Cold Atoms in Optical Lattices:

A versatile system to explore few- and many-body physics in periodic potentials

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Outline

- The Hubbard model for atoms
  - *Optical dipole potential*
  - *Cold bosonic atoms in a tight-binding periodic potential*
  - *The second quantized Hamiltonian*

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  - *Bloch band of a homogeneous lattice*
  - *Tilted lattice: Wannier-Stark ladder*
  - *Weak parabolic confinement: Discrete HO*

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  - *Bound states: Effective dimers*
  - *Three-atom states: Bound trimers*

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  - *Three-atom states: Bound trimers*
- Many body physics of the Hubbard model
  - *Superfluid and Mott-Insulating phases for bosons*
  - *Metal and Insulating phases for fermions*

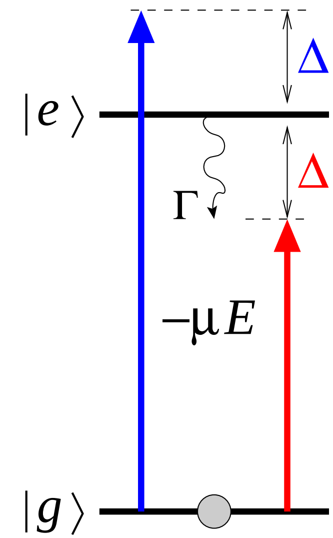
The Hubbard model for atoms

Optical dipole potential

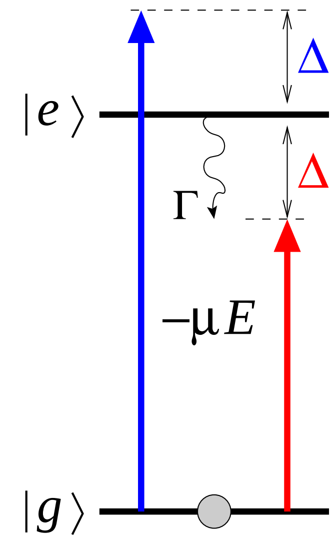
Atom with $|g\rangle \leftrightarrow |e\rangle$ frequency ω_{eg} in laser field $E = E_0 e^{-i\omega t}$

Dipole coupling $-\mu E$ (with μ el.-dip. matrix element for $|g\rangle \leftrightarrow |e\rangle$)

$\Rightarrow$ detuning $\boxed{\Delta = \omega - \omega_{eg}}$ recoil energy $\boxed{E_r = \frac{\hbar^2 k^2}{2M}}$



Optical dipole potential



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$|\Delta| \gg \mu E_0/\hbar, \Gamma \quad \Rightarrow \quad |g\rangle \rightarrow |e\rangle$ non-resonant

Second-order perturbation theory $\Rightarrow$ ac Stark shift of $|g\rangle$

$\boxed{V_{\mathrm{dip}}(\mathbf{r}) = \frac{|\mu E(\mathbf{r})|^2}{\hbar\Delta} = -\frac{1}{2}\alpha(\omega) I(\mathbf{r})}$ with polarizability $\alpha(\omega) = \frac{3\pi c^2}{\omega_{eg}^3} \frac{\Gamma}{\omega_{eg} - \omega}$

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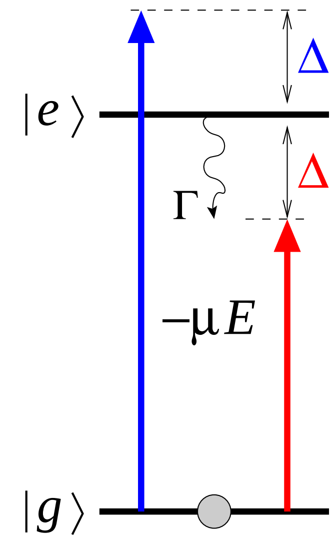

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- Blue detuned laser $\Delta > 0 \Rightarrow V_{\text{dip}}(\mathbf{r}) > 0$: low-field seeking atoms
- Red detuned laser $\Delta < 0 \Rightarrow V_{\text{dip}}(\mathbf{r}) < 0$: high-field seeking atoms

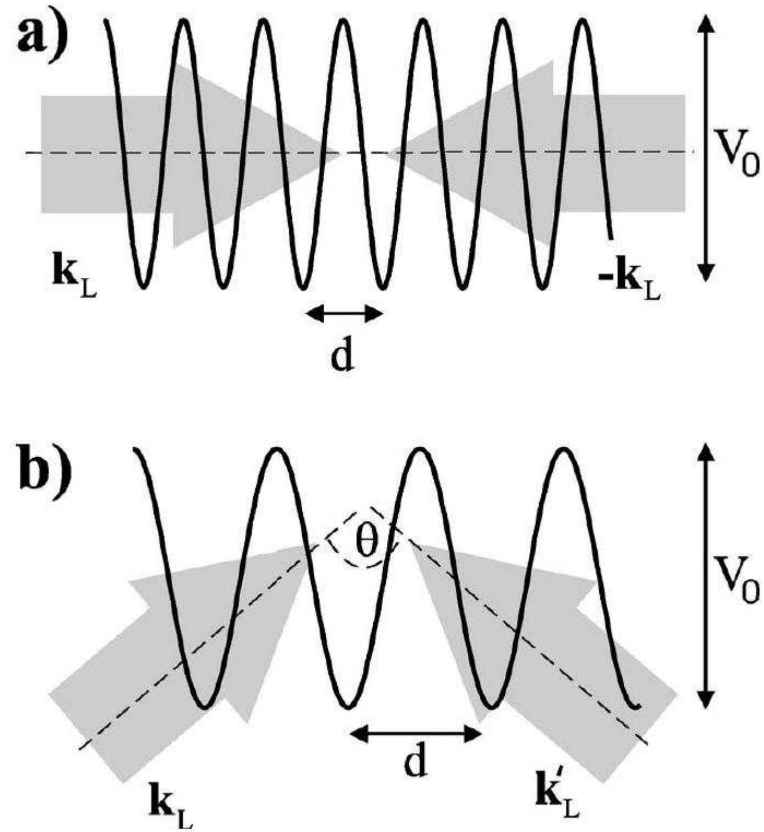
Optical lattice potential

1D Optical lattice

$$V_{\rm OL}(x) = V_0 \sin^2(\frac{\pi}{d}x)$$

with

$$V_0 = sE_r \quad \& \quad d = \frac{\pi}{k_L^x} \quad [k_L^x = k_L \sin(\frac{\theta}{2})]$$



[from: Morsch, Oberthaler, RMP 78, 179 (2006)]

Optical lattice potential

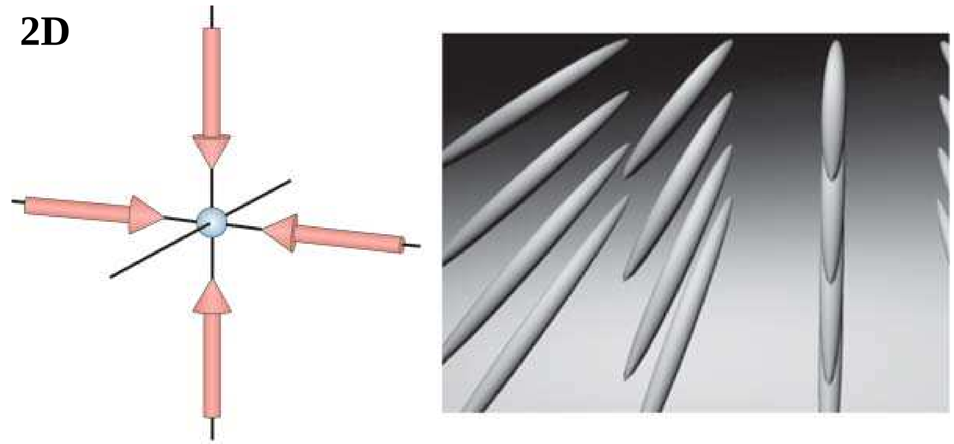
2D & 3D Optical lattice

$$V_{\mathrm{OL}}(\mathbf{r}) = \sum_{\xi=x,y,(z)} V_{0\xi} \sin^2(\tfrac{\pi}{d}\xi)$$

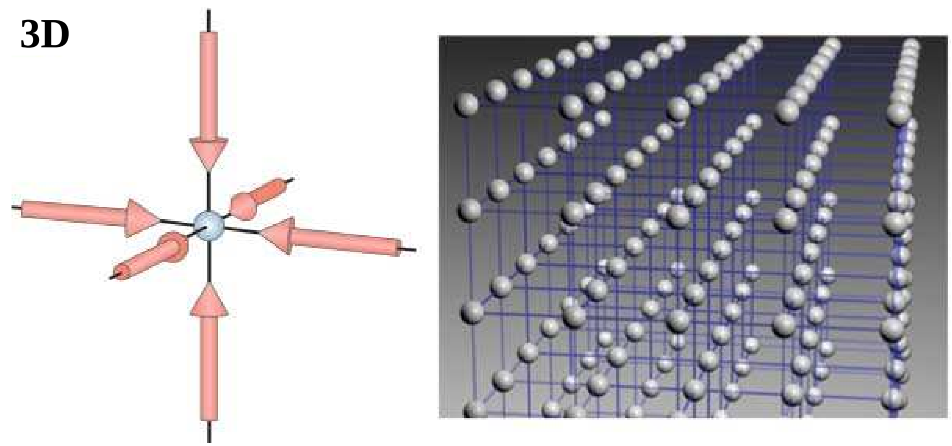
with

$$V_{0\xi} = s_\xi E_r$$

2D



3D



[from: Bloch, Dalibard, Zwerger, RMP 80, 885 (2008)]

Atom in a lattice

Stationary Schrödindeg equation (1D)

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V_{\mathrm{OL}}(x)\right]\psi(x) = E\psi(x) \qquad V_{\mathrm{OL}}(x) = V_{\mathrm{OL}}(x+d)$$ – periodic

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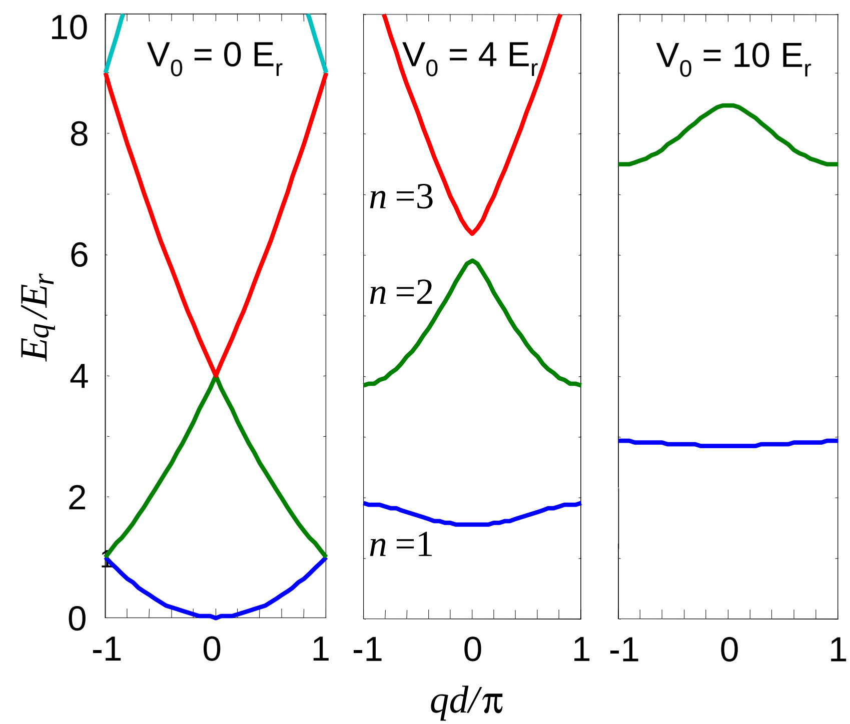
$\Rightarrow$ **Bloch theorem**: $\psi(x)=\psi_{n,q}(x)$ are Bloch functions (“plane-waves”)

$\psi_{n,q}(x)=e^{iqx}\,u_{n,q}(x)$ with $E_{n,q}$ energy, $q\in[-\frac{\pi}{d},\frac{\pi}{d}]$ quasimomentum

$[u_{n,q}(x)=u_{n,q}(x+d)]$



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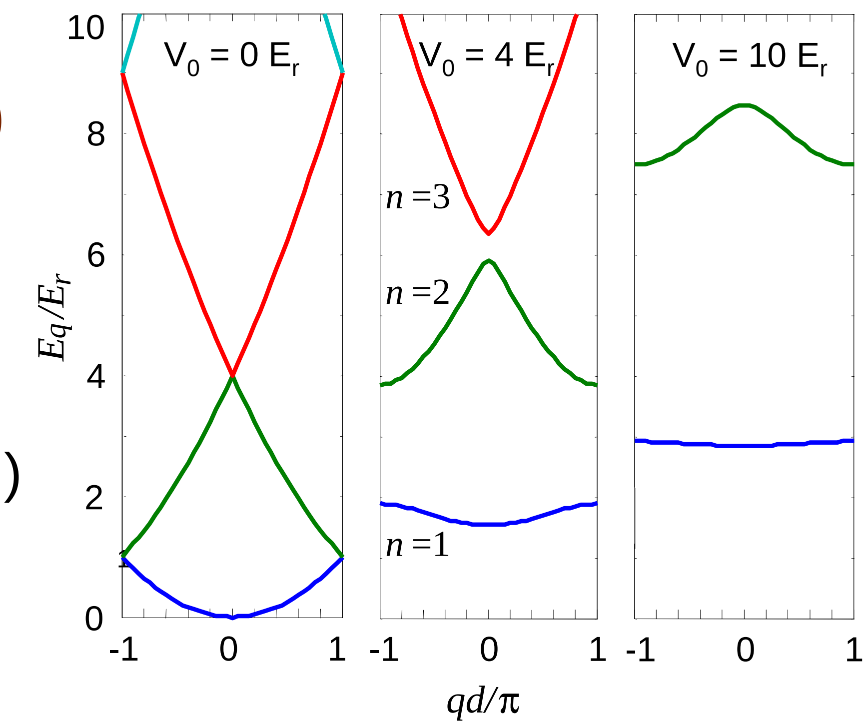


