Few- and many-body physics of interaction-bound atoms in optical lattices

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Outline

Bose-Hubbard model

- Single particle in a lattice
- Two-particle states in a lattice: dimers
- Three-particle states in a lattice: trimers
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Bose-Hubbard model

- Single particle in a lattice
- Two-particle states in a lattice: dimers
- Three-particle states in a lattice: trimers

Many-body physics of tightly-bound dimers

- Effective Hamiltonian
- Repulsively bound dimers: droplets (FM)
- Attractively bound dimers: checkerboard crystal (AFM)
Bose-Hubbard Hamiltonian

Neutral bosons in tight-binding periodic potential

\[ H = \sum_j \epsilon_j \hat{n}_j - J \sum_{\langle j,i \rangle} b_j^\dagger b_i + \frac{U}{2} \sum_j \hat{n}_j (\hat{n}_j - 1) \]

\( \epsilon_j \ (= 0) \): single-particle energy

\( b_j \) (\( b_j^\dagger \)): boson annihilation (creation) operator at site \( j \)

\( \hat{n}_j \equiv b_j^\dagger b_j \): number operator

\( J \ (> 0) \): inter-site tunneling

\( U \propto a \): on-site interaction (\( U > 0 \) repulsion; \( U < 0 \) attraction)

Single particle in a lattice (1D)

State vector

\[ |\psi\rangle = \sum_j \psi(x_j) |x_j\rangle \]

Difference equation

\[ -J \left[ \psi(x_{j-1}) + \psi(x_{j+1}) \right] = E^{(1)} \psi(x_j) \]
Single particle in a lattice (1D)

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Difference equation

\[-J \left[ \psi(x_{j-1}) + \psi(x_{j+1}) \right] = E^{(1)} \psi(x_j)\]

Solution

\[ \psi_q(x_j) = e^{iqx_j} \]

Dispersion relation

\[ E_q^{(1)} = -2J \cos(qd) \]
Two particles in Hubbard model (1D)

State vector

\[ |\Psi\rangle = \sum_{j,j'} \Psi(x_j, y_{j'}) |x_j, y_{j'}\rangle \]

Recurrence relation

\[ -J \left[ \Psi(x_{j-1}, y_{j'}) + \Psi(x_{j+1}, y_{j'}) + \Psi(x_j, y_{j'-1}) + \Psi(x_j, y_{j'+1}) \right] + U \delta_{j,j'} \Psi(x_j, y_{j'}) = E^{(2)} \Psi(x_j, y_{j'}) \]
Two particles in Hubbard model (1D)

State vector

\[ |\Psi\rangle = \sum_{j,j'} \Psi(x_j, y_{j'}) |x_j, y_{j'}\rangle \]

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\[-J \left[ \Psi(x_{j-1}, y_{j'}) + \Psi(x_{j+1}, y_{j'}) + \Psi(x_j, y_{j'-1}) + \Psi(x_j, y_{j'+1}) \right] + U \delta_{jj'} \Psi(x_j, y_{j'}) = E^{(2)} \Psi(x_j, y_{j'}) \]

\[ R = \frac{1}{2} (x + y) \text{ center of mass} \& r = x - y \text{ relative coordinates} \]

Two-particle wavefunction (with \( K \) center-of-mass quasimomentum)

\[ \Psi(x, y) = e^{iKR} \psi_K(r) \]

Recurrence relation (with \( J_K \equiv 2J \cos(Kd/2) \) and \( r_i = d_i \ (i = j - j') \))

\[-J_K \left[ \psi_K(r_{i-1}) + \psi_K(r_{i+1}) \right] + U \delta_{r0} \psi_K(r_i) = E^{(2)}_K \psi_K(r_i) \]

Solution: Scattering states

Relative coordinate wavefunction

\[ \psi_{K,k}(r_i) = \cos(\sqrt{k} |r_i| + \delta_{K,k}) \]

with \( \delta_{K,k} \) scattering phase shift

\[ \tan(\delta_{K,k}) = -\frac{U \csc(kd)}{4J \cos(Kd/2)} \]
Solution: Scattering states

Relative coordinate wavefunction

\[ \psi_{K,k}(r_i) = \cos(k|r_i| + \delta_{K,k}) \]

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Generalized 1D scattering lengths

\[ a_K = -\lim_{kd \to 0} \frac{\partial \delta_{K,k}}{\partial k} = \mp \frac{2J_K}{U} \]
Solution: Scattering states

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Generalized 1D scattering lengths

\[ a_K = -\lim_{kd \to 0} \frac{\partial \delta_{K,k}}{\partial k} = \mp \frac{2J_K}{U} d \]

