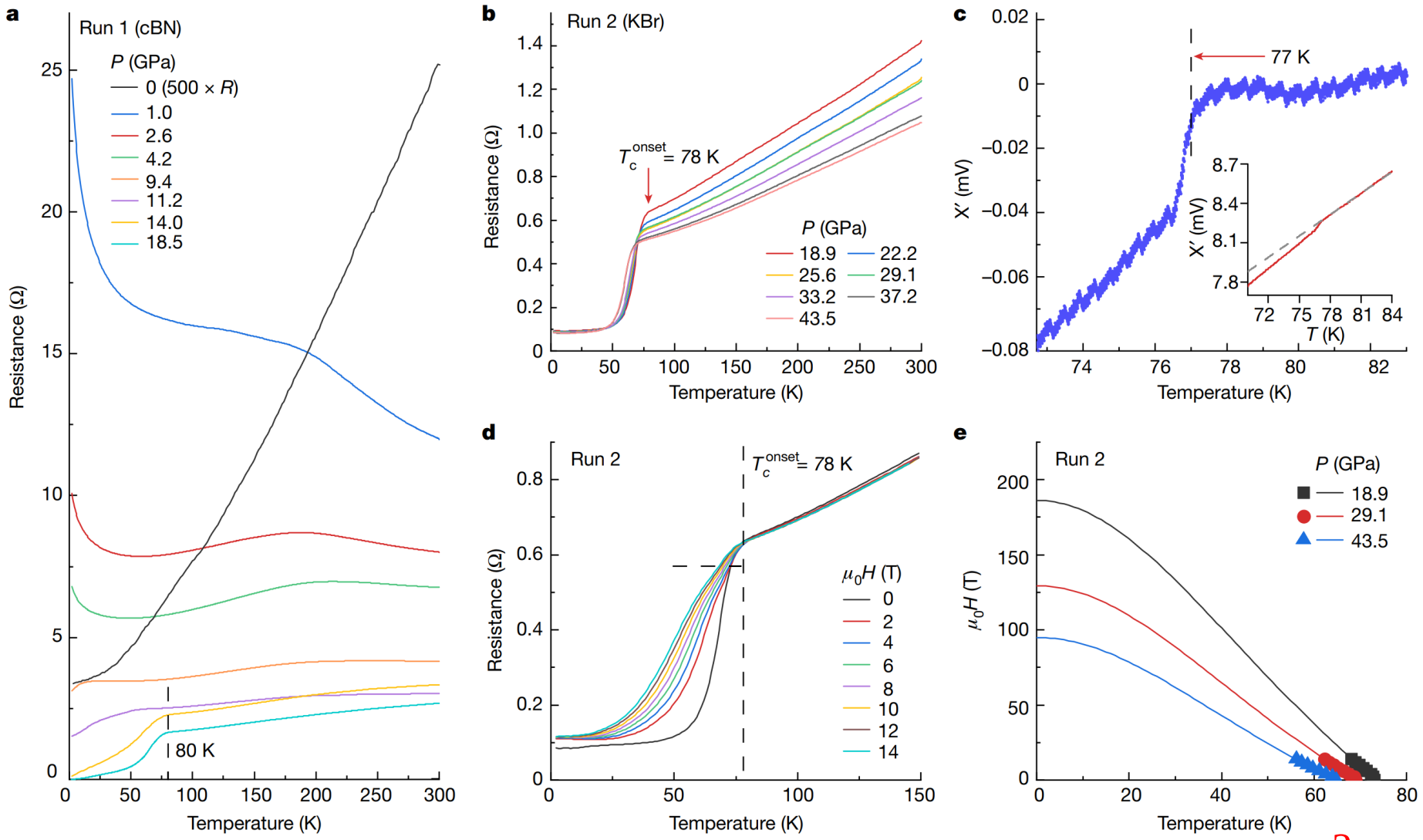
Orbital-selective Superconductivity in the Pressurized Bilayer Nickelate $La_3Ni_2O_7$: An Infinite Projected Entangled-Pair State Study

arXiv:2311.05491(2023)