Change of basis (Fourier transform)

Bloch functions (“plane waves”)

$$\psi_{n,q}(x) = \sum_j w_{n,j}(x)e^{iqdj}$$

Wannier functions (“localized” $\sim dj = x_j$)

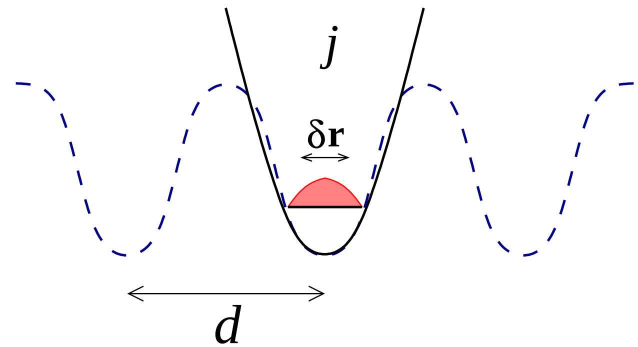
$$w_{n,j}(x) = w_n(x - dj)$$

$[w_n(x - x_j) = \frac{1}{2\pi}\int \mathrm{d}q\, e^{-ix_j q}\, \psi_{n,q}(x)]$

Atom in a nearly-harmonic potential

Deep OL potential $V_0 \gg E_r$ **(**$s \gg 1$**)** **and** $k_B T \ll \hbar\nu$ **(lowest BB** $n = 1$**)**

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r} \sim \mathbf{r}_j)\right]\phi(\mathbf{r}) = \hbar\nu\,\phi(\mathbf{r}),$$



$$V(\mathbf{r} \sim \mathbf{r}_j) \simeq \frac{M\nu^2}{2}(\mathbf{r} - \mathbf{r}_j)^2 \quad \text{with} \quad \nu \simeq \sqrt{\frac{2V_0\pi^2}{Md^2}}$$

$\Rightarrow$ Ground state of the harmonic oscillator

$$\phi(\mathbf{r} \sim \mathbf{r}_j) = \left(\frac{1}{\pi\delta r^2}\right)^{3/4} \exp\left[-\frac{(\mathbf{r} - \mathbf{r}_j)^2}{2\delta r^2}\right] \quad \text{with} \quad \delta r^2 \simeq \frac{\hbar}{M\nu}$$

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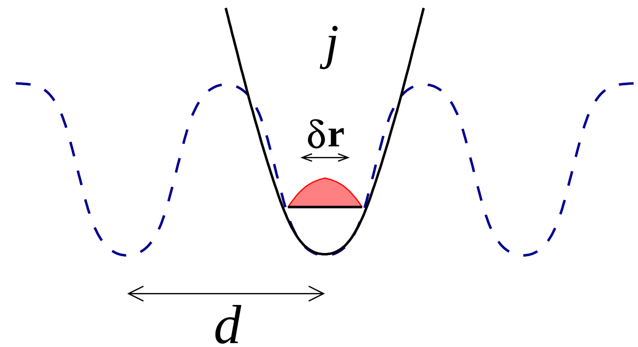

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Localized Wannier function $\boxed{w_j(\mathbf{r}) \simeq \phi(\mathbf{r} \sim \mathbf{r}_j)}$

(tight-binding approximation)

Hamiltonian for bosonic atoms

Boson field operator $\hat{\psi}(\mathbf{r})$: $\int d^3r\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) = \hat{N}$, $[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r'})] = \delta(\mathbf{r} - \mathbf{r'})$

Hamiltonian

$$H = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2M}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right] \hat{\psi}_i(\mathbf{r}) + \frac{g}{2}\int d^3r\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})$$

with $V_{\text{ext}}(\mathbf{r}) = V_{\mathrm{OL}}(\mathbf{r}) + V_{\mathrm{T}}(\mathbf{r})$ & $g = \frac{4\pi a_s \hbar^2}{M}$ (a_s: s-wave scattering length)

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Second quantization $\boxed{\hat{\psi}(\mathbf{r}) = \sum_j \hat{b}_j\, w_j(\mathbf{r})}$

with

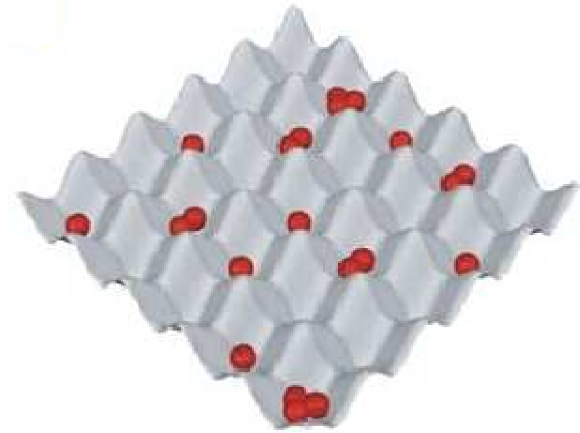
$\hat{b}_j$ ($\hat{b}_j^\dagger$): boson annihilation (creation) operator at site j ($[\hat{b}_j, \hat{b}_{j'}^\dagger] = \delta_{jj'}$)

$\hat{b}_j^\dagger \hat{b}_j \equiv \hat{n}_j$: number operator at site j

$\Downarrow$

Bose-Hubbard (second quantized) Hamiltonian

Neutral atoms in deep optical lattice



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

with

Single-particle energy

$$\varepsilon_j = \int d^3r\, V_{\mathrm{T}}(\mathbf{r}) |w_j(\mathbf{r})|^2 \simeq V_{\mathrm{T}}(\mathbf{r}_j)$$

Tunneling (hopping) between i & j

$$J = \int d^3r\, w_i^*(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2M} + V_{\mathrm{OL}}(\mathbf{r}) \right] w_j(\mathbf{r}) \simeq \frac{4}{\sqrt{\pi}} E_r s^{3/4}\, e^{-2\sqrt{s}}$$

On-site interaction ($U > 0$ repulsion; $U < 0$ attraction)

$$U = g \int d^3r\, |w_j(\mathbf{r})|^4 \simeq \frac{4\pi a_s \hbar^2}{M} \left(\frac{1}{\sqrt{2\pi} \delta r^3} \right)^3$$

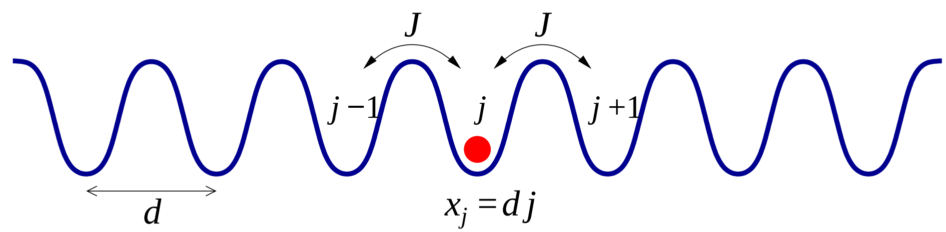
Jaksch et al, Phys. Rev. Lett. **81**, 3108 (1998)

Single atom in a lattice

Single particle in homogeneous lattice (1D)

Hamiltonian ($\varepsilon_j = 0$)

$$H = -J \sum_j \left(|x_j\rangle\langle x_{j+1}| + |x_{j+1}\rangle\langle x_j| \right)$$



State vector

$$|\psi\rangle = \sum_j \psi(x_j)\,|x_j\rangle$$

$\boxed{H\,|\psi\rangle = E^{(1)}\,|\psi\rangle}$ $\Rightarrow$ Difference equation

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

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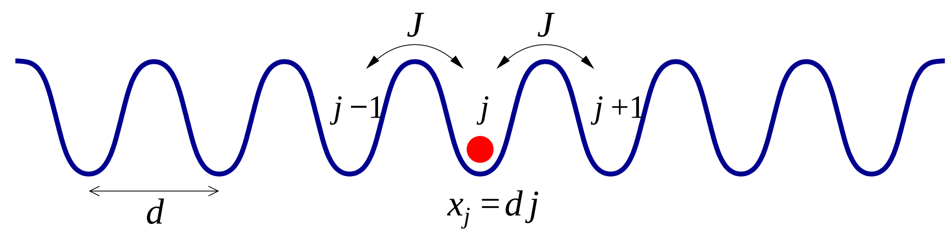

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Solution [infinite lattice (PBC)]

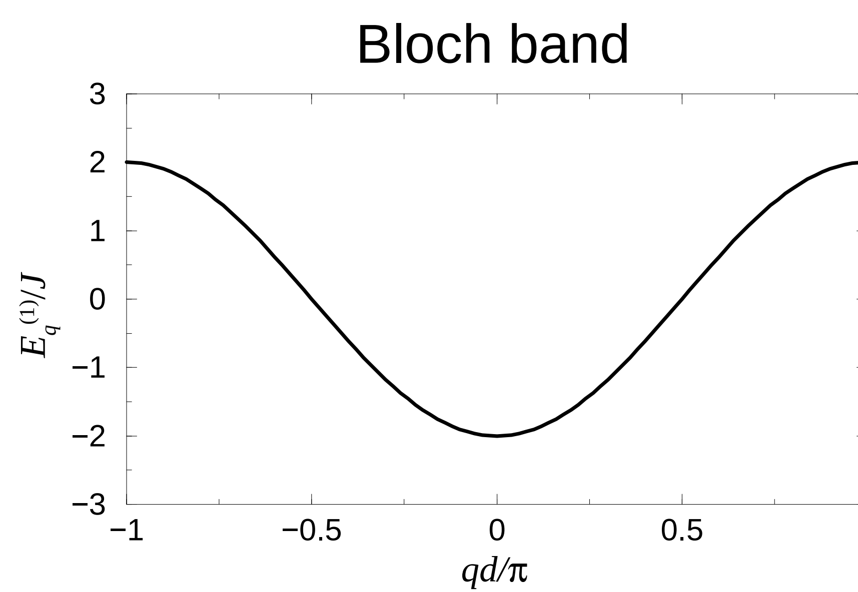
$$\psi_q(x_j) = e^{iqx_j}$$

$$\Rightarrow\ |\psi_q\rangle = \sum_j e^{iqx_j}\,|x_j\rangle$$

Dispersion relation $[q \in [-\frac{\pi}{d}, \frac{\pi}{d}]]$

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

$$E_q^{(1)} \in [-2J, 2J]$$



Single particle in homogeneous lattice (1D)

Hamiltonian ($\varepsilon_j = 0$)

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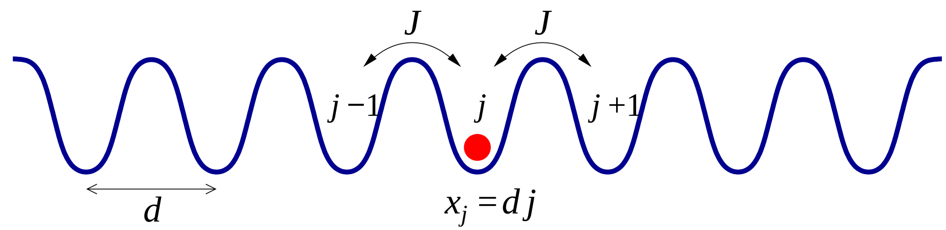


$$\boxed{H\,|\psi\rangle = E^{(1)}\,|\psi\rangle}$$ $\Rightarrow$ Difference equation

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

Solution [finite lattice (N sites)]

$$\psi_k(x_j) = \sin\left[\frac{\pi(k+1)j}{N+1}\right]$$

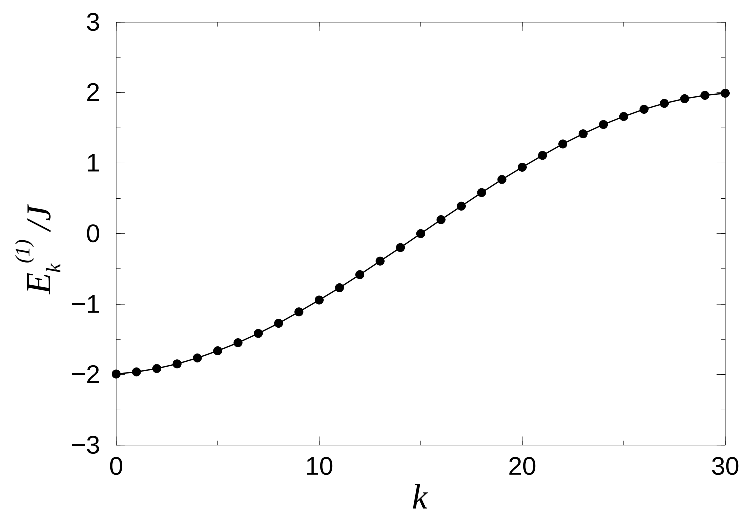
$$\Rightarrow\ |\psi_k\rangle = \sqrt{\frac{2}{N+1}} \sum_{j=1}^{N} \sin\left[\frac{\pi(k+1)j}{N+1}\right]\, |x_j\rangle$$

