Simulating the solid state with cold atoms:

how to get a quantitative phase diagram

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Outline

- “Artificial crystals of light”?
- The issue of inhomogeneity
- Getting the numbers out: finite-size and finite-curvature scaling
- A demonstration (with numerical data replacing experimental ones)
- Conclusions and outlook

“Artificial crystals of light”?

1995: Bose-Einstein condensation achieved in trapped gases of ultra-cold (< 1 μK) atoms

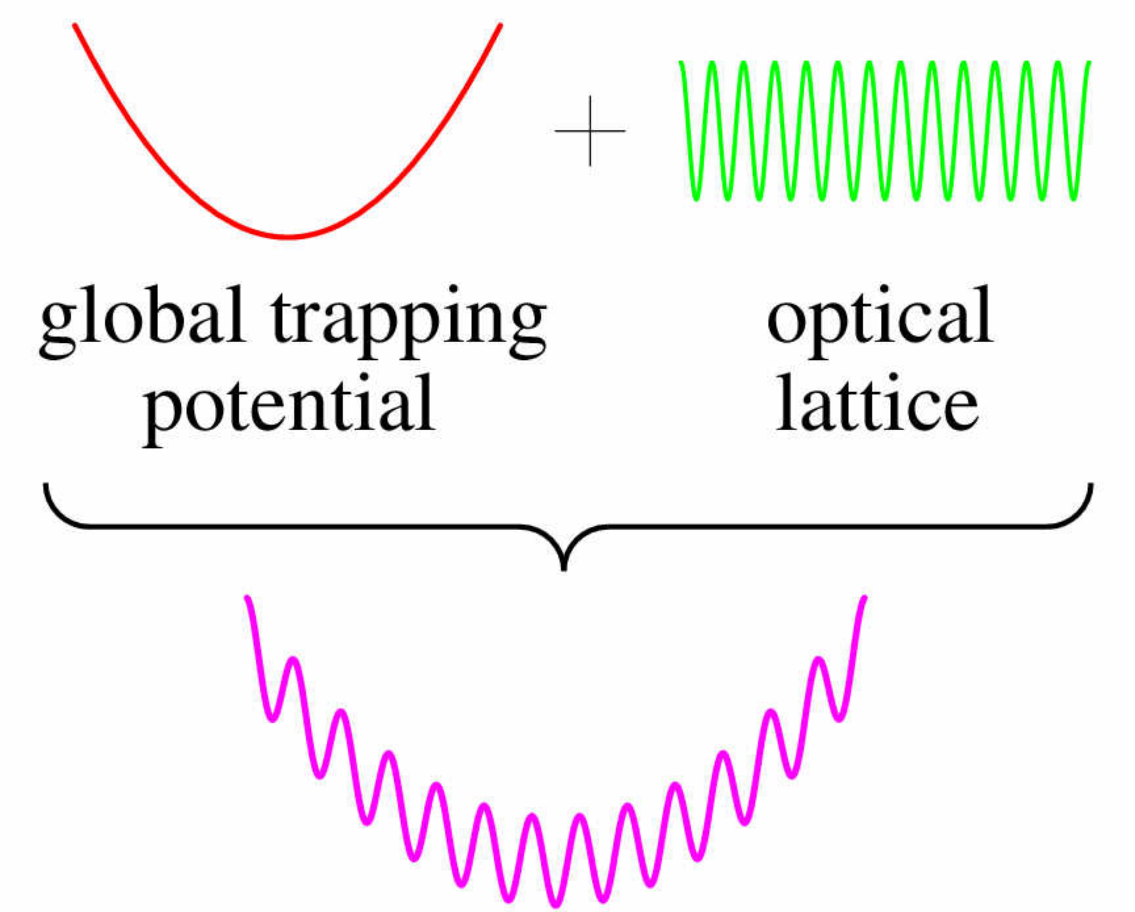
Last few years: Optical lattices – laser standing waves applied to the atom gas. Atoms hopping from site to site of lattice ↔ electrons hopping from site to site of a material?

