Density-dependent processes of dipolar molecules in an optical lattice

<u>Tomasz Sowiński</u>[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

The Institute of Photonic Sciences

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Bosons in optical lattice

- **Hamiltonian of the system**

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

- **Lattice potential**

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

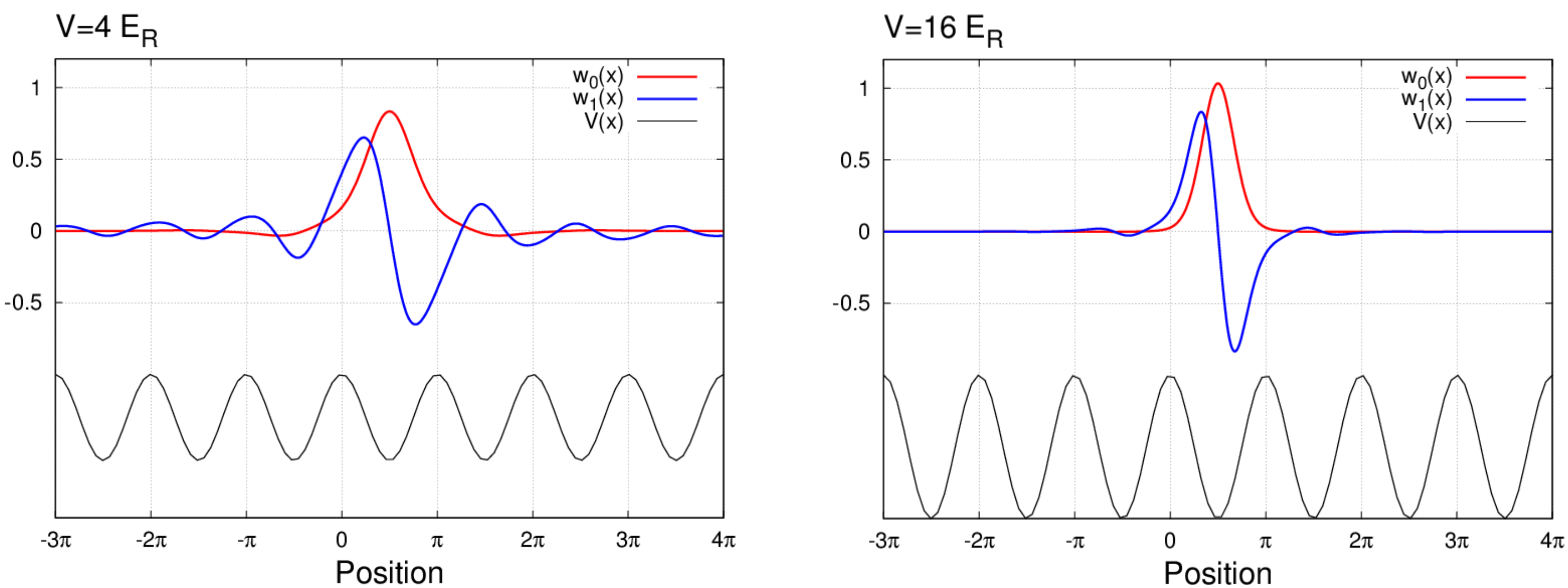
- **Natural units of the problem**
  - laser wave length $\lambda/2\pi$
  - lattice flattening $\kappa = \dfrac{\hbar\Omega}{2E_R}$
  - recoil energy $E_R = \dfrac{2\pi^2\hbar^2}{m\lambda^2}$