Spectrum of scattering states

\[ E_{K,k}^{(2)} = -4J \cos(Kd/2) \cos(kd) \]

Density of states

\[ \rho(E, K) \propto \frac{1}{\sqrt{[4J \cos(Kd/2)]^2 - E^2}} \]
Solution: Interaction-bound states

**Repulsive interaction** $U > 0$

**Relative coordinate wavefunction**

$$\psi_K(r_i) = \frac{\sqrt{U_K}}{4U_K^2 + 1} \left( U_K - \sqrt{U_K^2 + 1} \right) |i|$$

with $U_K \equiv U/(2J_K)$ & $J_K \equiv 2J \cos(Kd/2)$

**Dimer dispersion relation**

$$E_K^B = \sqrt{U^2 + 4J_K^2} \quad \Rightarrow$$

- $E_{\pi/d}^B = |U| = U$
- $E_0^B = \sqrt{U^2 + 16J^2}$
Solution: Interaction-bound states

**Attractive interaction** \( U < 0 \)

**Relative coordinate wavefunction**

\[
\psi_K(r_i) = \frac{\sqrt{\mathcal{U}_K}}{4 \sqrt{\mathcal{U}_K^2 + 1}} \left( \sqrt{\mathcal{U}_K^2 + 1} - |\mathcal{U}_K| \right)
\]

with \( \mathcal{U}_K \equiv (U/2J_K) \& J_K \equiv 2J \cos(Kd/2) \)

**Dimer dispersion relation**

\[
E_K^B = -\sqrt{U^2 + 4J_K^2} \implies
\]

- \( E_0^B = -\sqrt{U^2 + 16J^2} \)
- \( E_{\pi/d}^B = -|U| = U \)
Solution: Interaction-bound states

**Strong interaction** \(|U| > J\)

**Relative coordinate wavefunction**

\[ \psi_K(r_i) \simeq \sqrt{\frac{U^2 - J^2}{U^2 + J^2}} \left( -\frac{J_K}{U} \right) |i| \]

localization length \(\zeta \leq \left[2 \ln\left(U/2J\right)\right]^{-1}\)

\(\zeta < 1\) for \(U/J > 2\sqrt{e}\) \(\Rightarrow\)

**Tightly-bound dimer**

**Dimer dispersion relation**

\[ E^B_K \simeq (U - 2\tilde{J}) - 2\tilde{J}\cos(Kd) \]

with \((U - 2\tilde{J})\) dimer "internal" energy \(\tilde{J} \equiv -2J^2/U\) effective tunneling rate
Solution: Interaction-bound states

Strong interaction $|U| > J$

Relative coordinate wavefunction

$$\psi_K(r_i) \simeq \sqrt{\frac{U^2 - J^2_K}{U^2 + J^2_K}} \left( -\frac{J_K}{U} \right) |i|$$

localization length $\zeta \leq \left[2 \ln(U/2J)\right]^{-1}$

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Tightly-bound dimer

Dimer dispersion relation

$$E^B_K \simeq (U - 2\tilde{J}) - 2\tilde{J} \cos(Kd)$$

with $(U - 2\tilde{J})$ dimer “internal” energy

$\tilde{J} \equiv -2J^2/U$ effective tunneling rate

Effective dimer Hamiltonian

$$H_{\text{eff}} = (U - 2\tilde{J}) \sum_j \hat{m}_j - \tilde{J} \sum_j (c_j^{\dagger}c_{j+1} + c_{j+1}^{\dagger}c_j)$$
Repulsively bound atom pair: Experiment

Single dimer

Three particles in Hubbard model (1D)

Complete three-body spectrum $[U = -10J]$
Three particles in Hubbard model (1D)

Three-body continuum

\[ E_{c3} = \epsilon(k_1) + \epsilon(k_2) + \epsilon(K - k_1 - k_2) \]

\[ \epsilon(k) = -2J \cos(k) \]

\[ K = k_1 + k_2 + k_3 \]
Three particles in Hubbard model (1D)

Three-body continuum

\[ E_{c3} = \epsilon(k_1) + \epsilon(k_2) + \epsilon(K - k_1 - k_2) \]
\[ \epsilon(k) = -2J \cos(k) \quad K = k_1 + k_2 + k_3 \]

Two-body continuum

\[ E_{c2} = \epsilon^{(2)}(Q) + \epsilon(K - Q) \]
\[ \epsilon^{(2)}(Q) = \text{sgn}(U) \sqrt{U^2 + [4J \cos(Q/2)]^2} \]
\[ \simeq (U - 2\tilde{J}) - 2\tilde{J} \cos(Q) \]
Three particles in Hubbard model (1D)

