



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

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Greece



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



- 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

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

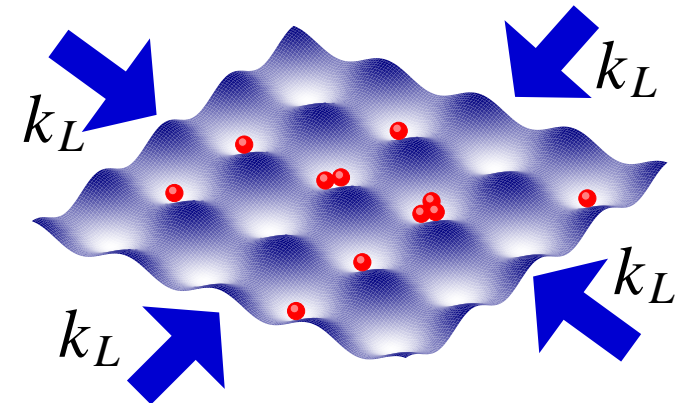
ε_j ($= 0$): single-particle energy

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)



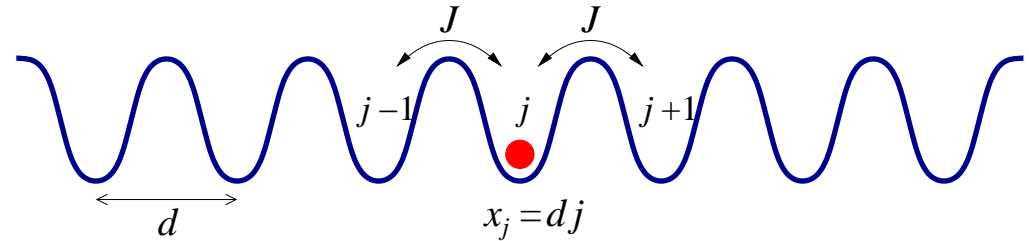
[atoms in deep optical lattice]

Single particle in a lattice (1D)



State vector

$$|\psi\rangle = \sum_j \psi(x_j) |x_j\rangle \quad \Downarrow$$



Difference equation

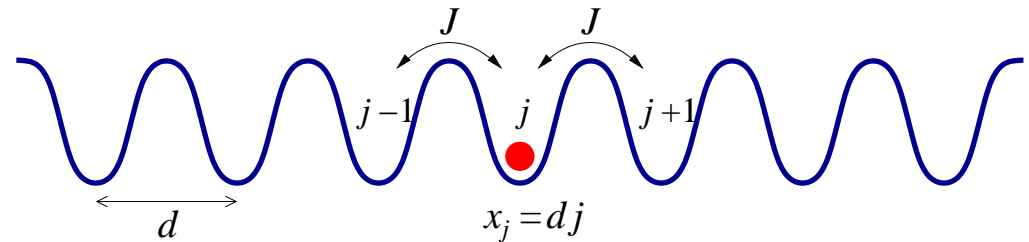
$$-J[\psi(x_{j-1}) + \psi(x_{j+1})] = E^{(1)} \psi(x_j)$$

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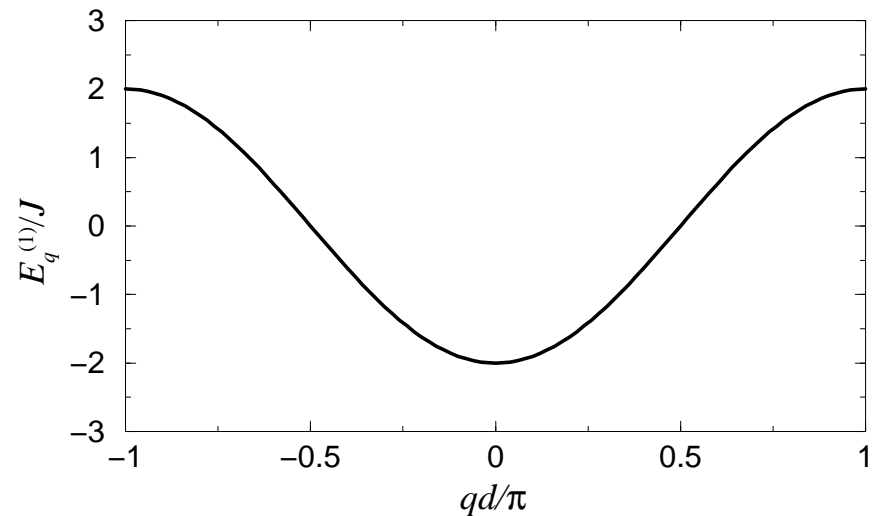
Solution

$$\psi_q(x_j) = e^{iqx_j}$$

Dispersion relation

$$E_q^{(1)} = -2J \cos(qd)$$

Bloch band

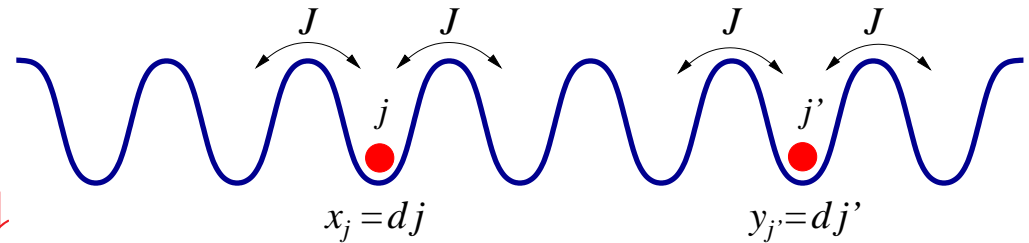


Two particles in Hubbard model (1D)



State vector

$$|\Psi\rangle = \sum_{j,j'} \Psi(x_j, y_{j'}) |x_j, y_{j'}\rangle \quad \Downarrow$$



Recurrence relation

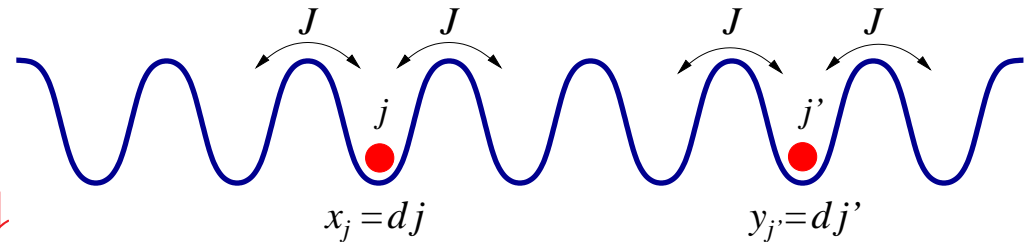
$$-J[\Psi(x_{j-1}, y_{j'}) + \Psi(x_{j+1}, y_{j'}) + \Psi(x_j, y_{j'-1}) + \Psi(x_j, y_{j'+1})] \\ + U\delta_{jj'}\Psi(x_j, y_{j'}) = E^{(2)}\Psi(x_j, y_{j'})$$

Two particles in Hubbard model (1D)



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

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 $r_i = di$ ($i = j - j'$))

$$-J_K [\psi_K(r_{i-1}) + \psi_K(r_{i+1})] + U \delta_{r0} \psi_K(r_i) = E_K^{(2)} \psi_K(r_i)$$

Solution: Scattering states



Relative coordinate wavefunction

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

with $\delta_{K,k}$ scattering phase shift

$$\tan(\delta_{K,k}) = -\frac{U \csc(kd)}{4J \cos(Kd/2)}$$

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Generalized 1D scattering lengths

$$a_K = -\lim_{kd \rightarrow \frac{0}{\pi}} \frac{\partial \delta_{K,k}}{\partial k} = \mp \frac{2J_K}{U} d$$

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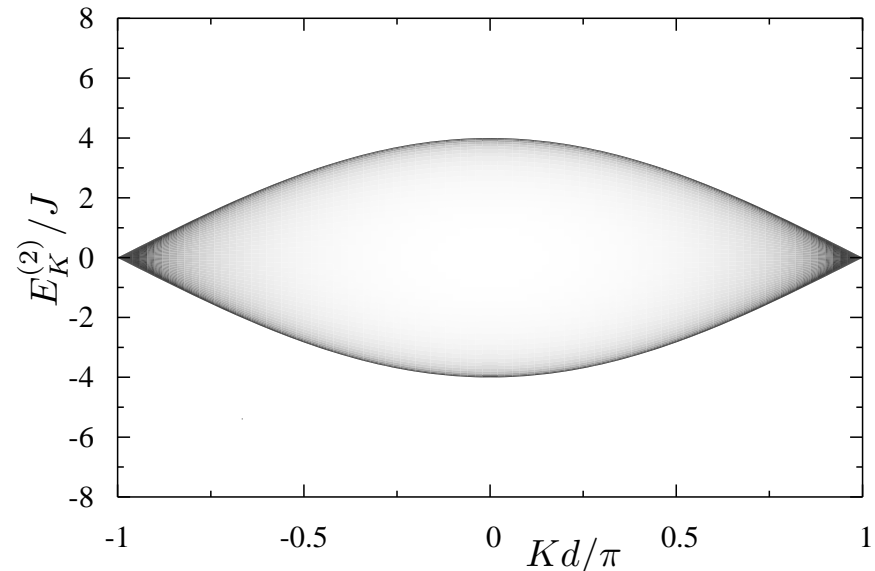
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Spectrum of scattering states

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

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

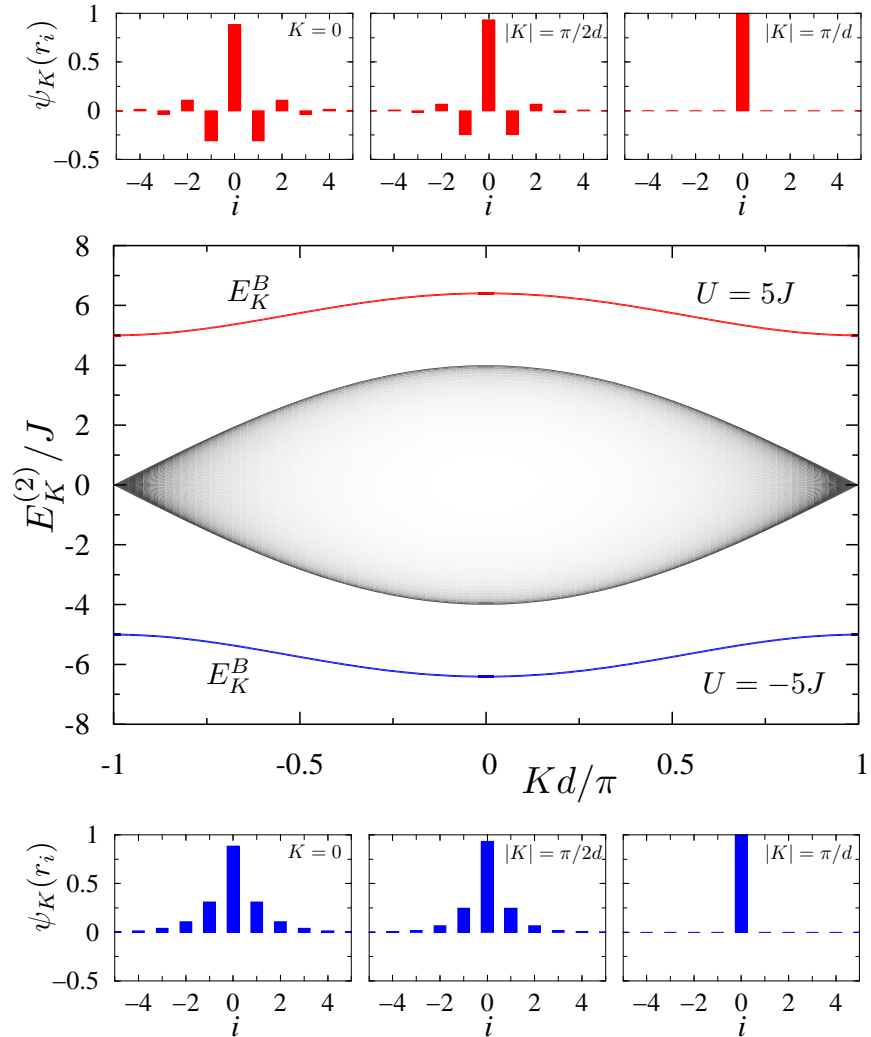
$$\psi_K(r_i) = \frac{\sqrt{\mathcal{U}_K}}{\sqrt[4]{\mathcal{U}_K^2 + 1}} \left(\mathcal{U}_K - \sqrt{\mathcal{U}_K^2 + 1} \right)^{|i|}$$

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

Dimer dispersion relation

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

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



Solution: Interaction-bound states



Attractive interaction $U < 0$

Relative coordinate wavefunction

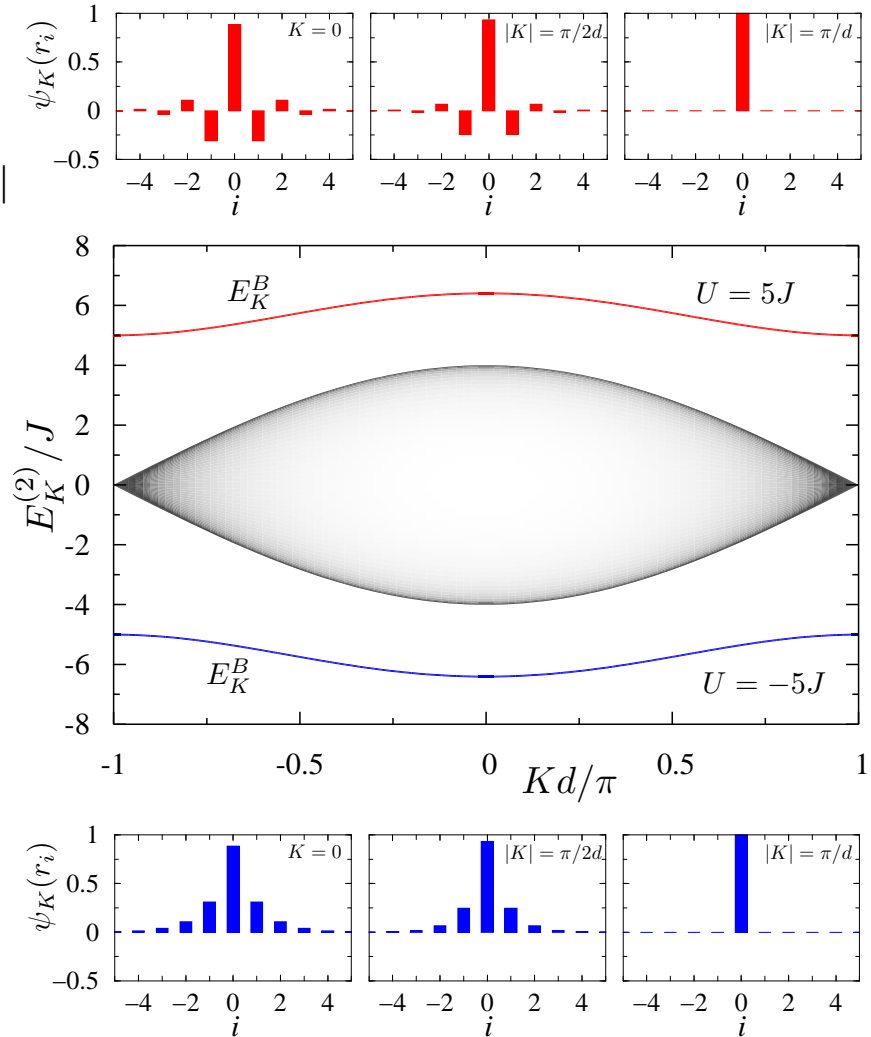
$$\psi_K(r_i) = \frac{\sqrt{U_K}}{\sqrt[4]{U_K^2 + 1}} \left(\sqrt{U_K^2 + 1} - |U_K| \right)^{|i|}$$