Wannier functions

- **Convenient basis**

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

α denotes appropriate Bloch band



Field operator decomposition

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

the lowest band approximation

- **Single particle Hamiltonian**

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

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

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

summation over nearest neighbours of ***i***

Field operator decomposition

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

the lowest band approximation

- **Interaction Hamiltonian**

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

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

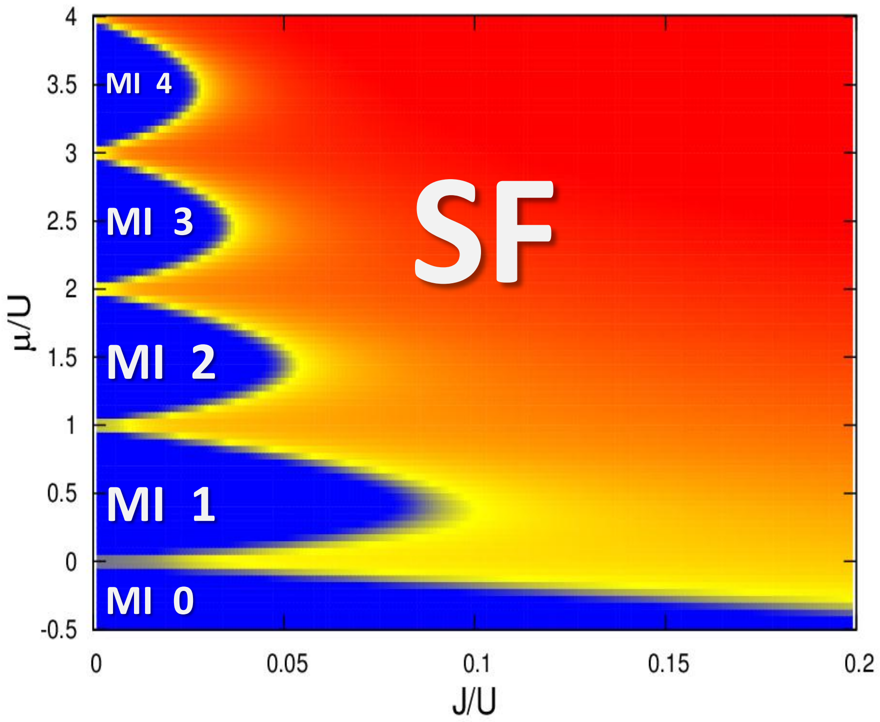
$$= \frac{\mathbf{U}}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i + \mathbf{V}\sum_i\sum_{\langle j\rangle}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_i\hat{a}_j + \ldots$$

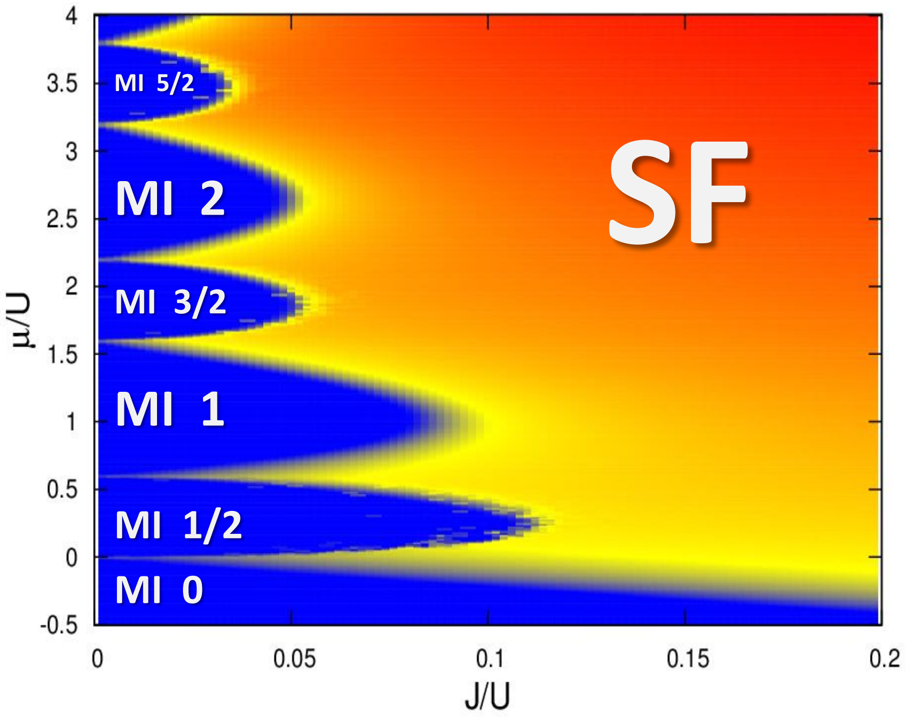
sufficient approximation when we consider short range interactions

density-density interaction between neighbouring sites

Bose-Hubbard models

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





V = 0

V > 0

Long range interactions

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

lowest band approximation

- **Interaction Hamiltonian**

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

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

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

taking into account only one additional term is not consistent!

