RPA Studies of the Dynamic Response of Ultracold Atoms in 1D Optical Lattices

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Outline

- Bose-Hubbard Model & Spectroscopy
- Equations of Motion (EOM)
- Random Phase Approximation (RPA)...
- ... and the Bose-Hubbard Model
- Results
Bose-Hubbard Model

\[ H = -J \sum_{i=1}^{I} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2} \sum_{i=1}^{I} n_i(n_i - 1) \]

\( I \) sites, \( N \) particles, interaction strength \( U \), tunneling strength \( J \)

\( T = 0 \)

optical lattice
Bose-Hubbard Model

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\( I \) sites, \( N \) particles, interaction strength \( U \), tunneling strength \( J \)

\( T = 0 \)

optical lattice

tunneling

on-site interaction

3 sites, 3 particles, interaction strength, tunneling strength
Bose-Hubbard Model

\[ H = -J \sum_{i=1}^{I} (a_{i}\dagger a_{i+1} + a_{i+1}\dagger a_{i}) + \frac{U}{2} \sum_{i=1}^{I} n_{i}(n_{i} - 1) \]

\( I \) sites, \( N \) particles, interaction strength \( U \), tunneling strength \( J \)

\( T = 0 \)

optical lattice
Bose-Hubbard Model

$I$ sites, $N$ particles, interaction strength $U$, tunneling strength $J$

\[ H = -J \sum_{i=1}^{I} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2} \sum_{i=1}^{I} n_i(n_i - 1) \]

number-state representation

\[ |\phi\rangle = \sum_{\{n_1, \ldots, n_I\}} c_i^\phi |n_1, \ldots, n_I\rangle, \quad \sum_{i} n_i = N \]
Spectroscopy via Lattice Modulation

static lattice potential

\[ V(x) = V_0 \sin^2(kx) \]
Spectroscopy via Lattice Modulation

static lattice potential

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amplitude modulated lattice

\[ V(x, t) = V_0[1 + F \sin(\omega t)] \sin^2(kx) \]
Spectroscopy via Lattice Modulation

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

amplitude modulated lattice
$V(x, t) = V_0 [1 + F \sin(\omega t)] \sin^2(kx)$

exact time-evolution

$I = N = 10$
$U/J = 20$

Spectroscopy via Lattice Modulation

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amplitude modulated lattice
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linearized Hamiltonian
\[ H_{\text{lin}}(t) = H_0 + \sin(\omega t)(\lambda H_0 - \kappa H_J) \]

Spectroscopy via Lattice Modulation

static lattice potential

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linearized Hamiltonian

\[ H_{\text{lin}}(t) = H_0 + \sin(\omega t) \left( \lambda H_0 - \kappa H_J \right) \]

transition amplitudes

\[ |\langle 0 | \kappa H_J | \nu \rangle|^2 \]
From the Schrödinger Equation to the Equations of Motion (EOM)

Schrödinger equation
\[ H |\nu\rangle = E_\nu |\nu\rangle \]

phonon operators
\[ Q^\dagger_\nu |0\rangle = |\nu\rangle \]
\[ Q_\nu |0\rangle = 0 \]

variations \( \delta Q \)
exhaust the whole Hilbert space

\[ \langle 0 | [\delta Q, [H, Q^\dagger_\nu]] |0\rangle = (E_\nu - E_0) \langle 0 | [\delta Q, Q^\dagger_\nu] |0\rangle \]

- “complicated” reformulation of the Schrödinger equation
- requires the groundstate

- offers “handles” for approximations: phonon operators and restriction of the variations
Approximation of the Phonon Operators

systematic approach
expand phonon operators in terms of particle-hole (de-) excitations $c_k^\dagger (c_k)$

simplest expansions of phonon operators

Tamm-Dancoff Approximation (TDA)

$$Q_{\nu}^\dagger = \sum_k X_k^{(\nu)} c_k^\dagger$$

1 particle - 1 hole excitations

Random Phase Approximation (RPA)

$$Q_{\nu}^\dagger = \sum_k X_k^{(\nu)} c_k^\dagger - \sum_k Y_k^{(\nu)} c_k$$

1 particle - 1 hole excitations + de-excitations

higher RPAs
Particle-Hole Operators and the Bose-Hubbard Model

- **Filling factor**: $N/I = 1$
- **Strongly interacting**: $U \gg J$

**Ground-state approximation**

$|\text{RPA, } 0\rangle \approx |1, 1, \ldots, 1\rangle$
Particle-Hole Operators and the 
Bose-Hubbard Model

system properties
- filling factor \( \frac{N}{I} = 1 \)
- strongly interacting \( U \gg J \)

naive ansatz
- \( c_{ij} = a_i^\dagger a_j \)
- \( c_{ij} = a_j^\dagger a_i \)

ground-state approximation
- \( |\text{RPA}, 0\rangle \approx |1, 1, \cdots, 1\rangle \)
Particle-Hole Operators and the Bose-Hubbard Model

system properties

- filling factor $N/I = 1$
- strongly interacting $U \gg J$

naive ansatz

\[
\begin{align*}
\hat{c}_{ij} &= \hat{a}_{i}^\dagger \hat{a}_j \\
\hat{c}_{ij} &= \hat{a}_{j}^\dagger \hat{a}_i
\end{align*}
\]

just hopping in opposite directions

ground-state approximation

\[|\text{RPA}, 0\rangle \approx |1, 1, \ldots, 1\rangle\]
Particle-Hole Operators and the Bose-Hubbard Model

system properties
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 Particle-Hole Operators and the Bose-Hubbard Model