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

Dimer dispersion relation

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



Solution: Interaction-bound states

Strong interaction $|U| > J$

Relative coordinate wavefunction

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

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

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

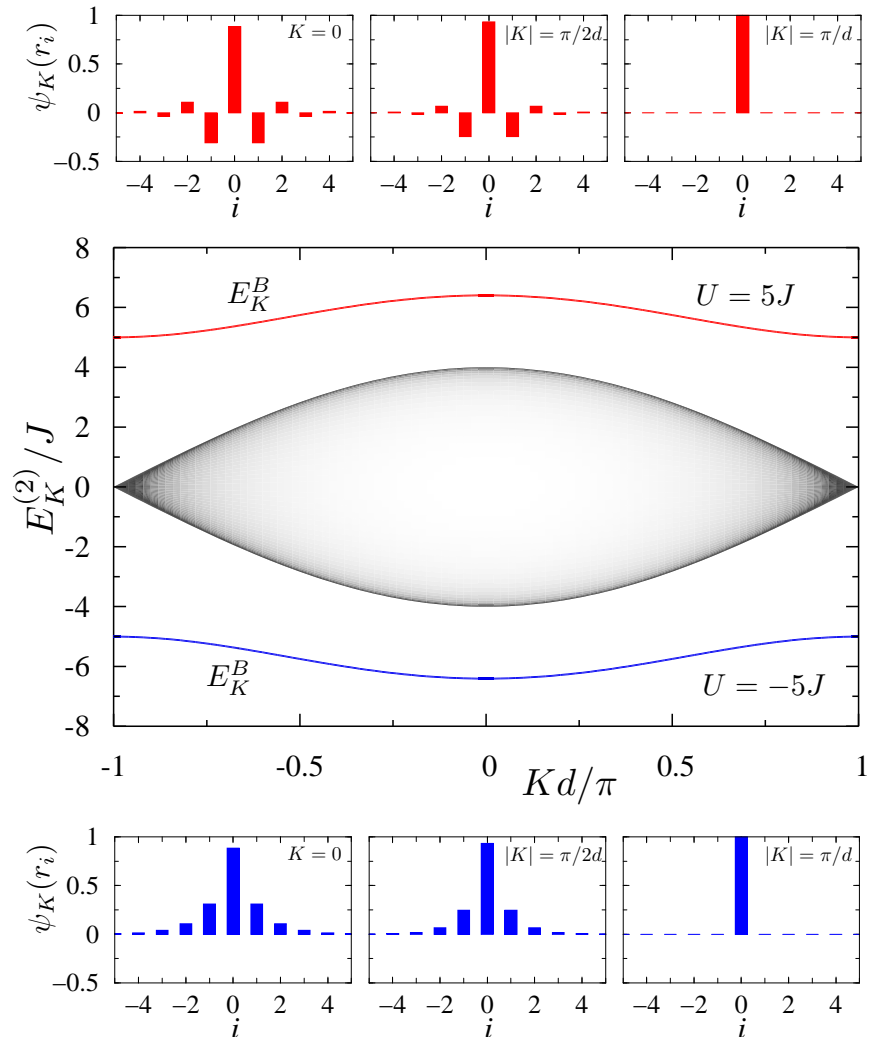
Tightly-bound dimer

Dimer dispersion relation

$$E_K^B \simeq (U - 2\tilde{J}) - 2\tilde{J} \cos(Kd)$$

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

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



Solution: Interaction-bound states



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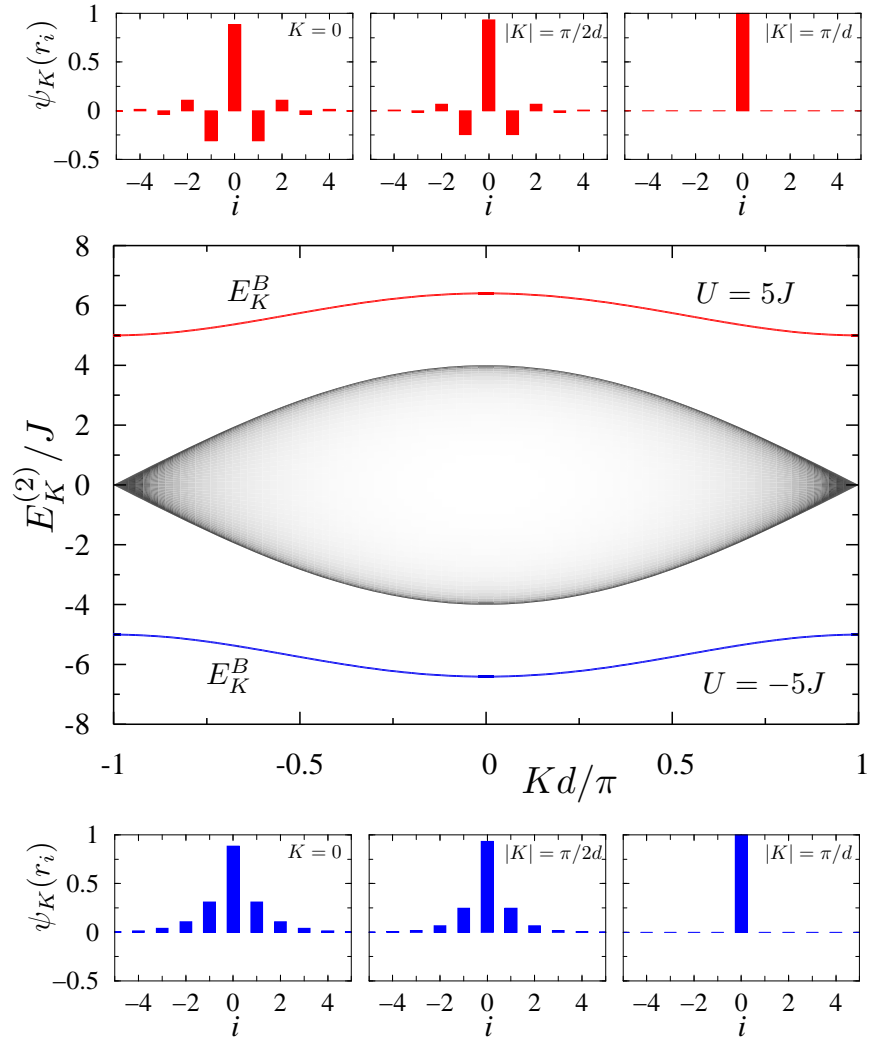
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Effective dimer Hamiltonian

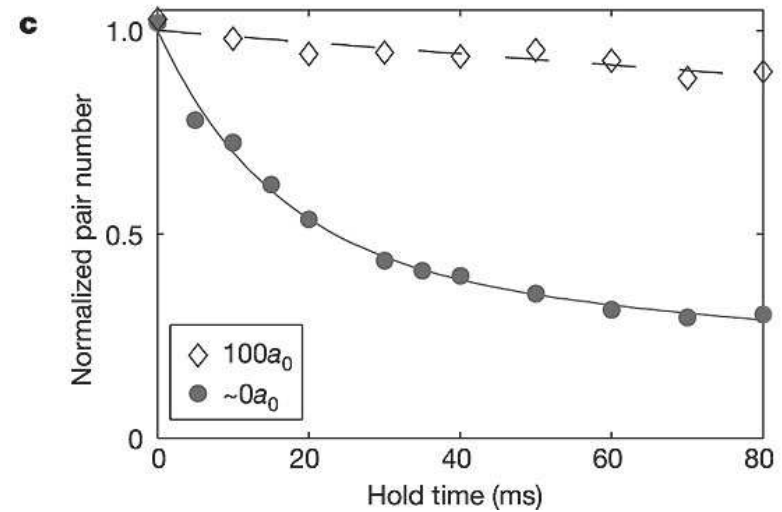
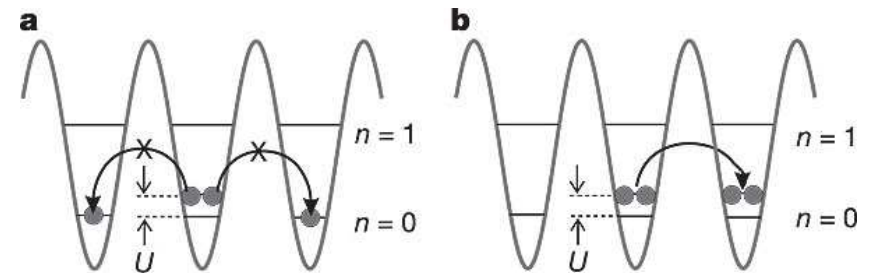
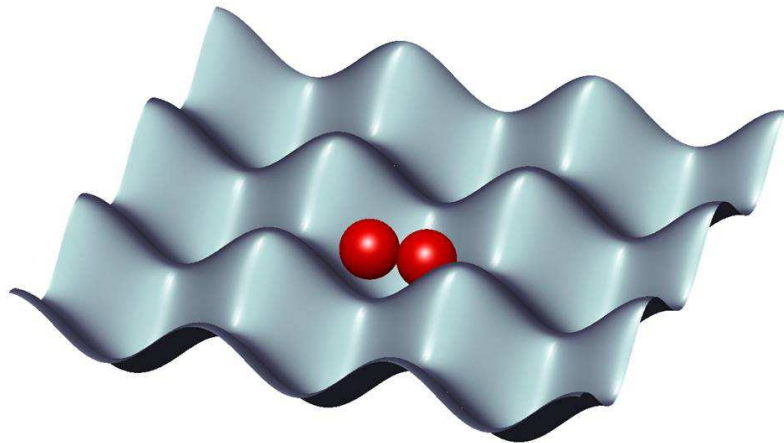
$$H_{\text{eff}} = (U - 2\tilde{J}) \sum_j \hat{m}_j - \tilde{J} \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j)$$



Repulsively bound atom pair: Experiment



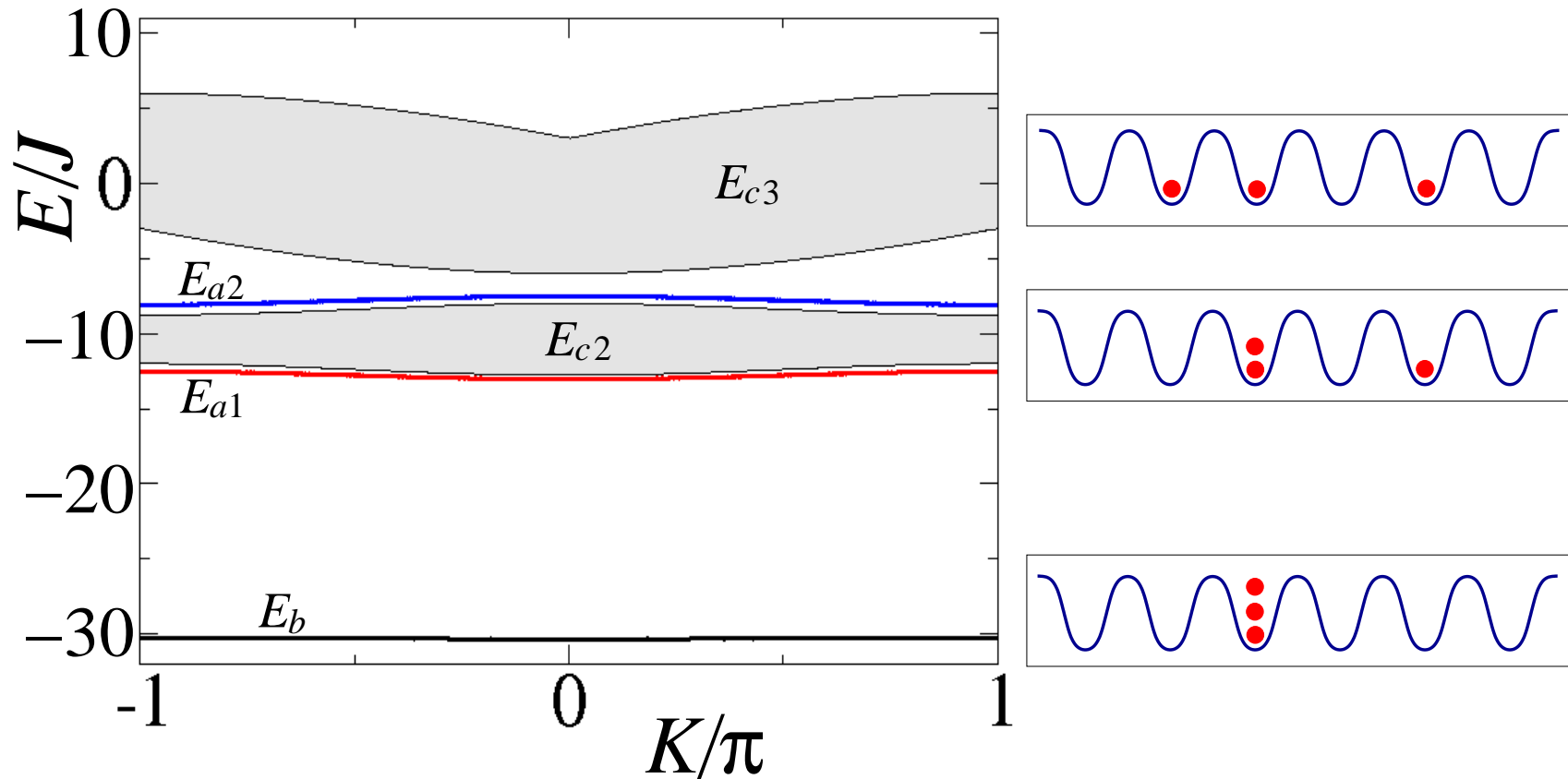
Single dimer



Three particles in Hubbard model (1D)



Complete three-body spectrum [$U = -10J$]



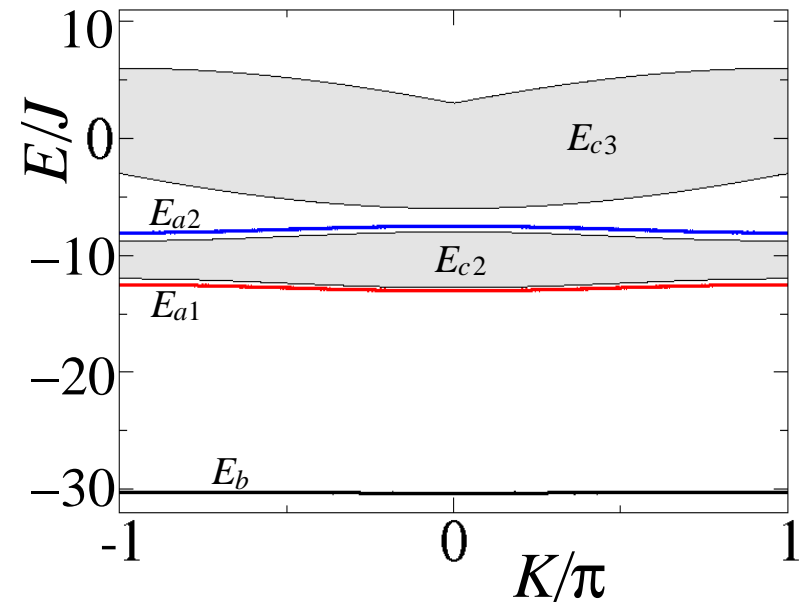
Three particles in Hubbard model (1D)



Three-body continuum

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

$$\epsilon(k) = -2J \cos(k) \quad K = k_1 + k_2 + k_3$$



Three particles in Hubbard model (1D)



