Density-dependent processes of dipolar molecules in an optical lattice

Tomasz Sowiński[1,2], Omjyoti Dutta[2], Philipp Hauke[2], Luca Tagliacozzo[2], Maciej Lewenstein[2]

[1] Institute of Physics of the Polish Academy of Sciences, Poland
[2] ICFO – The Institute of Photonic Sciences, Spain

Abstract

We study the extended Bose–Hubbard model describing an ultra-cold gas of dipolar molecules in an optical lattice, taking into account all on-site and nearest-neighbor interactions, including occupation-dependent tunneling and pair tunneling terms. We show that these terms lead to additional quantum phase transitions and can destroy insulating phases. These considerable changes of the phase diagram have to be taken into account in upcoming experiments with dipolar molecules.

Bosons in optical lattice — 1

- **Hamiltonian of the system**

$$\mathcal{H} = \int \mathrm{d}^3\boldsymbol{r}\ \Psi^\dagger(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\boldsymbol{r})\right]\Psi(\boldsymbol{r}) + \frac{1}{2}\iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\ \Psi^\dagger(\boldsymbol{r})\Psi^\dagger(\boldsymbol{r}')\mathcal{V}(\boldsymbol{r}-\boldsymbol{r}')\Psi(\boldsymbol{r}')\Psi(\boldsymbol{r})$$

- **Lattice potential**

$$V_{\mathrm{ext}}(\boldsymbol{r}) = V_0\left[\sin^2\frac{2\pi x}{\lambda} + \sin^2\frac{2\pi y}{\lambda}\right] + \frac{m\Omega^2}{2}z^2$$

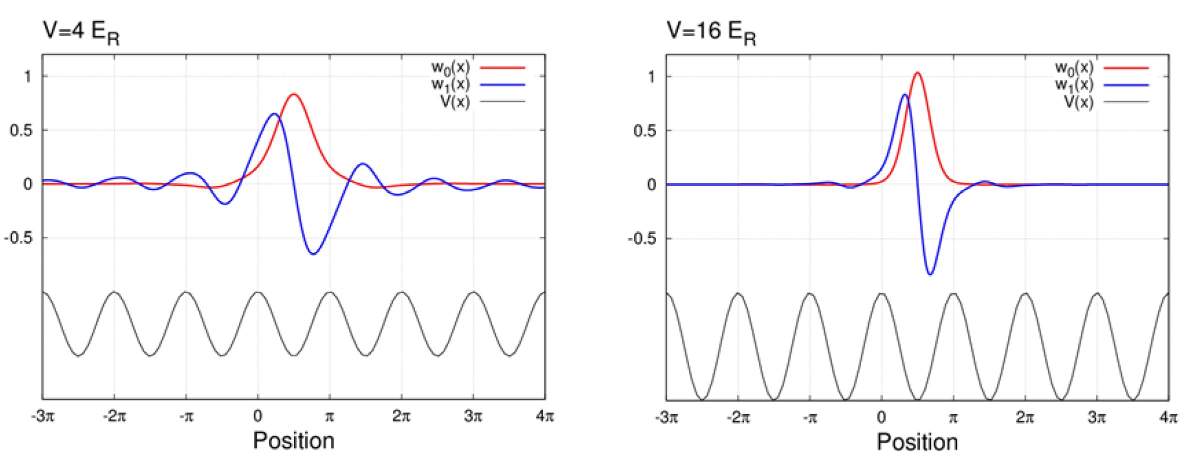
- **Natural units of the problem**
  - laser wave length $\lambda/2\pi$
  - lattice flattening $\kappa = \frac{\hbar\Omega}{2E_R}$
  - recoil energy $E_R = \frac{2\pi^2\hbar^2}{m\lambda^2}$

Wannier functions — 2

- **Convenient basis**

$\mathcal{W}_i^\alpha(\boldsymbol{r})$ wave function localized in i-th lattice site

α denotes appropriate Bloch band



Field operator decomposition — 3

$$\Psi(\boldsymbol{r}) = \sum_\alpha\sum_i \hat{a}_i^{(\alpha)}\mathcal{W}_i^\alpha(\boldsymbol{r}) \approx \sum_i \hat{a}_i\mathcal{W}_i(\boldsymbol{r})$$

the lowest band approximation

- **Single particle Hamiltonian**

$$\mathcal{H} = \int \mathrm{d}^3\boldsymbol{r}\ \Psi^\dagger(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\boldsymbol{r})\right]\Psi(\boldsymbol{r})$$

$$= \sum_{ij}\hat{a}_i^\dagger\hat{a}_j\int \mathrm{d}^3\boldsymbol{r}\ \mathcal{W}_i^*(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\boldsymbol{r})\right]\mathcal{W}_j(\boldsymbol{r})$$

$$= \mathbf{E}\sum_i \hat{a}_i^\dagger\hat{a}_i - \mathbf{J}\sum_i\sum_{\langle j\rangle}\hat{a}_i^\dagger\hat{a}_j + \ldots$$

