Quantum simulation of small-polaron formation with trapped ions

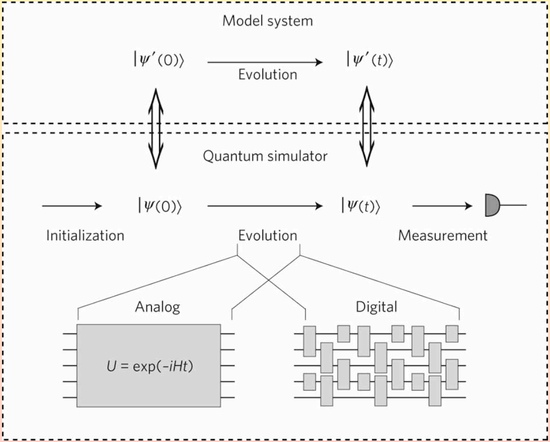
Vladimir M. Stojanović

UNIVERSITY OF BASEL

Control of Complex Quantum Systems workshop @ KITP

Analog and digital quantum simulations

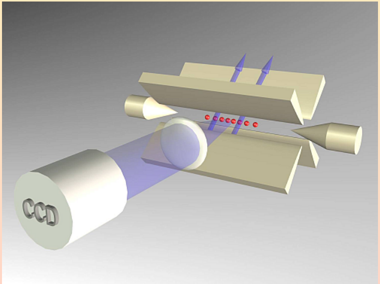
IDEA: (Feynman '81, Lloyd '96; see J. I. Cirac and P. Zoller, Nature Phys. 2012)
Simulate the dynamics of a complex quantum system using another system that is easier to manipulate and measure



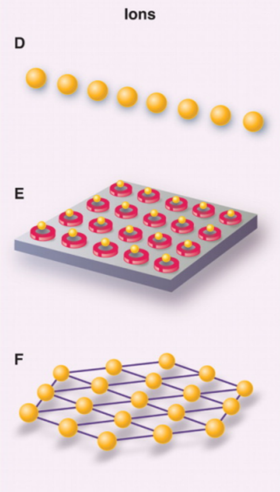
R. Blatt and C. F. Roos, Nature Phys. **8**, 277 (2012)

Analog quantum simulations with trapped ions

- sophisticated trapping & cooling
- single-ion addressability
- high-precision measurements
- internal states $\longrightarrow$ pseudospins



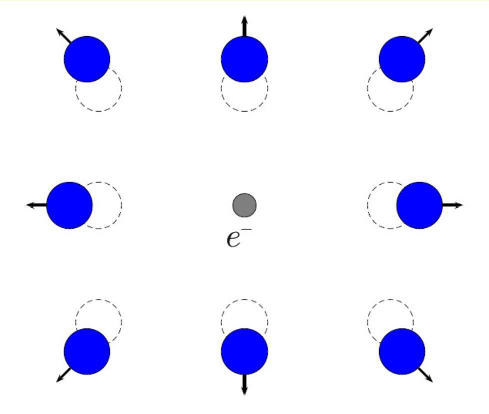
Source: R. Blatt's group (Innsbruck)



Buluta & Nori, Science '09

Review: C. Schneider, D. Porras, and T. Schaetz, Rep. Prog. Phys. **75**, 024401 (2012)

Small polarons: basics



D. Emin, 1982: "...A small polaron is an extra electron or a hole severely localized within a potential well that it creates by displacing the atoms that surround it..."

Polaron concept:

L. D. Landau (1933), polar semiconductors (alkali-halides)

Polarons also found in:

transition-metal oxides, glasses, undoped cuprates, some conductive polymers, etc.

main feature:

low-mobility ($\mu < 1\,\mathrm{cm}^2/\mathrm{Vs}$), increasing with temperature (at high temperatures)!

Generic coupled electron-phonon model

$$H = H_{\rm e} + H_{\rm ph} + H_{\text{e-ph}}$$

$$H_{\rm e} = -t \sum_i (c_{i+1}^\dagger c_i + \text{h.c.})$$

$$H_{\rm ph} = \sum_q \omega(q) b_q^\dagger b_q$$

translational invariance: $[H, \mathrm{K}] = 0$ regardless of the form of $H_{\text{e-ph}}$

$$\mathrm{K} = \sum_k k\, c_k^\dagger c_k + \sum_q q\, b_q^\dagger b_q$$

total crystal momentum operator

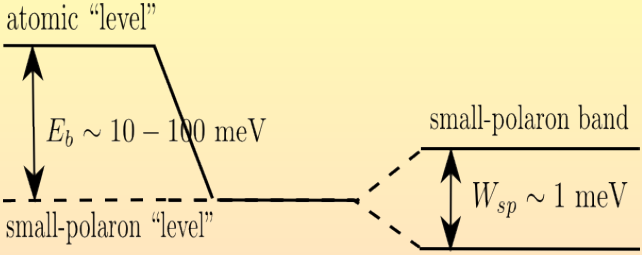
$$K|\psi_\kappa\rangle = \kappa\, |\psi_\kappa\rangle$$

$$H|\psi_\kappa\rangle = E_\kappa |\psi_\kappa\rangle$$

quasiparticle residue (spectral weight) at quasimomentum $\mathbf{k}$:

$$Z_{\mathbf{k}} \equiv |\langle \Psi_{\mathbf{k}} | \psi_{\mathbf{k}} \rangle|^2 \qquad (\, 0 < Z_{\mathbf{k}} < 1 \,)$$