Three-body continuum

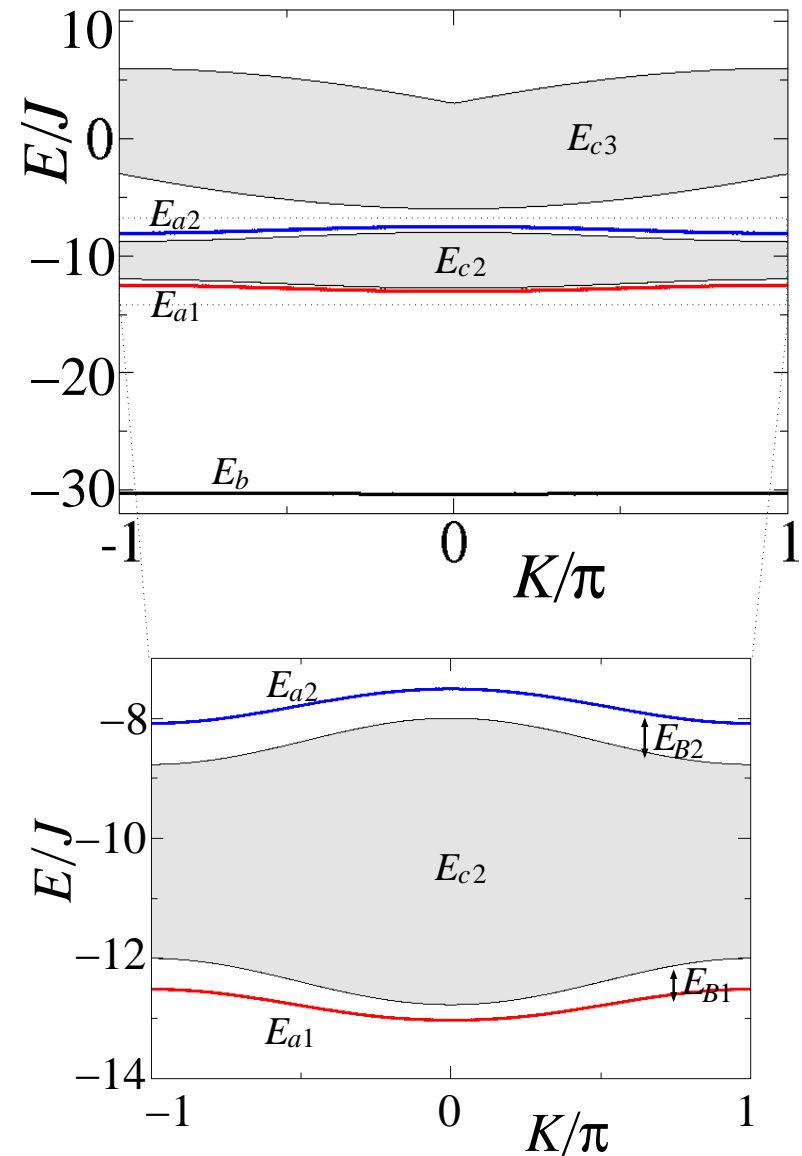
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Two-body continuum

$$E_{c2} = \epsilon^{(2)}(Q) + \epsilon(K - Q)$$

$$\begin{aligned} \epsilon^{(2)}(Q) &= \text{sgn}(U) \sqrt{U^2 + [4J \cos(Q/2)]^2} \\ &\simeq (U - 2\tilde{J}) - 2\tilde{J} \cos(Q) \end{aligned}$$



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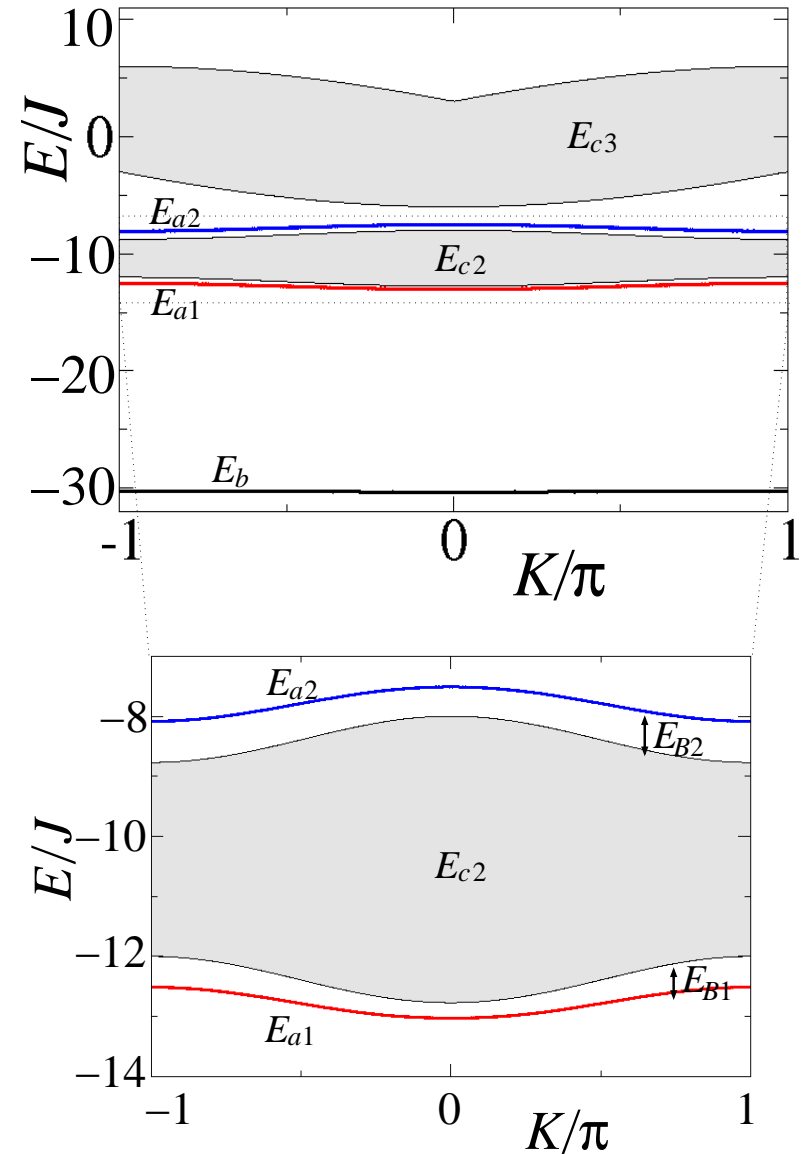
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Weakly-bound (off-site) trimers

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



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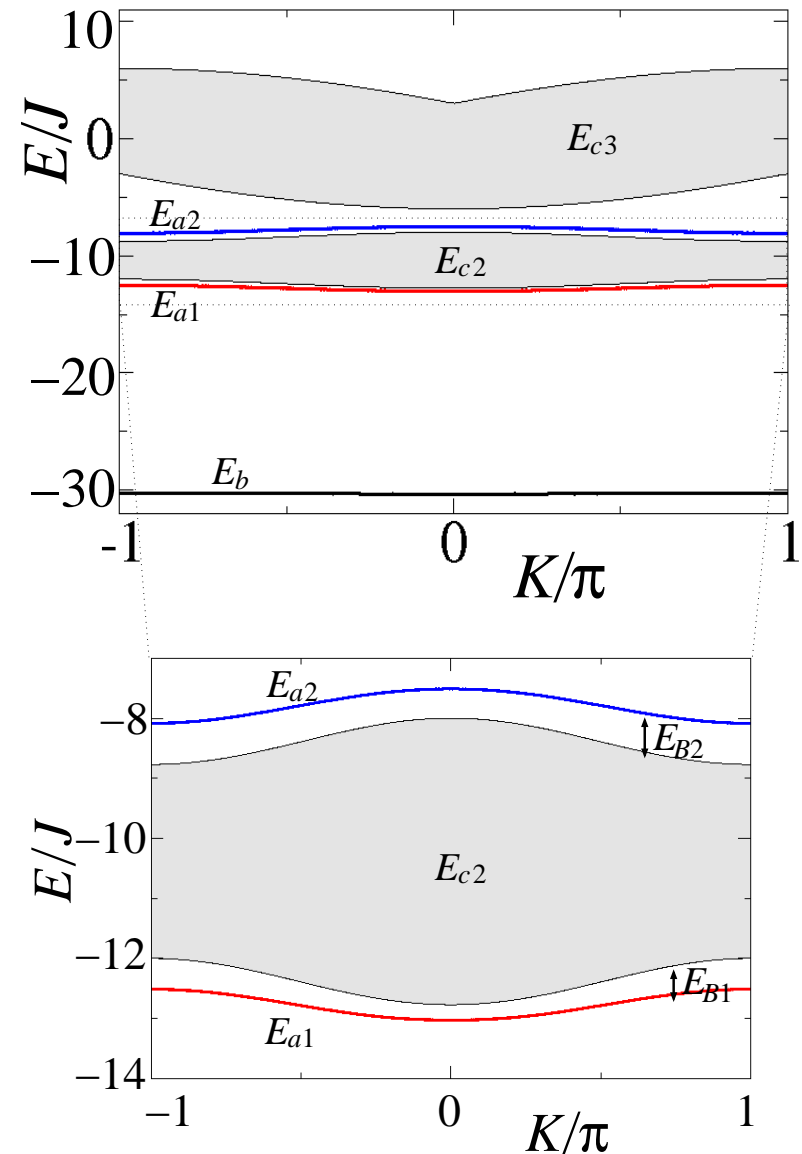
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Weakly-bound (off-site) trimers

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

Strongly-bound (on-site) trimer

$$E_b \simeq 3U$$



Formalism: Three-body bound states



State vector in momentum representation

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

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

with

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

$$I_E(k) \equiv \frac{U}{2\pi} \int_{-\pi}^{\pi} dq \frac{1}{\epsilon(k)+\epsilon(q)+\epsilon(K-k-q)-E} \\ = -\frac{\text{sgn}[E-\epsilon(k)]U}{\sqrt{[E-\epsilon(k)]^2 - 16J^2 \cos^2[(K-k)/2]}}$$

Formalism: Three-body bound states



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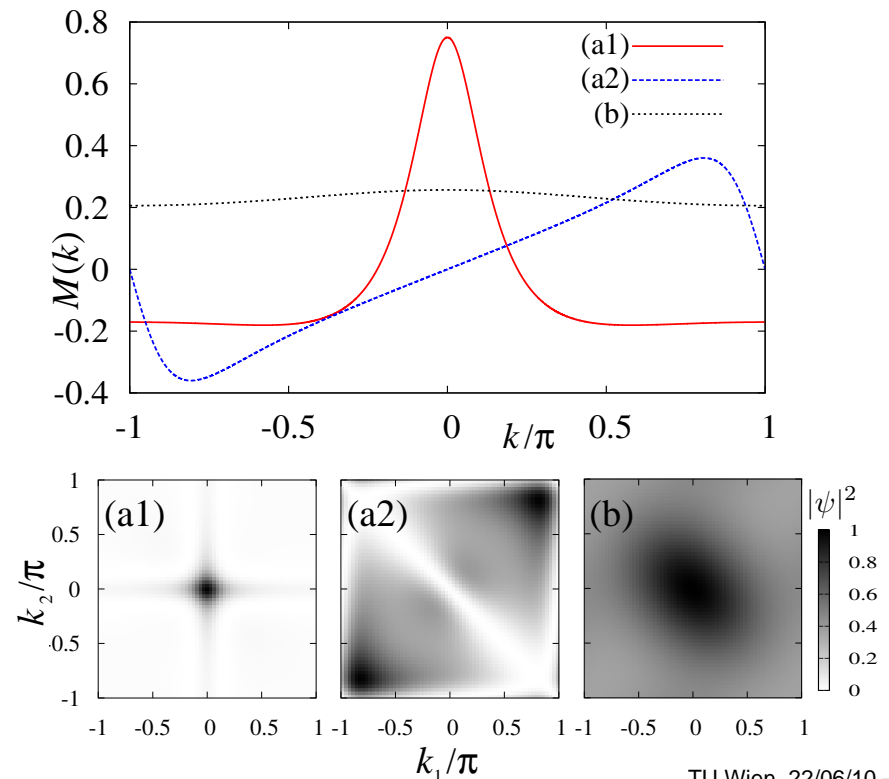
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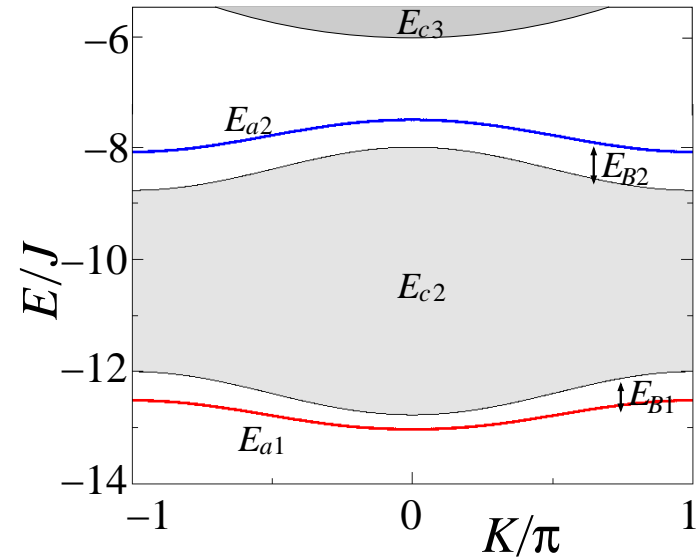
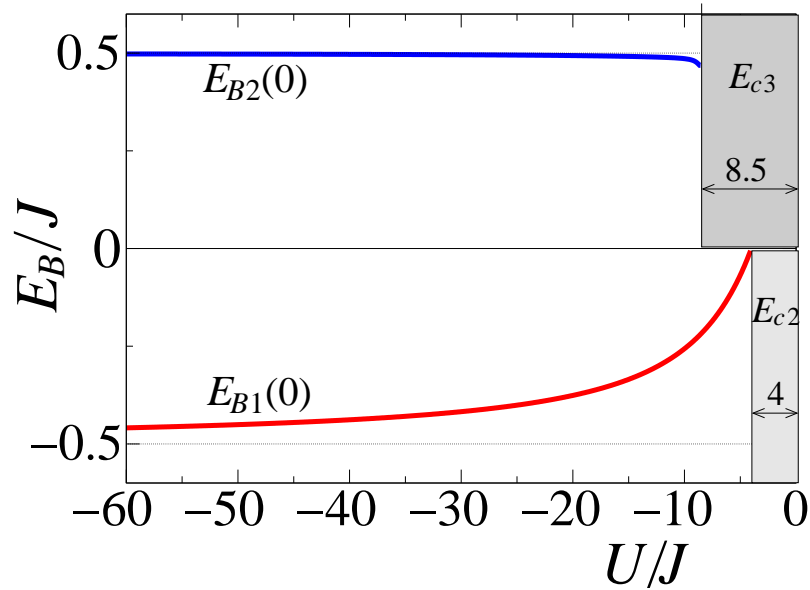
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Thresholds & limits of U



Binding energies



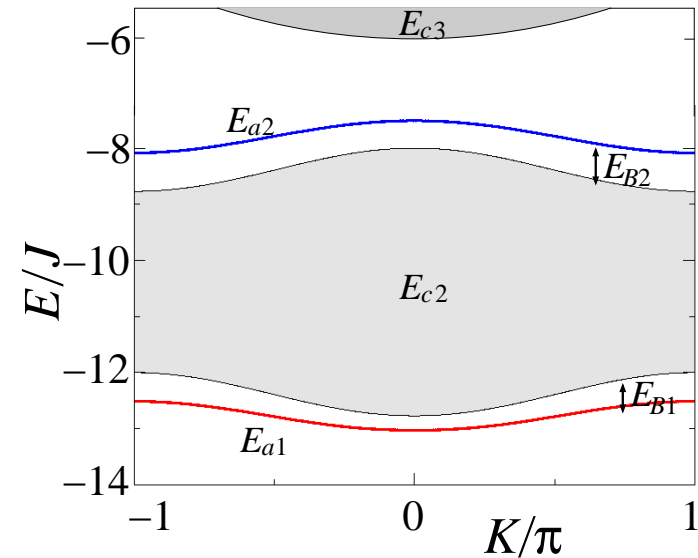
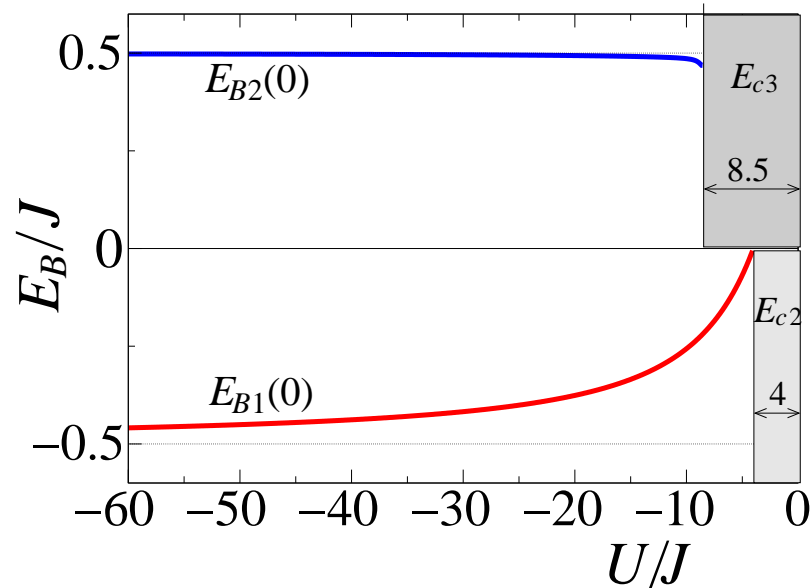
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Thresholds & limits of U