Energy eigenvalues [$0 \le k < N$]

$$E_k^{(1)} = -2J\cos\left[\frac{\pi(k+1)}{N+1}\right]$$

$$\lim_{N\to\infty} E_k^{(1)} = E_q^{(1)}$$

Bloch band ($N = 31$)



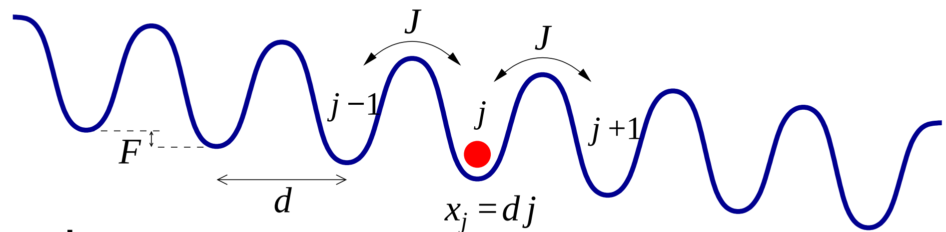
Single particle in tilted lattice (1D)

Hamiltonian ($\varepsilon_j = Fj$)

$$H = F \sum_j j \, |x_j\rangle\langle x_j| \, - J \sum_j (\, |x_j\rangle\langle x_{j+1}| \, + \, |x_{j+1}\rangle\langle x_j| \,)$$

State vector

$$|\psi\rangle = \sum_j \psi(x_j) \, |x_j\rangle$$



$$\boxed{H \, |\psi\rangle = E^{(1)} \, |\psi\rangle}$$ $\Rightarrow$ Difference equation

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

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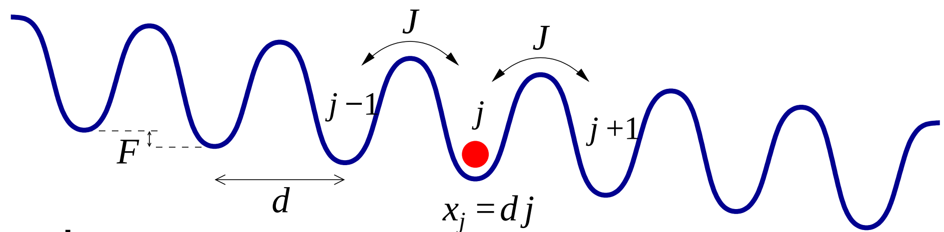

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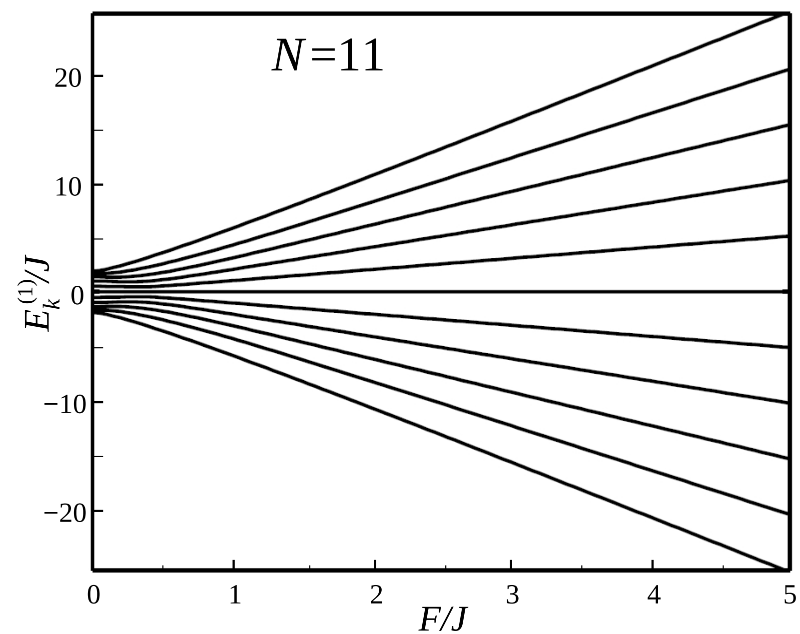
Bloch band $\longrightarrow$ Stark ladder



Solution

$$\psi_k(x_j) = \mathcal{J}_{j-k}(\tfrac{J}{2F})$$

$$\Rightarrow\ |\psi_k\rangle = \sum_j \mathcal{J}_{j-k}\Big(\frac{J}{2F}\Big)\,|x_j\rangle \xrightarrow{F>J} |x_k\rangle$$

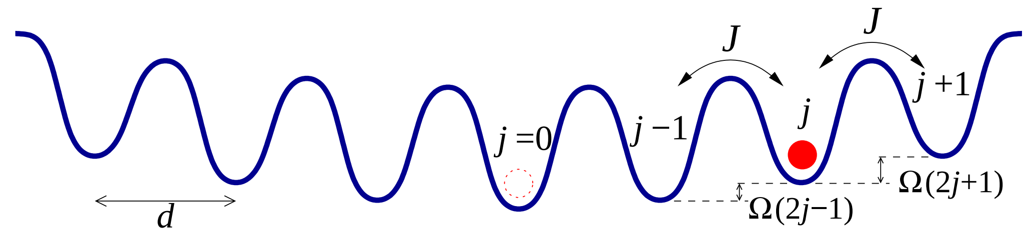
Energy eigenvalues $[k \in \mathbb{Z}]$

$$E_k^{(1)} \xrightarrow{F\neq 0} Fk$$ Stark ladder

$$\Rightarrow\ \tau_{\rm B} = \frac{2\pi\hbar}{F}$$ period of Bloch oscillations

Single particle in lattice & parabolic potential (1D)

Hamiltonian ($\varepsilon_j = \Omega j^2$)



$$H = \Omega \sum_j j^2 \, |x_j\rangle\langle x_j| \, - J \sum_j (\, |x_j\rangle\langle x_{j+1}| \, + \, |x_{j+1}\rangle\langle x_j| \,)$$

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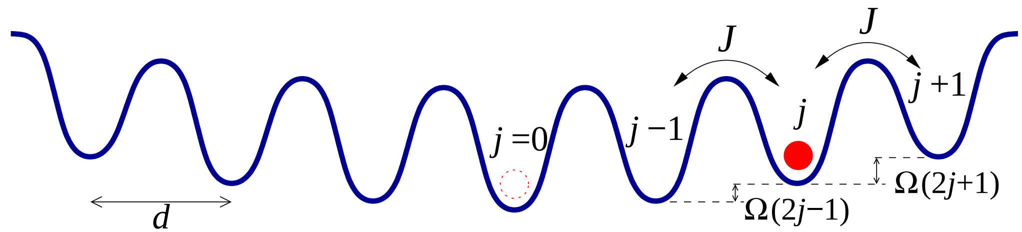
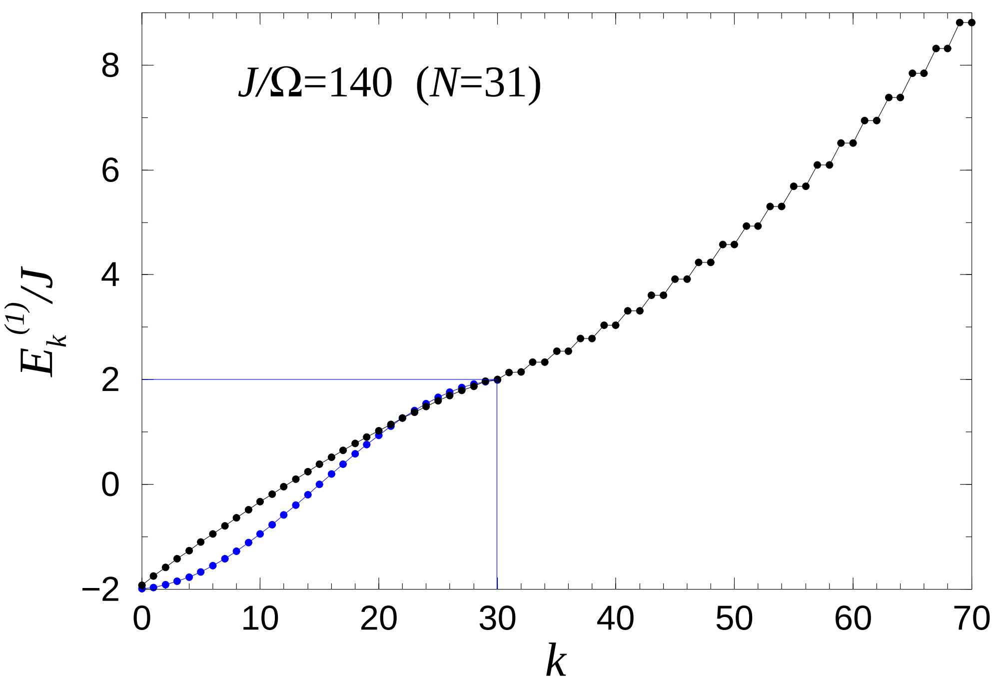


$$H = \Omega \sum_j j^2 \, |x_j\rangle\langle x_j| \; - \; J \sum_j \big(\, |x_j\rangle\langle x_{j+1}| \; + \; |x_{j+1}\rangle\langle x_j| \, \big)$$

Spectrum of H:



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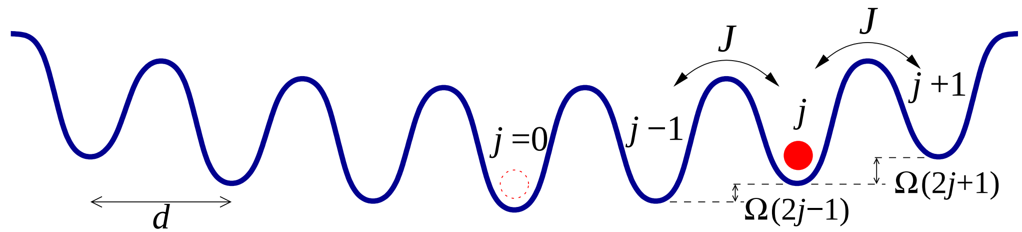


$$H = \Omega \sum_j j^2 \,|x_j\rangle\langle x_j| \,-\, J \sum_j \big(|x_j\rangle\langle x_{j+1}| + |x_{j+1}\rangle\langle x_j| \big)$$

Spectrum of H:

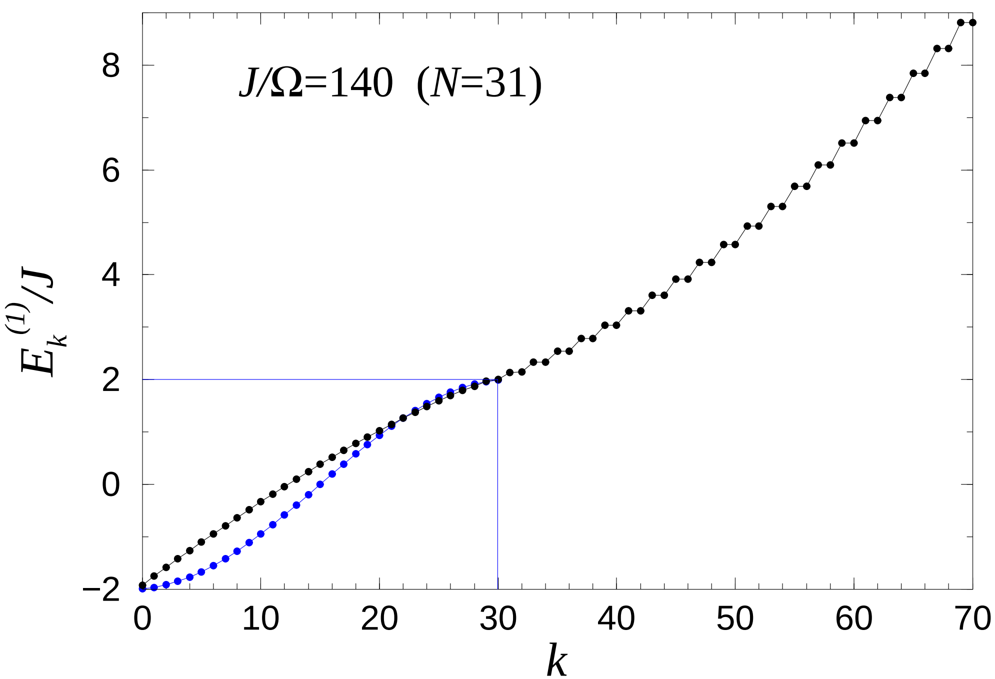
(i) Modified Bloch band

$$\boxed{-2J \le E_k^{(1)} \le 2J}$$

@ $j = 0, \pm 1, \ldots$ with $\Omega j^2 < 2J$

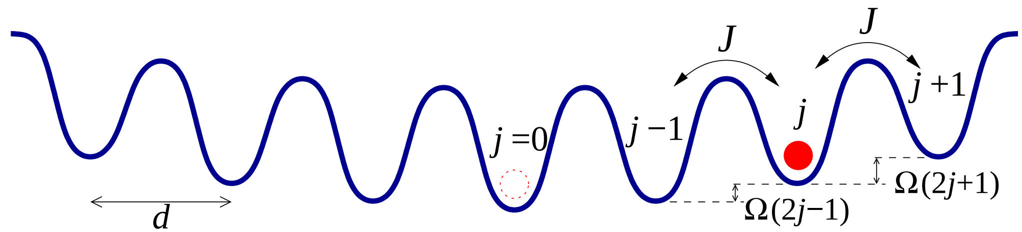
$\Rightarrow E_0^{(1)}, E_1^{(1)}, \ldots, E_{N-1}^{(1)}$

