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Moiré atoms, Wigner molecules, and emergent Kagome lattice

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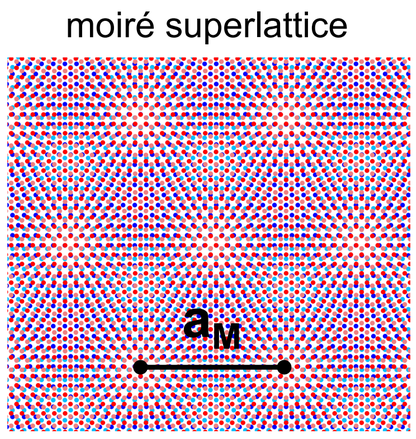
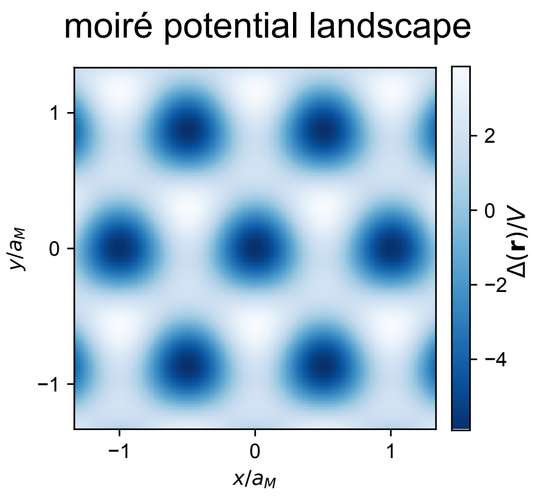
Q: What happens in semiconductor moiré superlattices at higher filling factors ≥ 1 per potential minimum where interaction and moiré potential energies are frustrated?

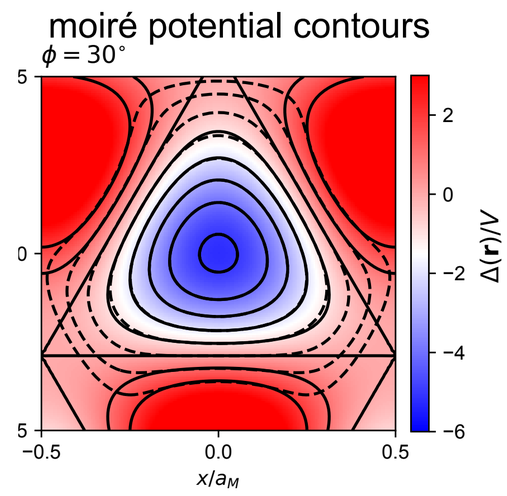
Model: 2DEG + smooth periodic potential

$$H = \sum_i \frac{p_i^2}{2m} + \Delta(r_i) + \sum_{i \neq j} \frac{e^2}{\epsilon |r_i - r_j|}$$

$$\Delta(r) = -2V \sum_{i=1,3,5} \cos(g_i \cdot r + \phi)$$







"moiré atom" = local minimum of moiré potential
= parabolic quantum dot + trigonal moiré crystal field