summation over nearest neighbours of *i*

Long range interactions — 4

$$\Psi(\boldsymbol{r}) = \sum_\alpha\sum_i \hat{a}_i^{(\alpha)}\mathcal{W}_i^\alpha(\boldsymbol{r}) \approx \sum_i \hat{a}_i\mathcal{W}_i(\boldsymbol{r})$$

lowest band approximation

- **Interaction Hamiltonian**

$$\mathcal{H} = \frac{1}{2}\iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\ \Psi^\dagger(\boldsymbol{r})\Psi^\dagger(\boldsymbol{r}')\mathcal{V}(\boldsymbol{r}-\boldsymbol{r}')\Psi(\boldsymbol{r}')\Psi(\boldsymbol{r})$$

$$= \frac{1}{2}\sum_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l\iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\ \mathcal{W}_i^*(\boldsymbol{r})\mathcal{W}_j^*(\boldsymbol{r}')\mathcal{V}(\boldsymbol{r}-\boldsymbol{r}')\mathcal{W}_k(\boldsymbol{r}')\mathcal{W}_l(\boldsymbol{r})$$

$$= \frac{\mathbf{U}}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i + \mathbf{V}\sum_i\sum_{\langle j\rangle}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_i\hat{a}_j + \ldots$$

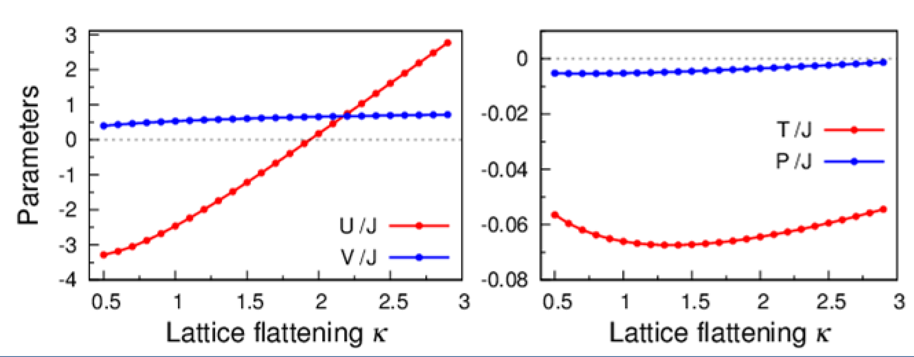
$$-\mathbf{T}\sum_i\sum_{\langle j\rangle}\hat{a}_i^\dagger(\hat{a}_i^\dagger\hat{a}_i + \hat{a}_j^\dagger\hat{a}_j)\hat{a}_j + \frac{\mathbf{P}}{2}\sum_i\sum_{\langle j\rangle}\hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_j\hat{a}_j + \ldots$$

Studied Hamiltonian — 5

$$\mathcal{H} = \mathbf{E}\sum_i \hat{a}_i^\dagger\hat{a}_i - \mathbf{J}\sum_{\{ij\}}\hat{a}_i^\dagger\hat{a}_j + \frac{\mathbf{U}}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \mathbf{V}\sum_{\{ij\}}\hat{n}_i\hat{n}_j - \mathbf{T}\sum_{\{ij\}}\hat{a}_i^\dagger(\hat{n}_i + \hat{n}_j)\hat{a}_j + \frac{\mathbf{P}}{2}\sum_{\{ij\}}\hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_j\hat{a}_j$$

- **Considered interaction**

$$\mathcal{V}(\boldsymbol{r}-\boldsymbol{r}') = \gamma\left(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^3} - 3\frac{(z-z')^2}{|\boldsymbol{r}-\boldsymbol{r}'|^5}\right) + g\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')$$



$\gamma = 1$

$V_0 = 6E_R$

Physical realization — 6

- **Two dimensionless parameters**

$$g = 16\pi^2\frac{a_s}{\lambda} \qquad \gamma = d^2\frac{m}{\hbar^2\epsilon_0\lambda}$$

s-wave scattering length; electric dipole moment

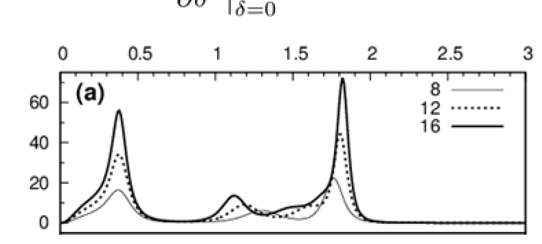
- **Model assumptions**
  - optical lattice laser wave length λ = 790 nm
  - mass ~ mass of the RbCs molecule
  - scattering length ~ 100 Bohr Radius ⟶ $g \approx 1$
  - dipole moment up to 3 debye ⟶ γ up to 470