$N = 2\lfloor j_{\max} \rfloor + 1$ with $j_{\max} \simeq 1.3\sqrt{\frac{J}{\Omega}}$



Single particle in lattice & parabolic potential (1D)

Hamiltonian ($\varepsilon_j = \Omega j^2$)



$$H = \Omega \sum_j j^2 \,|x_j\rangle\langle x_j| \, - J \sum_j (\,|x_j\rangle\langle x_{j+1}| \, + \, |x_{j+1}\rangle\langle x_j| \,)$$

Spectrum of H:

(ii) Localized states

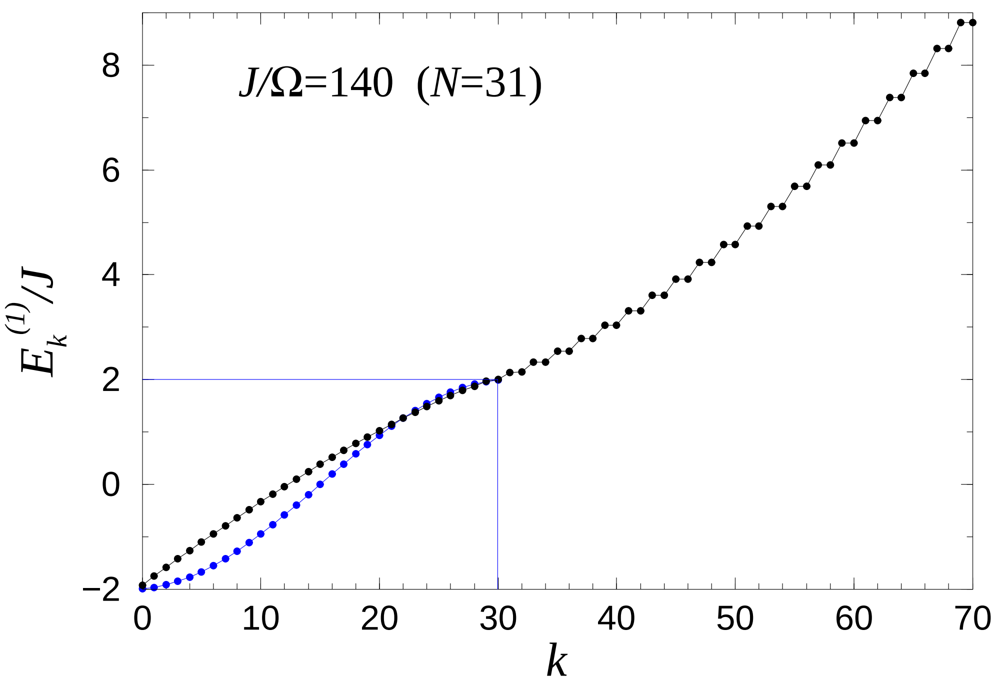
$\boxed{E_k^{(1)} > 2J}$ for $k \geq N$

$\Rightarrow E_{k,k'}^{(1)} \simeq \Omega j^2$ double-degenerate

$|\psi_{k,k'}\rangle \simeq \, |x_{\pm|j|}\rangle$

with ($|j| > j_{\max}$)

$k = 2|j| + 1 \;\;\&\;\; k' = 2|j| + 2$



Discrete harmonic oscillator

- $E_0^{(1)}, E_1^{(1)}, \ldots, E_{N-1}^{(1)}$ approx. linear (HO) spectrum:

$$E_k^{(1)} \approx -2J + \hbar\omega\,(k + \tfrac{1}{2}) \qquad \text{[with } \hbar\omega = 2\sqrt{\Omega J}\text{]}$$

$$|\psi_k\rangle \approx \mathcal{N} \sum_j (2^k k!)^{-1/2} e^{-\zeta_j^2/2} H_k(\zeta_j)\,|1_j\rangle \qquad \text{[with } \zeta_j = j\,\sqrt[4]{\Omega/J}\text{]}$$

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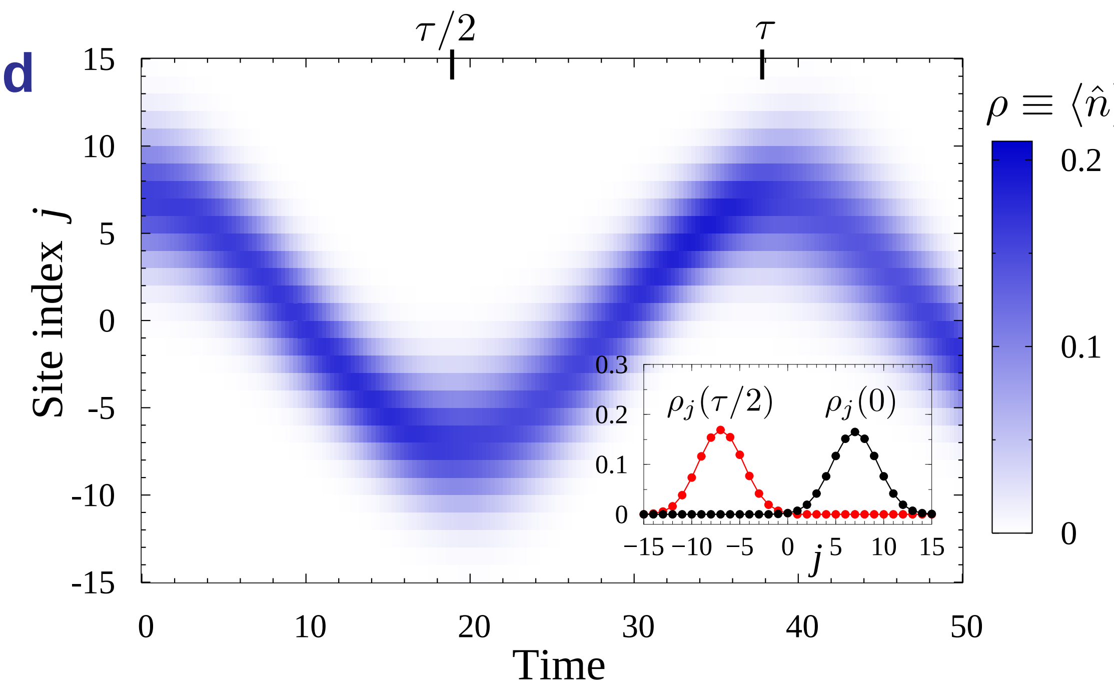
WP oscillations with period

$$\tau \simeq \frac{2\pi}{\omega} = \frac{\pi\hbar}{J}\sqrt{\frac{J}{\Omega}}$$

Initial state

$$|\psi(t=0)\rangle = |\psi_0^{(j'=7)}\rangle$$

$$= \sqrt[8]{\frac{\Omega}{\pi^2 J}}\sum_j e^{-\zeta_{j-j'}^2/2}\,|x_j\rangle$$



Valiente, Petrosyan, EPL **83**, 30007 (2008)

Two bosonic atoms in a lattice

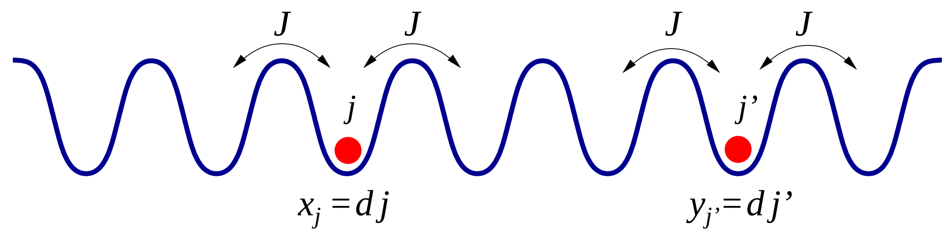
Two particles in Hubbard model (1D)

Hamiltonian ($\varepsilon_j = 0$)

$$H = -J \sum_j (|x_j\rangle\langle x_{j+1}| + |x_{j+1}\rangle\langle x_j|) - J \sum_j (|y_j\rangle\langle y_{j+1}| + |y_{j+1}\rangle\langle y_j|)$$
$$+U \sum_j |x_j, y_j\rangle\langle x_j, y_j|$$

State vector

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



$$\boxed{H\,|\psi\rangle = E^{(2)}\,|\psi\rangle}$$ $\Rightarrow$ Recurrence relation

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

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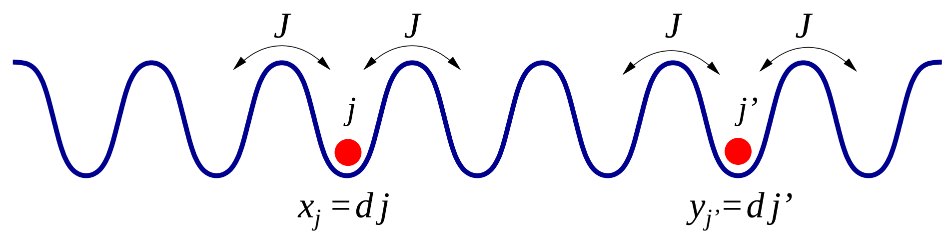

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$$+U\delta_{jj'}\Psi(x_j, y_{j'}) = E^{(2)}\,\Psi(x_j, y_{j'})$$

$R = \frac{1}{2}(x+y)$ 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 $r_i = di$ ($i = j - j'$))

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

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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- $U \to 0 \quad [\delta_{K,k} = 0] \Rightarrow \psi_{K,k}(r_i) = \cos(k|r_i|)$: noninteracting bosons
- $|U| \to \infty \ [\delta_{K,k} = \frac{\pi}{2}] \Rightarrow \psi_{K,k}(r_i) = \sin(k|r_i|)$: "fermionized" bosons [$\psi_{K,k}(0) = 0$]

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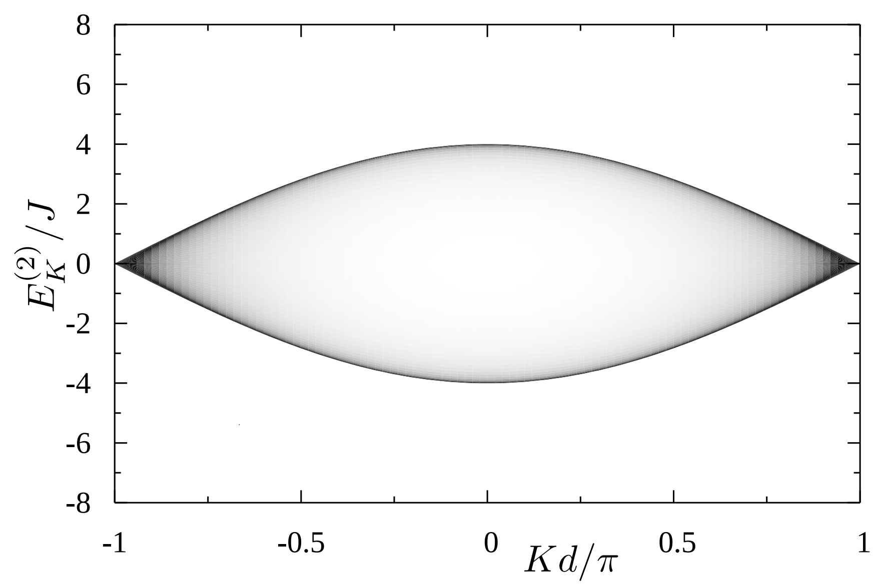
Spectrum of scattering states

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

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

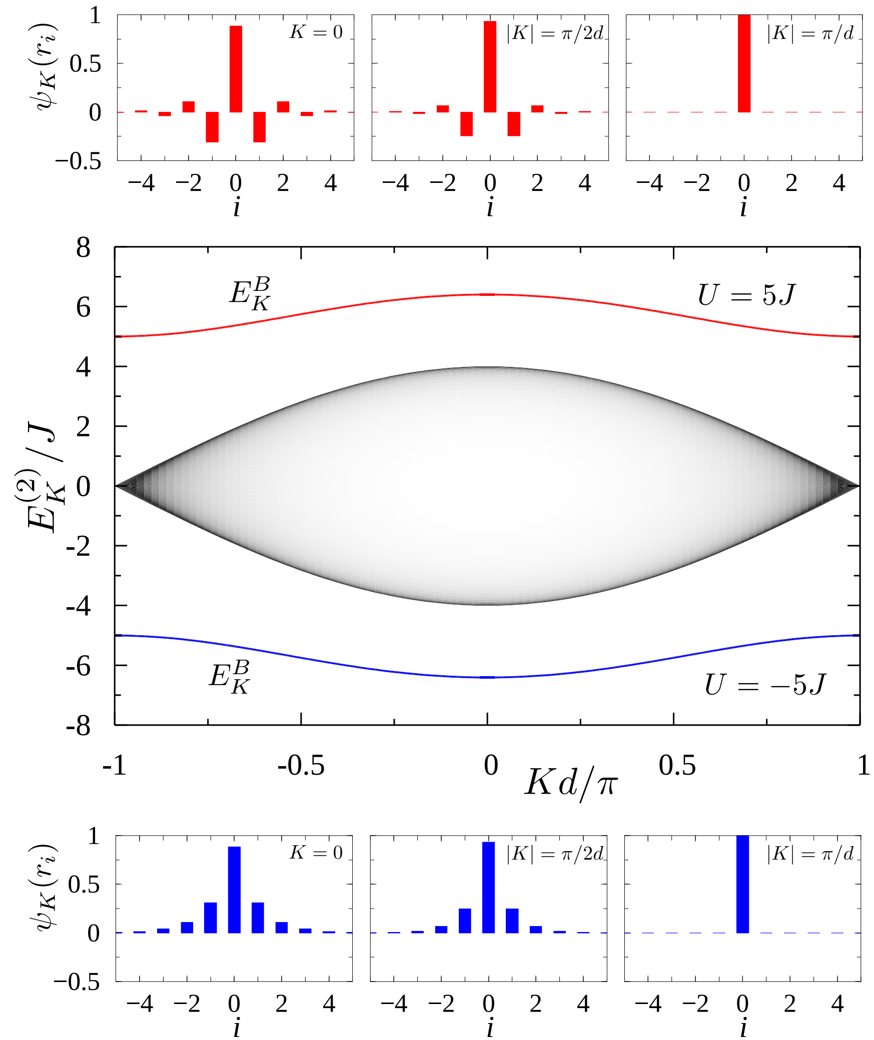
$$\psi_K(r_i) = \frac{\sqrt{\mathcal{U}_K}}{\sqrt[4]{\mathcal{U}_K^2+1}} \left(\mathcal{U}_K - \sqrt{\mathcal{U}_K^2 + 1}\right)^{|i|}$$

