Optical Lattices with Large Scattering length

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Idea

"Is the study of few-body physics limited to the measurement of loss rates?" (R. Grimm)

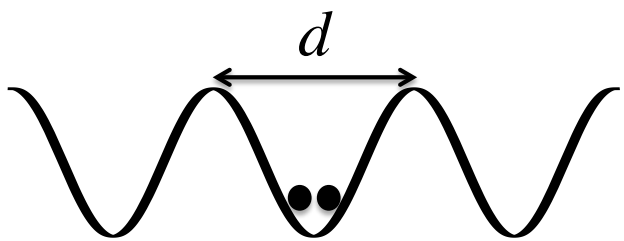
Is the use of optical lattices limited to the emulation of the Hubbard model?

Use optical lattice to provide stability against losses and few-body physics to introduce new ideas to atoms in optical lattices $\Rightarrow$ new tool for *many-body* physics.

Idea

Hubbard model in an optical lattice (OL) needs weak interactions $a \ll d$

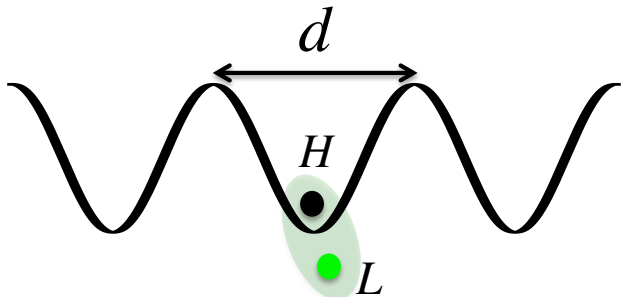
- not to occupy higher bands
- so that U, J are calculated perturbatively



Idea

Here: OLs with $a \gtrsim d$ keeping the single band approach.

- One atomic species confined to the OL
- second species interacts with the first one but is untrapped
- second species forms *bound states* with the first and is trapped only by interactions
- requires achieving $a \sim d$: Feshbach resonance with good magnetic field control



Similar ideas in few-body systems: Y. Nishida and S. Tan (2011); Y. Nishida (2010); T. Yin et al (2011)

See also: M. Antezza and Y. Castin (2006); D. Petrov et al (2008).

Idea

Why? Brings new non-lattice degrees of freedom going beyond the conventional Hubbard model.

Also few-body physics in a new setting: "molecules" with enhanced stability due to the lattice (strongly suppresses three-body losses)

$a \sim 600$nm already achieved in a narrow resonance (~ 1G) in a ^{6}Li-^{40}K mixture (C. Kohstall et al 2012)

Example of application

Implement an *electron-phonon quantum simulator*:

Trapped atoms (Heavy - mass M)

- "ions"
- in a deep OL such that their wave functions do not overlap and their statistics are unimportant
- without the "electrons" they would oscillate at the lattice onsite frequency (flat phonon dispersion)

Untrapped atoms (Light - mass m)

- "electrons"
- spin polarized fermions
- interact with heavy atoms creating phonon dispersion, Peierls instability, polaron physics, etc.

Calculations I

$M \gg m$: Born-Oppenheimer Approximation - but not necessary...

Wave function of N_l light and N_h heavy atoms:

$$\Psi = \psi\left(\{\mathbf{R}\}\right)\chi\left(\{\mathbf{R}\},\{\mathbf{r}\}\right)$$

$\mathbf{R}, \mathbf{r}$ heavy and light coordinates, χ Slater determinant of N_l light atom states ϕ:

$$\phi(\mathbf{r}) \propto \sum_{j=1}^{N_h} c_j \mathrm{e}^{-\kappa\|\mathbf{R}_j-\mathbf{r}\|}/\|\mathbf{R}_j-\mathbf{r}\|$$

κ, c_j determined by the Bethe-Peierls boundary conditions.