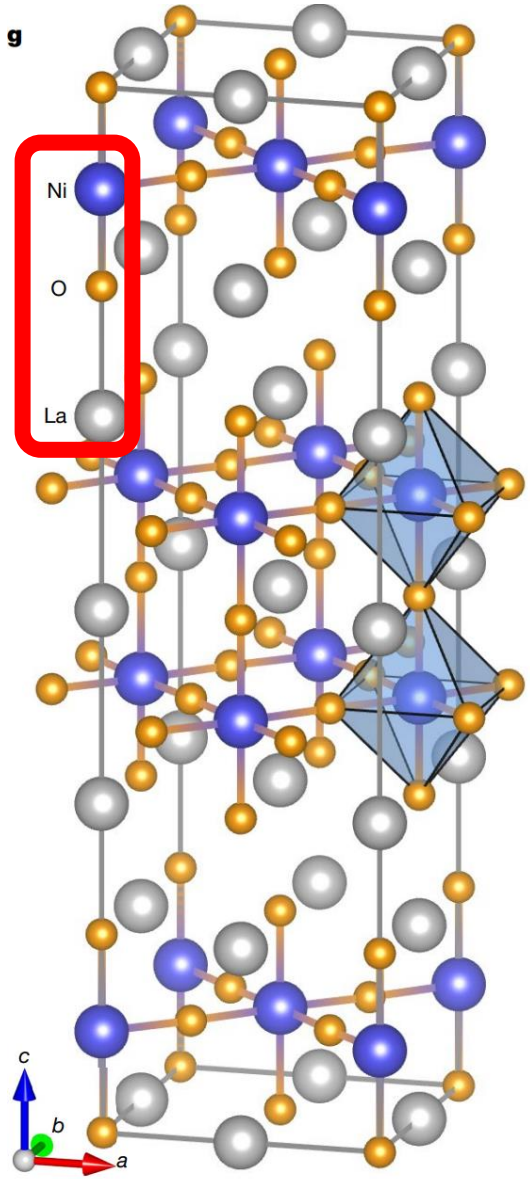
Xing-Yu Zhang

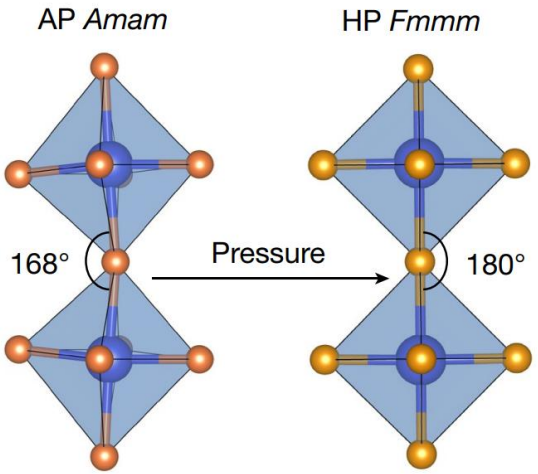
$La_3Ni_2O_7$ Superconduct under pressure