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

Dimer dispersion relation

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

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



Solution: Interaction-bound states

Attractive interaction $U < 0$

Relative coordinate wavefunction

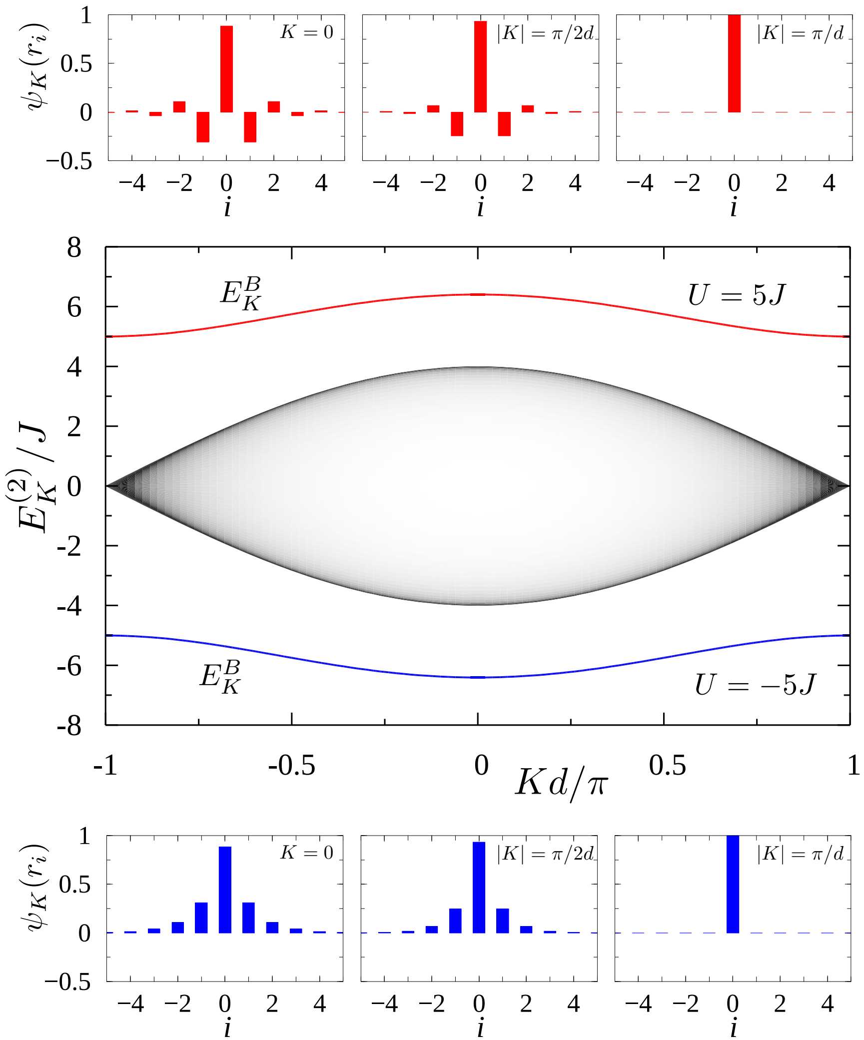
$$\psi_K(r_i) = \frac{\sqrt{\mathcal{U}_K}}{\sqrt[4]{\mathcal{U}_K^2+1}} \left(\sqrt{\mathcal{U}_K^2+1} - |\mathcal{U}_K|\right)^{|i|}$$

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

Dimer dispersion relation

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

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



Solution: Interaction-bound states

Strong interaction $|U| > J$

Relative coordinate wavefunction

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

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

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

Tightly-bound dimer

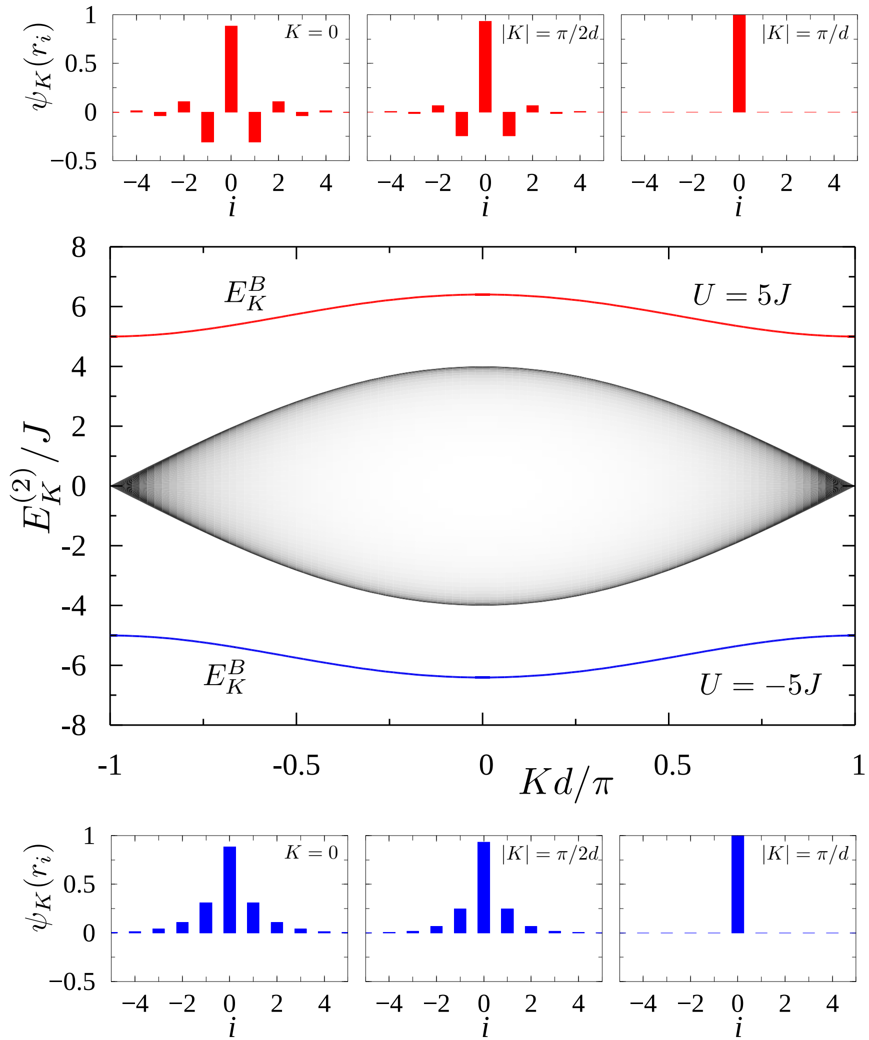
Dimer dispersion relation

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

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

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

$\Downarrow$



Valiente, Petrosyan, JPB **41**, 161002 (2008)

Effective dimer Hamiltonian

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

with

$\hat{c}_j$ ($\hat{c}_j^\dagger$) dimer annihilation (creation) & $\hat{m}_j \equiv \hat{c}_j^\dagger \hat{c}_j$ number operators at site j

$\tilde{J} \equiv -\frac{2J^2}{U}$ effective tunneling rate; $(U - 2\tilde{J})$ dimer "internal" energy

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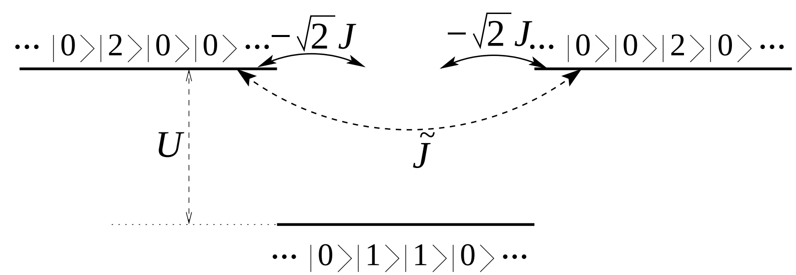
Second-order perturbation theory:



Energies of $|2,0\rangle$ & $|0,2\rangle$ differ from $|1,1\rangle$ by U

For $\frac{J}{|U|} \ll 1$ transition $|2,0\rangle \rightarrow |1,1\rangle$ is non-resonant

$\Rightarrow$ On-site interaction $U (\gtrless 0)$ binds two atoms into a **dimer**

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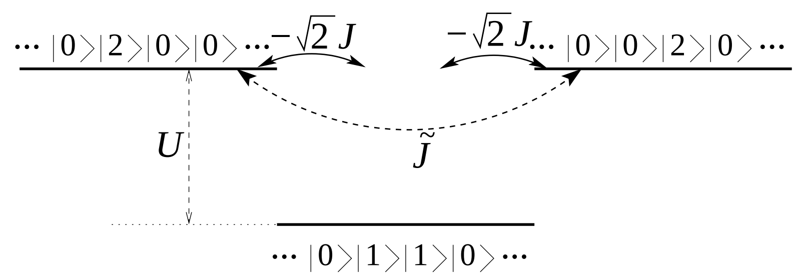

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$\Rightarrow$ On-site interaction $U(\gtrless 0)$ binds two atoms into a **dimer**

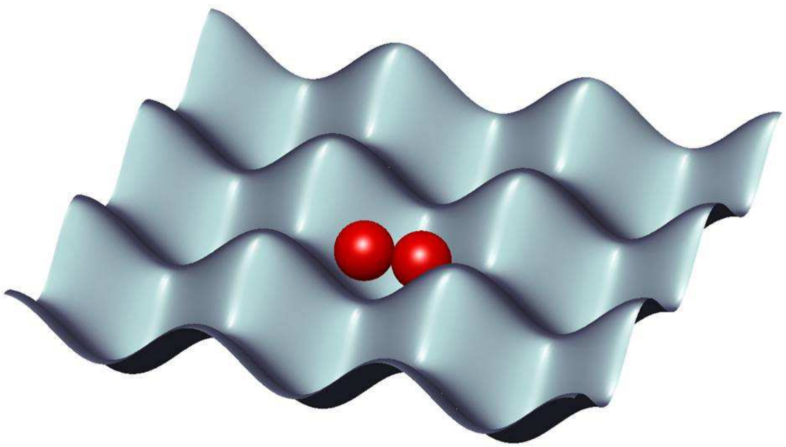
But $|2,0\rangle \rightarrow |1,1\rangle \rightarrow |0,2\rangle$ is resonant (second order in J)

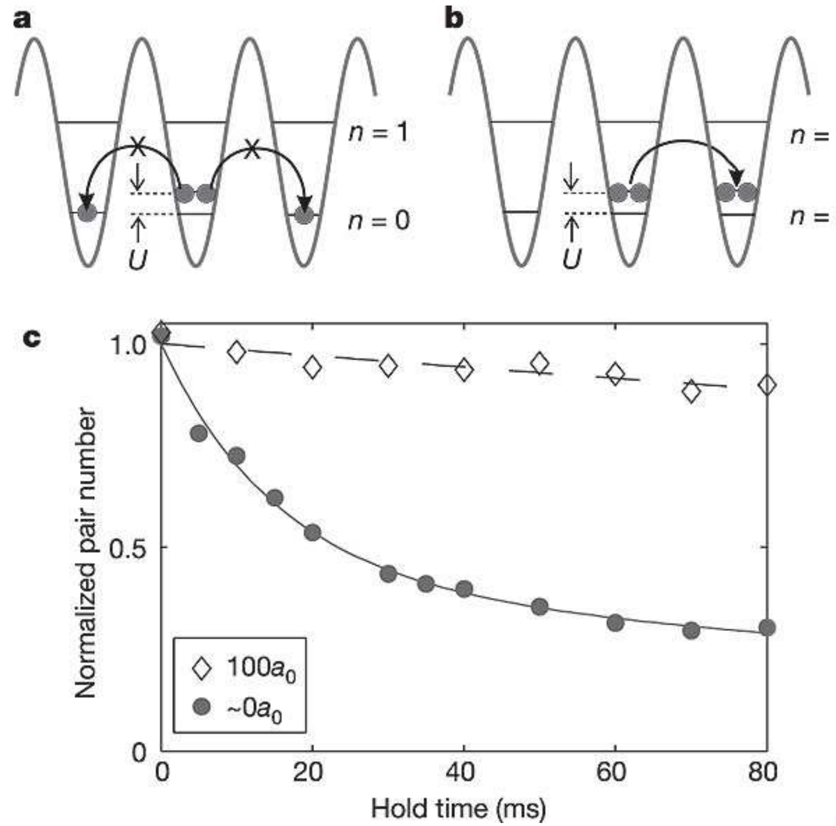
$\Rightarrow$ $\tilde{J} = -\frac{2J^2}{U}(\ll J)$ effective (second-order) tunneling rate for **dimer**