The energy of each orbital is

$E(\kappa) = -\hbar^2\kappa^2/2m < 0$ so that total interaction energy is $\sum_{i=1}^{N_l} E(\kappa_i)$

Calculations II

The BP conditions lead to

$$\left(\kappa - \frac{1}{a}\right) c_i = \sum_{j=1}^{N_h} \frac{\mathrm{e}^{-\kappa \|\mathbf{R}_j - \mathbf{R}_i\|}}{\|\mathbf{R}_j - \mathbf{R}_i\|} c_j$$

The trapping potential of the heavy atoms is a 1D lattice tightly confined radially:

$$V = \frac{1}{2} M \omega_\perp^2 (x^2 + y^2) + V_0 \cos^2(\pi z/d)$$

Note that $\omega_\perp \gg \omega_z$ where ω_z is the onsite lattice oscillation frequency so wave function tightly confined in two directions on each site - motion essentially 1D.

Recoil energy $E_R \equiv \pi^2 E_d m/M$
KE of light atoms $\sim E_d \equiv \hbar^2/2md^2$

Calculations III

Need to reduce losses so minimise overlap of heavy atom wave functions by keeping V_0 large - heavy atoms are localised at the lattice site minima: implements Kronig-Penney model with δ-function potentials (A. Berezin, PRB **33** 2122 (1986)).

Periodic boundary conditions + Bloch's theorem

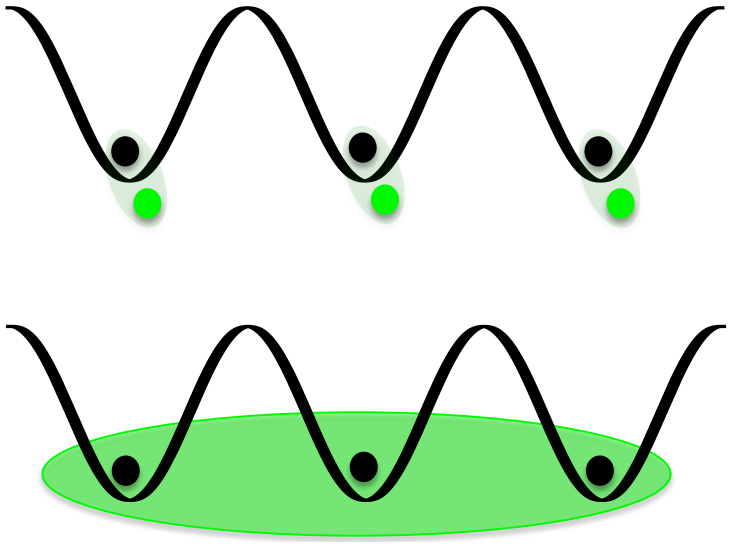
$$c_j = \exp(ik\|\mathbf{R}_j\|) \text{ with } \exp(ikdN_h) = 1$$

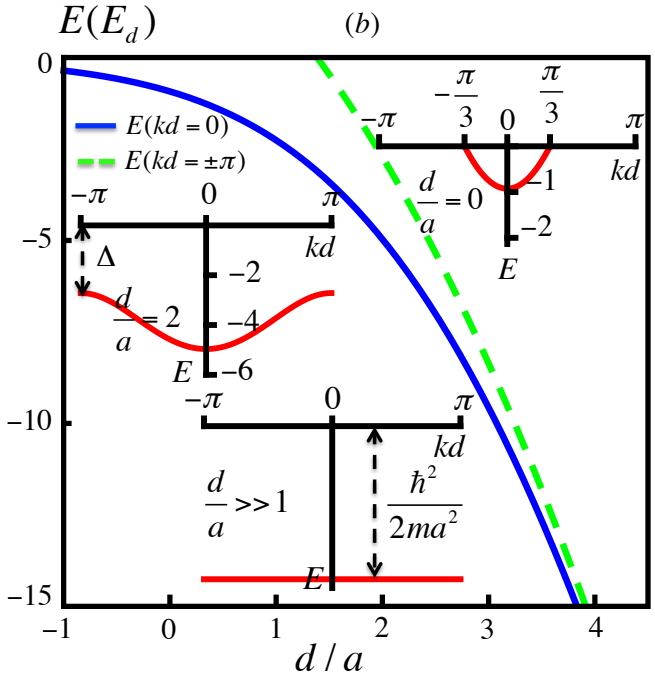
where k is the light atom lattice wave vector.