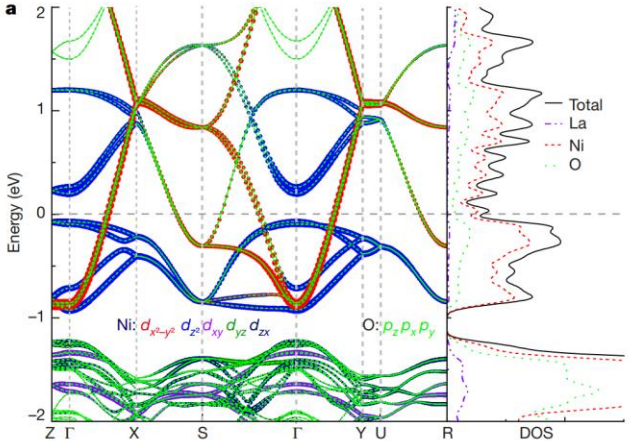


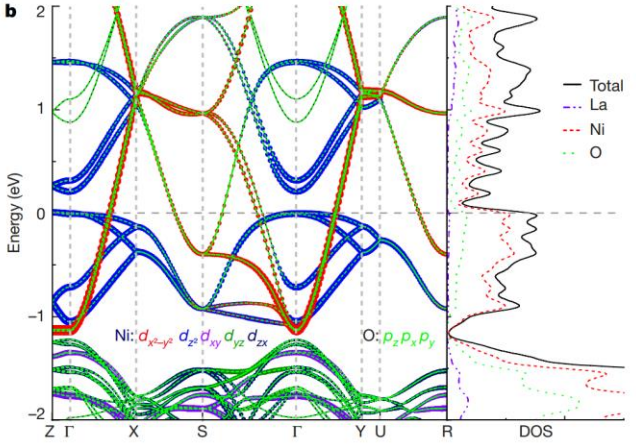
Sun, Nature 621, 493 (2023)