[& $2\tilde{J}$ second-order dimer level shift: $(U - 2\tilde{J})$]

Repulsively bound atom pair: Experiment

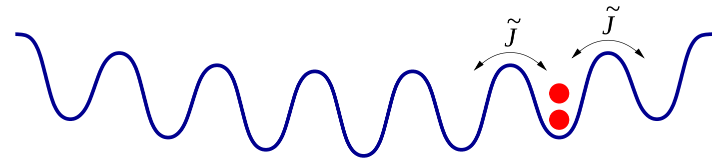
Single dimer





Winkler et al, Nature **441**, 853 (2006)

Dimer in lattice and parabolic potential



Hamiltonians

(a) $H \quad = \sum_j \left[\Omega j^2 \hat{n}_j + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) - J(\hat{b}_j^\dagger \hat{b}_{j+1} + \hat{b}_{j+1}^\dagger \hat{b}_j)\right]$

(b) $H_{\text{eff}} = \sum_j \left[\tilde{\Omega} j^2 \hat{m}_j + (U - 2\tilde{J})\hat{m}_j - \tilde{J}(\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j)\right]$

$[\tilde{\Omega} = 2\Omega, \quad \hat{m}_j = \frac{1}{2}\hat{n}_j \ \& \ \rho^D = \frac{1}{2}\rho]$

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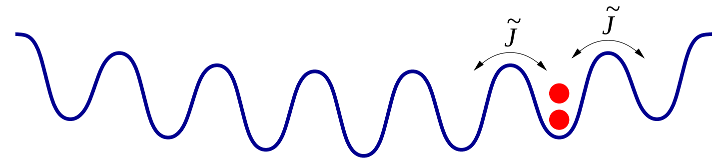

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WP oscillations with period

$$\tau^D \simeq \frac{2\pi}{\omega^D} = \frac{\pi\hbar}{\tilde{J}}\sqrt{\frac{\tilde{J}}{\tilde{\Omega}}} = \frac{\pi\hbar}{2J}\sqrt{\frac{U}{\Omega}}$$

$$[\hbar\omega^D = 2\sqrt{\tilde{\Omega}\tilde{J}}]$$

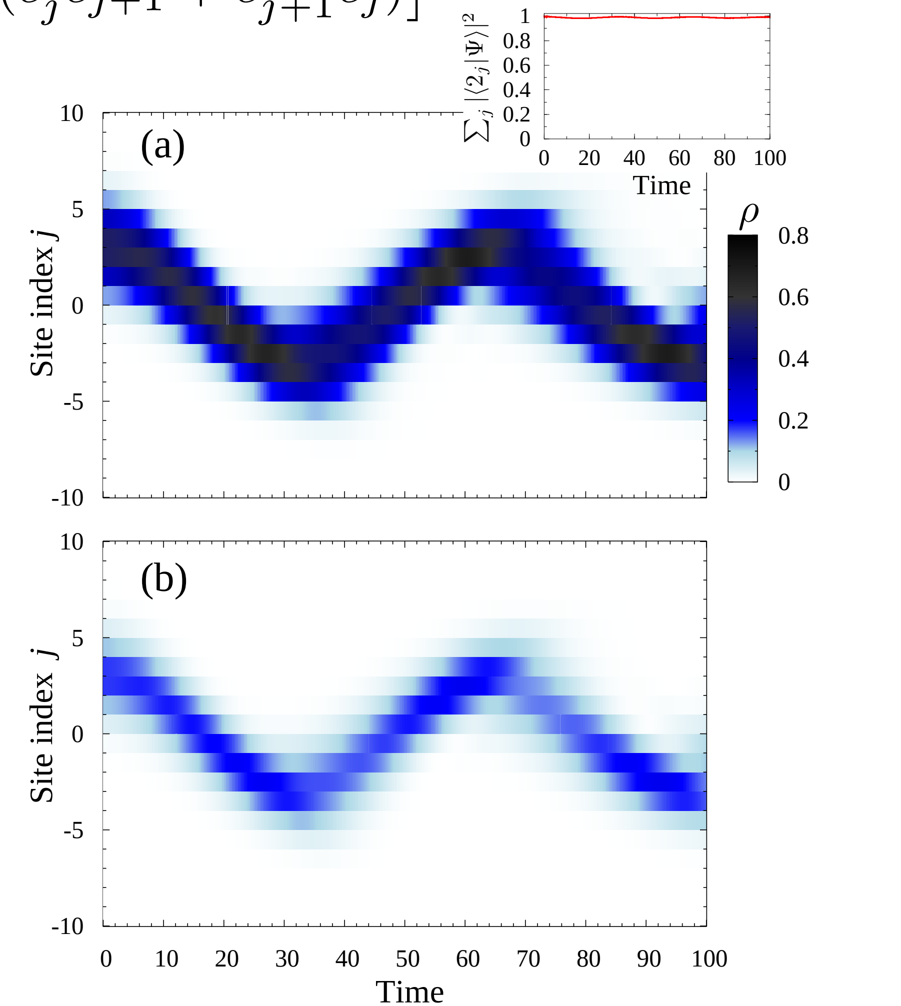
Initial state (shifted dimer ground state $|\Psi_0\rangle$)

$$|\Psi(t=0)\rangle = |\Psi_0^{(j'=3)}\rangle$$

$$= \sqrt[8]{\frac{\tilde{\Omega}}{\pi^2|\tilde{J}|}} \sum_j e^{-\xi_{j-j'}^2/2} e^{i\pi j} \, |1_j^D\rangle$$

$$= \sqrt[8]{\frac{\Omega|U|}{\pi^2 J^2}} \sum_j e^{-\xi_{j-j'}^2/2} (-1)^j \, |2_j\rangle$$

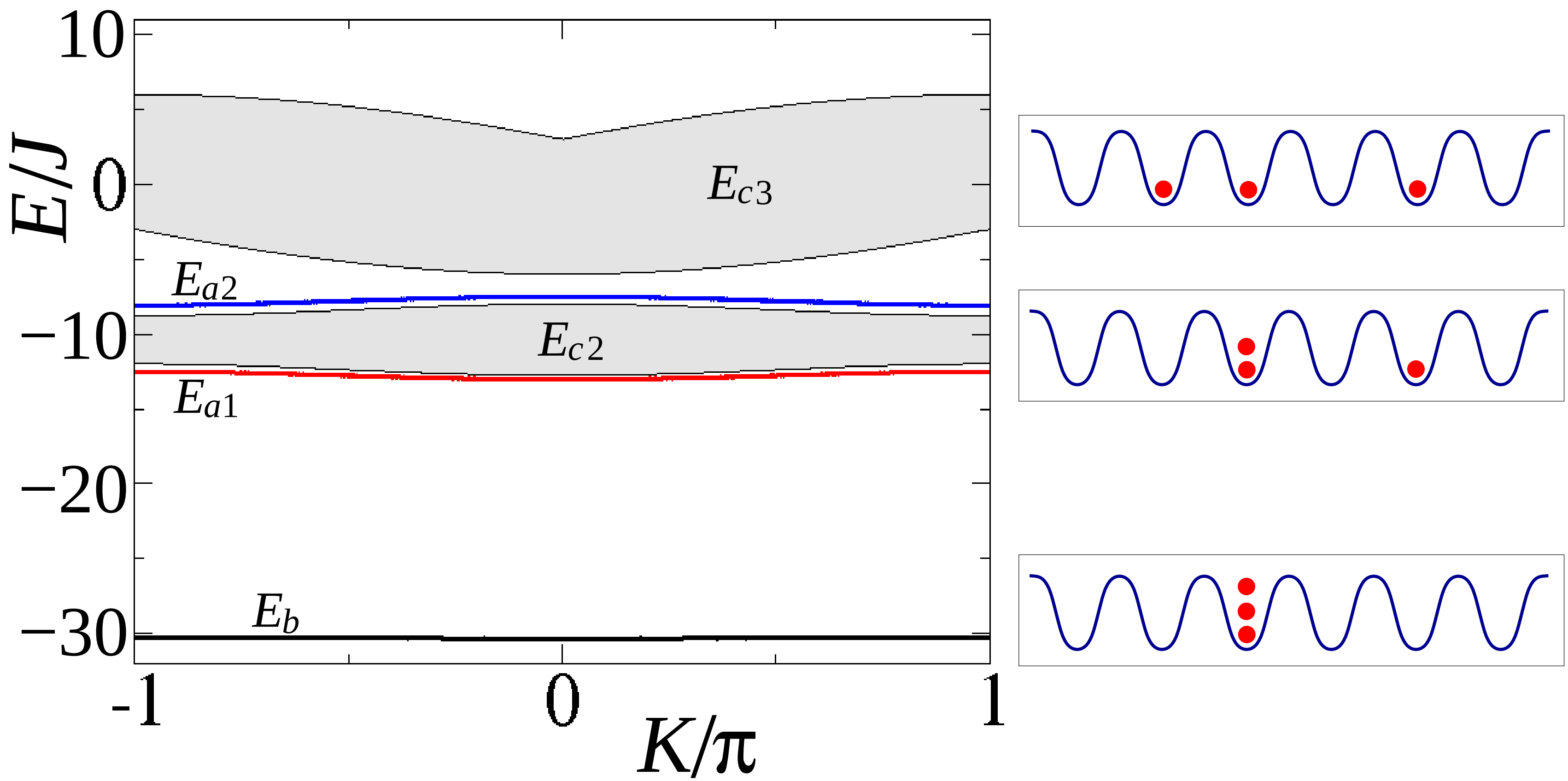
Parameters $\quad \frac{U}{J} = 10, \quad \frac{J}{\Omega} = 140 \Rightarrow N^D \simeq 11$



Valiente, Petrosyan, EPL **83**, 30007 (2008)

Three particles in Hubbard model (1D)

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



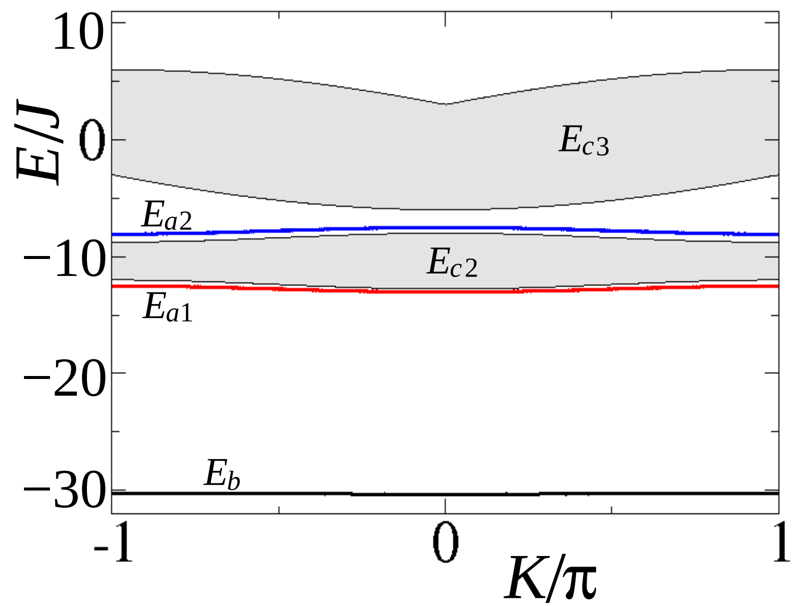
Valiente, Petrosyan, Saenz, arXiv:0907.3111

Three particles in Hubbard model (1D)

Three-body continuum

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

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



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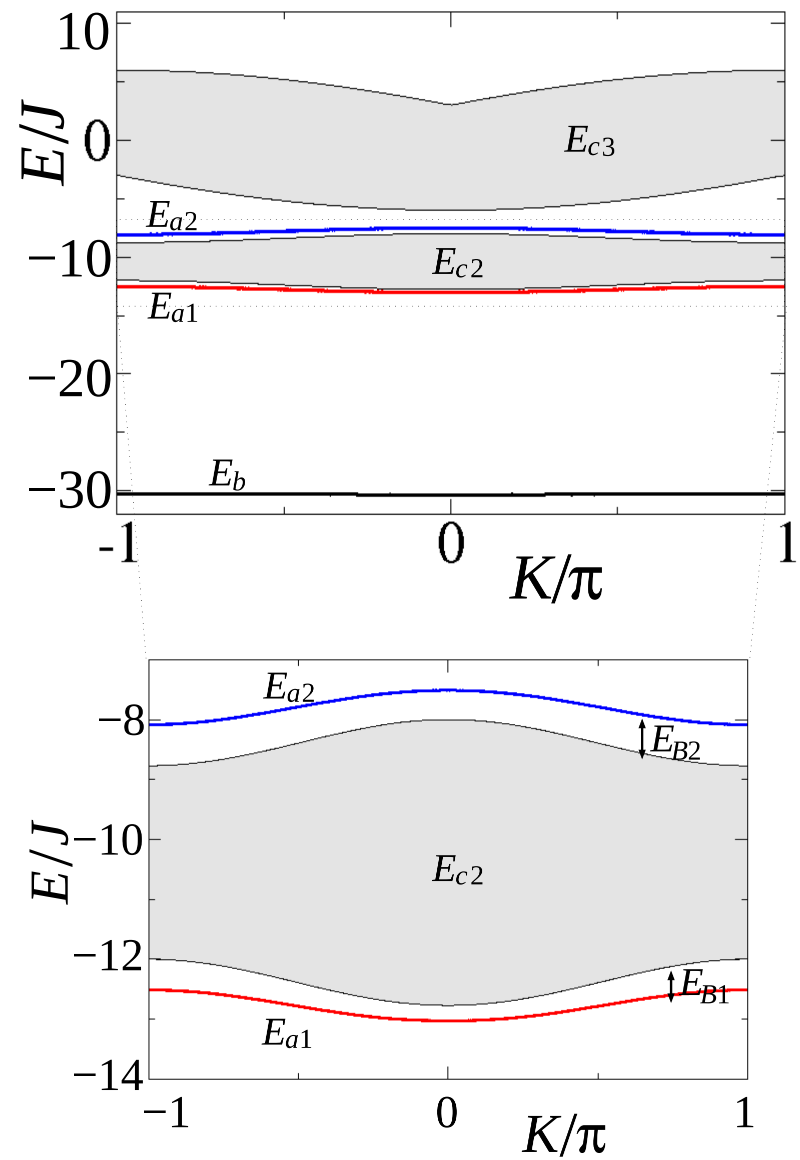
Two-body continuum