The resulting "electron" band is quite different from that of a standard Hubbard model

$$E(k) = -E_d \operatorname{arccosh}^2\left(\frac{e^{d/a}}{2} + \cos(kd)\right)$$

Band structure





- Full-filled deep "BEC limit" ($a \to 0^+$): tightly bound dimers of energy $-\hbar^2/2ma^2$, flat dispersion, no dimer overlap.
- a increases from 0^+: bandwidth increases, E_{gap} decreases until disappearing at $d/a = \ln 4 \simeq 1.39$.
- Unitarity: bandwidth$= 0.93E_d$ with Fermi surface at $k = \pm\pi/3d$ (1/3 light atoms remain bound).
- For any value of d/a there is still a fraction of bound atoms although it becomes very small on the "BCS" side.

Validity of BOA and losses

Importance of the nonadiabatic terms

(full band) transfer of light atoms into the continuum due to phonons. But, if $E_{\rm gap} \gtrsim 0$ forbidden by energy conservation: localized hole leads to an attraction between heavy atoms $\sim E_d e^{-d/a}$. But, for $V_0 = 25E_R$ and $M/m \simeq 10$, lattice potential is stronger ($\sim 10E_R \sim 10E_d$) so lattice deformation is very small: true gap $\sim$ band gap.

Losses

1. Formation of few-body states of size a: Already in Feshbach bound states so losses are only excitation of light atoms into the continuum due to collisions with phonons - *evaporative cooling* - tunable since it depends strongly $E_{\rm gap}$/(electron-phonon coupling strength).

2. Relaxation to deep bound states: light-light-heavy losses (h-h-l forbidden due to lattice). Rate of formation $\sim E_d(R_e/a)^4 \exp(-2d/a)/\hbar$ where R_e is the range of the interatomic potential (Petrov et al). For the gapped case d/a=2, relaxation time $\gtrsim$10s for a ^{6}Li-^{40}K mixture.

Novelties in this setup

New type of lattice It allows us to create a lattice for the light species using lasers which only trap the heavy atoms

Evaporative cooling At finite temperatures, atoms with large kinetic energy can escape to continuum: natural evaporative cooling process (assuming thermalization mechanism e.g. via collisions with heavy atoms)

Tunneling physics At very low temperatures and for small enough gaps, light atoms can in principle tunnel out of the band which might lead to interesting analogies with tunnelling problems in solid state physics

Phonons

We can simulate both *transverse* and *longitudinal* phonons

Longitudinal Phonons

Heavy atom lattice frequency shifted from $\omega_z = \sqrt{4V_0 E_R}$ due to light atoms. At $d/a = 2$ we can neglect next-nearest neighbours:

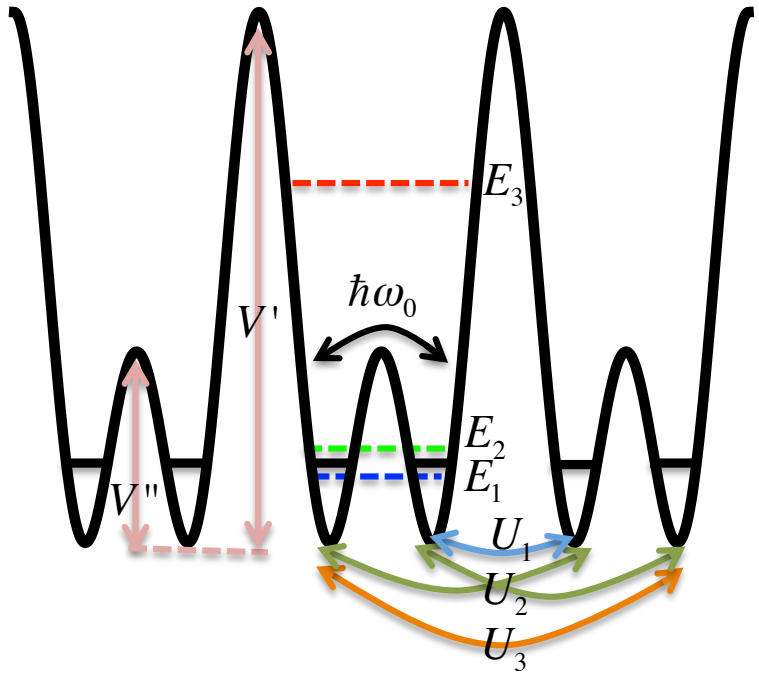
$$U(R) = 2\frac{\hbar^2}{ma^2}\mathrm{e}^{-2R/a}(R/a)^{-1}\left(1 - \frac{(R/a)^{-1}}{2}\right)$$