Three-body continuum

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Weakly-bound (off-site) trimers

\[ E_{a1(2)} \simeq U + O(J) \]
Three particles in Hubbard model (1D)

Three-body continuum

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Weakly-bound (off-site) trimers

\[ E_{a1(2)} \simeq U + O(J) \]

Strongly-bound (on-site) trimer

\[ E_b \simeq 3U \]
Formalism: Three-body bound states

State vector in momentum representation

\[ |\psi\rangle = \frac{1}{(2\pi)^{3/2}} \int \int \int_{\Omega^3} dk_1 dk_2 dk_3 \psi(k_1, k_2, k_3) |k_1, k_2, k_3\rangle \quad k_j \in \Omega \equiv [-\pi, \pi] \]
Formalism: Three-body bound states

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\[ H |\psi\rangle = E |\psi\rangle \Rightarrow \psi(k_1, k_2, k_3) = -\frac{M(k_1) + M(k_2) + M(k_3)}{\epsilon(k_1) + \epsilon(k_2) + \epsilon(k_3) - E} \]

with

\[ M(k)[1 + I_E(k)] = -\frac{U}{\pi} \int_{-\pi}^{\pi} dq \frac{M(q)}{\epsilon(k) + \epsilon(q) + \epsilon(K - k - q) - E} \]

\[ I_E(k) \equiv \frac{U}{2\pi} \int_{-\pi}^{\pi} dq \frac{1}{\epsilon(k) + \epsilon(q) + \epsilon(K - k - q) - E} \]

\[ = -\frac{\text{sgn}[E - \epsilon(k)] U}{\sqrt{[E - \epsilon(k)]^2 - 16J^2 \cos^2 [(K - k)/2]}} \]

Mattis, Rev. Mod. Phys. 58, 361 (1986)
Formalism: Three-body bound states

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\[ |\psi\rangle = \frac{1}{(2\pi)^{3/2}} \int \int \int_{\Omega^3} dk_1 dk_2 dk_3 \psi(k_1, k_2, k_3) |k_1, k_2, k_3\rangle \quad k_j \in \Omega \equiv [-\pi, \pi] \]

\[ H |\psi\rangle = E |\psi\rangle \Rightarrow \psi(k_1, k_2, k_3) = -\frac{M(k_1) + M(k_2) + M(k_3)}{\epsilon(k_1) + \epsilon(k_2) + \epsilon(k_3) - E} \]

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\[ M(k)[1 + I_E(k)] = -\frac{U}{\pi} \int_{-\pi}^{\pi} dq \frac{M(q)}{\epsilon(k) + \epsilon(q) + \epsilon(K-k-q) - E} \]

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\[ = -\frac{\text{sgn}[E-\epsilon(k)]U}{\sqrt{[E-\epsilon(k)]^2 - 16J^2 \cos^2 [(K-k)/2]} \]
Thresholds & limits of $U$

$E_B^1(K) = E_{a1}(K) - E_{c2}(K, Q = 0)$

$E_B^2(K) = E_{a2}(K) - E_{c2}(K, Q = \pi)$
Thresholds & limits of $U$

\[ E_{B1}(K) = E_{a1}(K) - E_{c2}(K, Q = 0) \]

\[ E_{B2}(K) = E_{a2}(K) - E_{c2}(K, Q = \pi) \]

For $|U| \lesssim 4J \Rightarrow E_{a1} \rightarrow E_{c2}$ ($E_{B1} \rightarrow 0$: Scattering resonance)
Thresholds & limits of $U$

For $|U| \lesssim 4J \Rightarrow E_{a1} \rightarrow E_{c2}$ \hspace{0.5cm} (For $|U| \lesssim 8J$ $E_{c2} \cap E_{c3} \neq 0$)

$E_{B1}(K) = E_{a1}(K) - E_{c2}(K, Q = 0)$

$E_{B2}(K) = E_{a2}(K) - E_{c2}(K, Q = \pi)$
Thresholds & limits of $U$

\[
\begin{align*}
E_{B1}(K) &= E_{a1}(K) - E_{c2}(K, Q = 0) \\
E_{B2}(K) &= E_{a2}(K) - E_{c2}(K, Q = \pi)
\end{align*}
\]

For $|U| \lessapprox 4J$ $\Rightarrow$ $E_{a1} \rightarrow E_{c2}$ ($E_{B1} \rightarrow 0$: Scattering resonance)