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

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



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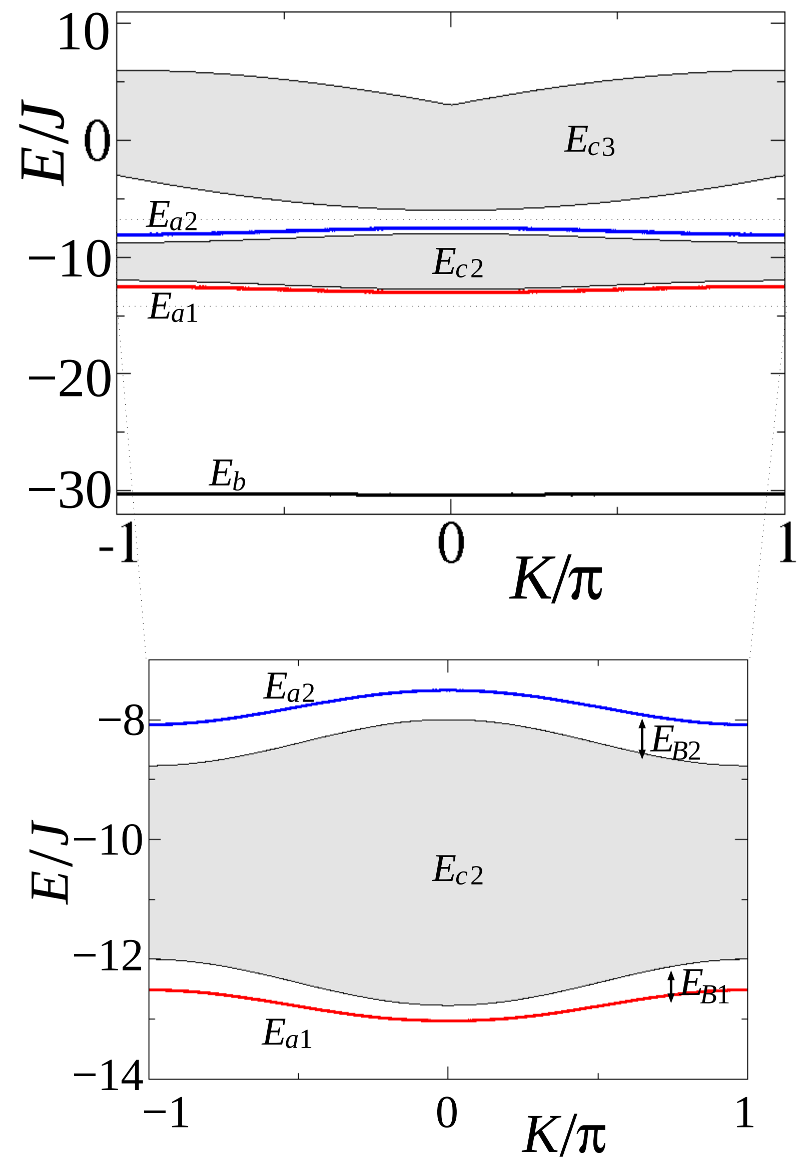

Weakly-bound (off-site) trimers

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

- Effective dimer-monomer exchange $2J$

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

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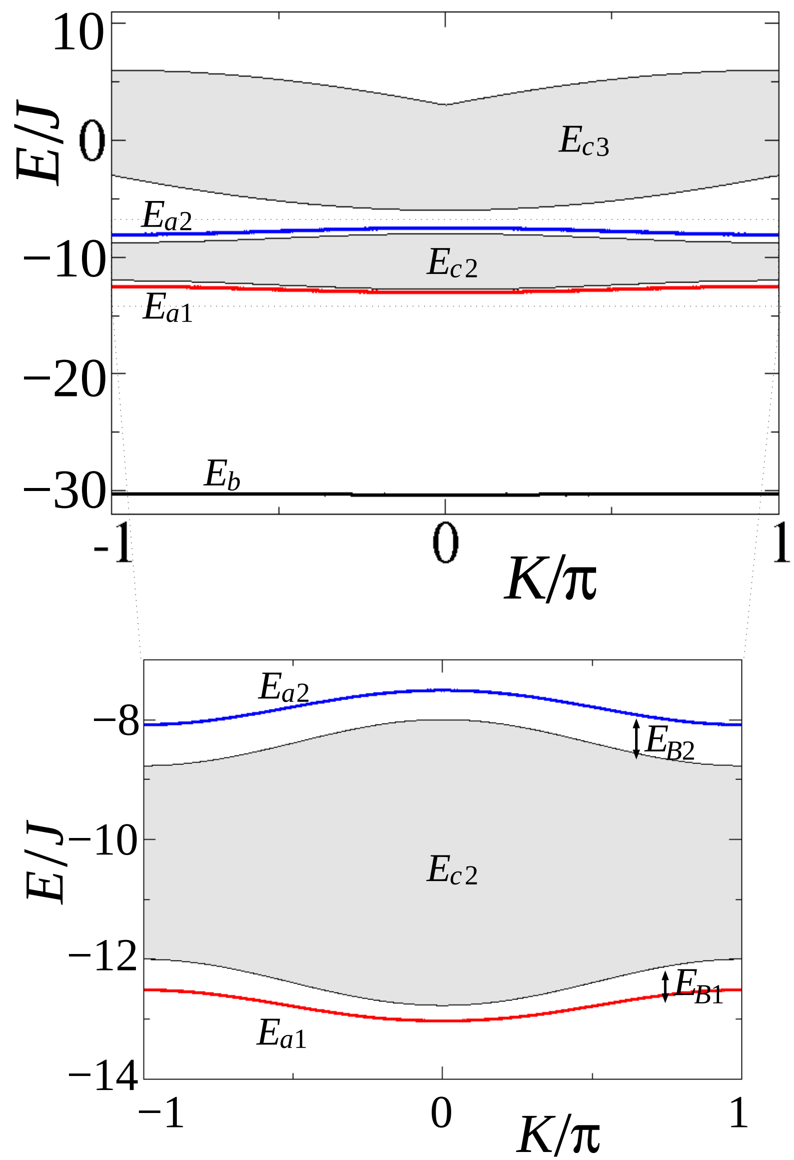
Weakly-bound (off-site) trimers

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

- Effective dimer-monomer exchange $2J$

Strongly-bound (on-site) trimer

$$E_b \simeq 3U$$



Many-body physics of the Hubbard model

Superfluid and Mott-Insulating phases for bosons

Bose-Hubbard Hamiltonian

$$H = \sum_j \varepsilon_j \hat{n}_j - J \sum_{\langle j,i \rangle} \hat{b}_j^\dagger \hat{b}_i + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1) \qquad (U > 0)$$

$\boxed{\varepsilon_j \to -\mu_j}$ [μ_j — local chemical potential for grand canonical ensemble]

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$\boxed{\varepsilon_j \to -\mu_j}$ [μ_j — local chemical potential for grand canonical ensemble]

- $U \gg J(\to 0)$

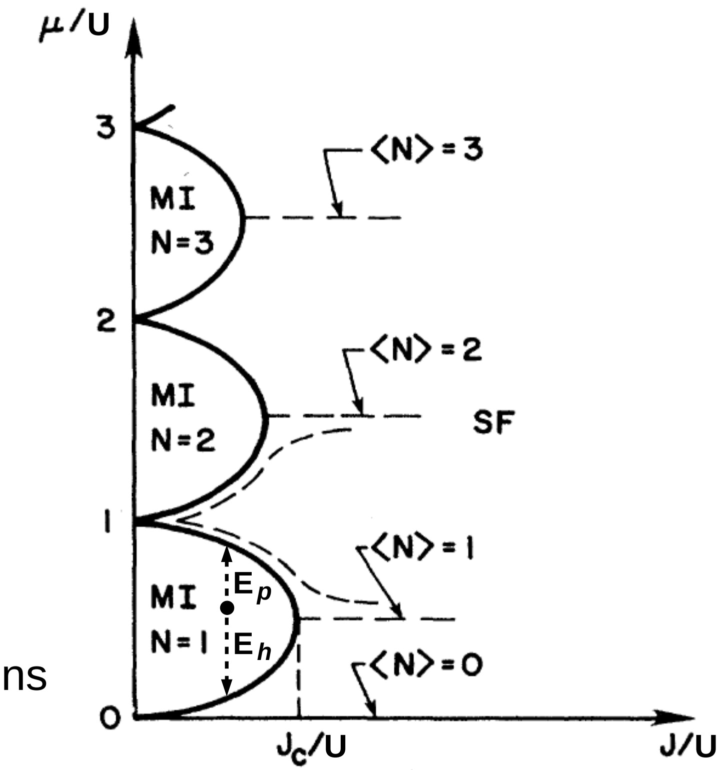
  Energy per site: $E(n) = -\mu n + \frac{1}{2} U n(n-1)$

  $\min E(n) \Rightarrow n - 1 < \frac{\mu}{U} < n \quad (n = 0 \text{ for } \mu < 0)$

  Mott insulating phase with $n =$ integer

  $|\Psi_{\text{MI}}\rangle = \ldots |n\rangle_{j-2} |n\rangle_{j-1} |n\rangle_j |n\rangle_{j+1} |n\rangle_{j+2} \ldots$

  - Local number- (Fock-) state with no coherence
  - Energy gap $E_{p,h} \sim U$ for *particle* and *hole* excitations
  - Vanishing compressibility $\frac{\partial \langle n \rangle}{\partial \mu} = 0$



[From Fisher et al., PRB 40, 546 (1989)]

Superfluid and Mott-Insulating phases for bosons

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$\boxed{\varepsilon_j \to -\mu_j}$ [μ_j — local chemical potential for grand canonical ensemble]

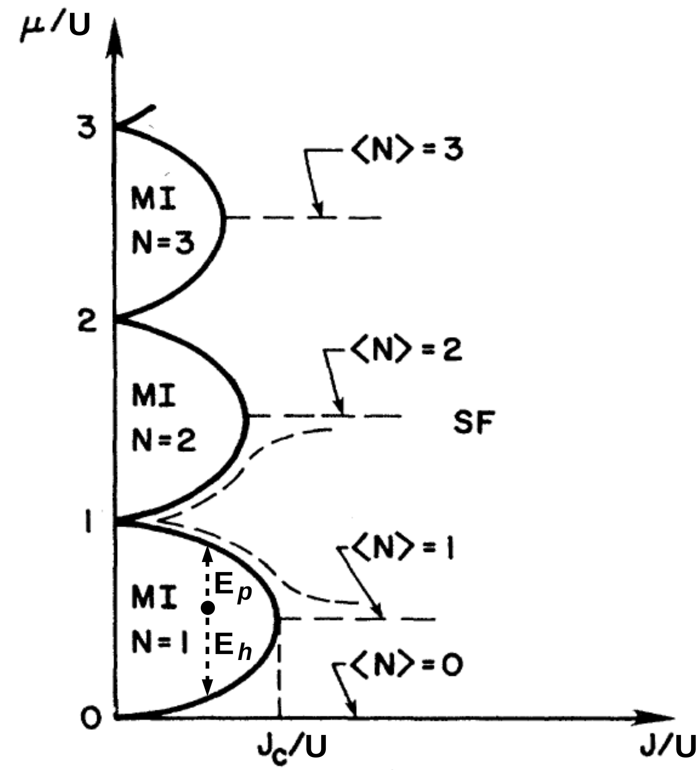
- $J > J_c(\sim U)$ [MF: $J_c(\langle n \rangle = 1) \simeq \frac{U}{5.8 \cdot 2D}$]

  Kinetic Energy $E_q \propto J > U$

  Superfluid (BEC) phase

  $|\Psi_{\text{MI}}\rangle \simeq \prod_j \sum_n c_n \, |n\rangle_j \stackrel{U \to 0}{\longrightarrow} \prod_N \, |\psi_q\rangle = \prod_j \, |\alpha\rangle_j$

