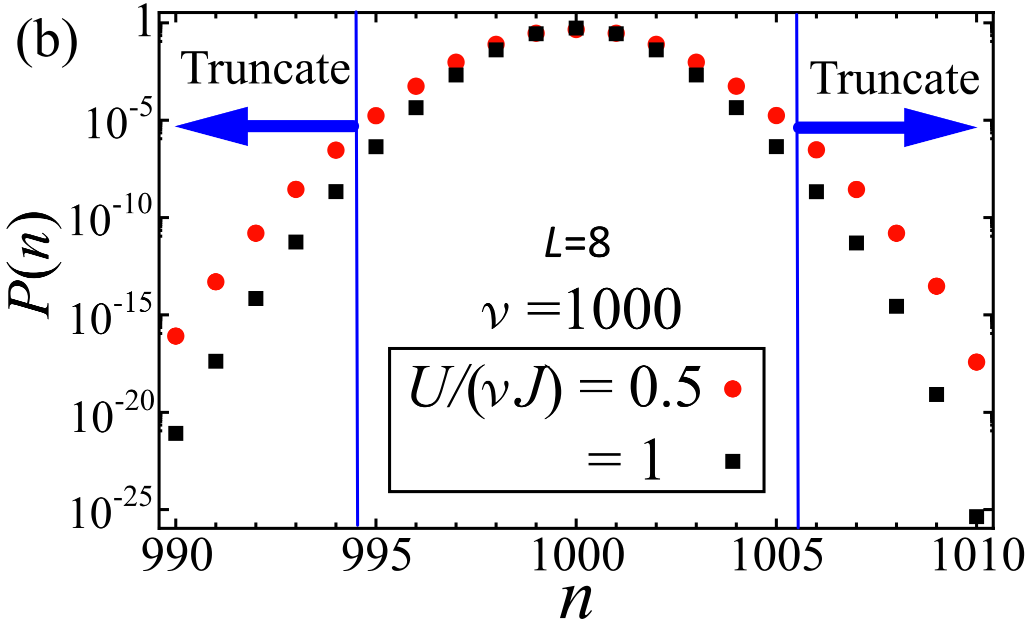
where $\nu = N/L\,,E_{\rm J} = \sqrt{\nu J U}$

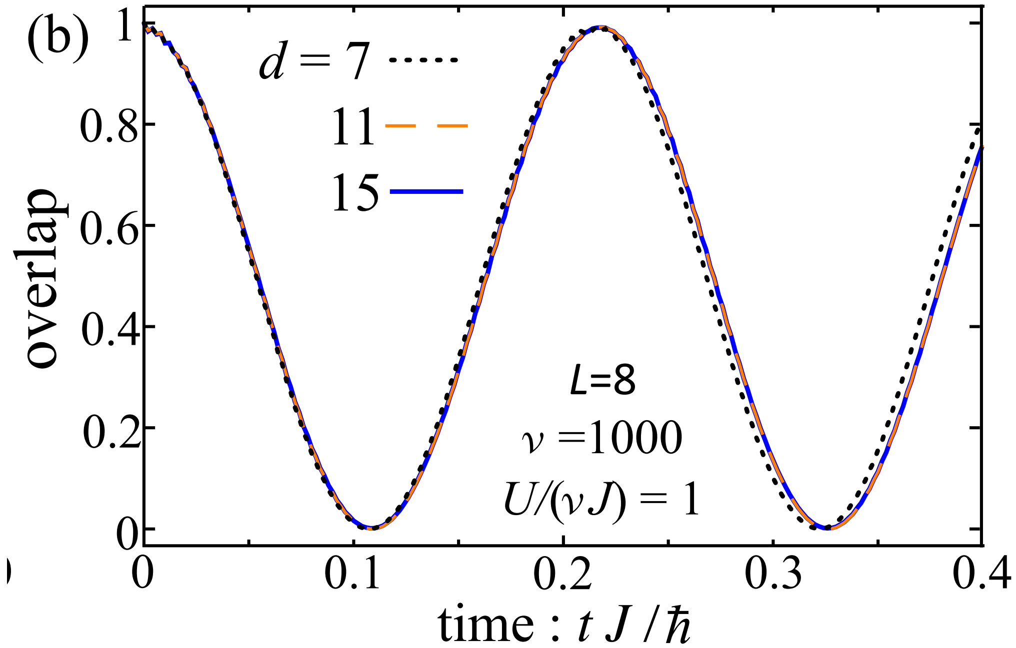


For $\nu = 1000$, as h_e decreases the error also decreases such that it is within 10% when $h_e \lesssim 0.7$.