Advantages: Not limited to what chemistry deigns to provide – lattices can be arbitrary, and arbitrarily clean (or dirty!)

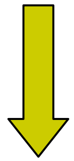
Achievements: Observed several phases known from condensed matter (superfluid, Mott insulator, metal)

Immanuel Bloch (2004): “artificial crystals of light”

The issue of inhomogeneity



Filling fraction varies with position

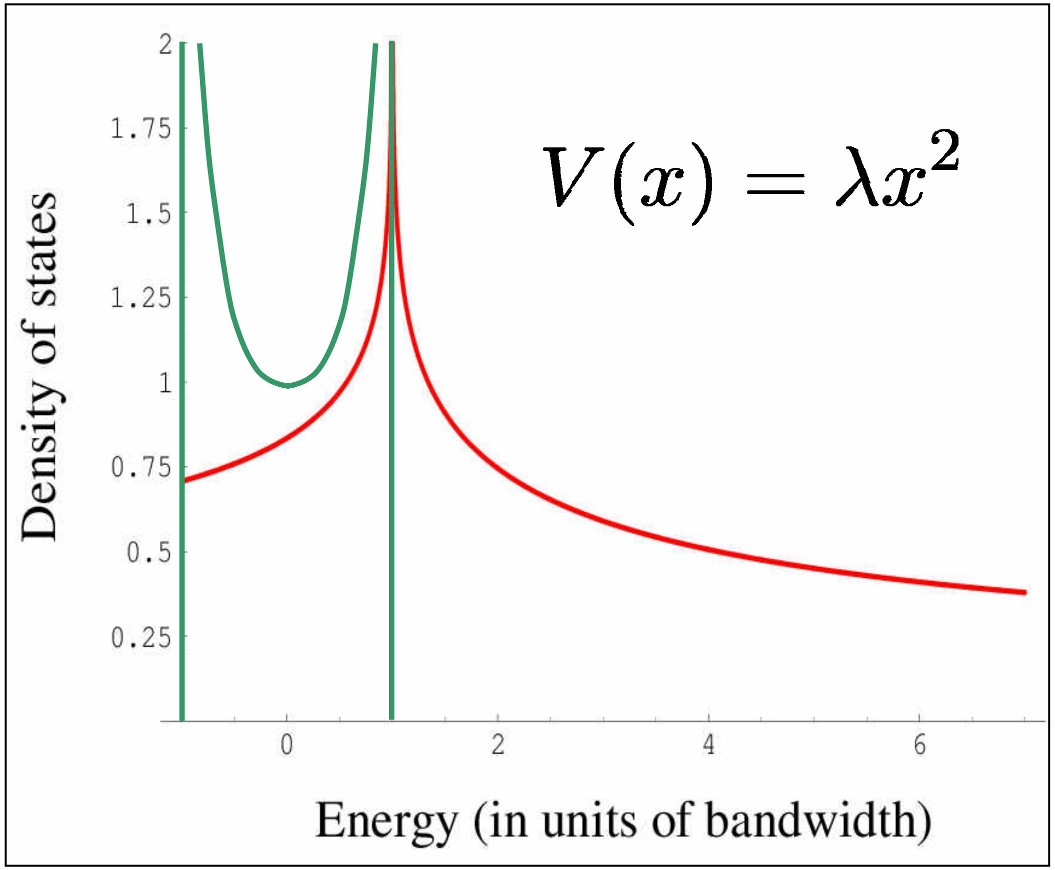


Phase transition is an interface that sweeps through the system

(This is not what happens in a bulk material!)