$La_3Ni_2O_7$ structure





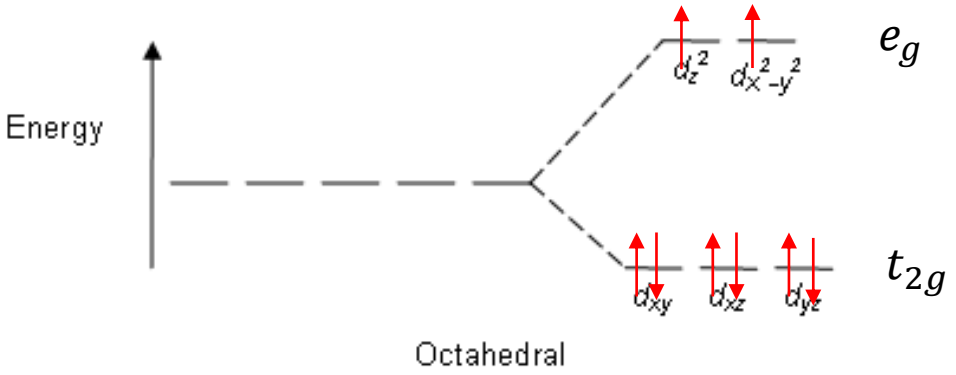




Ni-28: [Ar] $3d^8\ 4s^2$ or [Ar] $3d^9\ 4s^1$

+3 +2.5 -2

$La_3Ni_2O_7$



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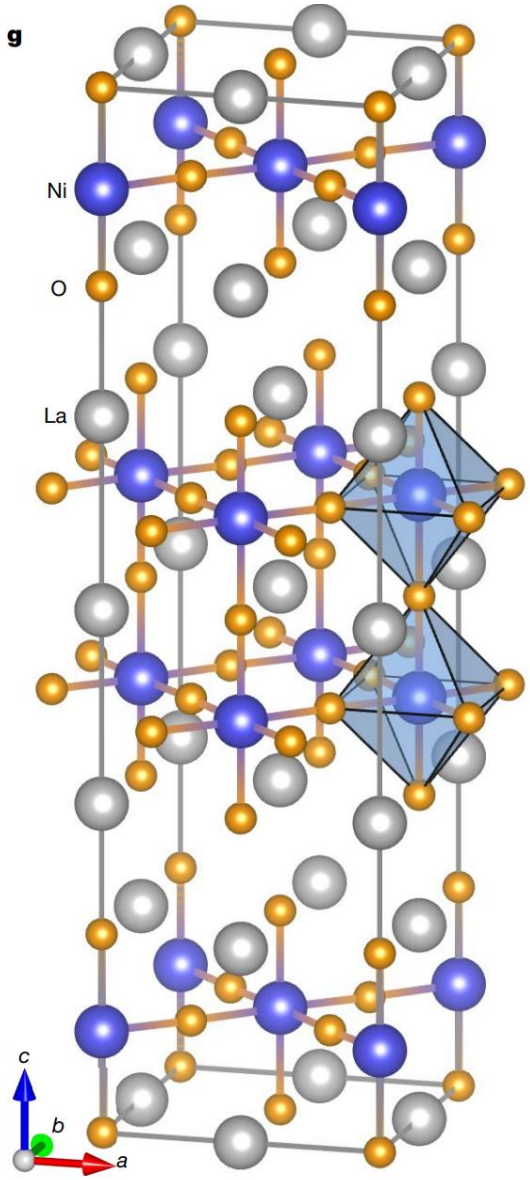
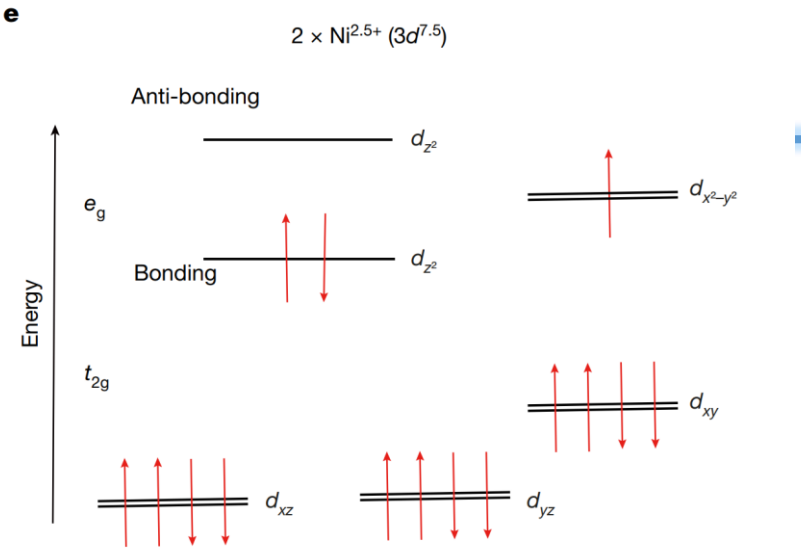
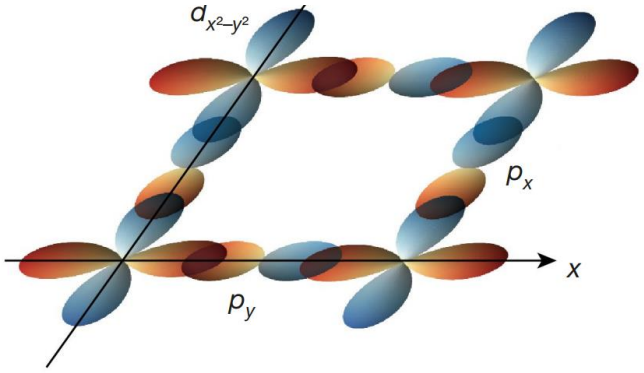
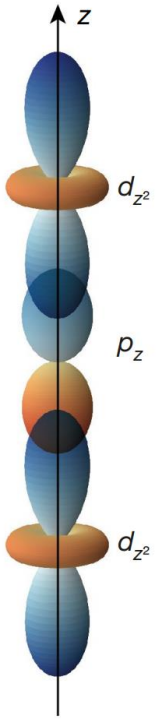
$La_3Ni_2O_7$ orbitals