The error for $\nu = 10$ is significantly larger and does not depend even monotonically on h_e. This means that at this filling the mapping to the quantum rotor model is invalid.

Note: Bose-Hubbard model with high filling factors





Outline:

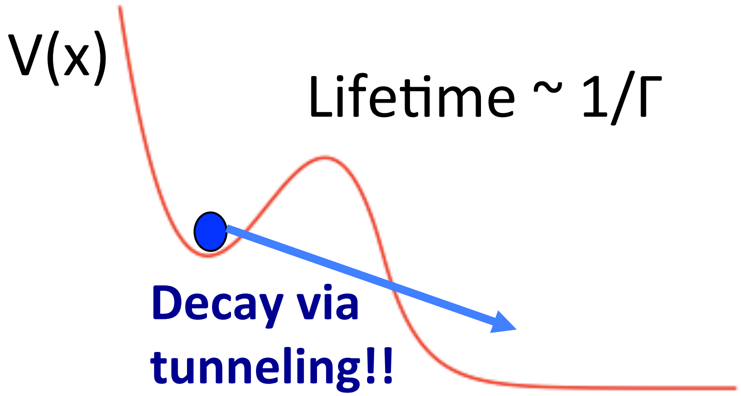
1. Time-evolving block decimation (TEBD)

2. Cold atom systems and motivation of this work

3. Coherent quantum phase slips:
   Quantitative comparison with instanton techniques
   Danshita and Polkovnikov, PRB 82, 094304 (2010)

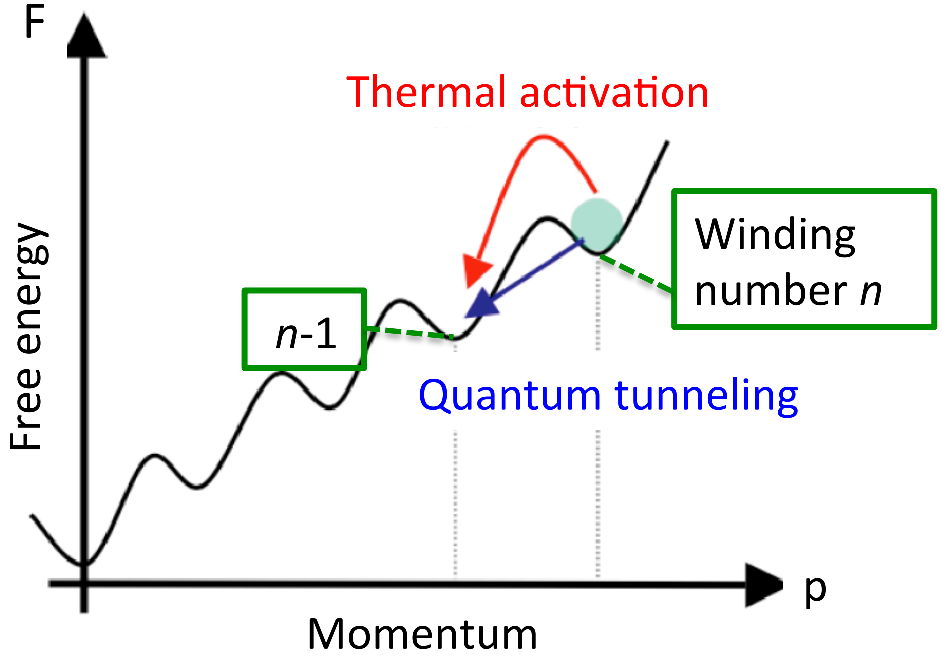
4. Superflow decay via quantum phase slips:
   Testing a scaling formula
   Danshita and Polkovnikov, PRA 85, 023638 (2012)