For $|U| \lessapprox 8.5J$ $\Rightarrow$ $E_{a2} \in E_{c3}$ (for $|U| \leq 8J$ $E_{c2} \cap E_{c3} \neq 0$)

\[
\begin{align*}
\lim_{U \rightarrow -\infty} E_{B1} &= -\frac{J}{2} \\
\lim_{U \rightarrow -\infty} E_{B2} &= \frac{J}{2}
\end{align*}
\]
Effective Hamiltonian for dimer+monomer

\[ H_{\text{eff}} = H_1 + H_2 + H_{\text{int}} \]

for \(|U| > 8J\) \((E_{c2} \cap E_{c3} = 0)\)
Effective Hamiltonian for dimer+monomer

\[ H_{\text{eff}} = H_1 + H_2 + H_{\text{int}} \quad \text{for} \quad |U| > 8J \quad (E_{c2} \cap E_{c3} = 0) \]

Monomer (single-particle) Hamiltonian

\[ H_1 = -J \sum_j (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) \]
Effective Hamiltonian for dimer+monomer

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Monomer (single-particle) Hamiltonian

\[ H_1 = -J \sum_j (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) \]

Dimer (bound pair) Hamiltonian

\[ H_2 = (U - 2\tilde{J}) \sum_j \hat{m}_j - \tilde{J} \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \]
Effective Hamiltonian for dimer+monomer

\[ H_{\text{eff}} = H_1 + H_2 + H_{\text{int}} \quad \text{for} \quad |U| > 8J \quad (E_{c2} \cap E_{c3} = 0) \]

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\[ H_1 = -J \sum_j (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) \]

Dimer (bound pair) Hamiltonian

\[ H_2 = (U - 2\tilde{J}) \sum_j \hat{m}_j - \tilde{J} \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \]

Dimer-monomer interaction

\[ H_{\text{int}} = \tilde{V} \sum_j \hat{m}_j \hat{n}_{j+1} - W \sum_j (c_j^\dagger b_j^\dagger c_{j+1} b_{j+1} + c_j^\dagger b_{j+1}^\dagger c_j b_{j+1}) \]

\[ \tilde{V} = -7J^2/2U: \text{nearest-neighbor interaction} \]

\[ W = 2J: \text{(particle) exchange interaction} \]
Effective Hamiltonian for dimer+monomer

\[ H_{\text{eff}} = H_1 + H_2 + H_{\text{int}} \quad \text{for} \quad |U| > 8J \quad (E_{c2} \cap E_{c3} = 0) \]

Monomer (single-particle) Hamiltonian

\[ H_1 = -J \sum_j (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) \]

Dimer (bound pair) Hamiltonian

\[ H_2 = (U - 2\tilde{J}) \sum_j \hat{m}_j - \tilde{J} \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \]

Dimer-monomer interaction

\[ H_{\text{int}} = \tilde{V} \sum_j \hat{m}_j \hat{n}_{j+1} \]
\[ -W \sum_j (c_{j+1}^\dagger b_j^\dagger c_j b_{j+1} + c_j^\dagger b_{j+1}^\dagger c_{j+1} b_j) \]

\[ \tilde{V} = -7J^2/2U \]: nearest-neighbor interaction

\[ W = 2J \]: (particle) exchange interaction
Solution: Bound states \((K = 0, \pm \pi)\)

State vector

\[
|\Psi\rangle = \sum_{j_1 \neq j_2} \Psi(j_1, j_2) |j_1, j_2\rangle
\]

with

\[
\Psi(j_1, j_2) = e^{iK(j_1+j_2)/2} e^{-i\delta_K j_r} \phi_K(j_r) \quad (j_r \equiv j_1 - j_2 \quad \tan(\delta_K) = \tan(\frac{K}{2}) \frac{J-J}{J+J})
\]
Solution: Bound states \((K = 0, \pm \pi)\)

State vector

\[
|\Psi\rangle = \sum_{j_1 \neq j_2} \Psi(j_1, j_2) |j_1, j_2\rangle
\]

with

\[
\Psi(j_1, j_2) = e^{iK(j_1+j_2)/2}e^{-i\delta j_r \phi_K(j_r)} \quad (j_r \equiv j_1 - j_2 \quad \tan(\delta_K) = \tan(\frac{K}{2}) \frac{J_0 - j}{J_0 + j})
\]