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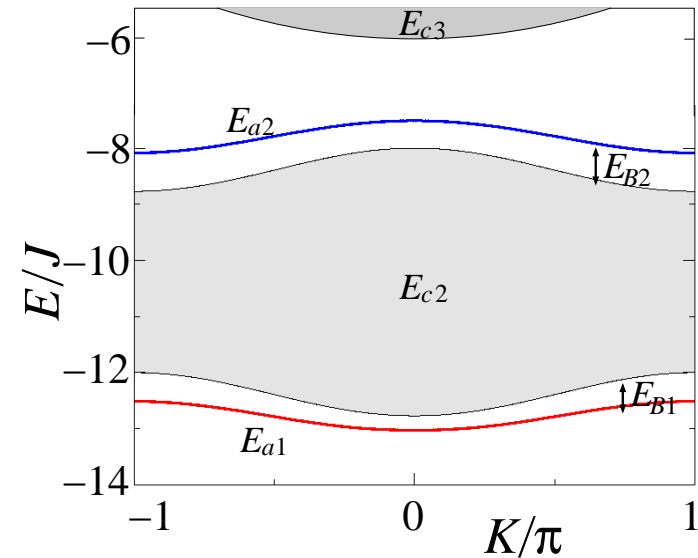
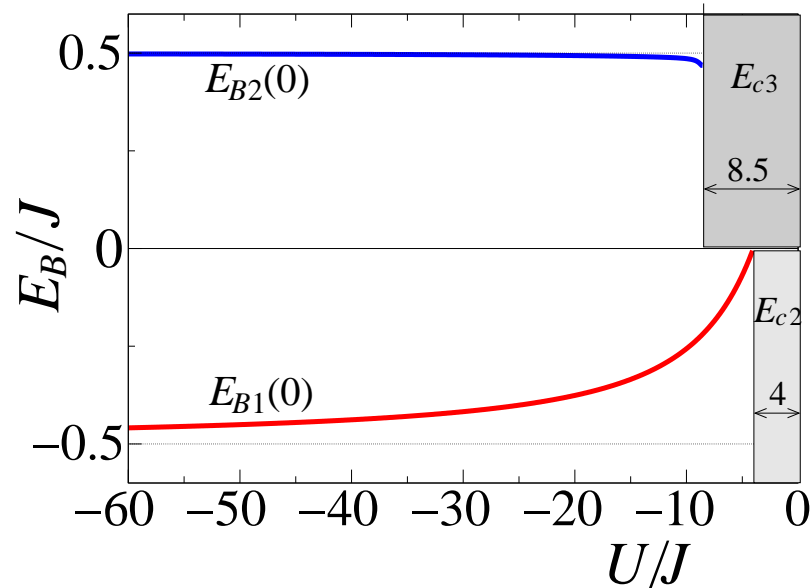
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For $|U| \lesssim 4J \Rightarrow E_{a1} \rightarrow E_{c2}$ ($E_{B1} \rightarrow 0$: Scattering resonance)

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Binding energies



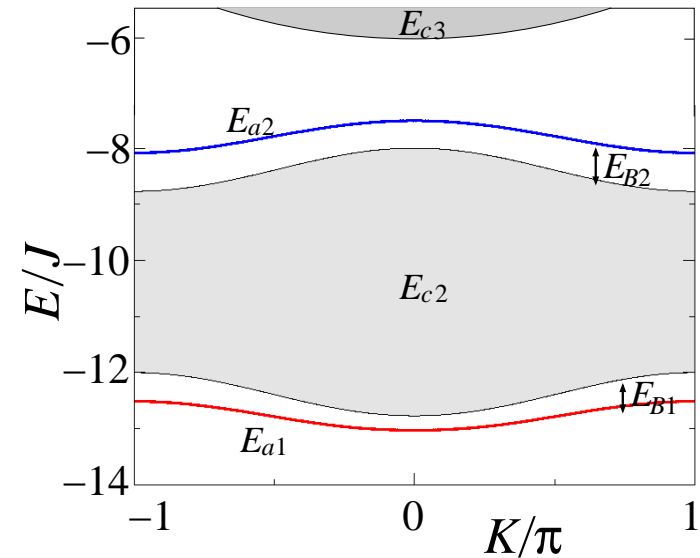
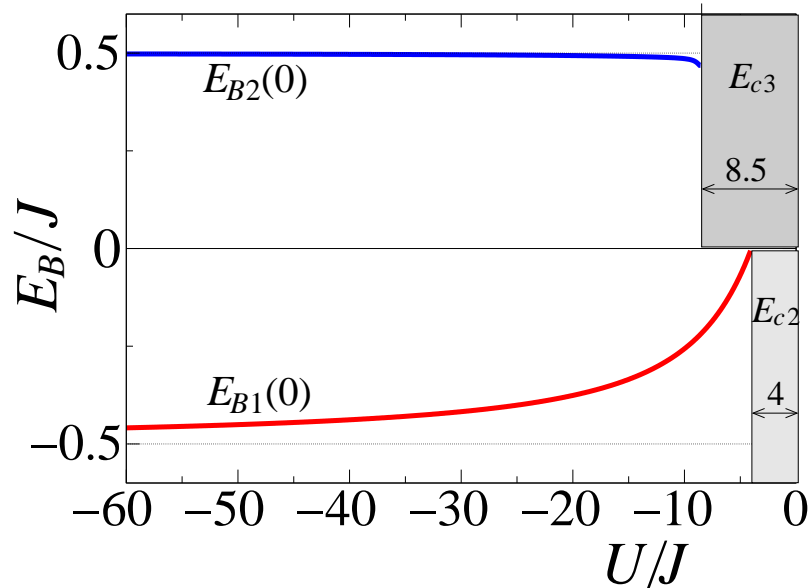
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For $|U| \lesssim 8.5J \Rightarrow E_{a2} \in E_{c3}$ (for $|U| \leq 8J$ $E_{c2} \cap E_{c3} \neq \emptyset$)

Thresholds & limits of U

Binding energies



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• $\lim_{U \rightarrow -\infty} E_{B1} = -\frac{J}{2}$

• $\lim_{U \rightarrow -\infty} E_{B2} = \frac{J}{2}$

Effective Hamiltonian for dimer+monomer



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

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Monomer (single-particle) Hamiltonian

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

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Dimer-monomer interaction

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

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

$W = 2J$: (particle) exchange interaction

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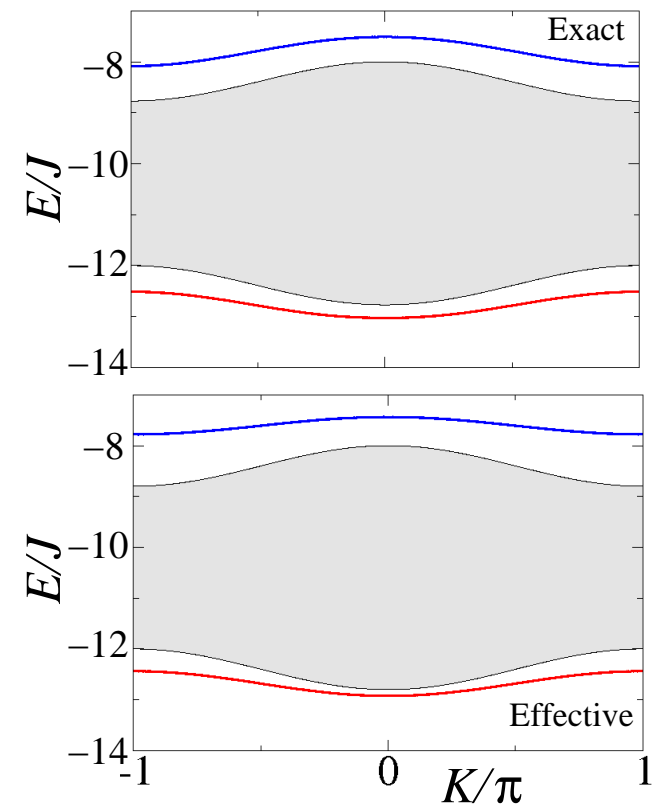
Dimer-monomer interaction

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dimer-monomer spectrum



Solution: Bound states ($K = 0, \pm\pi$)

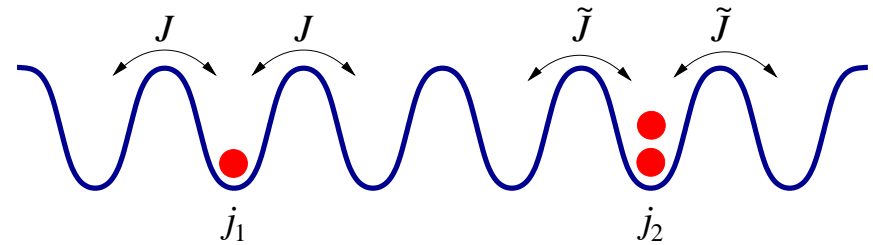


State vector

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

with

$$\Psi(j_1, j_2) = e^{iK(j_1+j_2)/2} e^{-i\delta_K j_r} \phi_K(j_r) \quad (j_r \equiv j_1 - j_2 \quad \tan(\delta_K) = \tan\left(\frac{K}{2}\right) \frac{J-\tilde{J}}{J+\tilde{J}})$$



Solution: Bound states ($K = 0, \pm\pi$)

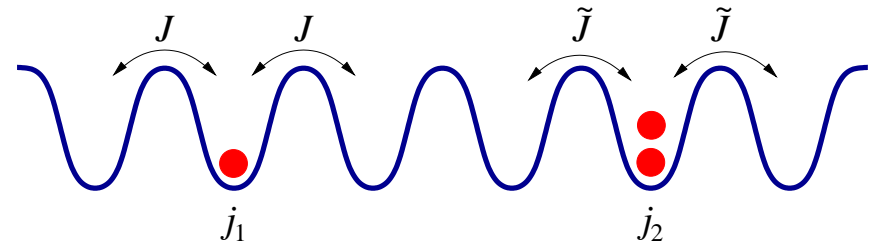


State vector

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

$$\phi_K(0) = 0$$

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

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

$$\text{with } \bar{J}_K \equiv \sqrt{J^2 + \tilde{J}^2 + 2J\tilde{J} \cos(K)} \quad W_K \equiv W \cos(K) \quad \bar{E} \equiv E - (U - 2\tilde{J})$$

$$\bar{J}_{0,\pi} = J \pm \tilde{J}$$

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)

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

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

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

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



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\Rightarrow Exchange interaction $W = 2J$ binds dimer and monomer

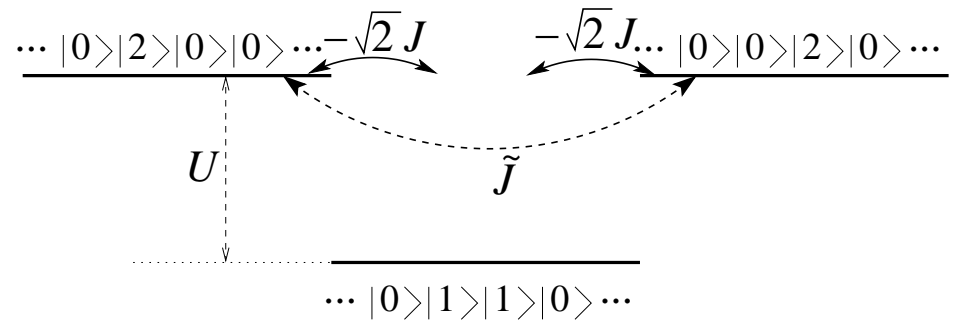


Many-body physics of tightly-bound dimers

Interaction-bound atom pair—Dimer



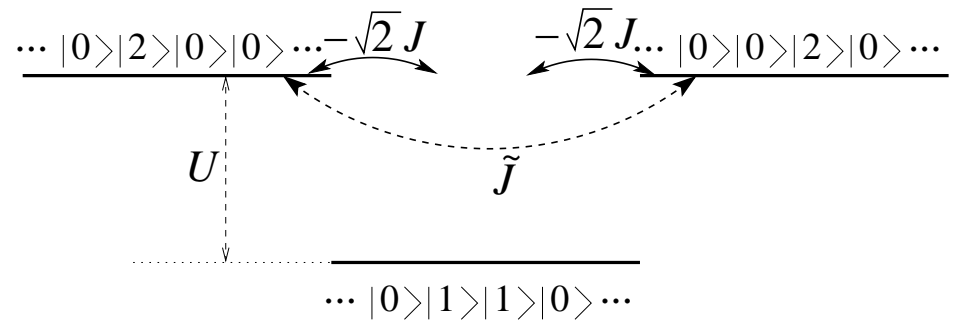
Energies of $|2, 0\rangle$ & $|0, 2\rangle$ are
larger (smaller) than of $|1, 1\rangle$ by U



Interaction-bound atom pair—Dimer



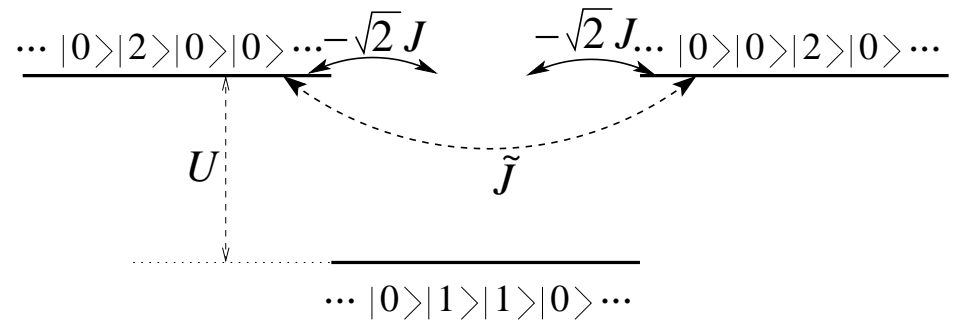
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For $|U|/J \gg 1 \Rightarrow |2, 0\rangle \rightarrow |1, 1\rangle$ is **non-resonant**

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

Interaction-bound atom pair—Dimer



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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 ($|U| \gg J$)

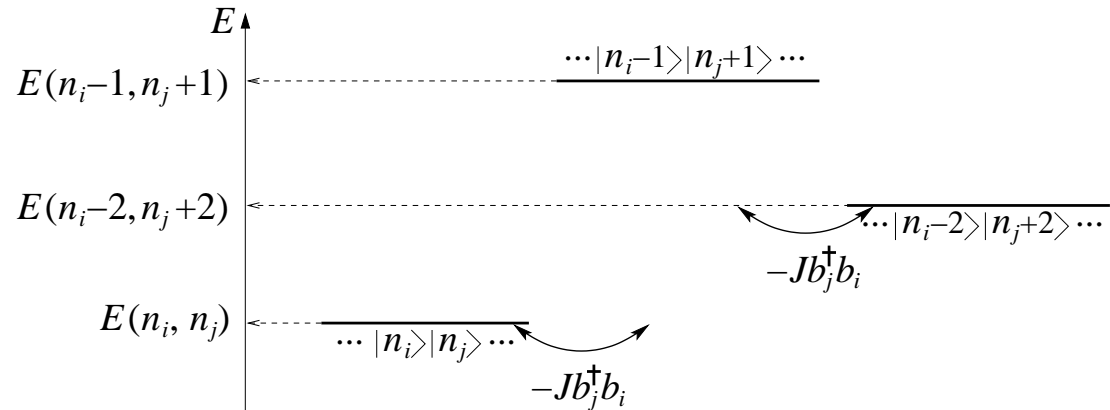


Define

$$c_j = \frac{1}{\sqrt{2(\hat{n}_j+1)}} b_j^2, \quad c_j^\dagger$$

$$\hat{m}_j = c_j^\dagger c_j$$

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



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 $\hat{S}(\hat{m}_j, \hat{m}_i) + \hat{S}(\hat{m}_i, \hat{m}_j) = \frac{2\hat{m}_j^2 + 2\hat{m}_i^2 + \hat{m}_j + \hat{m}_i}{1 - 4(\hat{m}_j - \hat{m}_i)^2}$