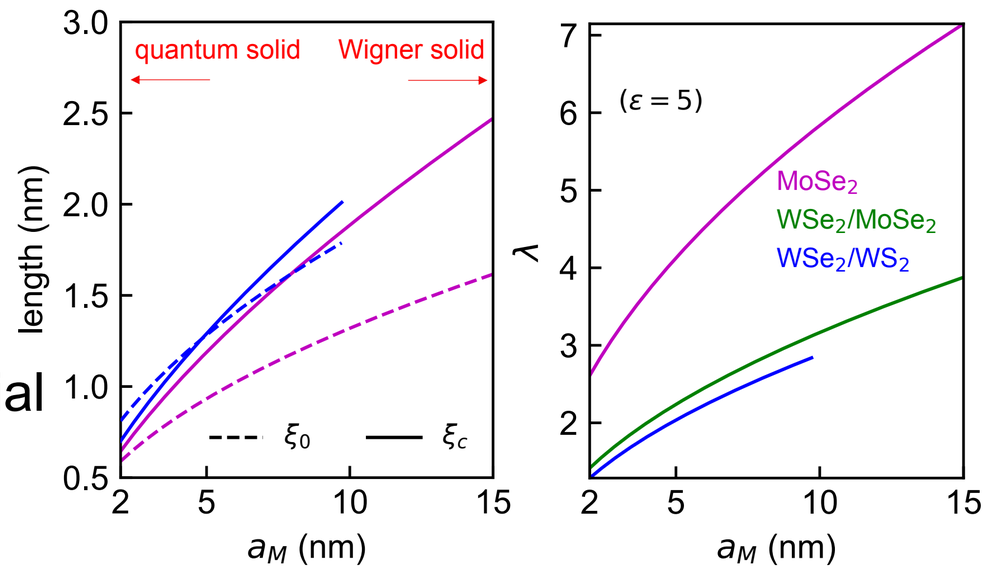
$$\Delta(r) = \frac{1}{2} k r^2 + c_3 \sin(3\theta) r^3 + \cdots$$

3 key length scales:

-ξ_0: radius of one-electron ***quantum*** oscillator wavefunction

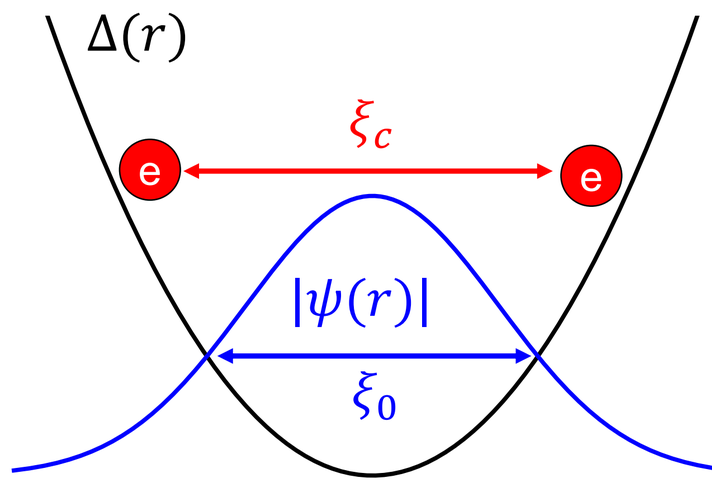
-ξ_c: radius of two ***classical*** point charges in parabolic potential with Coulomb repulsion

-a_M: distance between moiré atoms



Atomic coupling constant: $\lambda = \frac{coulomb\ energy}{bandgap} = \frac{e^2/(\epsilon \xi_0)}{\hbar \omega} = (\xi_c/\xi_0)^3$

$$\xi_0 = \left[\frac{\hbar^2}{mk}\right]^{\frac{1}{4}} \propto a_M^{1/2} \qquad \xi_c = \left[\frac{e^2}{2\epsilon k}\right]^{\frac{1}{3}} \propto a_M^{2/3}$$



Hierarchy of length scales $\xi_0 \ll \xi_c \ll a_M$ realized in limit $a_M \to \infty$

Atomic limit: $\xi_0, \xi_c \ll a_M$

Classical limit: $\xi_0 \ll \xi_c, a_M$

Exact diagonalization of isolated moiré atom

- Evolution from "Schrödinger atom" to "Wigner molecule"
- Wigner molecules are observable with STM

Moiré solids ($\max(\xi_0, \xi_c) \sim a_M$)

- Phase factor ϕ shapes moiré potential landscape
- Self-consistent Hartree-Fock solution for $\phi = 60º$ has Kagome lattice charge density and quasiparticle bands, whereas moiré potential minima form honeycomb lattice!
- Competition between interaction and moiré potential energy causes electrons to localize to *saddle point*s of moiré potential