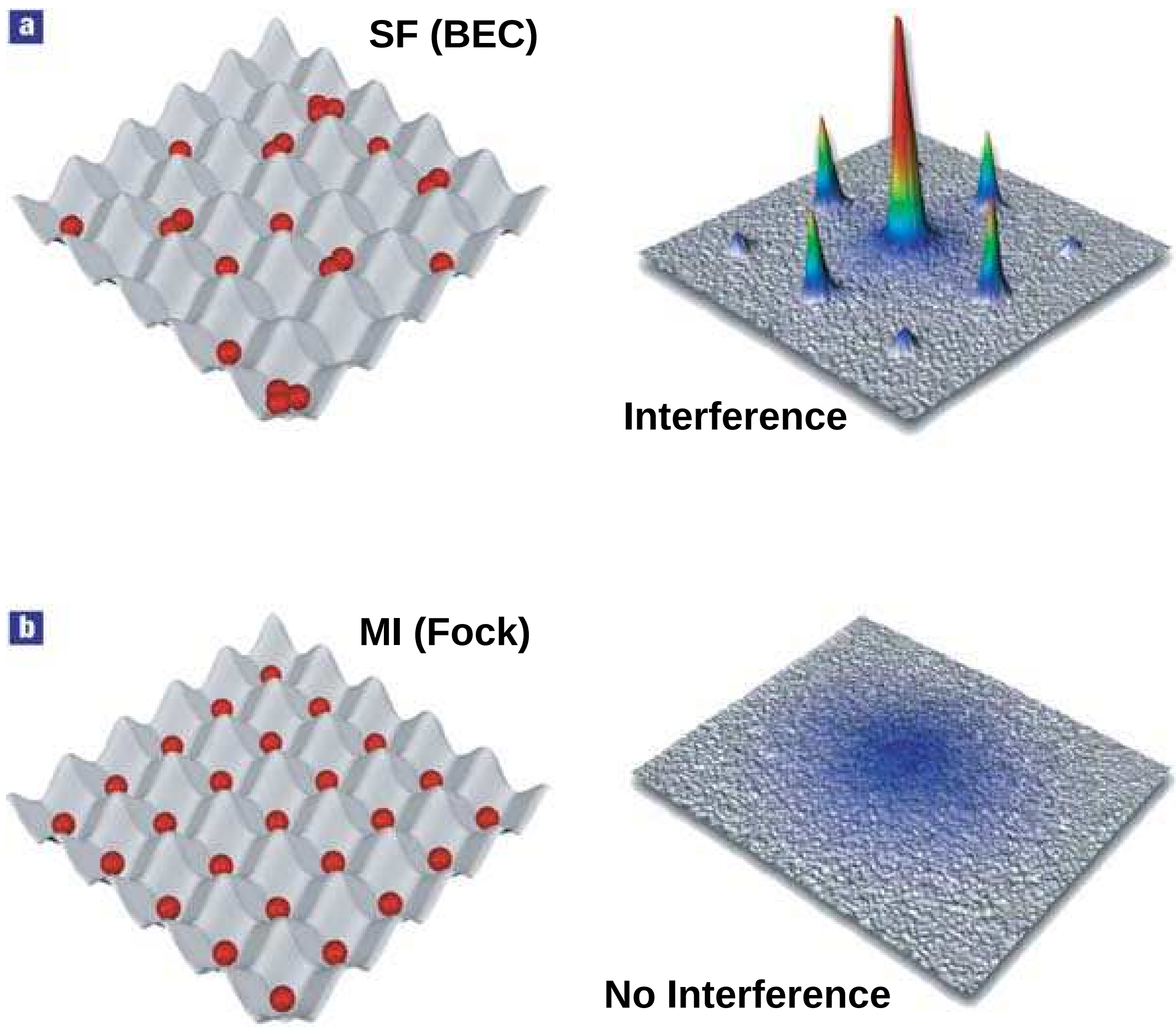
  - Long range coherence $\langle \hat{b}_j^\dagger \hat{b}_i \rangle \neq 0 \Rightarrow$ Interference
  - Gapless excitations
  - Finite compressibility $\frac{\partial \langle n \rangle}{\partial \mu} > 0$



[From Fisher et al., PRB 40, 546 (1989)]

Superfluid and Mott-Insulating phases for bosons

Experimental observation of *Quantum Phase Transition*



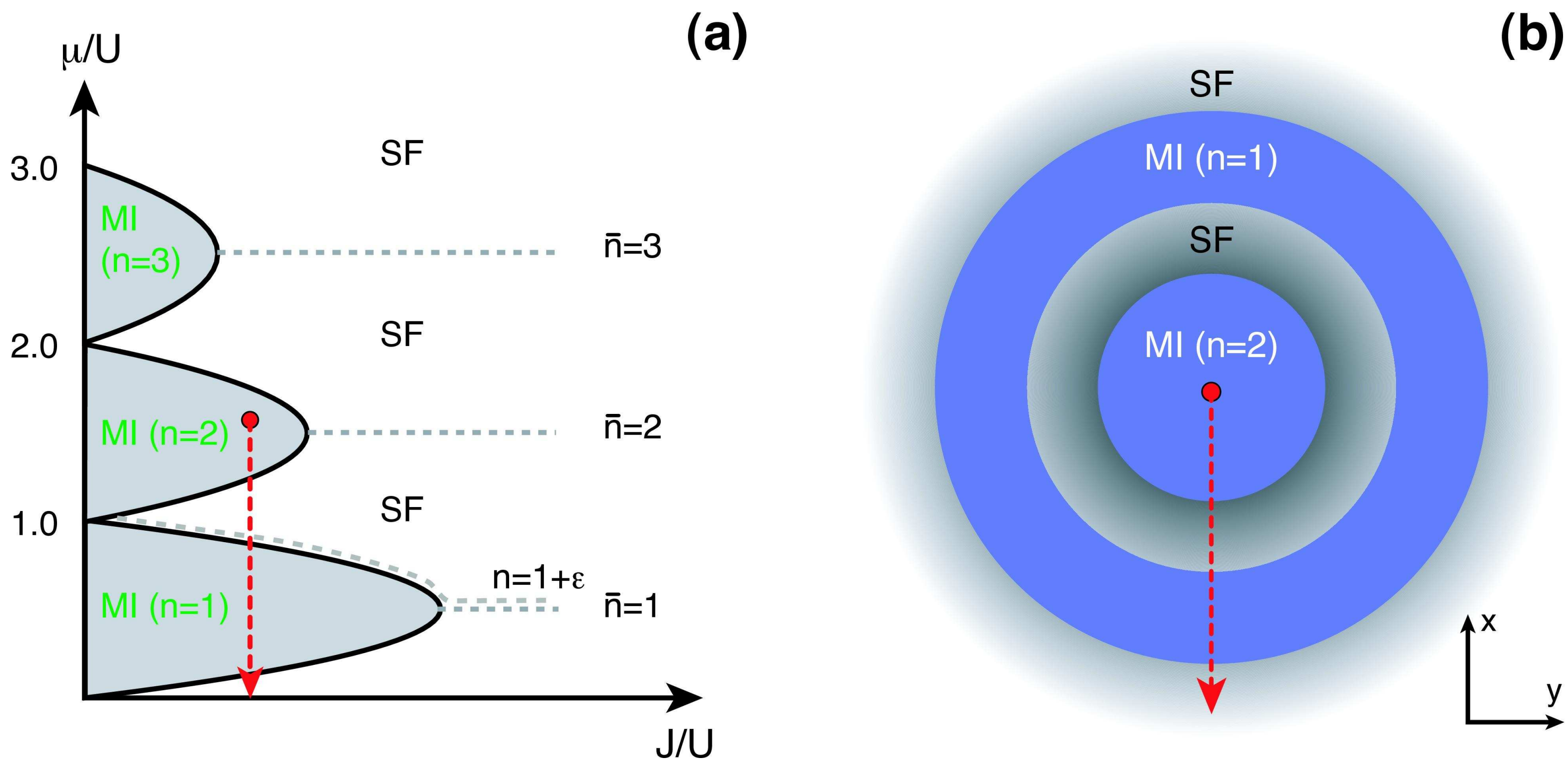
Shallow OL: $\boxed{J \gtrsim U}$

Deep OL: $\boxed{U \gg J}$

[From I. Bloch, Nature Phys. 1, 23 (2005)]

Superfluid and Mott-Insulating phases for bosons

In-trap density & phase distribution (OL + HP)



[from: Bloch, Dalibard, Zwerger, RMP 80, 885 (2008)]

Metal and Insulating phases for fermions

Fermi-Hubbard Hamiltonian $[\{\hat{f}_{j,\sigma}, \hat{f}^{\dagger}_{j',\sigma'}\} = \delta_{jj'}\delta_{\sigma\sigma'} \quad \hat{n}_{j,\sigma} = \hat{f}^{\dagger}_{j,\sigma}\hat{f}_{j,\sigma}(= 0, 1)]$

$$H = \sum_j \varepsilon_j(\hat{n}_{j,\downarrow} + \hat{n}_{j,\uparrow}) - J \sum_{\substack{\langle j,i\rangle \\ \sigma=\downarrow,\uparrow}} \hat{f}^{\dagger}_{j,\sigma}\hat{f}_{i,\sigma} + U \sum_j \hat{n}_{j,\downarrow}\hat{n}_{j,\uparrow} \qquad (U > 0)$$

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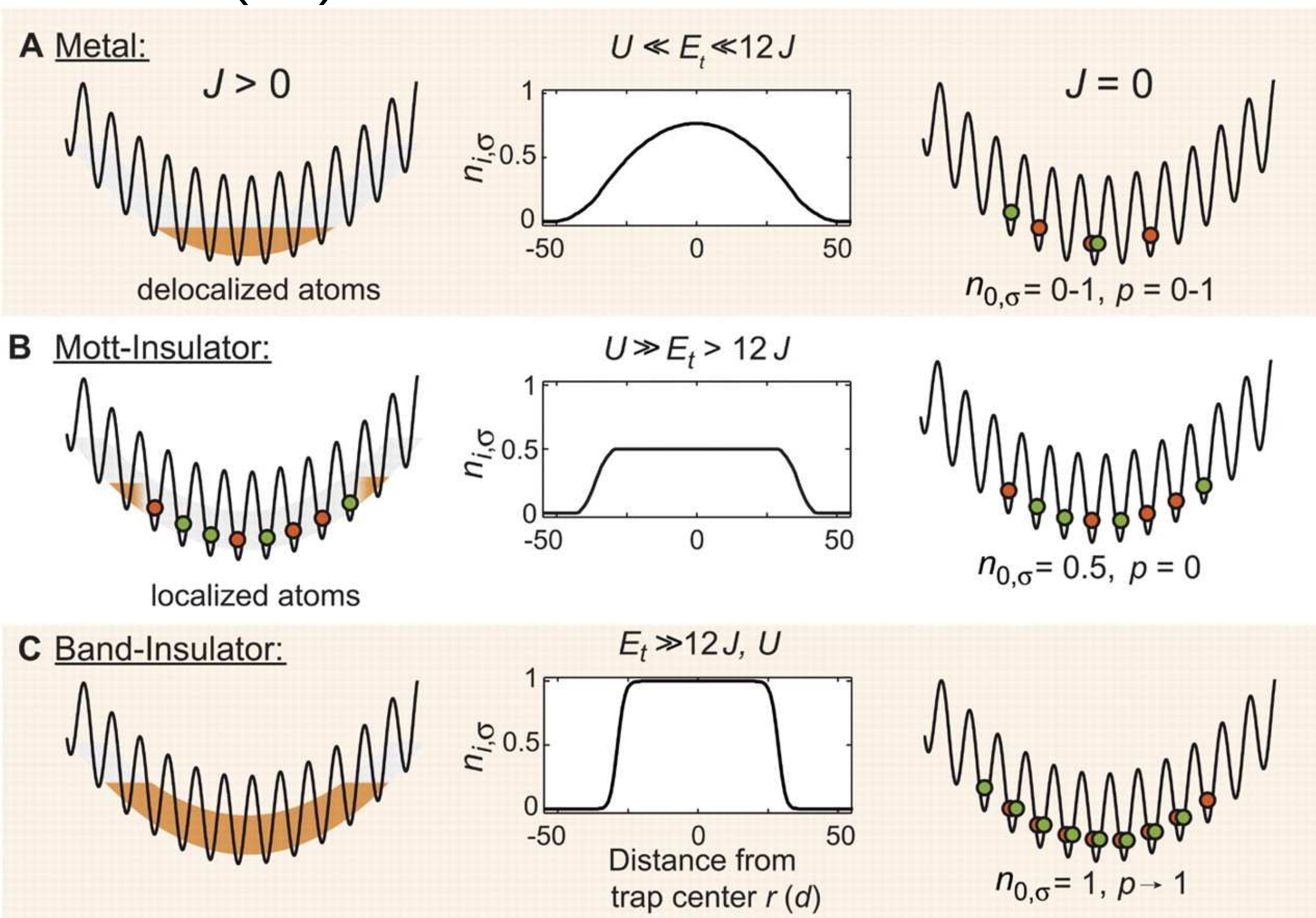
OL + HP (3D)



[from: Schneider et al., Science 322, 1520 (2008)]

Kinetic energy

$E_q \simeq 3 \cdot 4J$

Trap (Fermi) energy

$E_t = \Omega[3N_\sigma/2\pi]^{2/3}$

with

$\varepsilon_j = \Omega(j_x^2 + j_y^2 + j_z^2)$

Summary

- Cold atoms in optical lattice potentials can implement important models of cond.-mat. physics (Hubbard, Heisenberg spin-$\frac{1}{2}$, etc.)
- Interacting atom pairs can form tightly-bound dimers in a lattice
  - Dimer-monomer (particle) exchange interaction can bind them into trimers
- Many-body dynamics in a lattice can exhibit quantum phase transitions

Summary

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Further reading

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M.P.A. Fisher, P.B. Weichman, G. Grinstein, and D.S. Fisher, Phys. Rev. B **40**, 546 (1989)

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F.H.L. Essler et al., *The one-dimensional Hubbard model* (Cambridge University press, 2005)