The starkness of the problem

Example: non-interacting particles in optical lattice plus harmonic trap



This form of the DoS is universal for arbitrarily small (non-zero) trap amplitude

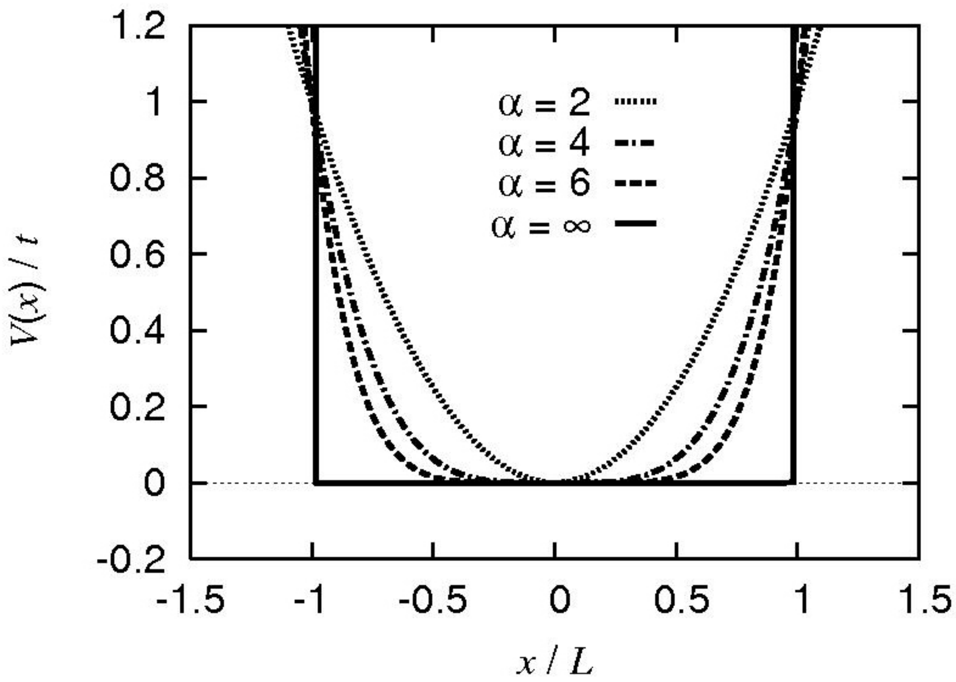
$\lambda \rightarrow 0$ limit is singular!

see C. H. and J. Quintanilla, *Phys. Rev. Lett.* **93**, 080404 (2004)

Finite-curvature scaling

Behaviour is not governed by the amplitude of the trapping potential, but by the power law.

Suggests a sequence of potentials approaching the hard-wall limit (which applies in crystals):



$$V_{\mathrm{trap}}(x) = t\left|\frac{x}{L}\right|^{\alpha}$$

see C. H. and J. Quintanilla, *Physica B* 378-380, 1035 (2006)

Experimental procedure

To determine (for example) the phase diagram of the Hubbard model:

1. Set up the optical lattice system with a particular trap power-law (α), box-size (L), and filling (f).

2. Drop the trap, and measure total energy.

3. (Finite-size scaling.) Repeat steps 1 and 2, increasing L until convergence is achieved – or experimental limits exceeded.

4. (Finite-curvature scaling.) Repeat steps 1 to 3, increasing α until convergence is achieved – or experimental limits exceeded.

5. Repeat steps 1 to 4 for various filling fractions. Under ideal circumstances, this yields $E(f)$ as $L,\alpha \rightarrow \infty$.