Recurrence relations for relative coordinate wavefunction \((|j_r| > 1)\)

\[
\phi_K(0) = 0
\]

\[
\tilde{J}_K [\phi_K(j_r + 1) + \phi_K(j_r - 1)] + \tilde{E} \phi_K(j_r) = 0
\]

\[
\tilde{J}_K \phi_K(\pm 2) + W_K \phi_K(\mp 1) + [\tilde{E} - \tilde{V}] \phi_K(\pm 1) = 0
\]

with \(\tilde{J}_K \equiv \sqrt{J^2 + \tilde{J}^2 + 2J\tilde{J} \cos(K)} \quad W_K \equiv W \cos(K) \quad \tilde{E} \equiv E - (U - 2\tilde{J}) \quad \tilde{J}_0,\pi = J \pm \tilde{J}\)
Solution: Bound states \( (K = 0, \pm \pi) \)

Exponential ansatz \( \phi_K(j_r > 0) \propto \alpha_K^{j_r-1} \)

& \( \phi_K(-j_r) = \pm \phi_K(j_r) \) ("+" symmetric (triplet); "−" antisymmetric (singlet) solutions)

\[ \Rightarrow \alpha_K^{(\pm)} = -\frac{\bar{J}_K}{V \mp W_K} \text{ with } \bar{E}_{a_1(2)} = -\frac{\bar{J}_K [1 + (\alpha_K^{(\pm)})^2]}{\alpha_K^{(\pm)}} \]
Solution: Bound states \( (K = 0, \pm \pi) \)

Exponential ansatz \( \phi_K(j_r > 0) \propto \alpha_K^{j_r^{-1}} \)

\& \( \phi_K(-j_r) = \pm \phi_K(j_r) \) \( (“+” \text{ symmetric (triplet); “−” antisymmetric (singlet) solutions}) \)

\[ \Rightarrow \alpha_K^{(\pm)} = -\frac{\tilde{J}_K}{V \mp W_K} \text{ with } \tilde{E}_{a1(2)} = -\frac{\tilde{J}_K[1+(\alpha_K^{(\pm)})^2]}{\alpha_K^{(\pm)}} \]

Bound states \( (|\alpha_K^{(\pm)}| < 1) \)

- \( |\tilde{V} \mp W_K| > \tilde{J}_K \Rightarrow |\tilde{V} \mp 2J| > J \pm \tilde{J} \)

For \( U \gg J \quad E_{B1(2)} = \tilde{E}_{a1(2)} \mp 2\tilde{J}_K \simeq \mp \frac{J}{2} \quad (\tilde{V} \ll J) \)
Solution: Bound states $(K = 0, \pm \pi)$

Exponential ansatz $\phi_K(j_r > 0) \propto \alpha_K^{j_r - 1}$

& $\phi_K(-j_r) = \pm \phi_K(j_r)$ ("+" symmetric (triplet); "−" antisymmetric (singlet) solutions)

$\Rightarrow \quad \alpha_K^{(\pm)} = -\frac{\tilde{J}_K}{\tilde{V} \mp W_K}$

with $\tilde{E}_{a1(2)} = -\frac{\tilde{J}_K [1 + (\alpha_K^{(\pm)})^2]}{\alpha_K^{(\pm)}}$

Bound states ($|\alpha_K^{(\pm)}| < 1$)

- $|\tilde{V} \mp W_K| > \tilde{J}_K \quad \Rightarrow \quad |\tilde{V} \mp 2J| > J \pm \tilde{J}$

For $U \gg J \quad E_{B1(2)} = \tilde{E}_{a1(2)} \mp 2\tilde{J}_K \simeq \mp \frac{J}{2} \quad (\tilde{V} \ll J)$

$\Rightarrow$ Exchange interaction $W = 2J$ binds dimer and monomer
Many-body physics of tightly-bound dimers
Interaction-bound atom pair—Dimer

Energies of $|2, 0\rangle$ & $|0, 2\rangle$ are larger (smaller) than of $|1, 1\rangle$ by $U$
Interaction-bound atom pair—Dimer

Energies of $|2,0\rangle$ & $|0,2\rangle$ are larger (smaller) than of $|1,1\rangle$ by $U$

For $|U|/J \gg 1 \Rightarrow |2,0\rangle \rightarrow |1,1\rangle$ is non-resonant

On-site interaction (repulsion $U > 0$) binds two atoms into a dimer
Interaction-bound atom pair—Dimer

Energies of $|2, 0\rangle$ & $|0, 2\rangle$ are larger (smaller) than of $|1, 1\rangle$ by $U$

For $|U|/J \gg 1 \Rightarrow |2, 0\rangle \rightarrow |1, 1\rangle$ is non-resonant

On-site interaction (repulsion $U > 0$) binds two atoms into a dimer

But $|2, 0\rangle \rightarrow |1, 1\rangle \rightarrow |0, 2\rangle$ is resonant (second order in $J$)