Long range interactions

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

lowest band approximation

- **Interaction Hamiltonian**

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

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

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

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

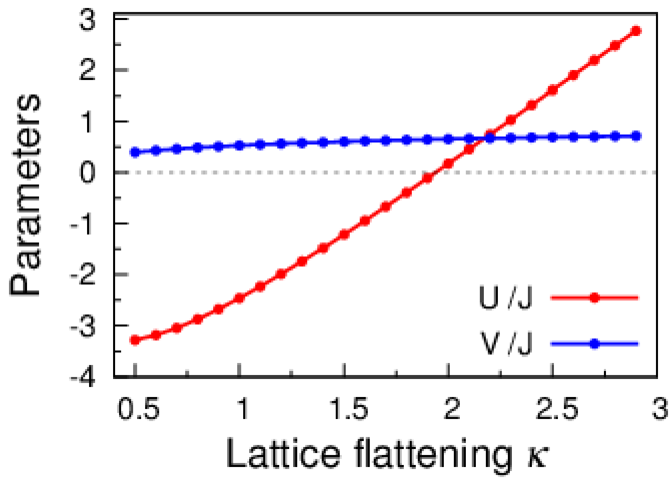
Studied Hamiltonian

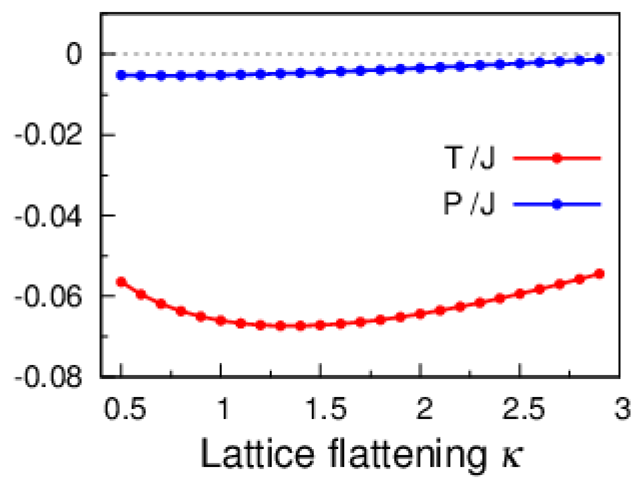
$$\mathcal{H} = \mathbf{E}\sum_i \hat{a}_i^\dagger \hat{a}_i - \mathbf{J}\sum_{\{ij\}} \hat{a}_i^\dagger \hat{a}_j + \frac{\mathbf{U}}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \mathbf{V}\sum_{\{ij\}} \hat{n}_i \hat{n}_j$$

$$-\mathbf{T}\sum_{\{ij\}} \hat{a}_i^\dagger(\hat{n}_i + \hat{n}_j)\hat{a}_j + \frac{\mathbf{P}}{2}\sum_{\{ij\}} \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_j \hat{a}_j$$