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- 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

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

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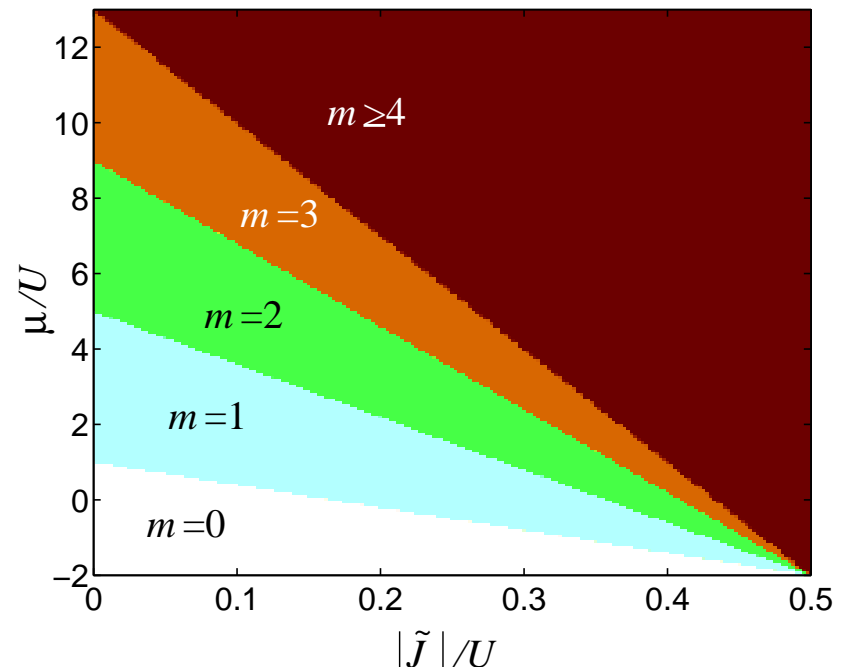
1D Phase Diagram [$\mu - \tilde{J}$]

Grand canonical ensemble

H_{eff} with uniform chem. potential

$$\mu = -2\varepsilon$$

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



Only uniform commensurate filling (incompressible phases)

Single dimers per site ($U \gtrsim 0$)



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

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

Similar to Extended Hubbard Model (nearest-neighbor interaction)

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

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

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

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

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$$\text{Since } \frac{1}{4} < 1 \Rightarrow H_{XXZ} \simeq H_{\text{Ising}} = 2h_z \sum_j \sigma_j^z + \tilde{J} \sum_{\langle j,i \rangle} \sigma_j^z \sigma_i^z$$

Droplets in a lattice ($U > 0$)

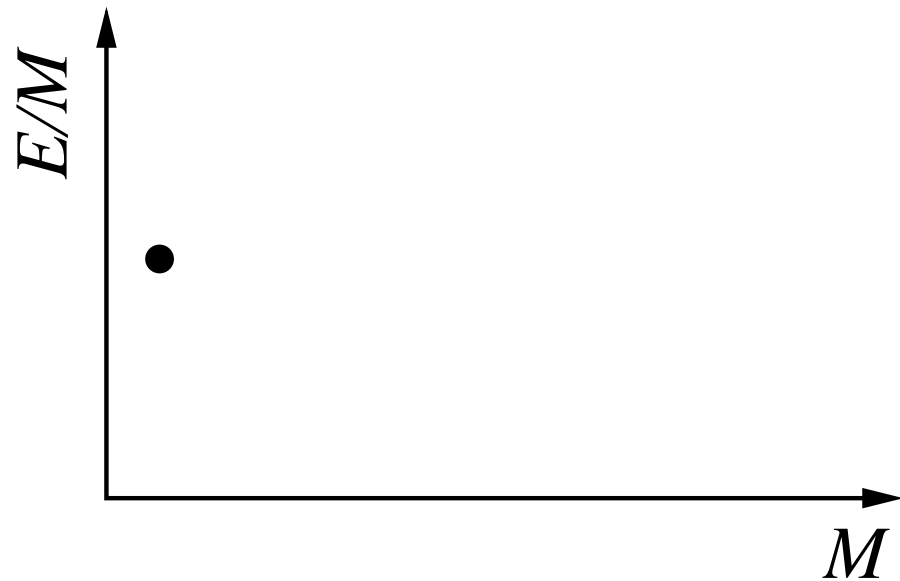
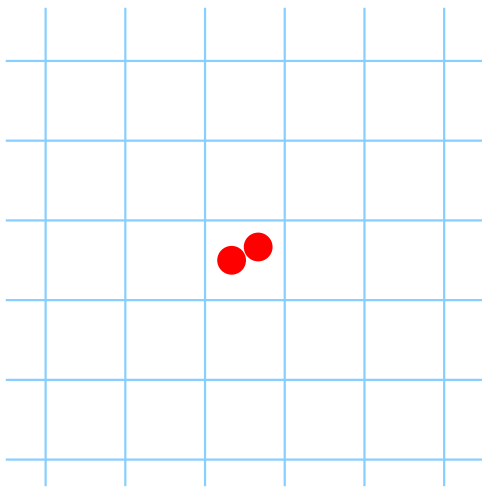


Strong dimer-dimer attraction ($8\tilde{J} > \tilde{J}$)

Droplets in a lattice ($U > 0$)



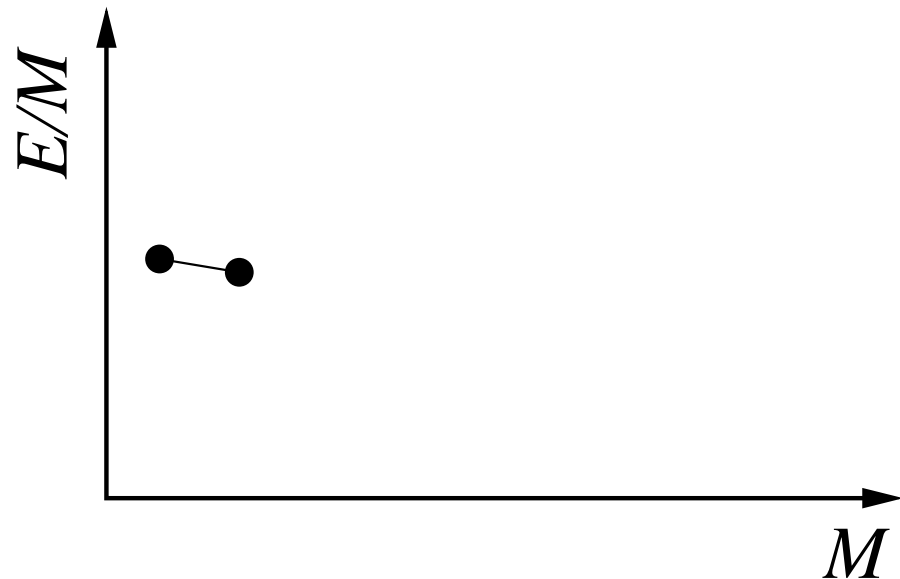
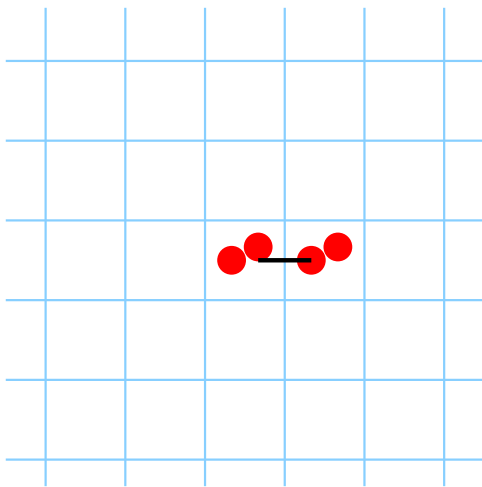
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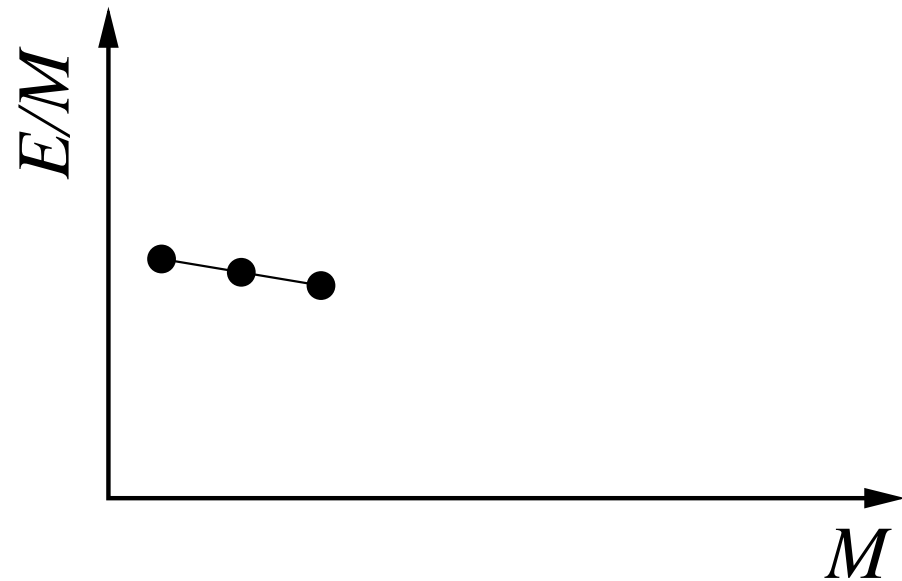
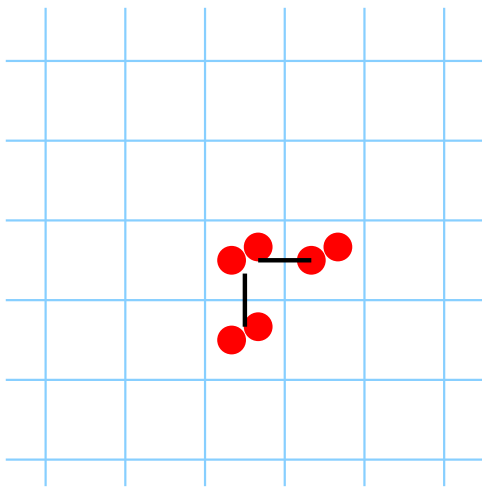
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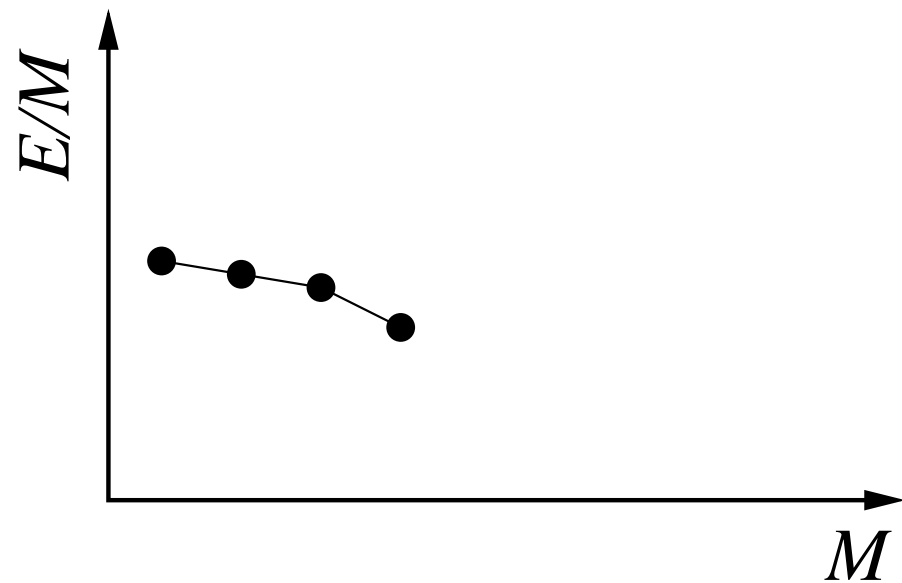
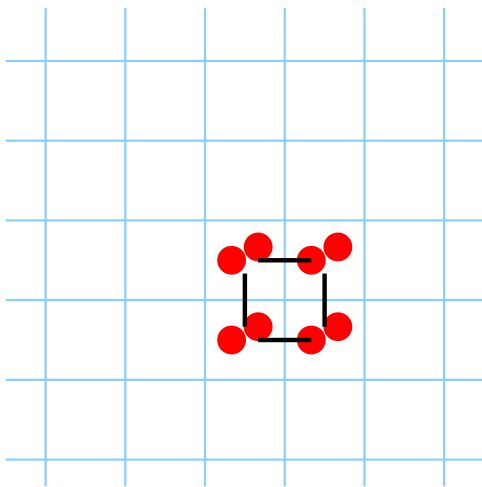
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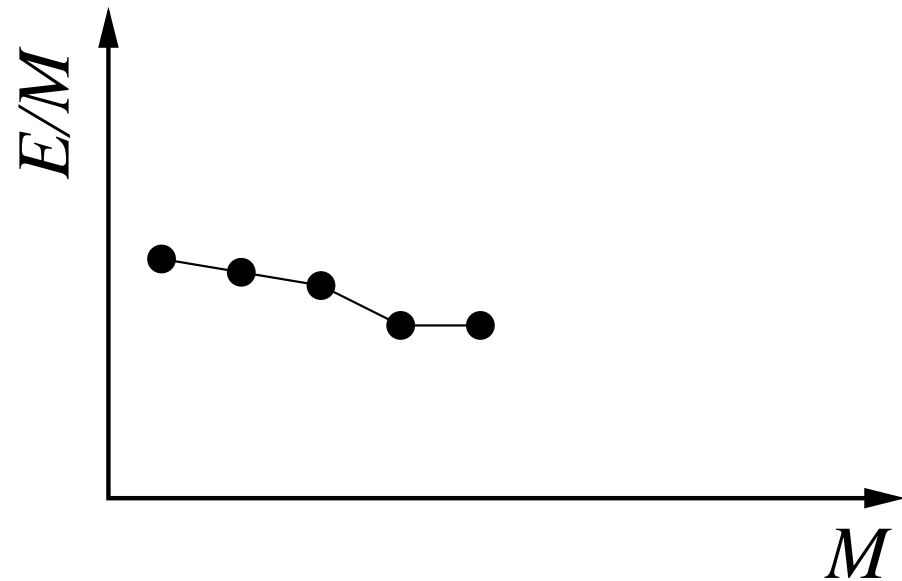
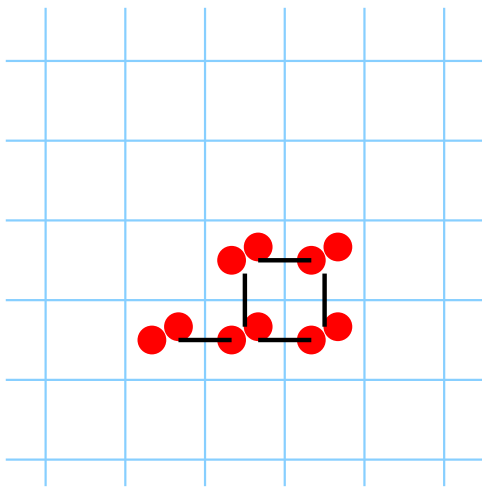
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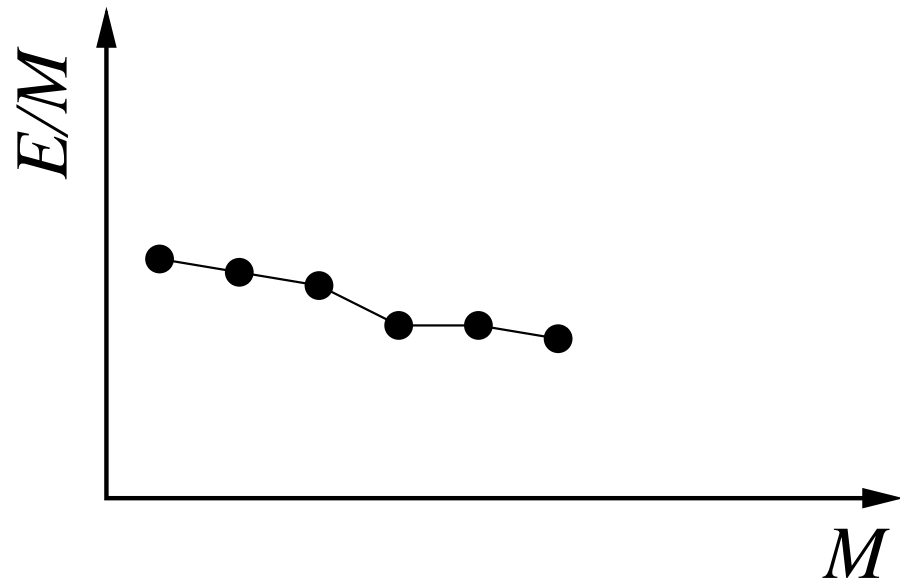
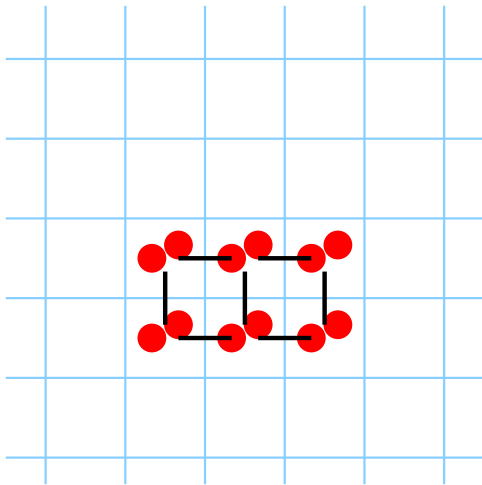
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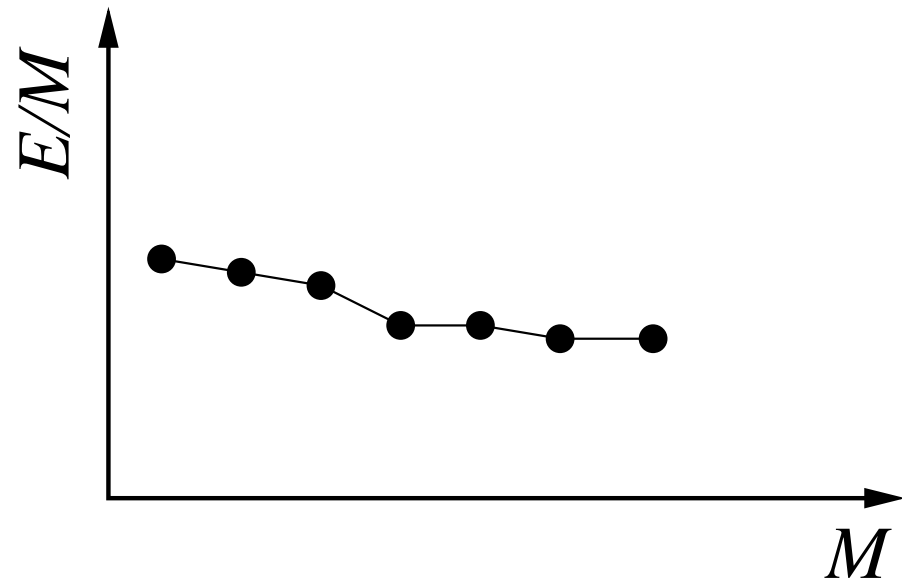
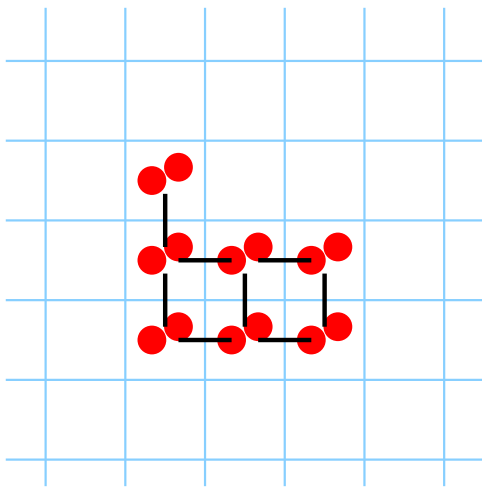
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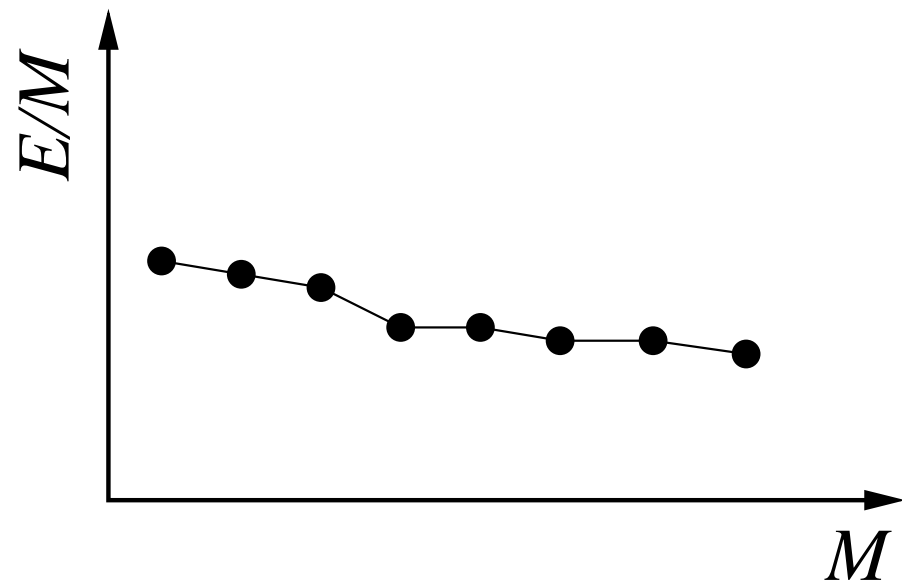
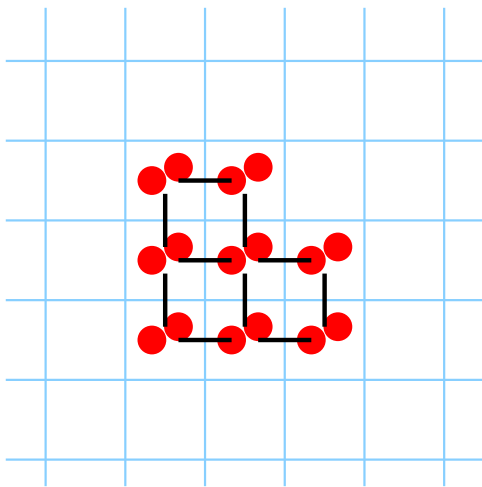
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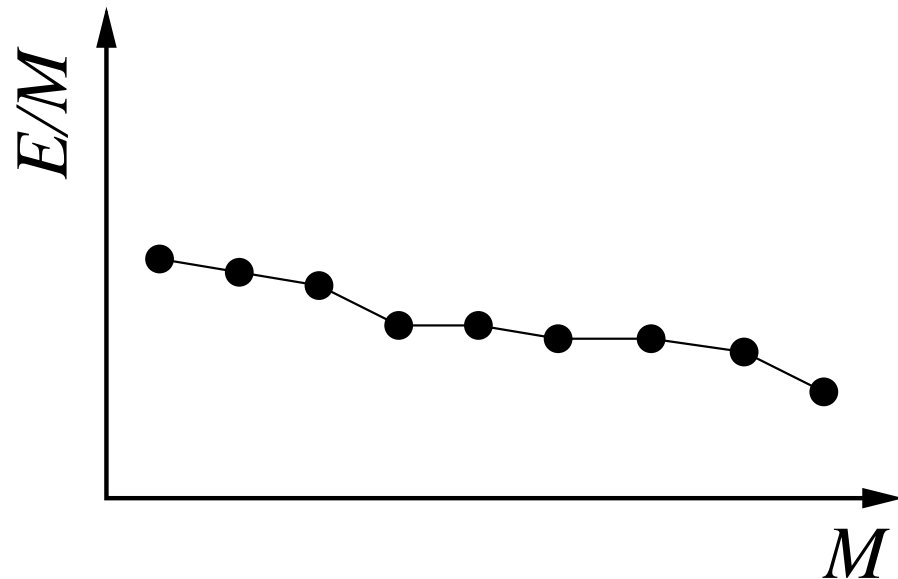
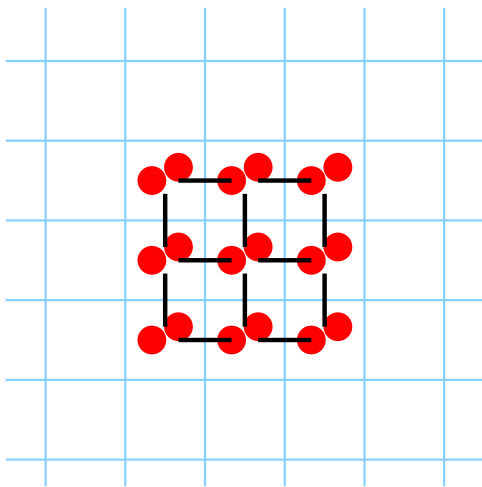
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Droplets in a lattice ($U > 0$)