5. Conclusions



Note:
Similar dynamics have been studied using iTEBD.
Schachenmayer, Pupillo, and Daley, NJP (2010)

4.1. Overview of supercurrent decay via phase slips

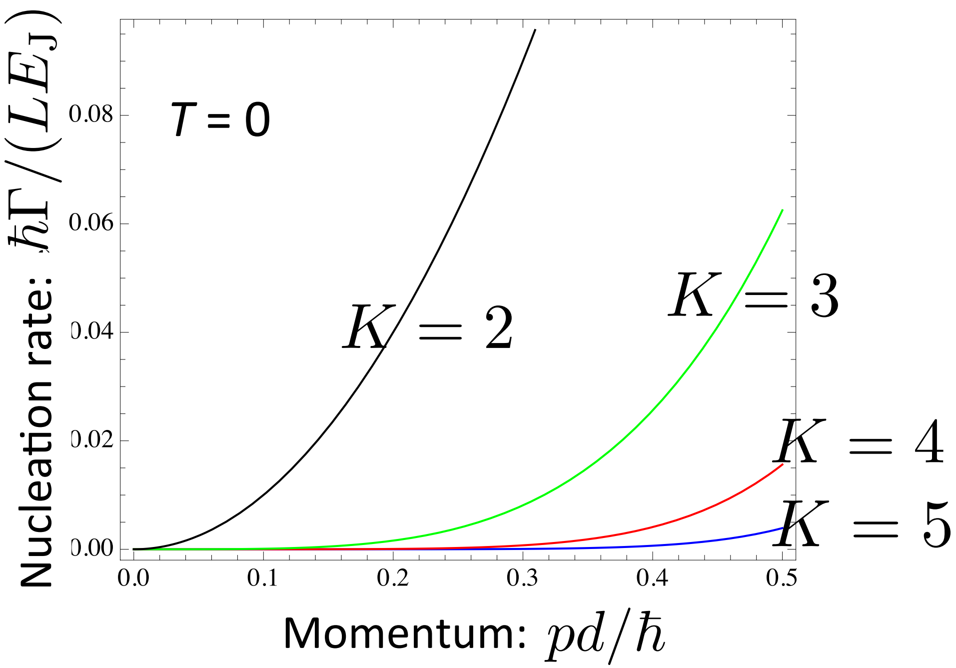


The instanton method gives the nucleation rate for a phase slip:

$$\Gamma \propto L \times p^{2K-2}$$

for small p

K: Luttinger parameter



1/*K* quantifies the strength of quantum fluctuations from classical wave.

▪ Tomonaga-Luttinger liquid

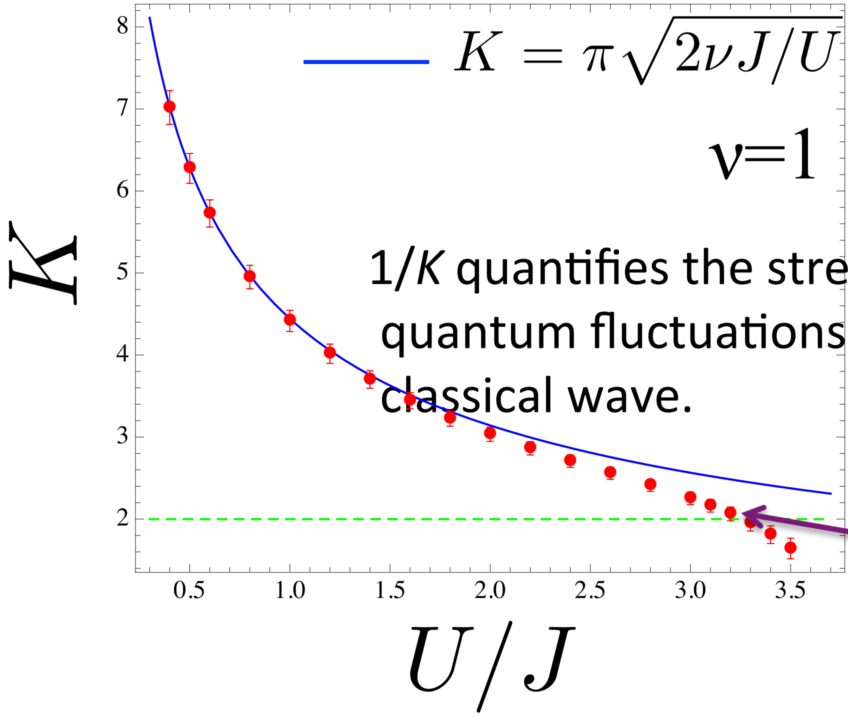
Euclidean action for the TL liquid:

$$S_{\rm TL} = \frac{\hbar K}{2\pi}\int dx \int d\tau \left[\frac{1}{c_{\rm s}}\left(\frac{\partial\theta}{\partial\tau}\right)^2 + c_{\rm s}\left(\frac{\partial\theta}{\partial x}\right)^2\right]$$

K : TL parameter

θ : phase of the bosonic field, $c_{\rm s}$: sound velocity,

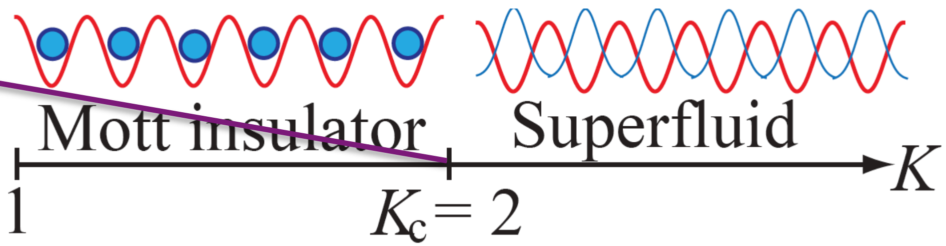
If one starts with the Bose-Hubbard model and $U/(\nu J) \lesssim 1$,



$$c_{\rm s} \simeq \sqrt{2\nu J U}\, d/\hbar$$

1/*K* quantifies the strength of quantum fluctuations from classical wave.

$$K \simeq \pi\sqrt{2\nu J/U} \sim \frac{\text{healing length}}{\text{interparticle distance}}$$