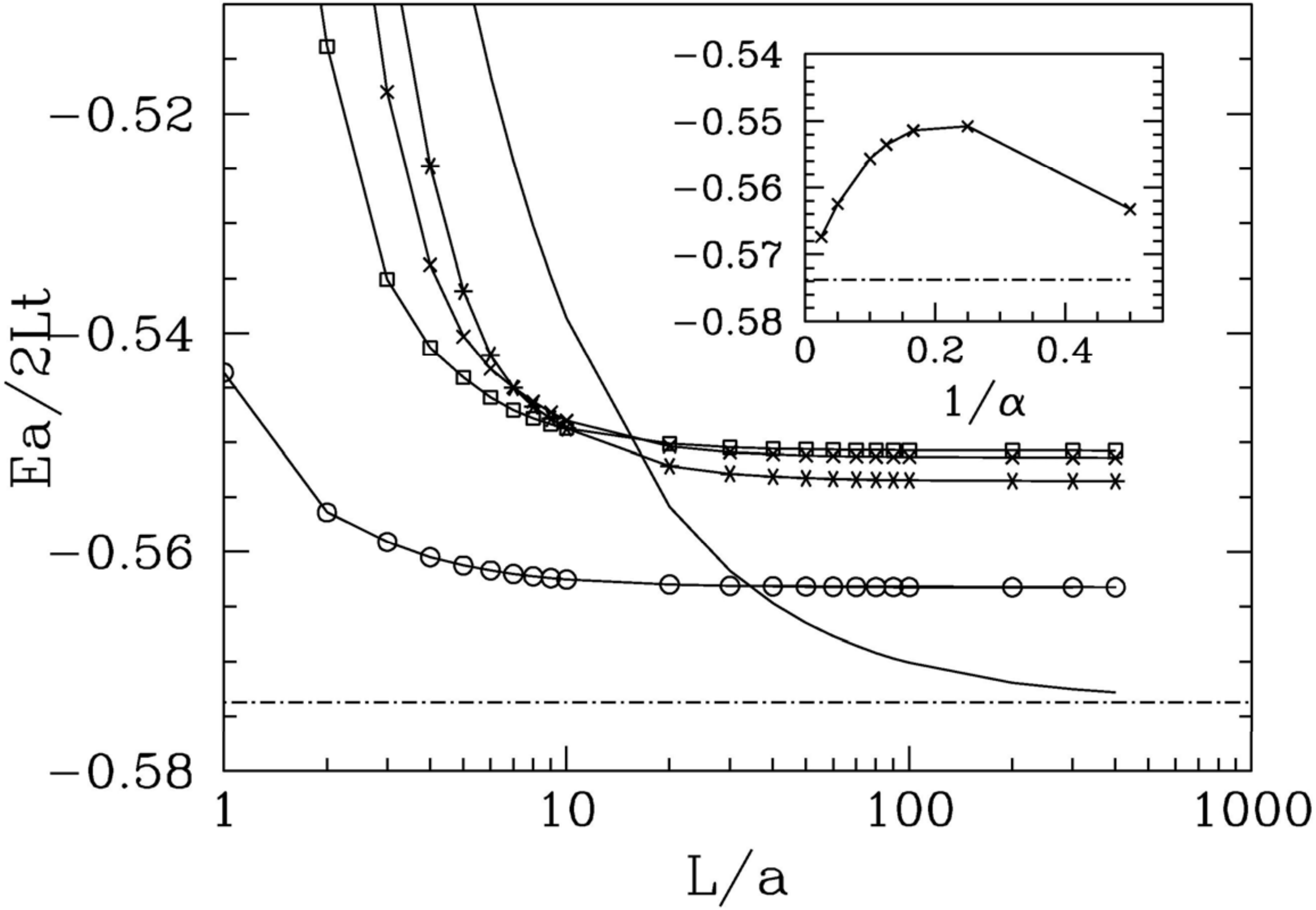
6. Numerically differentiate the curve – jumps indicate phase transitions!