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 ferromagnetic spin domain

Attractively-bound dimers ($U < 0$)



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

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

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

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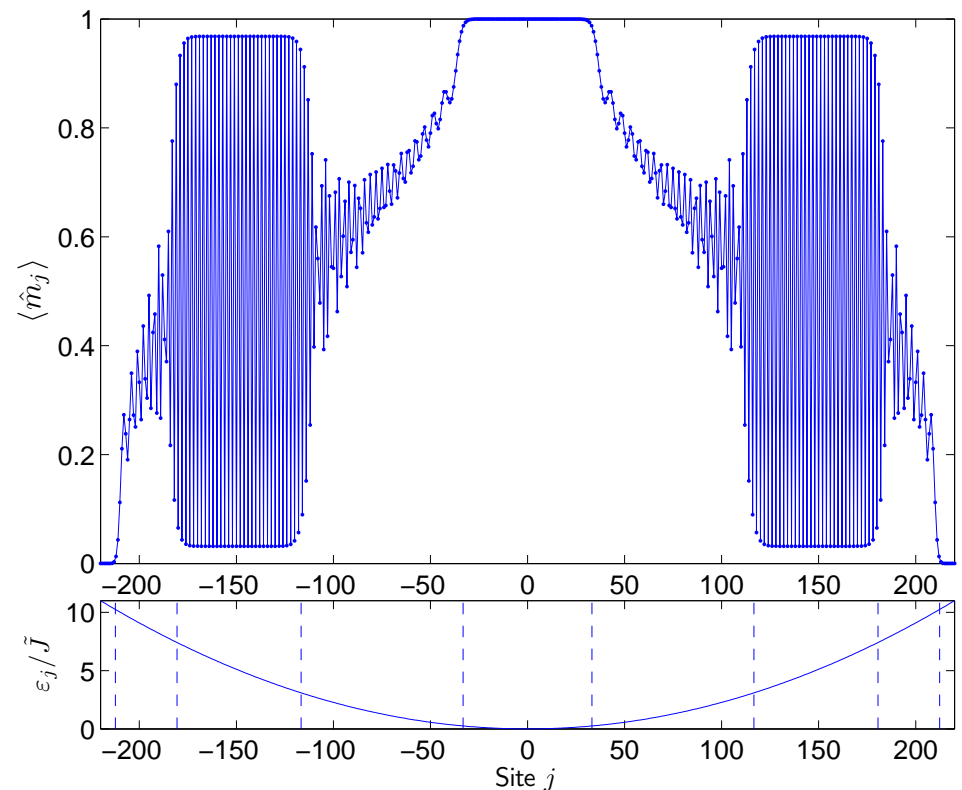
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Extended Hubbard Model with $\tilde{J} > 0$ (nearest-neighbor repulsion)

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 ($U < 0$)



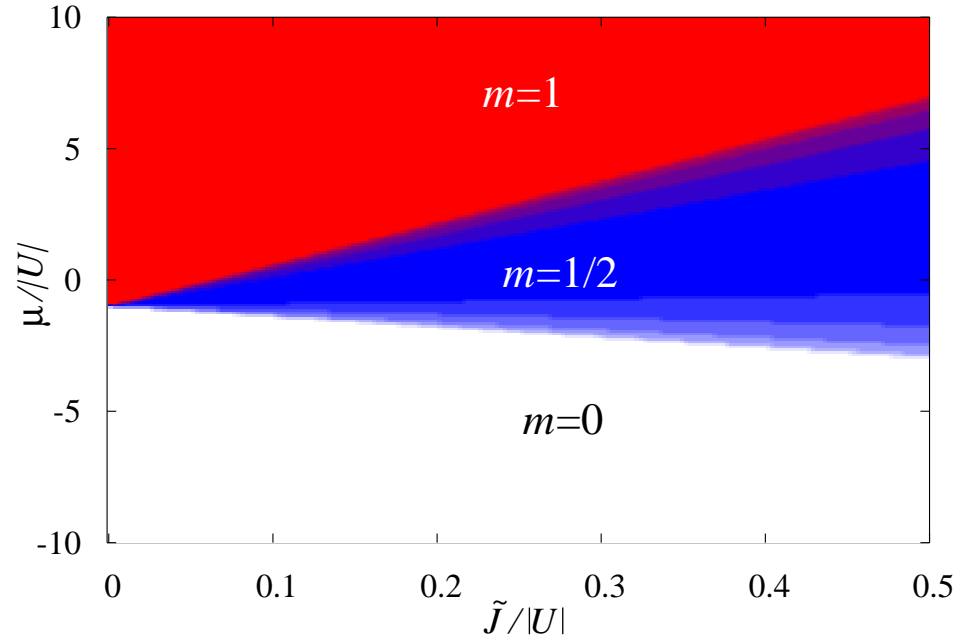
1D Phase Diagram [$\mu - \tilde{J}$]

Grand canonical ensemble

H_{eff} with uniform chem. potential

$$\mu = -2\varepsilon$$

Exact diagonalization for 10 sites



Attractively-bound dimers ($U < 0$)



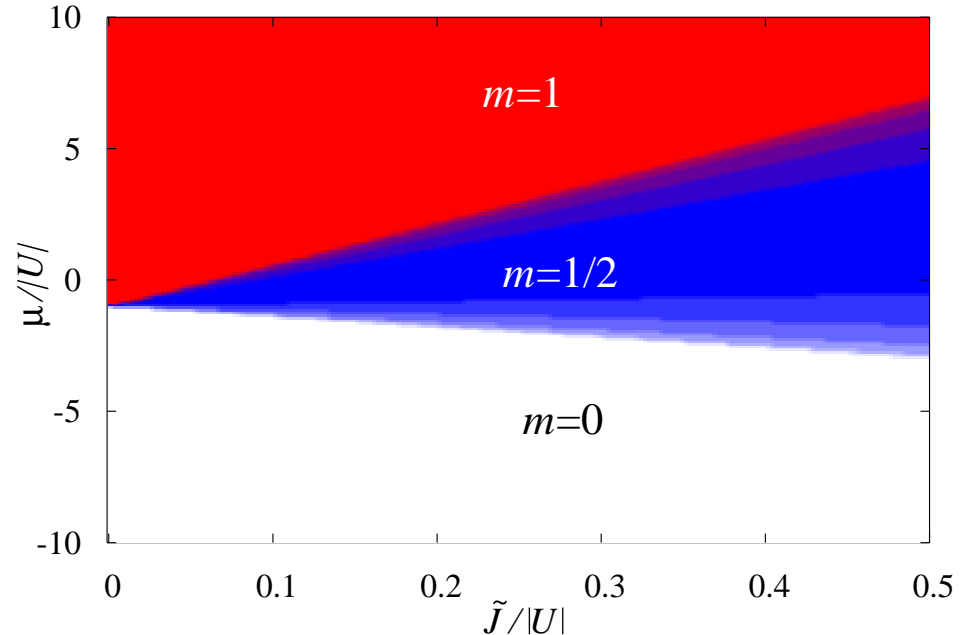
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$m = 0, m = \frac{1}{2}, m = 1$ incompressible phases:

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

$0 < m < \frac{1}{2}$ & $\frac{1}{2} < m < 1$ compressible (supersolid) phases

Attractively-bound dimers ($U < 0$)