Effective tunneling rate for dimer $|2, 0\rangle \rightarrow |0, 2\rangle$ is $\tilde{J} = -\frac{2J^2}{U}$

Slow dynamics ($|\tilde{J}| \ll J$)
Effective Hamiltonian for dimers \((|U| \gg J)\)

Define
\[
c_j = \frac{1}{\sqrt{2(n_j+1)}} b_j^2, \quad c_j^\dagger
\]
\[
\hat{m}_j = c_j^\dagger c_j
\]
\[
\tilde{J} = -\frac{2J^2}{U}
\]

Adiabatic elimination of nonresonant states \(|n_{i\pm 1}\rangle|n_{j \mp 1}\rangle\) \((n_l = 2m_l)\)
Effective Hamiltonian for dimers ($|U| \gg J$)

Effective Hamiltonian for paired bosons in a periodic potential

$$H_{\text{eff}} = 2\varepsilon \sum_j \hat{m}_j + U \sum_j \hat{m}_j (2\hat{m}_j - 1) - \tilde{J} \sum_{\langle j, i \rangle} c_j^\dagger \hat{T}(\hat{m}_j, \hat{m}_i) c_i + \tilde{J} \sum_{\langle j, i \rangle} \hat{S}(\hat{m}_j, \hat{m}_i)$$

Kinetic Energy

$$\hat{T}(\hat{m}_j, \hat{m}_i) = \delta_{\hat{m}_i \hat{m}_j} \sqrt{(2\hat{m}_j + 1)(2\hat{m}_i + 1)}$$

Potential Energy

$$\hat{S}(\hat{m}_j, \hat{m}_i) + \hat{S}(\hat{m}_i, \hat{m}_j) = \frac{2\hat{m}_j^2 + 2\hat{m}_i^2 + \hat{m}_j + \hat{m}_i}{1 - 4(\hat{m}_j - \hat{m}_i)^2}$$
Effective Hamiltonian for dimers \((|U| \gg |J|)\)

Effective Hamiltonian for paired bosons in a periodic potential

\[
H_{\text{eff}} = 2\varepsilon \sum_{j} \hat{m}_j + U \sum_{j} \hat{m}_j (2\hat{m}_j - 1) - \tilde{J} \sum_{\langle j,i \rangle} c_j^{\dagger} \hat{T}(\hat{m}_j, \hat{m}_i) c_i + \tilde{J} \sum_{\langle j,i \rangle} \hat{S}(\hat{m}_j, \hat{m}_i)
\]

- Kinetic Energy
  \[
  \hat{T}(\hat{m}_j, \hat{m}_i) = \delta_{\hat{m}_i \hat{m}_j} \sqrt{(2\hat{m}_j + 1)(2\hat{m}_i + 1)}
  \]

- Potential Energy
  \[
  \hat{S}(\hat{m}_j, \hat{m}_i) + \hat{S}(\hat{m}_i, \hat{m}_j) = \frac{2\hat{m}_j^2 + 2\hat{m}_i^2 + \hat{m}_j + \hat{m}_i}{1 - 4(\hat{m}_j - \hat{m}_i)^2}
  \]

- Nearest-neighbor attraction/repulsion > tunneling

\[
\frac{\text{Kin.En}}{\text{Pot.En}} = \frac{3(m + 1)(2m + 1)}{8(4m^2 + 6m + 3)} < 0.2 \quad (1D)
\]

Repulsively-bound dimers \((U > 0)\)

Nearest-neighbor interaction (potential) energy

\[
\tilde{J} \frac{2\hat{m}_j^2 + 2\hat{m}_i^2 + \hat{m}_j + \hat{m}_i}{1 - 4(\hat{m}_j - \hat{m}_i)^2} \quad \tilde{J} = -\frac{2J^2}{U} < 0
\]

- For \(m_i = m_j \rightarrow\) Attraction
- For \(m_i \neq m_j \rightarrow\) Repulsion

⇒ Dimer clustering into “droplets” with uniform filling!
Repulsively-bound dimers ($U > 0$)

Nearest-neighbor interaction (potential) energy

$$\tilde{J} \left( \frac{2\hat{m}_j^2 + 2\hat{m}_i^2 + \hat{m}_j + \hat{m}_i}{1 - 4(\hat{m}_j - \hat{m}_i)^2} \right)$$

$$\tilde{J} = -\frac{2J^2}{U} < 0$$

- For $m_i = m_j$ → Attraction
- For $m_i \neq m_j$ → Repulsion

$\Rightarrow$ Dimer clustering into “droplets” with uniform filling!