Bare-band electrons vs. small polarons



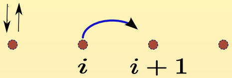
- small-polaron band center is shifted downwards by E_b (binding energy) from that of a bare electron
- small-polaron bandwidth (W_{sp}) is much smaller than W_e

Necessary condition for small-polaron formation:

$$E_b \geq W_e/2$$

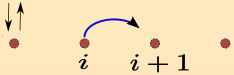
Molecular-crystal model and short range e-ph coupling

local (Holstein-type) coupling



$$\epsilon \rightarrow \epsilon + \alpha_H u_i$$

non-local (Peierls-type) coupling



$$t \rightarrow t + \alpha_P \left(u_{i+1} - u_i\right)$$

$$u_i \equiv \frac{1}{\sqrt{2m\omega}}(b_i^\dagger + b_i)$$

dimensionless couplings:

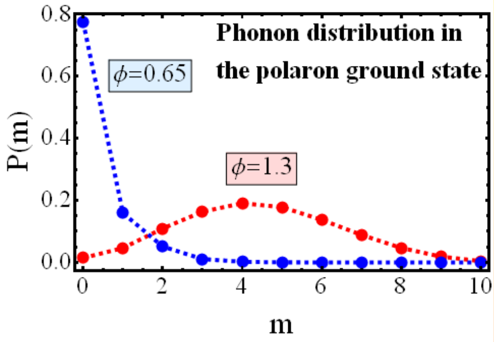
$$\frac{\alpha_{\mathrm{H}}}{\sqrt{2m\omega}} \equiv g\omega$$

$$\frac{\alpha_{\mathrm{P}}}{\sqrt{2m\omega}} \equiv \phi\omega$$

Holstein term: $$H_{\mathrm{g}} = g\omega \sum_i c_i^\dagger c_i (b_i^\dagger + b_i)$$

Peierls term: $$H_\phi = \phi\omega \sum_i (c_{i+1}^\dagger c_i + \mathrm{h.c.})(b_{i+1}^\dagger + b_{i+1} - b_i^\dagger - b_i)$$

Hilbert spaces and phonon ground-state distributions



need truncation (phonons !) of the original Hilbert space

$$\mathcal{H} = \mathcal{H}_{\rm e} \otimes \mathcal{H}_{\rm ph}$$

to states with the total of at most M phonons

$$|\Psi\rangle = \sum_{\mathbf{n},\mathbf{m}} C_{\mathbf{n},\mathbf{m}} \, |\mathbf{n}\rangle_{\rm e} \otimes |\mathbf{m}\rangle_{\rm ph}$$

Dimension of the truncated Hilbert space:

$N = 6$ sites, $M = 8$ phonons $\longrightarrow$ $D = 7722$

$M = 9$ phonons $\longrightarrow$ $D = 12012$

$M = 10$ phonons $\longrightarrow$ $D = 18018$

Toyozawa-type variational Ansatz: inner workings

Y. Toyozawa, Prog. Theor. Phys. **26**, 29 (1961)

Bloch wave-functions (eigenstates of the total crystal momentum):

$$|\psi_\kappa\rangle = N^{-1/2} \sum_n e^{i\kappa n} \, |\psi_\kappa(n)\rangle$$

"Wannier-like" function ($4N$ variational parameters):

$$|\psi_\kappa(n)\rangle = \sum_{m=-N/2}^{N/2-1} \Phi_\kappa(m) e^{i\kappa m} c^\dagger_{n+m} |0\rangle_{\mathrm{e}} \otimes |\xi_\kappa(n)\rangle_{\mathrm{ph}}$$

product of phonon coherent states:

$$|\xi_\kappa(n)\rangle_{\mathrm{ph}} \equiv \prod_l \exp\left(v_l^\kappa b^\dagger_{n+l} - v_l^{\kappa *} b_{n+l}\right) |0\rangle_{\mathrm{ph}}$$

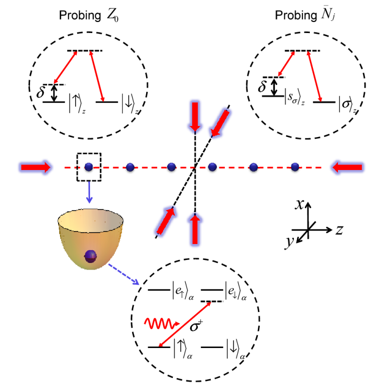
Holstein model: TA becomes exact in the limit of vanishing hopping!