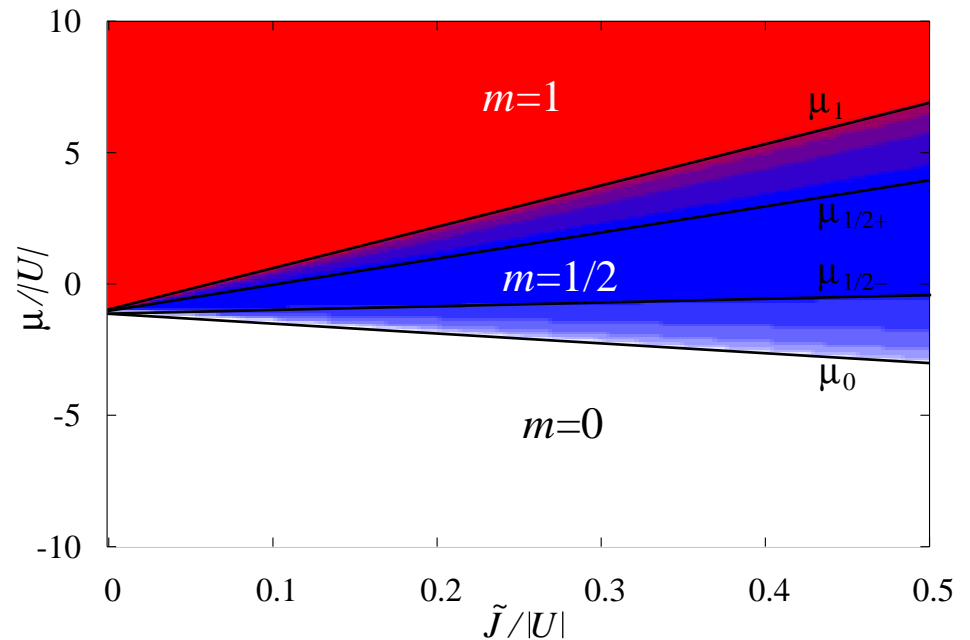
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Exact Bethe Ansatz solution

$$\mu_0 = U - 4\tilde{J} \quad \mu_1 = U + 16\tilde{J}$$

$$\mu_{1/2-} = U + 1.6836\tilde{J} \quad \mu_{1/2+} = U + 10.3164\tilde{J}$$

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

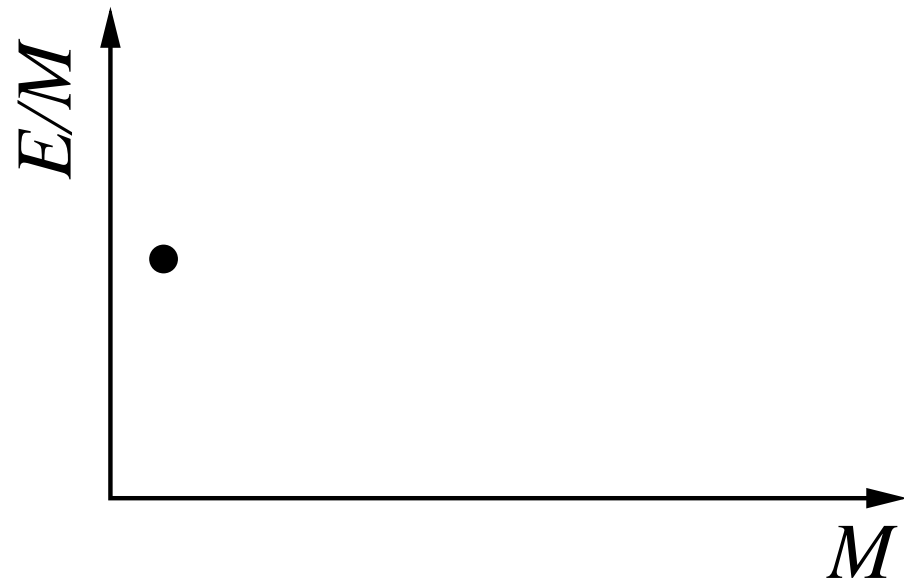
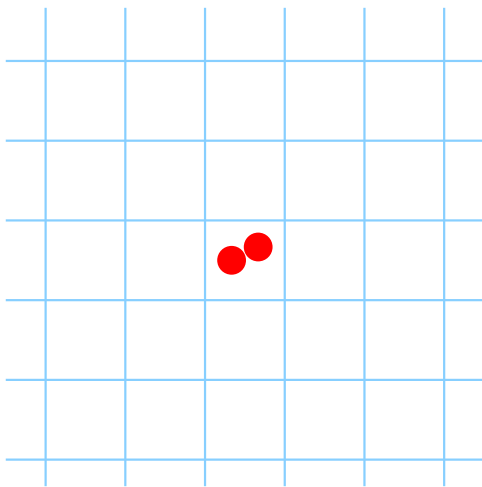


Strong dimer-dimer repulsion ($8\tilde{J} > \tilde{J}$)

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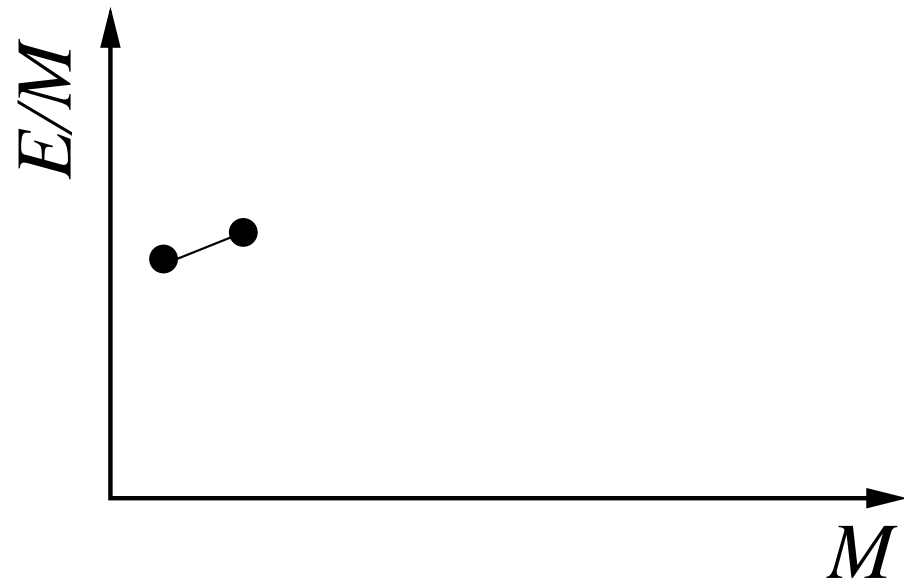
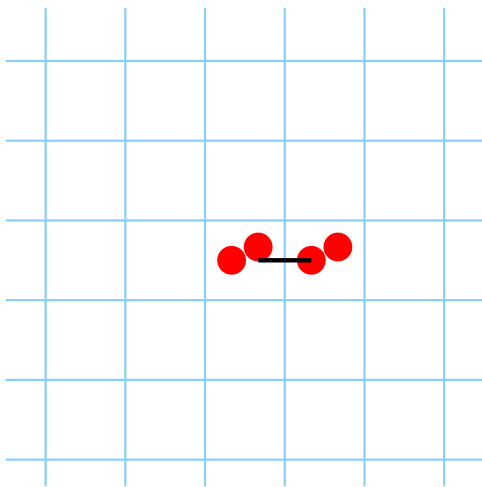
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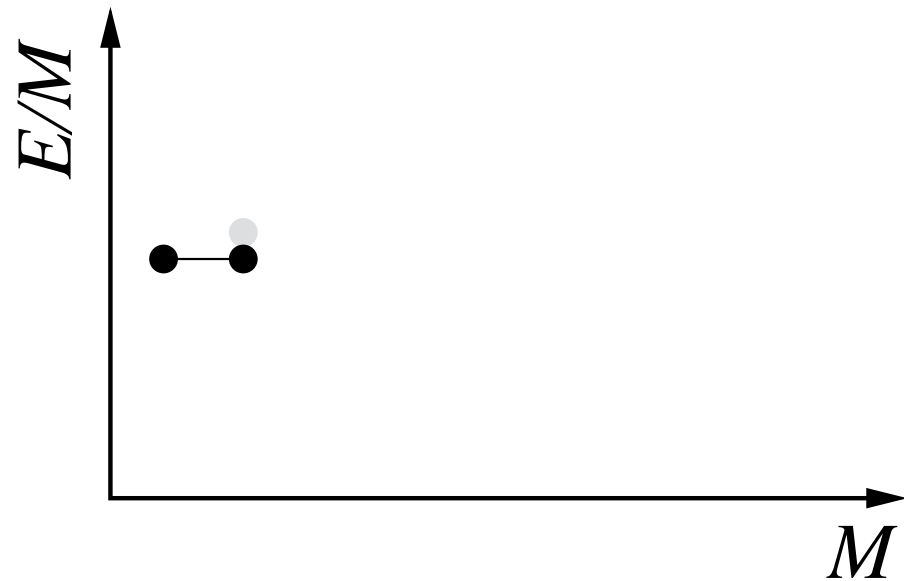
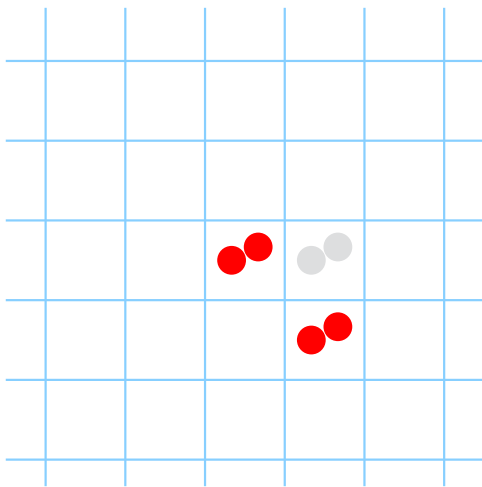
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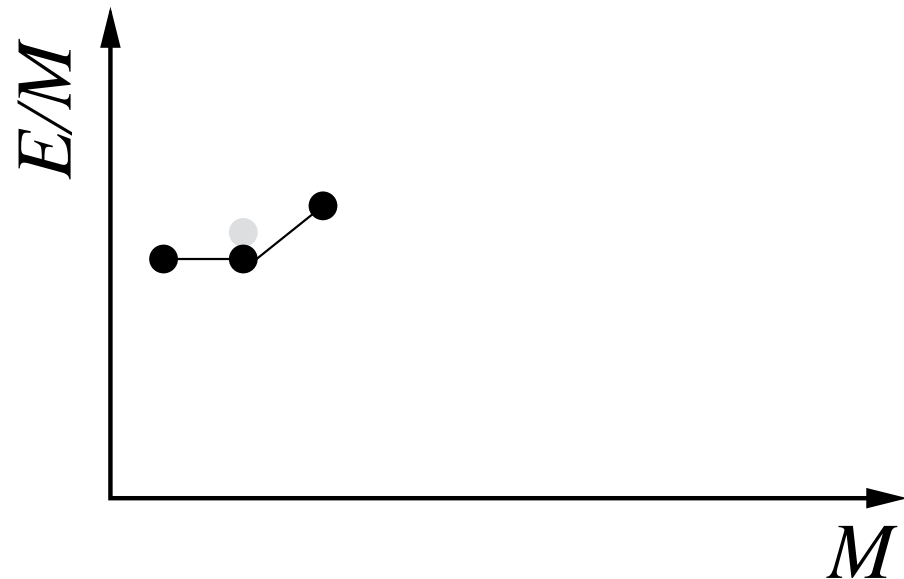
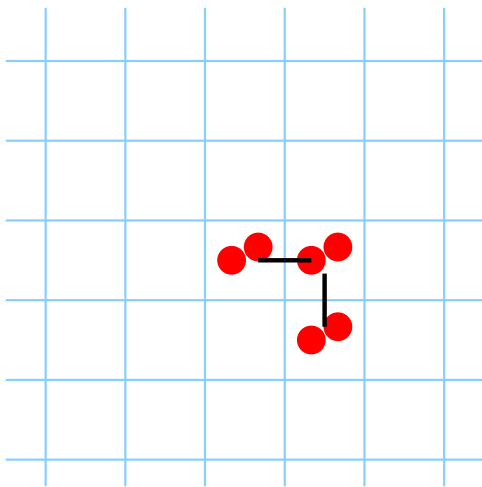
Strong dimer-dimer repulsion ($8\tilde{J} > \tilde{J}$)