System properties
- filling factor $N/I = 1$
- strongly interacting $U \gg J$

Naive ansatz
$c_{ij}^{\dagger} = a_i^{\dagger} a_j$
$c_{ij} = a_j^{\dagger} a_i$

Just hopping in opposite directions

Fails

$| \text{RPA, 0} \rangle \approx |1, 1, \ldots, 1 \rangle$

Ground-state approximation

Fails

$c_{ij}^{\dagger} = \frac{1}{\sqrt{2}} a_i^{\dagger} a_i^{\dagger} a_i a_j$
creates ph-excitation

$c_{ij} = \frac{1}{\sqrt{2}} a_j^{\dagger} a_i^{\dagger} a_i a_i$
destroys ph-excitation
EOM formulated as generalized eigenproblem

\[
\begin{pmatrix}
A & B \\
-B & -A
\end{pmatrix}
\begin{pmatrix}
X_\nu \\
Y_\nu
\end{pmatrix}
=
E_{\nu 0}
\begin{pmatrix}
S & -T \\
-T & S
\end{pmatrix}
\begin{pmatrix}
X_\nu \\
Y_\nu
\end{pmatrix}
\]
Solving RPA

EOM formulated as generalized eigenproblem

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Y_\nu
\end{pmatrix}
\]

\[
A_{kl} = \langle 0 | [c_k, H, c_l^\dagger] | 0 \rangle = A_{lk},
\]

\[
B_{kl} = -\langle 0 | [c_k, H, c_l] | 0 \rangle = B_{lk},
\]

\[
S_{kl} = \langle 0 | [c_k, c_l^\dagger] | 0 \rangle = S_{lk},
\]

\[
T_{kl} = \langle 0 | [c_k, c_l] | 0 \rangle = -T_{lk}
\]

\[
[A, H, B] := \frac{1}{2} ([A, [H, B]] + [[A, H], B])
\]
Solving RPA

EOM formulated as generalized eigenproblem

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\end{pmatrix}
\begin{pmatrix}
X_{\nu} \\
Y_{\nu}
\end{pmatrix}
\]

provides

- excitation energies \( E_{\nu 0} \)
- excited states \( |E_{\nu 0}\rangle \) via \( (X_{\nu}, Y_{\nu}) \)
Solving RPA

EOM formulated as generalized eigenproblem

\[
\begin{pmatrix}
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\end{pmatrix}
\begin{pmatrix}
X_{\nu} \\
Y_{\nu}
\end{pmatrix}
=
E_{\nu 0}
\begin{pmatrix}
S & -T \\
-T & S
\end{pmatrix}
\begin{pmatrix}
X_{\nu} \\
Y_{\nu}
\end{pmatrix}
\]

provides

- excitation energies \( E_{\nu 0} \)
- excited states \( |E_{\nu 0}\rangle \) via \( (X_{\nu}, Y_{\nu}) \)

strength function

\[
R(\omega) = \sum_{(\nu)} \delta(\omega - E_{\nu 0}) |\langle 0|\kappa H J|E_{\nu 0}\rangle|^2
\]
Solving RPA

EOM formulated as generalized eigenproblem

\[
\begin{pmatrix}
A & B \\
-B & -A
\end{pmatrix}
\begin{pmatrix}
X_\nu \\
Y_\nu
\end{pmatrix}
= E_{\nu_0}
\begin{pmatrix}
S & -T \\
-T & S
\end{pmatrix}
\begin{pmatrix}
X_\nu \\
Y_\nu
\end{pmatrix}
\]

provides

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- excited states \( |E_{\nu_0}\rangle \) via \((X_\nu, Y_\nu)\)

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R(\omega) = \sum_{(\nu)} \delta(\omega - E_{\nu_0}) |\langle 0 | \kappa H_J | E_{\nu_0} \rangle|^2
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transition amplitudes

excitation energies \( E_{\nu_0} \)
excited states \( |E_{\nu_0}\rangle \) via \((X_\nu, Y_\nu)\)
Results I: 1U Resonance Varying the System Size

- **I=N=20**
  - $U/J=15$
  - $R(\omega)$ in a.u.

- **I=N=30**
  - $U/J=15$
  - $R(\omega)$ in a.u.

- **I=N=40**
  - $U/J=20$
  - $R(\omega)$ in a.u.

$R(\omega)$ is the dynamic response of ultracold Bose gases in 1D optical lattices within the Generalized Random Phase Approximation (RPA), allowing for the computation of response functions based on the Taylor expansion in the modulation amplitude. The results are in excellent agreement with the exact time evolution, yielding a precise description of the system's dynamics.

(---) Random Phase Approximation
Results I: 1U Resonance Varying the System Size

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Results II: 1U Resonance Varying U/J

30 particles
30 sites

 centroid slipping-off $\omega = U$
towards superfluid regime
RPA offers numerically efficient access to the strength function (solving a single eigenproblem)

- can be easily extended via generalization of the phonon operators
  - adapt to other lattice topologies via additional matrix elements (e.g., superlattice potential)
  - improve on the resonance’s width via correlated ground-state