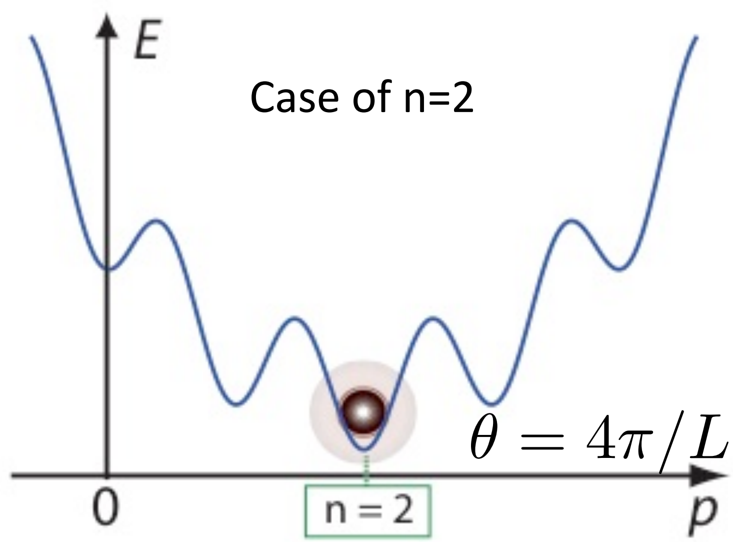


4.2. How to simulate the supercurrent dynamics

① Imaginary time evolution for $\theta = 2\pi n/L$

↓

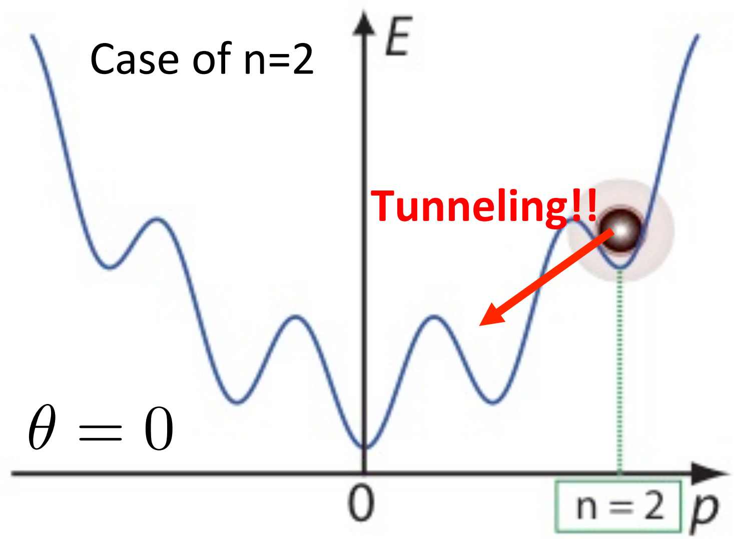
We obtain a state with n, $|\Phi_n\rangle$, where n is the winding number.



② Setting $\theta = 0$,

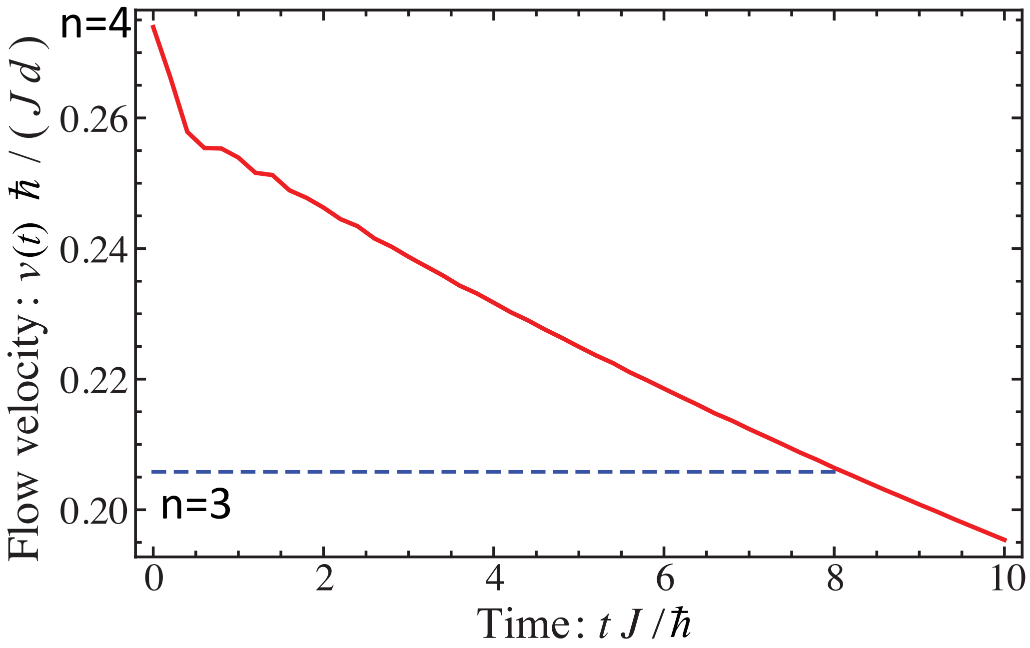
we calculate $e^{-iHt}|\Phi_n\rangle$

and necessary observables.