Quantum simulation of small Holstein polaron formation

VMS, T. Shi (MPQ), C. Bruder, and J. I. Cirac (MPQ), PRL **109**, 250501 (2012)

Goal: simulate the strong-coupling regime of the Holstein model using a linear array of ion microtraps

Previous proposals: F. Herrera and R. Krems, PRA **84**, 051401(R) (2011); J. P. Hague and C. MacCormick, NJP **14**, 033019 (2012)



Important points to address:

- realize strictly local e-ph coupling
- make phonons nearly dispersionless
- reach strong-coupling regime with realistic values of exp. parameters

Coupling internal states to motion in a nutshell

foundations: D. Porras and J. I. Cirac, PRL **92**, 207901 (2004)

basic mechanism: standing laser wave, detuned from a transition leads to a position and state-dependent conservative potential (**a.c.-Stark shift**)

$$V(x_\alpha) \propto \Omega^2(x_\alpha)/\Delta_\alpha \qquad \text{detuning: } \Delta_\alpha \equiv \omega_{L,\alpha} - \omega_0$$

Lamb-Dicke regime ($a \ll \lambda_L$):
linear expansion of $\Omega^2(x_\alpha)$ around the ion equilibrium positions

$$\Longrightarrow \quad H_I = \sum_{i,\alpha} F_\alpha q_i^\alpha (1 + \sigma_i^\alpha)$$

"pushing" force: $F_\alpha \propto G_\alpha^2 k_\alpha / 2\Delta_\alpha$

coupling of a spinless-fermion (Jordan-Wigner: $1 + \sigma_i^z \to 2c_i^\dagger c_i$)
excitation to longitudinal phonons ($q_i^z \propto b_i + b_i^\dagger$) is Holstein-like:

$$H_{\mathrm{e-ph}} \propto \sum_i c_i^\dagger c_i (b_i + b_i^\dagger)$$

Character of phonon modes and e-ph coupling

vibrational modes (transverse and longitudinal) result from:
trapping potentials + Coulomb repulsion between the ions

stiff limit: $\beta_\alpha \equiv \frac{e^2}{m\omega_\alpha^2 d_0^3} \ll 1$ (well-localized modes in direction α)

eliminate high-energy transverse phonons $\Longrightarrow$ for longitudinal ones (RWA)

$$H_L = \tilde{\omega}_z \sum_i b_i^\dagger b_i - \sum_{i \neq j} \frac{\tilde{\beta}_z \tilde{\omega}_z}{2\,|i-j|^3}(b_j^\dagger b_i + \text{H.c.}) \qquad (\,\tilde{\omega}_z \approx \omega_z\,)$$

nearly dispersionless (localized in real space) phonons $\Longrightarrow$ $J \ll \tilde{\omega}_z$

$$H_{\mathrm{e-ph}} = g\tilde{\omega}_z \sum_i c_i^\dagger c_i (b_i + b_i^\dagger)$$

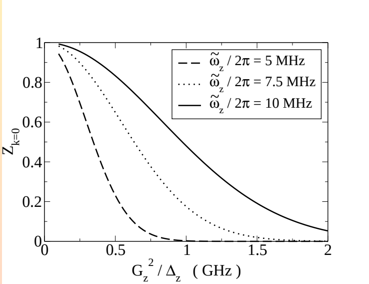
$$g = \frac{4\pi}{\tilde{\omega}_z}\frac{G_z^2}{\Delta_z} \times \frac{a}{d_0}$$

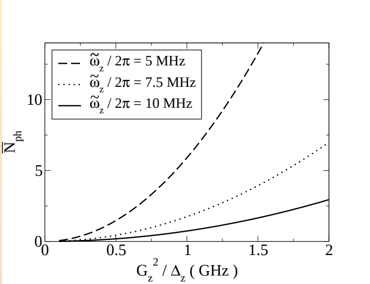
typical values:
$\omega_z/2\pi = 1 - 20$ MHz
$\Delta_z = 1000$ GHz,
$G_z = 10 - 100$ GHz

Polaron crossover

smooth crossover from a quasi-free excitation ($Z_{k=0}$ close to 1, $\bar{N}_{\text{ph}} \approx 0$) to a small polaron ($Z_{k=0} \approx 0$, $\bar{N}_{\text{ph}} \gtrsim 3$)

results from Toyozawa-Ansatz calculation on $N = 32$ sites ($J = 25$ KHz):





$$Z_{k=0} \equiv \frac{|\langle \Psi_{k=0} | \psi_{k=0} \rangle|^2}{\langle \psi_{k=0} | \psi_{k=0} \rangle}$$

$$\bar{N}_{\text{ph}} \equiv \langle \psi_{k=0} | \sum_i b_i^\dagger b_i \, | \psi_{k=0} \rangle$$

Conclusions & Outlook

- Small (Holstein) polaron physics can be simulated with trapped ions

  VMS, T. Shi, C. Bruder, and J. I. Cirac, PRL **109**, 250501 (2012)

- **Multiple-excitation regime**:
  exper. study of the density-driven destabilization of small polarons?

$$n_c \approx 1 - \frac{W_e}{2E_b} \qquad (E_b = g^2\omega)$$

- **Dynamics of small-polaron formation**:
  How rapidly upon creation of a bare excitation (excitation-phonon "interaction quench") the cloud of virtual phonons around it forms?

UNI BASEL