(Petrov et al) and heavy atom oscillation frequency becomes:

$$\omega = \sqrt{\omega_z^2 + \frac{2U''(R=2a)}{M}} \simeq \omega_z\left(1 + \frac{U''(R=2a)}{M\omega_z^2}\right)$$

This is approximately equivalent to estimating the square of the frequency shift of the π phonon i.e. $(\omega^2(q{=}\pi/d) - \omega_z^2)/\omega_z^2$ which is the square of the ratio of the phonon bandwidth to ω_z and is a dimensionless measure of the "electron"-phonon coupling strength. We find that, for $V_0{=}25E_R$ and therefore $\hbar\omega_z{=}10E_R$, the shift is $\simeq 0.001M/m$, i.e. in practice there will be no appreciable effect.

Double-well superlattice

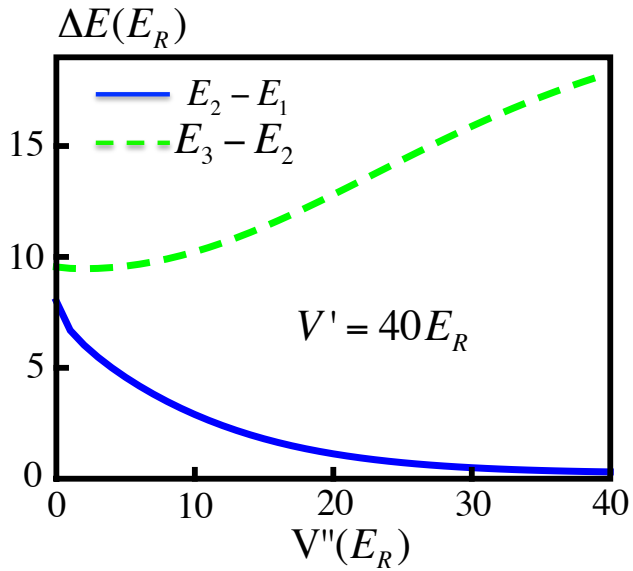


To overcome this difficulty we propose to use a lattice of double wells:

$$V = \frac{1}{2}M\omega_\perp^2(x^2+y^2) + V_0\cos^2(\pi z/d) + V_1\cos^2(2\pi z/d)$$

with $V''= V_1 - V_0/2 + V_0^2/16V_1$ and $V'=V_1 + V_0/2 + V_0^2/16V_1$. We can: 1) keep $d/a \sim O(1)$ and large V' (no tunnelling between double wells), and 2) tune $V''$to $\sim E_R$.

Double-well superlattice



We can restrict to the two lowest energy states $E_{1,2}$ of the double well with $V'' = 20E_R$ and $V' = 40E_R$, $E_3 - E_2 \simeq 14E_R \gg E_2 - E_1 \simeq 1E_R$.

Oscillation in the double well replaces the onsite oscillation so level splitting $\leftrightarrow \hbar\omega_z$.