- **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

- **Two dimensionless parameters**

$$g = 16\pi^2 \frac{a_s}{\lambda}$$

$$\gamma = d^2 \frac{m}{\hbar^2 \epsilon_0 \lambda}$$

s-wave scattering length

electric dipole moment

- **Model assumptions**

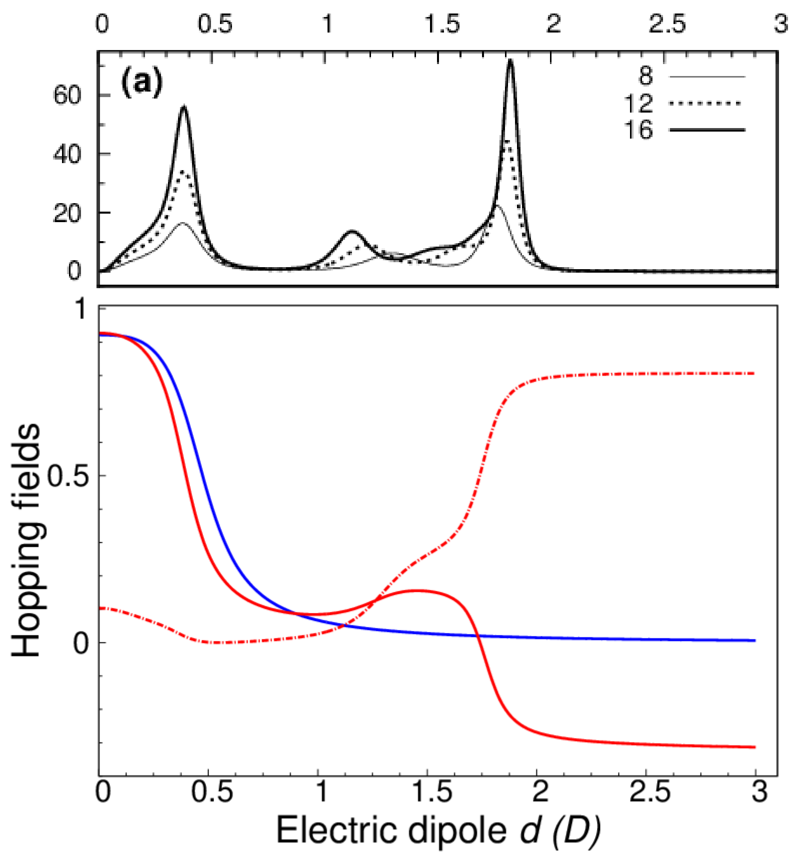
  - **optical lattice laser wave length λ = 790 nm**
  - **mass ~ mass of the RbCs molecule**
  - **scattering length ~ 100 Bohr Radius** ⟶ $g \approx 1$
  - **dipole moment up to 3 debye** ⟶ γ up to 470