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



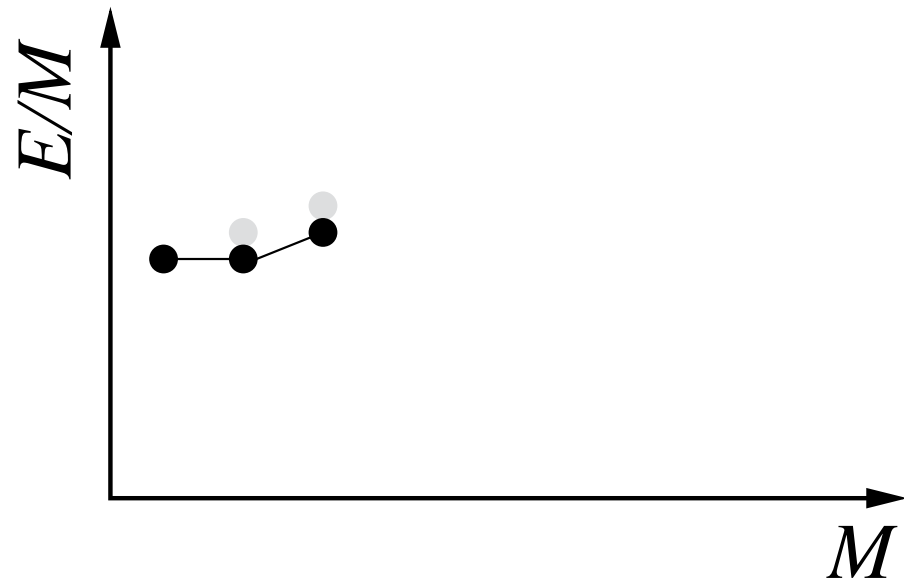
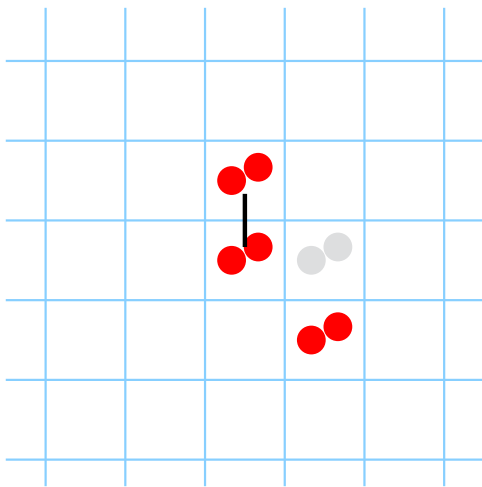
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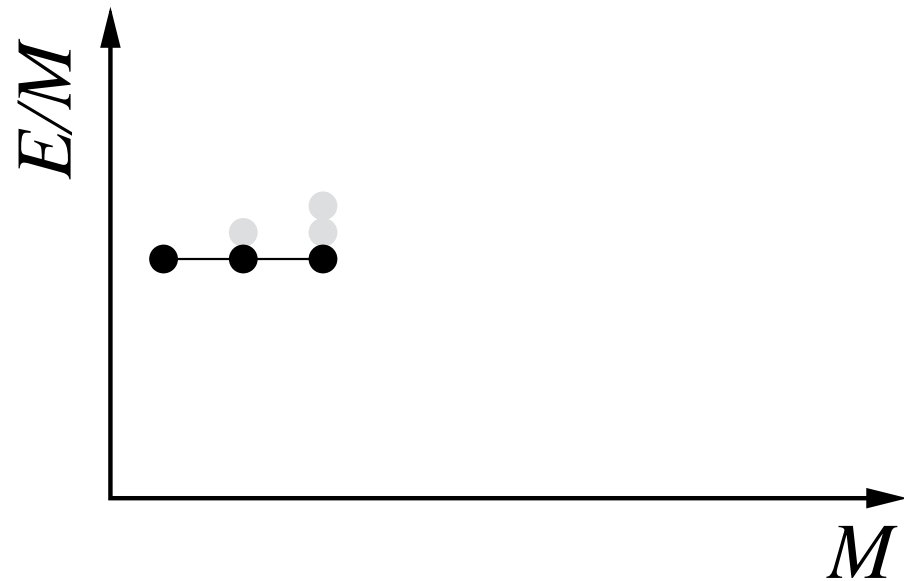
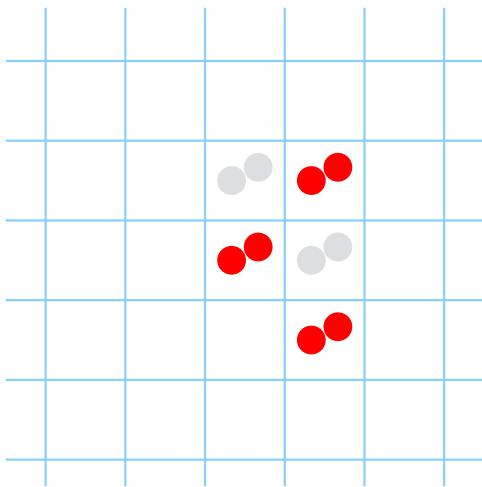
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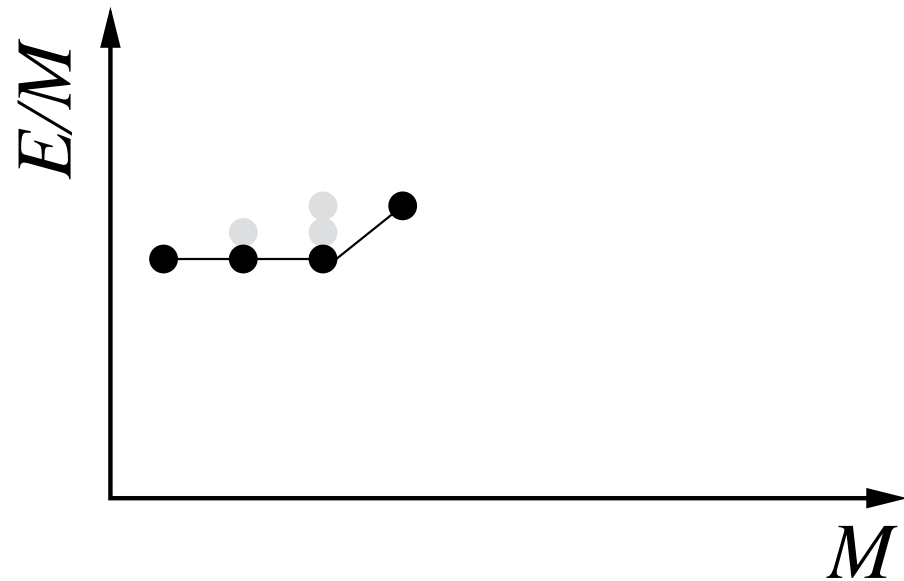
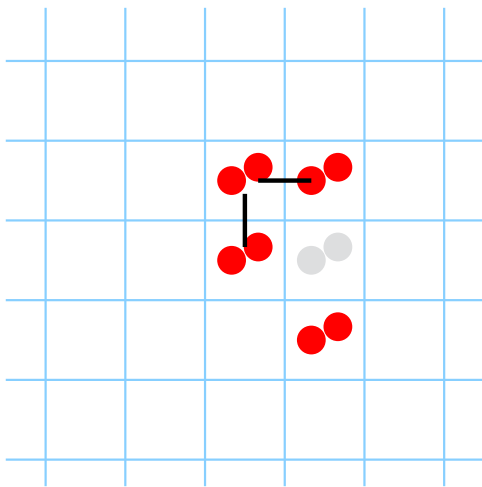
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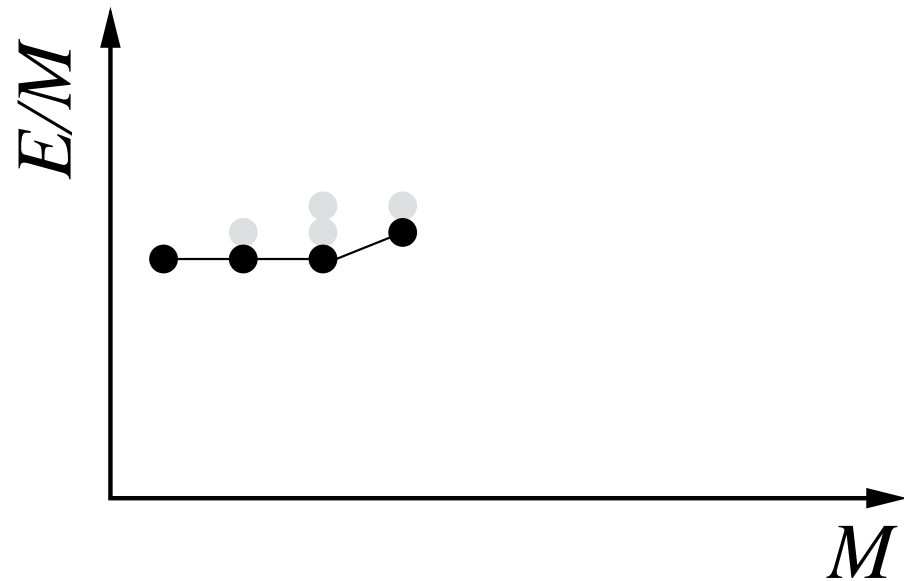
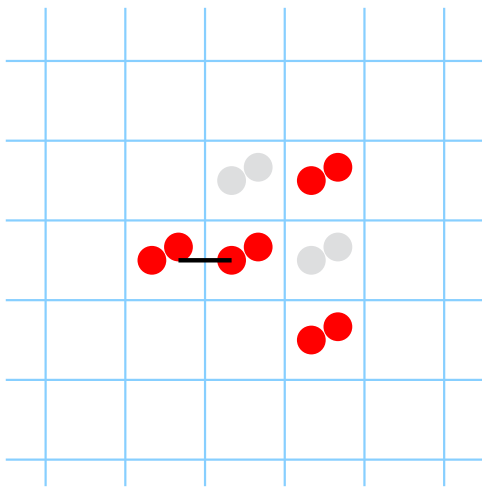
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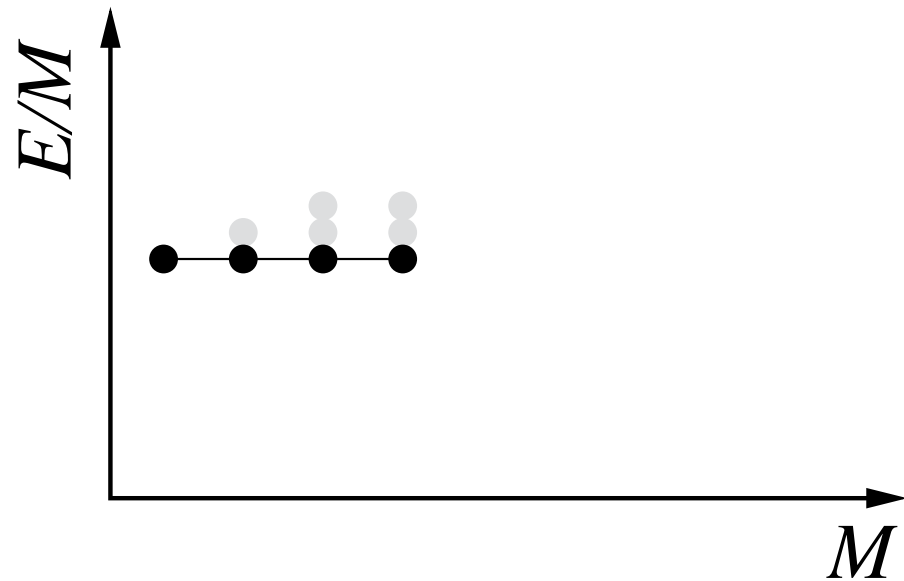
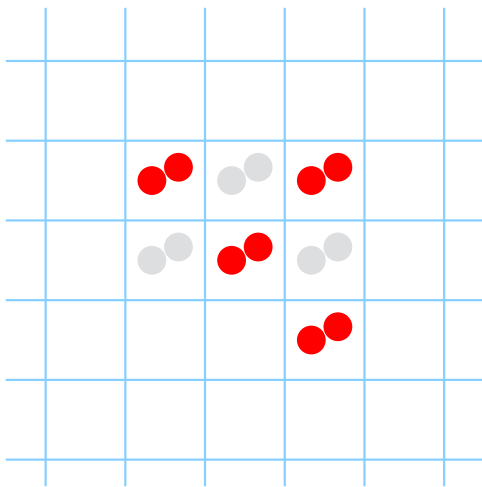
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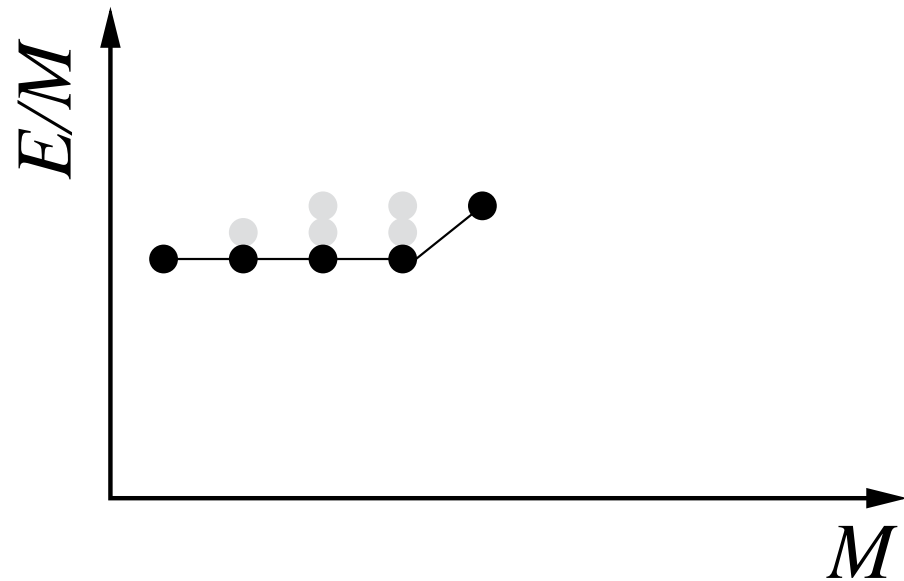
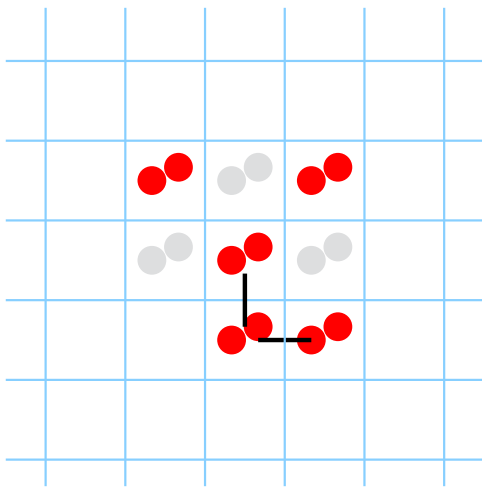
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Checkerboard crystal in a lattice ($U < 0$)



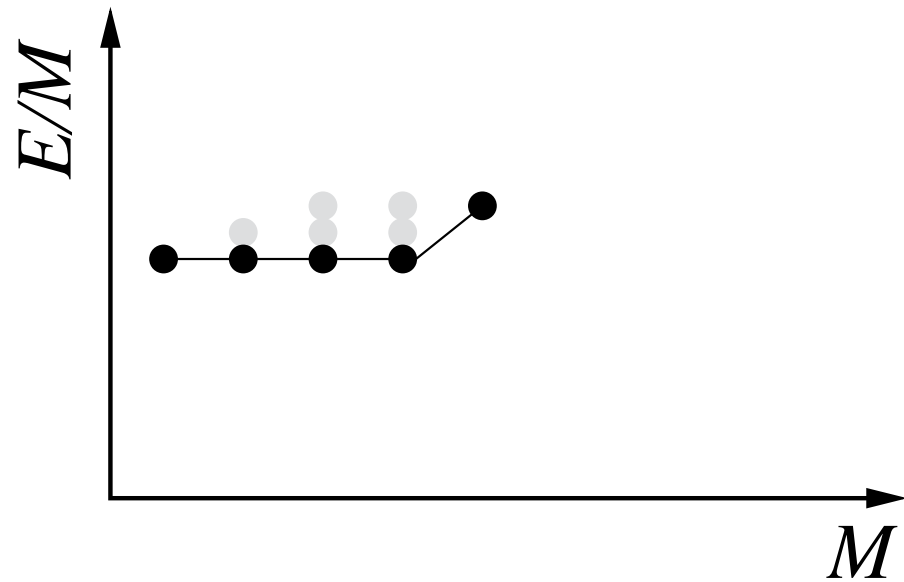
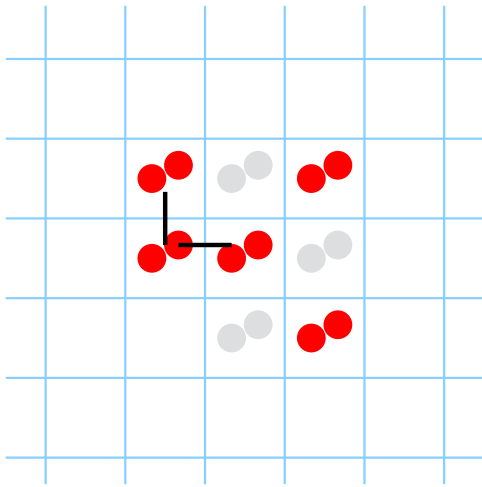
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Checkerboard crystal in a lattice ($U < 0$)



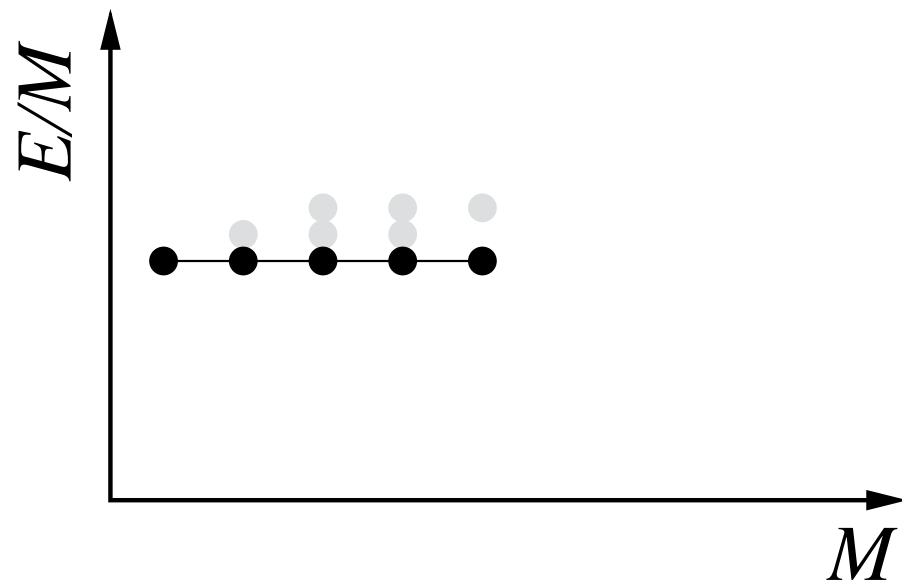
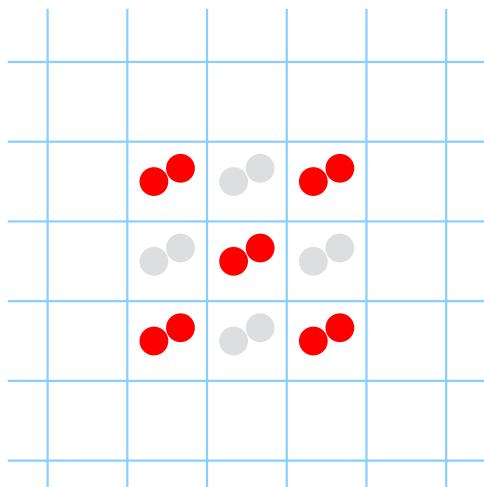
Strong dimer-dimer repulsion ($8\tilde{J} > \tilde{J}$)



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

Summary



- 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

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