CDW displacement is large ($\delta\langle z\rangle$ is $\simeq 0.2d$). Increases the "electron"-phonon coupling

Effective spin model

2 state approximation: Left/Right basis $\xi_{R,L}(\mathbf{R})$

$$\hat{H}_{\mathrm{BOA}} = \sum_{i=1}^{N_h} -\hbar\omega_z \left(\hat{a}^\dagger_{i,L}\hat{a}_{i,R} + \hat{a}^\dagger_{i,R}\hat{a}_{i,L}\right) + U_1 \hat{n}_{i,R}\hat{n}_{i+1,L}$$
$$+ U_2 \left(\hat{n}_{i,R}\hat{n}_{i+1,R} + \hat{n}_{i,L}\hat{n}_{i+1,L}\right) + U_3 \hat{n}_{i,L}\hat{n}_{i+1,R}$$

with

$$U_1 = \int d^3R_1 d^3R_2 |\xi_{i,R}(R_1)|^2 U(R_1 - R_2) |\xi_{i+1,L}(R_2)|^2$$

and similarly for U_2 and U_3.

Two states in each double well - map onto interacting spin-1/2 model using $\hat{\mathbf{S}}_i \equiv \left(\hat{a}^\dagger_{i,L}, \hat{a}^\dagger_{i,R}\right) \hat{\sigma} \left(\hat{a}_{i,L}, \hat{a}_{i,R}\right)^T$, chosen such that S_z points along the lattice.

Effective spin model

This leads to

$$\hat{H} = \sum_{i=1}^{N_h} -\hbar\omega_z \hat{S}_i^x + U_s \hat{S}_i^z \hat{S}_{i+1}^z + \text{ const}$$

where U_s=$(2U_2 - U_1 - U_3)/4$ and const $= (U_1 + 2U_2 + U_3)/4$, which is the Hamiltonian of the quantum Ising model in a purely transverse field $-\hbar\omega_z$ (Kivelson, Sachdev, Greiner et al) .

Heavy atom interaction energy (half band)

Half filled band leads to dimerisation of ion lattice. Calculation of band structure energy:

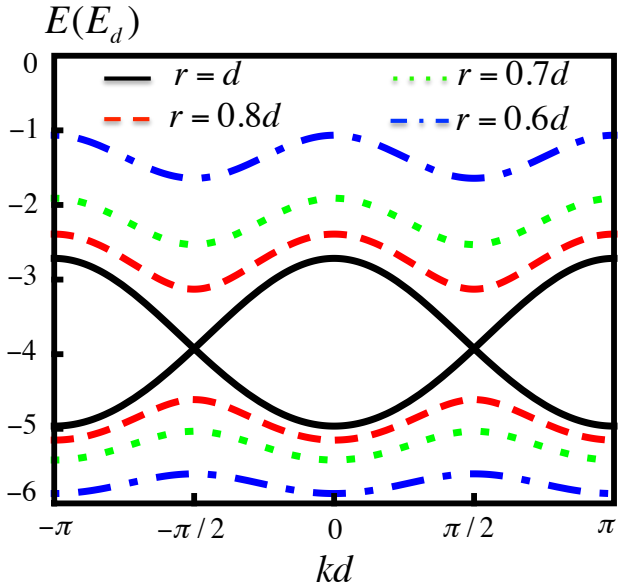
Each unit cell has two atoms - two bands from det[$\Xi(\kappa)$]=0, with

$$\Xi_{12} = \Xi_{21}^{*} = \frac{e^{-\kappa r}}{r} + \sum_{n=1}^{N_h/2} \left(e^{i2nk} \frac{e^{-\kappa(2nd+r)}}{2nd+r} + e^{-2ink} \frac{e^{-\kappa(2nd-r)}}{2nd-r} \right)$$

$$\Xi_{11} = \Xi_{22} = \left(\frac{1}{a} - \kappa \right) + \sum_{n=1}^{N_h/2} \left(2\cos(2nk) \frac{e^{-\kappa 2nd}}{2nd} \right)$$