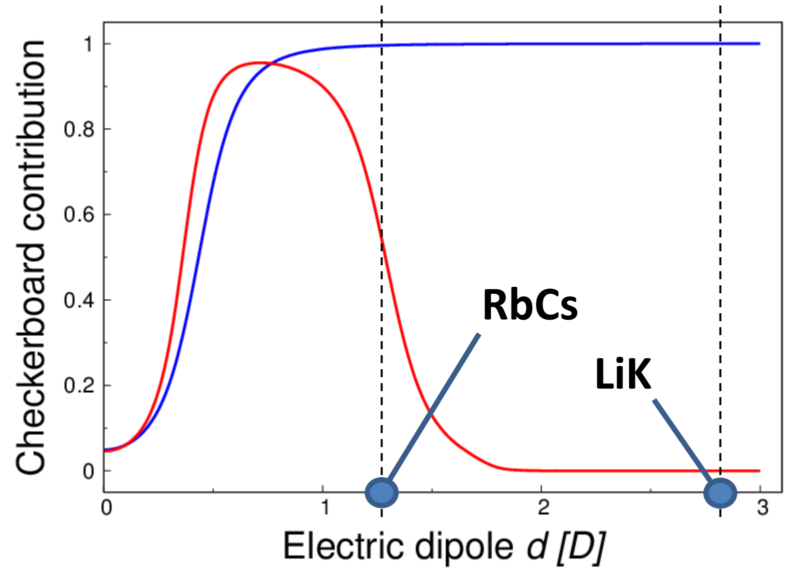
Half filled 1D system

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

- **Susceptibility**

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





BLUE - parameters T and P are neglected

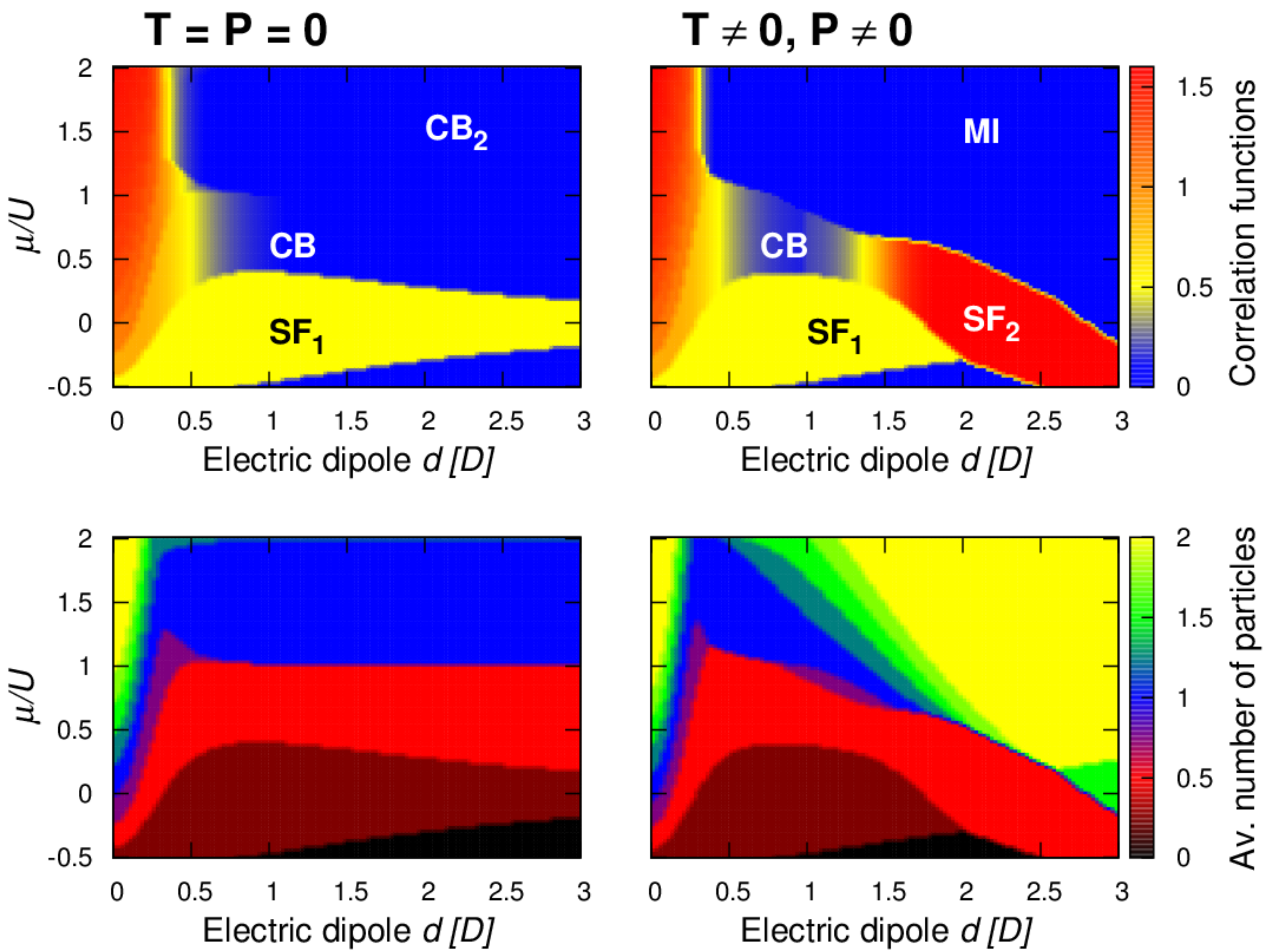
RED - whole Hamiltonian considered

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

Half filled system



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