Proof of the pudding…

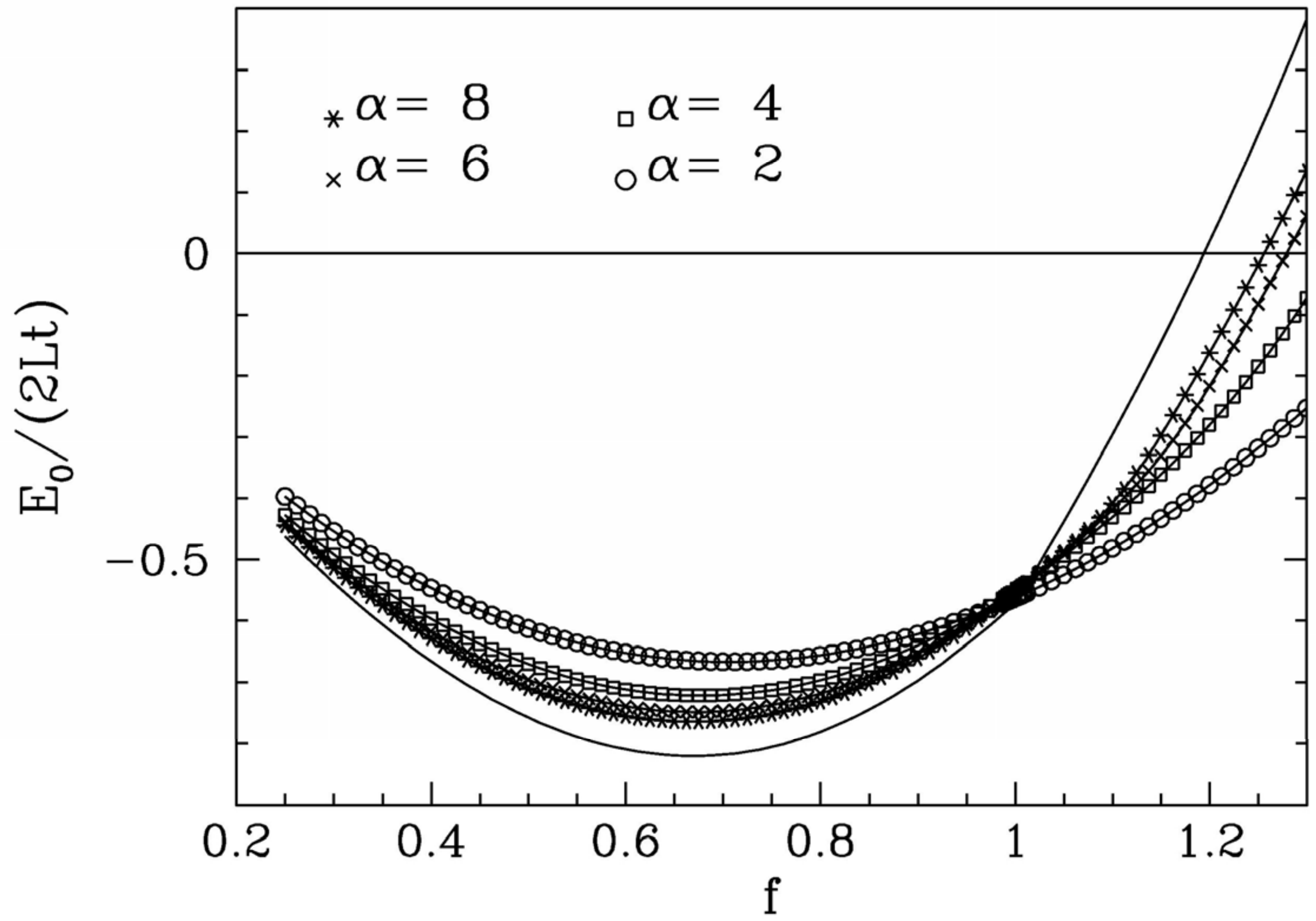
To test the procedure, do it for the 1D Hubbard model – there we can use numerical simulation results as ‘mock’ experimental data.

Simulations carried out with Bethe-Ansatz local density approximation (BA-LDA) by Campo and Capelle.