1D Phase Diagram $[\mu - \tilde{J}]$

Grand canonical ensemble

$H_{\text{eff}}$ with uniform chem. potential

$$\mu = -2\varepsilon$$

Exacts diagonalization for 5 sites ($0 \leq m \leq 4$)

Only uniform commensurate filling (incompressible phases)
Single dimers per site \((U \geq 0)\)

**Effective Hamiltonian** \((m = 0, 1 \ \forall \ j)\)

\[
H_{\text{eff}}^{(0,1)} = \left[ 2\varepsilon + U - 2d\tilde{J} \right] \sum_j \hat{m}_j - \tilde{J} \sum_{\langle j, i \rangle} c_j^{\dagger} c_i + 4\tilde{J} \sum_{\langle j, i \rangle} \hat{m}_j \hat{m}_i
\]

Similar to Extended Hubbard Model (nearest-neighbor interaction)
Single dimers per site ($U \geq 0$)

Effective Hamiltonian ($m = 0, 1 \ \forall \ j$)

$$H_{\text{eff}}^{(0,1)} = [2\varepsilon + U - 2d\tilde{J}] \sum_j \hat{m}_j - \tilde{J} \sum_{\langle j, i \rangle} c_j^\dagger c_i + 4\tilde{J} \sum_{\langle j, i \rangle} \hat{m}_j \hat{m}_i$$

Similar to Extended Hubbard Model (nearest-neighbor interaction)

Equivalent spin-$\frac{1}{2}$ XXZ model Hamiltonian ($|0_j\rangle \rightarrow |\downarrow_j\rangle, \ |1_j\rangle \rightarrow |\uparrow_j\rangle$)

$$H_{\text{XXZ}} = 2h_z \sum_j \sigma_j^z - \frac{1}{4}\tilde{J} \sum_{\langle j, i \rangle} (\sigma_j^x \sigma_i^x + \sigma_j^y \sigma_i^y) + \tilde{J} \sum_{\langle j, i \rangle} \sigma_j^z \sigma_i^z$$

$$h_z = \frac{1}{4} [2\varepsilon + U - 2d\tilde{J}] + 2d\tilde{J} \text{ – effective “magnetic field”}$$

$$\langle \sigma^z \rangle = [2\langle \hat{m} \rangle - 1] \text{ – fixed “magnetization” (averaged)}$$
Single dimers per site \((U \geq 0)\)

**Effective Hamiltonian** \((m = 0, 1 \ \forall \ j)\)

\[
H_{\text{eff}}^{(0,1)} = \left[ 2\varepsilon + U - 2d\tilde{J} \right] \sum_j \hat{m}_j - \tilde{J} \sum_{\langle j,i \rangle} c_j^{\dagger} c_i + 4\tilde{J} \sum_{\langle j,i \rangle} \hat{m}_j \hat{m}_i
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Similar to Extended Hubbard Model (nearest-neighbor interaction)

**Equivalent spin-\(\frac{1}{2}\) XXZ model Hamiltonian** \((|0_j\rangle \rightarrow |\downarrow_j\rangle, \ |1_j\rangle \rightarrow |\uparrow_j\rangle)\)

\[
H_{\text{XXZ}} = 2h_z \sum_j \sigma_j^z - \frac{1}{4} \tilde{J} \sum_{\langle j,i \rangle} \left( \sigma_j^x \sigma_i^x + \sigma_j^y \sigma_i^y \right) + \tilde{J} \sum_{\langle j,i \rangle} \sigma_j^z \sigma_i^z
\]

\[
h_z = \frac{1}{4} \left[ 2\varepsilon + U - 2d\tilde{J} \right] + 2d\tilde{J} - \text{effective "magnetic field"}
\]

\[
\langle \sigma^z \rangle = \left[ 2\langle \hat{m} \rangle - 1 \right] - \text{fixed "magnetization" (averaged)}
\]

Since \(\frac{1}{4} < 1 \Rightarrow H_{\text{XXZ}} \simeq H_{\text{Ising}} = 2h_z \sum_j \sigma_j^z + \tilde{J} \sum_{\langle j,i \rangle} \sigma_j^z \sigma_i^z\)
Droplets in a lattice \((U > 0)\)

**Strong dimer-dimer attraction** \((8\tilde{J} > \tilde{J})\)
Droplets in a lattice \((U > 0)\)

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Droplets in a lattice \((U > 0)\)

Strong dimer-dimer attraction \((8\tilde{J} > \tilde{J})\)

Spin-\(\frac{1}{2}\) model \((|0\rangle \rightarrow |\downarrow\rangle, |1\rangle \rightarrow |\uparrow\rangle) \Rightarrow \text{ferromagnetic spin domain}\)
Attractively-bound dimers \((U < 0)\)