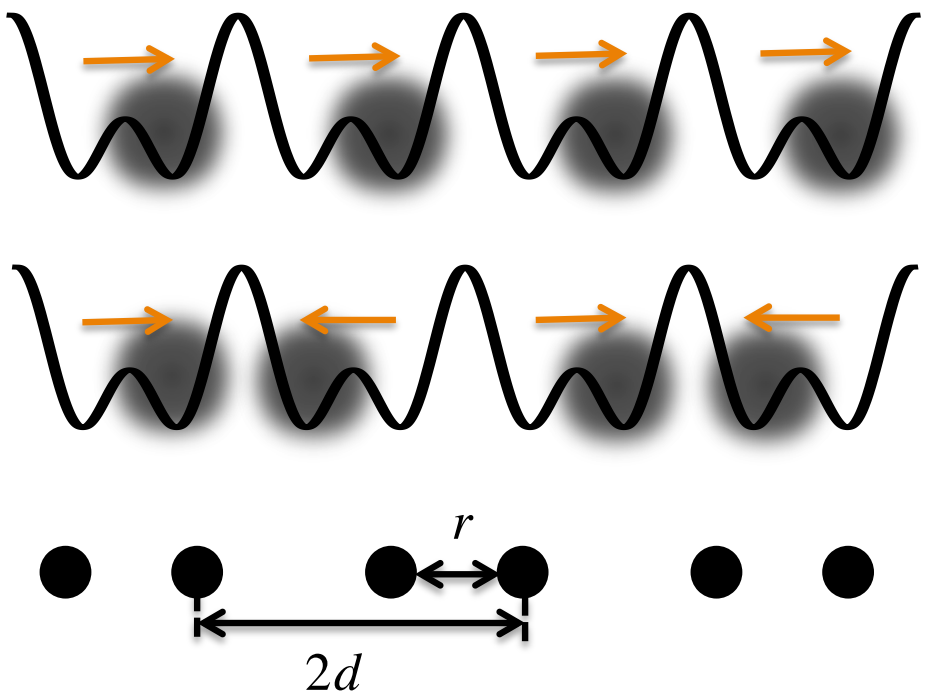
where r is the separation between the two atoms in the unit cell.

Heavy atom interaction energy (general case)



$r{=}d$: single band case; $r{<}d$: band split into higher (a) and lower (b) bands. Interaction energy: $V_{\mathrm{b}}(r)$ for a half-filled band and $V_{\mathrm{b}}(r) + V_{\mathrm{a}}(r)$ for full-filling where $V_{\mathrm{a(b)}}(r){=}\sum_k E_{\mathrm{a(b)}}(k, r)$ and $k{\in}[-\pi/2d, \pi/2d]$. We found empirically that V_b and V_a can be perfectly fitted with the symmetric (κ_+) and antisymmetric (κ_-) solutions of $\kappa_\pm \mp e^{-\kappa_\pm r}/r{=}1/a$

Effective spin model



Full band case - ferromagnetic phase: when $\hbar\omega_z \gg U_s$, the spins point along x and we recover the situation of the simple OL - phonon frequency $\sim\omega_z$. The electron-phonon coupling strength is very small:

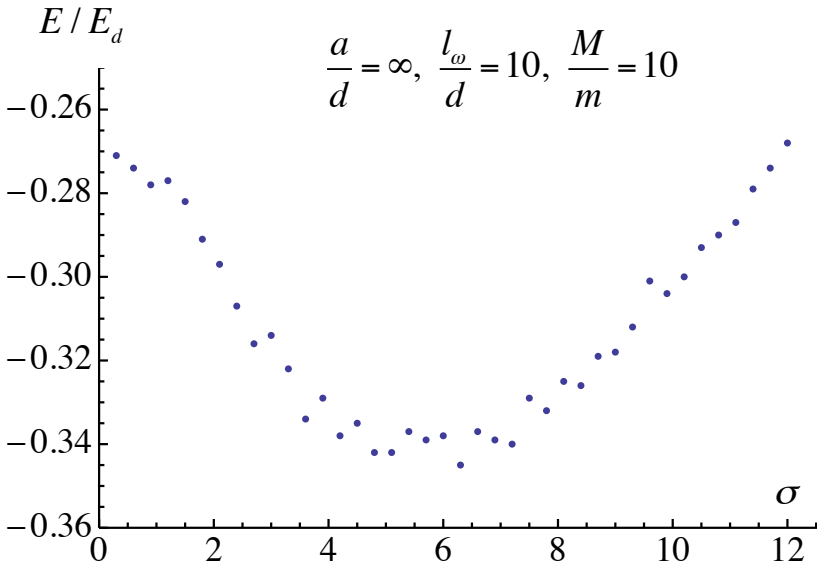
$$(\omega^2(q=\pi/d)-\omega_z^2)/\omega_z^2 \simeq (U_s/\hbar\omega_z)^2$$