Proof of the pudding…



Proof of the pudding…



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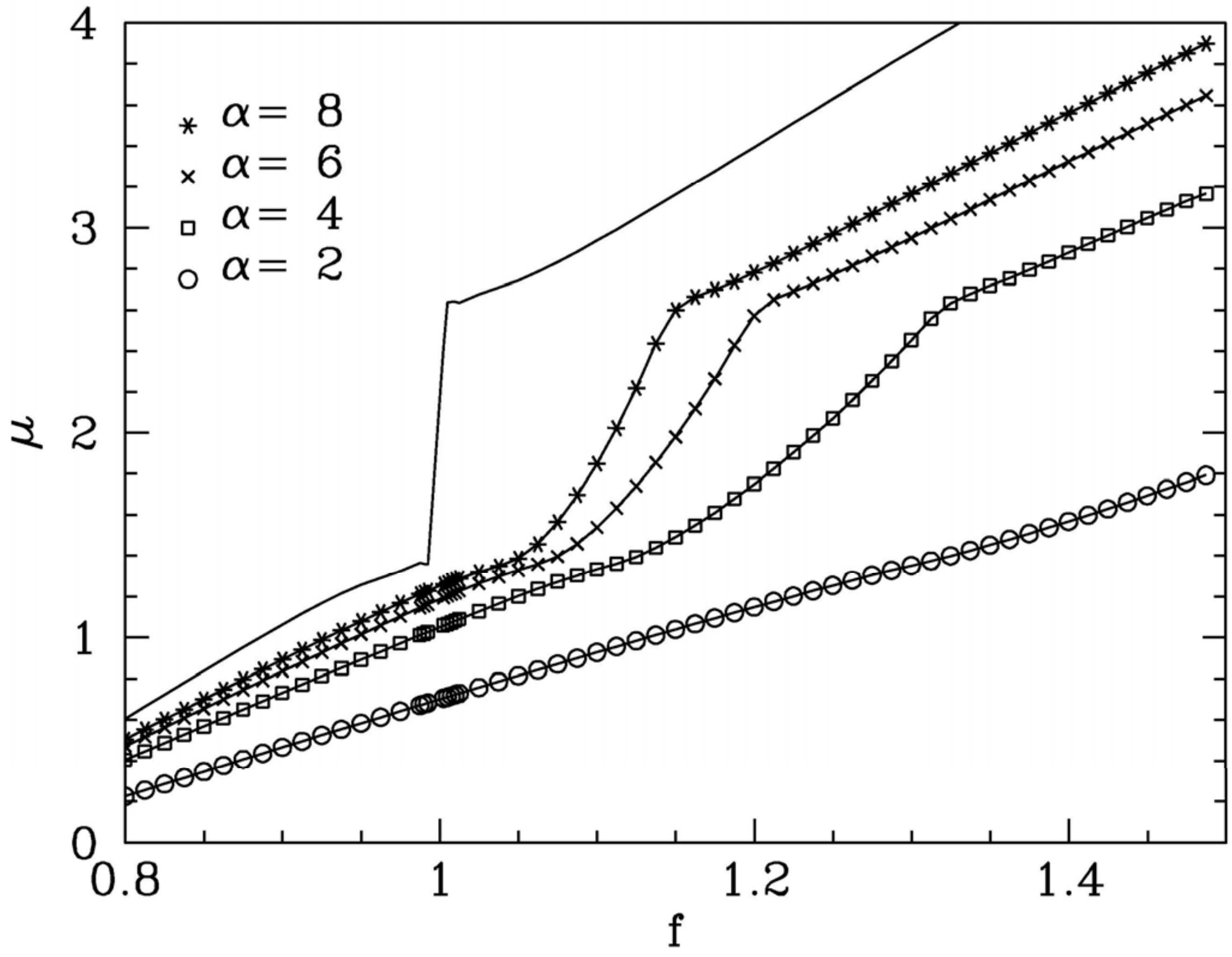