**Effective Hamiltonian** \((m = 0, 1 \ \forall \ j)\)

\[
H^{(0,1)}_{\text{eff}} = [2\varepsilon + U - 2d\tilde{J}] \sum_j \hat{m}_j - \tilde{J} \sum_{\langle j,i \rangle} c_j^\dagger c_i + 4\tilde{J} \sum_{\langle j,i \rangle} \hat{m}_j \hat{m}_i
\]

Extended Hubbard Model with \(\tilde{J} > 0\) (nearest-neighbor repulsion)
Attractively-bound dimers \((U < 0)\)

**Effective Hamiltonian** \((m = 0, 1 \ \forall \ j)\)

\[
H_{\text{eff}}^{(0,1)} = \left[2\varepsilon + U - 2d\tilde{J}\right] \sum_j \hat{m}_j - \tilde{J} \sum_{\langle j,i \rangle} c_j^\dagger c_i + 4\tilde{J} \sum_{\langle j,i \rangle} \hat{m}_j \hat{m}_i
\]

**Extended Hubbard Model with \(\tilde{J} > 0\) (nearest-neighbor repulsion)**

Dimer density in 1D lattice + weak harmonic potential

\[
2\varepsilon_j = \frac{j^2}{2200} \tilde{J}
\]

Ground state from DMRG calculation

Attractively-bound dimers ($U < 0$)

1D Phase Diagram [$\mu - \tilde{J}$]

Grand canonical ensemble

$H_{\text{eff}}$ with uniform chem. potential

$$\mu = -2\varepsilon$$

Exacts diagonalization for 10 sites
Attractively-bound dimers \( (U < 0) \)

### 1D Phase Diagram \([\mu - \tilde{J}]\)

Grand canonical ensemble

\[ H_{\text{eff}} \] with uniform chem. potential

\[ \mu = -2\varepsilon \]

Exacts diagonalization for 10 sites

\[ m = 0, m = \frac{1}{2}, m = 1 \] incompressible phases:

- \( m = 0 \) → \(|0\rangle |0\rangle |0\rangle |0\rangle\) empty (ferromagnetic) phase
- \( m = 1 \) → \(|1\rangle |1\rangle |1\rangle |1\rangle\) filled (ferromagnetic) phase
- \( m = \frac{1}{2} \) → \(|0\rangle |1\rangle |0\rangle |1\rangle\) “crystal” (anti-ferromagnetic) phase

\[ 0 < m < \frac{1}{2} \& \frac{1}{2} < m < 1 \] compressible (supersolid) phases
Attractively-bound dimers \((U < 0)\)

### 1D Phase Diagram \([\mu - \tilde{J}]\)

Grand canonical ensemble

\(H_{\text{eff}}\) with uniform chem. potential

\[
\mu = -2\varepsilon
\]

Exacts diagonalization for 10 sites

---

**Exact Bethe Ansatz solution**

\[
\begin{align*}
\mu_0 &= U - 4\tilde{J} \\
\mu_1 &= U + 16\tilde{J} \\
\mu_{1/2-} &= U + 1.6836\tilde{J} \\
\mu_{1/2+} &= U + 10.3164\tilde{J}
\end{align*}
\]

Yang, Yang, Phys. Rev. **150**, 327 (1966)
Checkerboard crystal in a lattice ($U < 0$)

Strong dimer-dimer repulsion ($8\tilde{J} > \tilde{J}$)
Checkerboard crystal in a lattice \((U < 0)\)

Strong dimer-dimer repulsion \((8\tilde{J} > \tilde{J})\)
Checkerboard crystal in a lattice \((U < 0)\)

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Checkerboard crystal in a lattice \((U < 0)\)

Strong dimer-dimer repulsion \((8\tilde{J} > \tilde{J})\)

Spin-\(\frac{1}{2}\) model \((|0\rangle \rightarrow |\downarrow\rangle, |1\rangle \rightarrow |\uparrow\rangle) \Rightarrow\) anti-ferromagnetic ordering
Interaction (attraction or repulsion) can bind particles together in a lattice

Strongly interacting pairs of particles form tightly-bound dimers

- Dimer-monomer (particle) exchange interaction can bind them into trimers

Collection of such dimers in a lattice can realize extended Hubbard (or spin-$\frac{1}{2}$ $XXZ$) model $\Rightarrow$ studies of many-body physics on a lattice
Interaction (attraction or repulsion) can bind particles together in a lattice

Strongly interacting pairs of particles form tightly-bound dimers
- Dimer-monomer (particle) exchange interaction can bind them into trimers

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