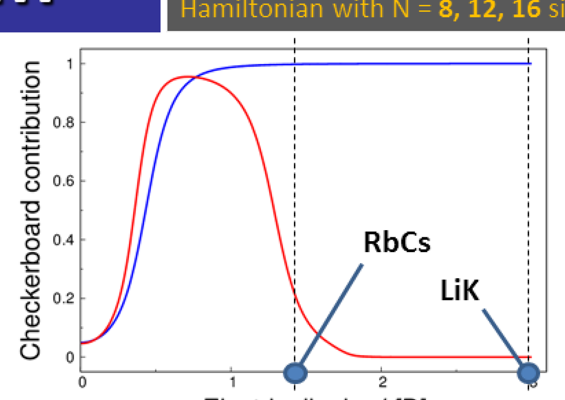
Half filled 1D system

METHOD: Exact diagonalization of the 1D Hamiltonian with N = 8, 12, 16 sites

- **Susceptibility**

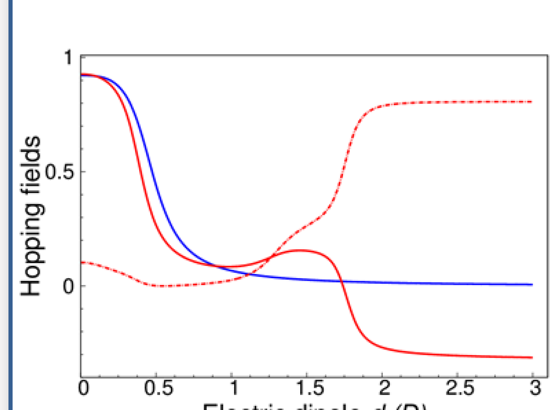
$$\chi = -\frac{\partial^2}{\partial\delta^2}\bigg|_{\delta=0}|\langle \mathrm{G}(d)|\mathrm{G}(d+\delta)\rangle|$$





BLUE - parameters T and P are neglected

RED - whole Hamiltonian considered

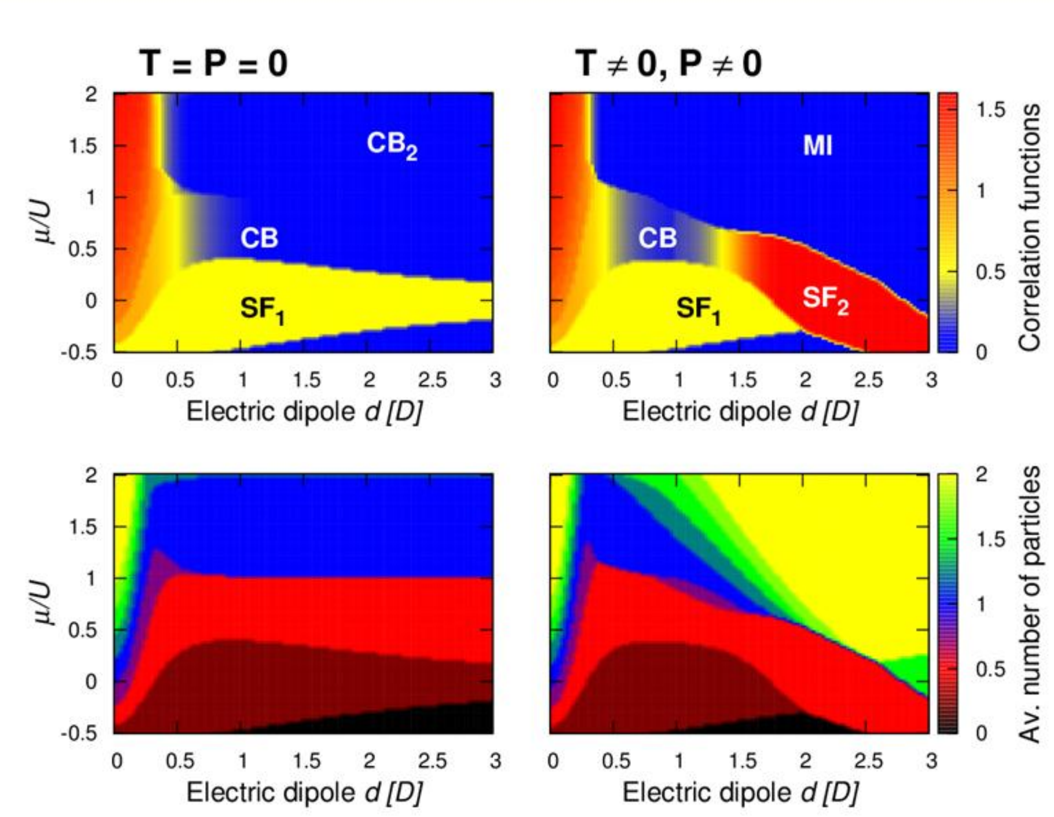


Hopping fields

$\phi_i = \sum_{\langle j\rangle}\langle a_j^\dagger a_i\rangle$ — single particle SF

$\Phi_i = \sum_{\langle j\rangle}\langle a_j^\dagger a_j^\dagger a_i a_i\rangle$ — double particle SF

Grand canonical phase diagram — 8



Summary

Commonly neglected terms in the extended Bose-Hubbard model for dipolar molecules can lead to NEW PHENOMENA

For a particular choice of optical lattice parameters **occupation-dependent tunneling** and **pair tunneling** destroy insulating checkerboard phases leading to a novel **two particle SF phase**.