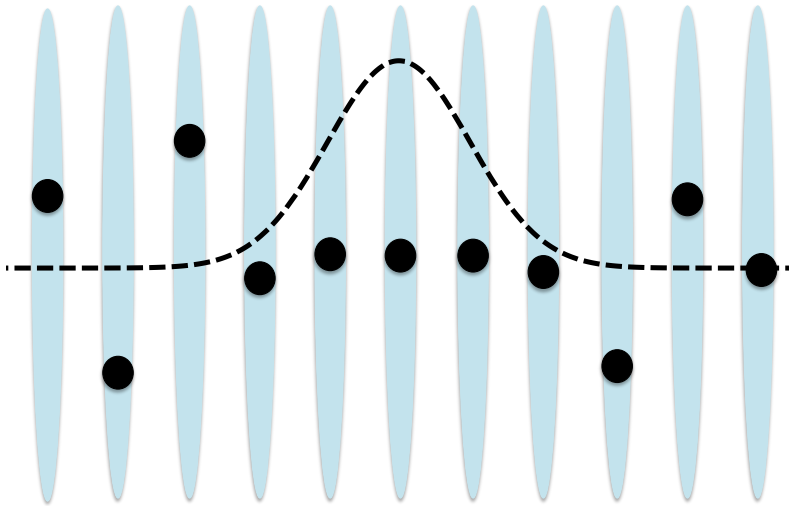
Half band case - antiferromagnetic phase: when $\hbar\omega_z \ll U_s$ emergence of a CDW from a Peierls instability.

Transverse Phonons

Simple experimental implementation: $\omega_\perp \ll \omega_z$ - single well deep lattice along z but weak confinement along x, y - effective 1D lattice 1 atom per site.

Example: Lattice polaron- chain of heavy atoms, 1 light atom - leads to localisation of light atom wave function





Beyond the Born-Oppenheimer Approximation

"Ion" motion uses a Hubbard-type (lattice model) description

Strength of this experimental system: *can actually simulate electrons and phonons*! - Light atoms are dynamical degrees of freedom too and not describable as lattice particles.

We can study:

- *dynamics* of the Peierls instability itself and the time-dependence of formation of the associated CDW
- "electron"-phonon scattering and transport phenomena, such as the mobility of electrons in holes in the presence of umklapp processes
- formation of light atom Cooper pairs due to phonon exchange and the SSH model
- the *lattice* polaron problem when only one light atom is present, propagating along the chain of heavy atoms

Experimental implementation

2D array of 1D tubes with a (super)lattice along each tube

Loading: Either 1) create the molecules with small a in the gas phase and then load them into a deep OL or 2) load the OL with heavy atoms, add gas of light atoms, form Feshbach molecules on each site through collisions.

Half-filled band preparation: start with full band then adiabatically increase a/d to close gap, lose half of the atoms and then decrease a/d to return to the gapped case.

CDW measurement (heavy atom dislocations): light scattering off heavy atoms gives peak with periodicity d but also secondary peak of CDW.

Light atom dislocation: use rf-spectroscopy to see energy distribution and Peierls gap.

Conclusions

Ideas from few-body physics can bring a new approach to atoms in OLs

Example: tunable lattice for the light atoms via interactions

Analog of an electron-phonon system

Future work: allow heavy atoms to tunnel, a case without parallel in solid state systems where the ions are fixed to the lattice sites.