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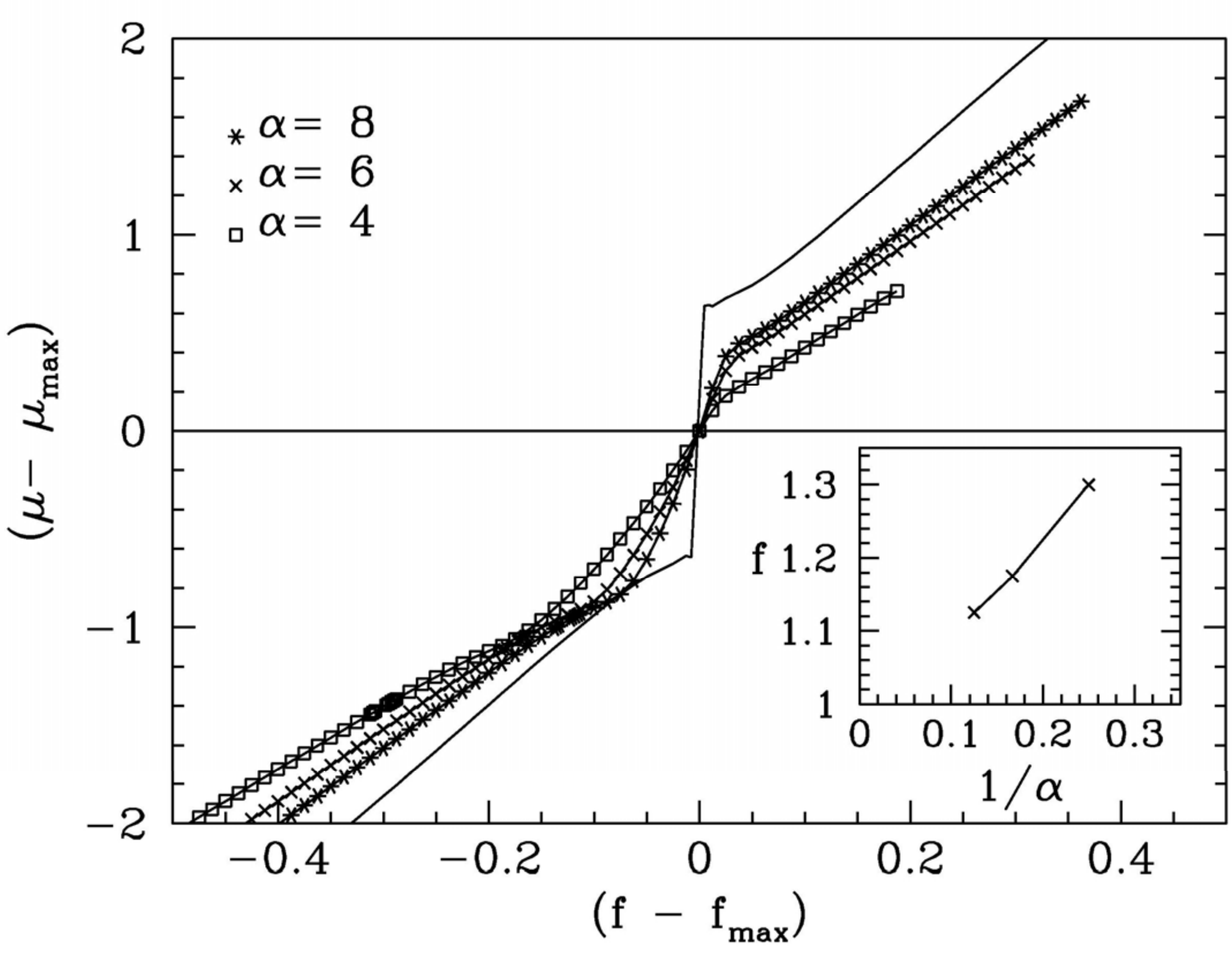

Conclusions and outlook

Conclusions:

1. Varying the trap power-law is crucial to quantitative simulations of the solid state using optical lattices.

2. Preliminary explorations suggest this is feasible if four or five successive power laws can be arranged.

Outlook:

3. More work needed on second-order transitions.

4. And if an experimentalist with a spare five minutes would like to set this up and run it, that'd be lovely…