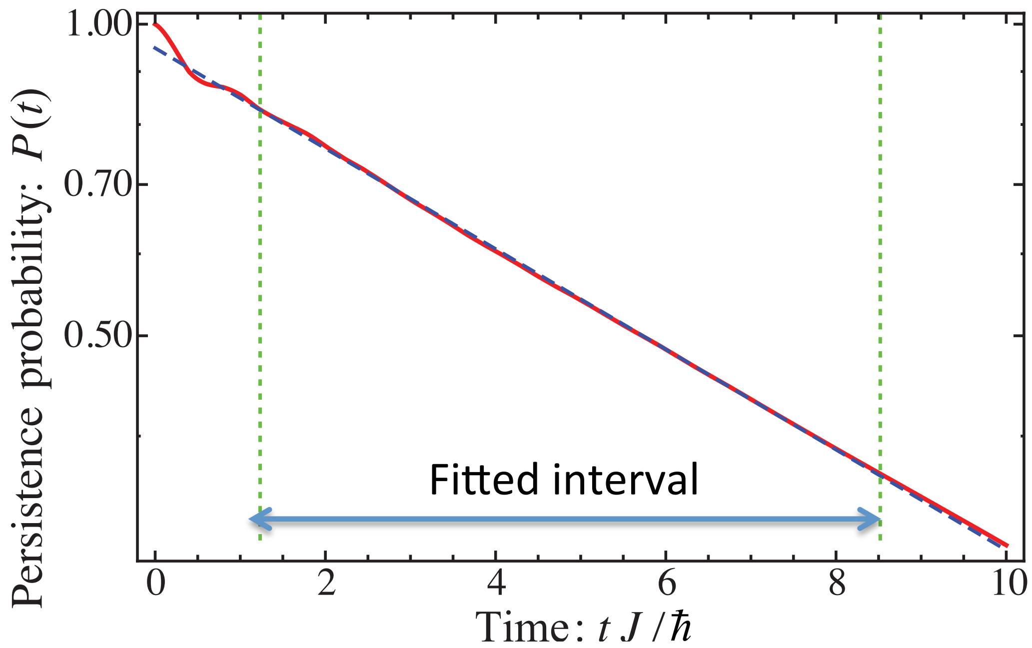
4.3. Extracting the nucleation rate Γ

$$U/J = 3$$
$$L = N = 160$$
$$n = 4\,(pd = \pi/20)$$



Flow velocity:

$$v = \frac{Jd}{i\hbar N}\sum_j \langle \hat{a}_j^\dagger \hat{a}_{j+1} - \text{h.c.}\rangle$$



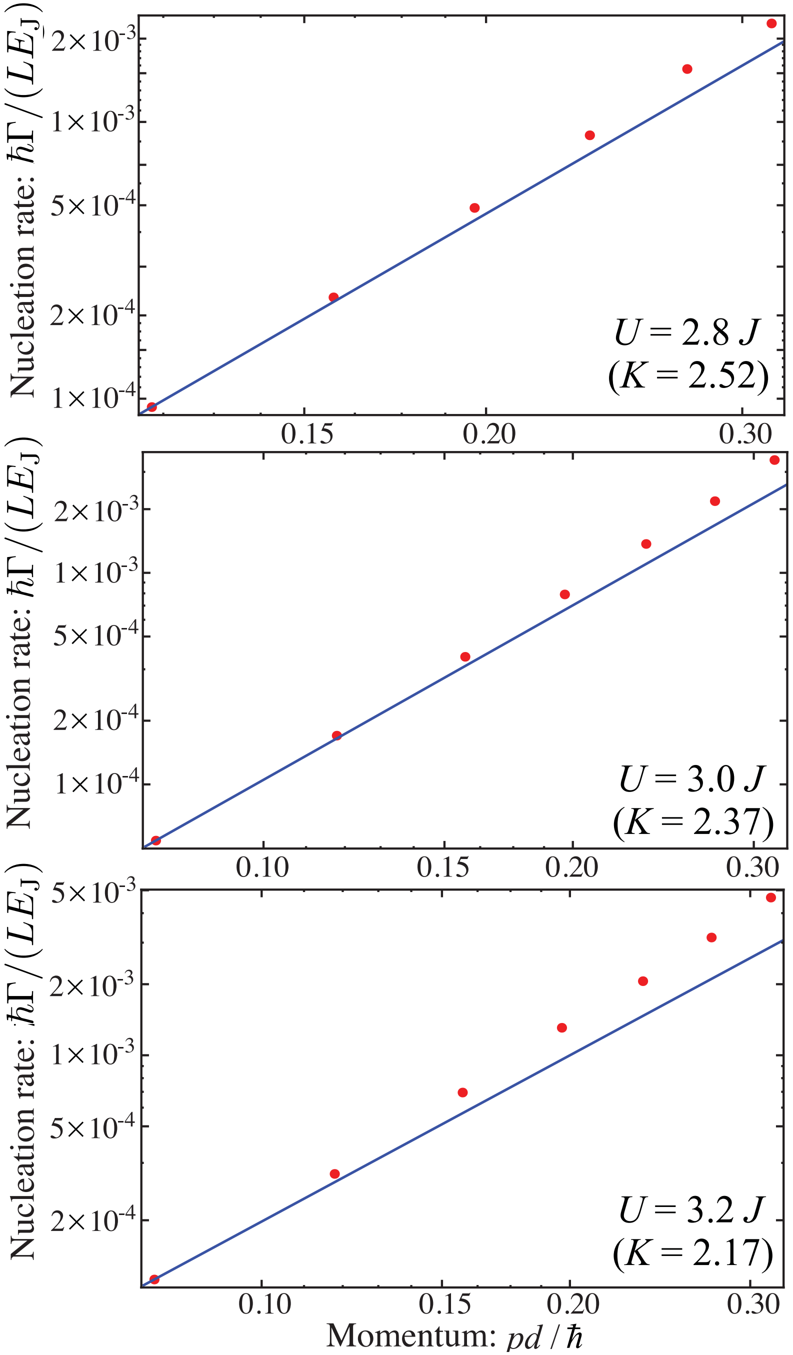
Persistence probability:

$$P(t) = |\langle\Psi(t)|\Psi(t=0)\rangle|^2$$

Fitting function:

$$f(t) = A\exp(-\Gamma t)$$

4.4. The nucleation rate Γ vs momentum p



Scaling formula from instanton:

$$\Gamma \propto L \times p^{2K-2}$$

for small p

The Luttinger parameter is taken from DMRG results by Kühner et al., PRB (2000)

TEBD results obey the scaling formula !!

Deviation for U=3.2J is relatively large, probably because it is close to the quantum phase-transition point (K=2).

5. Conclusions

We have successfully applied TEBD to a problem of macroscopic quantum tunneling.

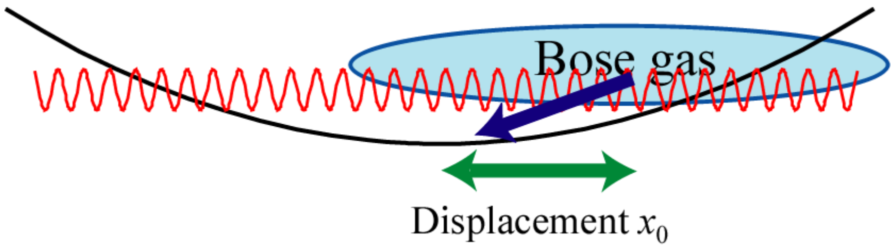
- We have reviewed TEBD for systems with periodic boundaries.
- From the persistence probability $P(t) = |\langle\Psi(t)|\Psi(t=0)\rangle|^2$ we have calculated the nucleation rate of quantum phase slips both for coherent oscillations and decay of metastable states.
- TEBD results are in good agreement with the instanton results in the semi-classical region.

Other twists of quantum phase slips:

- Determining the critical point for the superfluid-Mott insulator transition from the nucleation rate

Danshita and Polkovnikov, PRA 84, 063637 (2011)

- Interpreting an experiment on cold-atom transport [Fertig et al., PRL (2005)] in terms of quantum phase slips



Danshita, in preparation