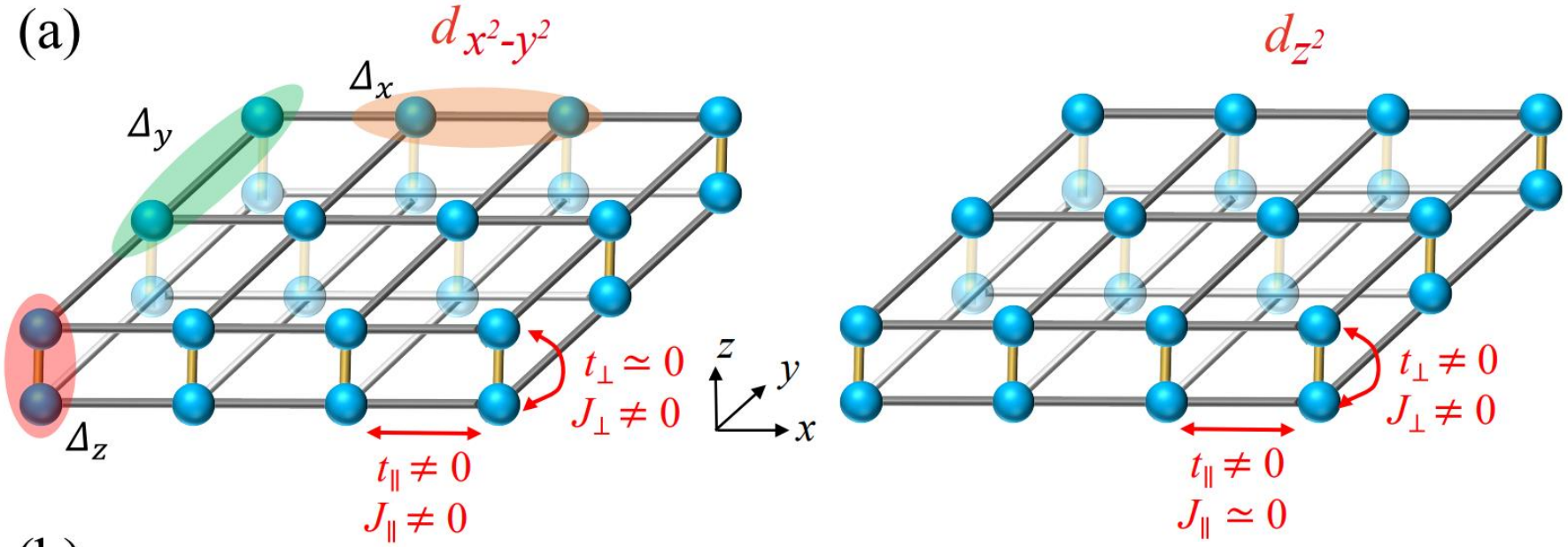


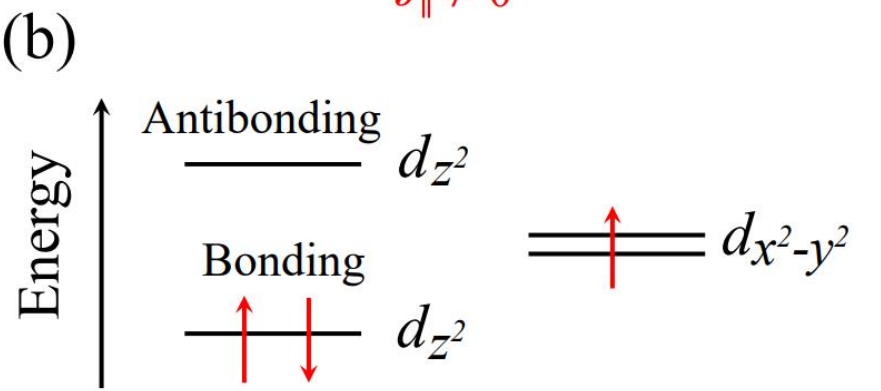






$d_{x^2-y^2}$ and d_{z^2} which responsible for SC order?





d_{z^2}: hybridize with $d_{x^2-y^2}$, which provide holes

$d_{x^2-y^2}$: Hund's rule located on the same site

Chen, arXiv:2311.05491(2023)

Different parameters for $d_{x^2-y^2}$ or d_{z^2}

$$
\begin{aligned}
H_{\text{bilayer}} &= -t_{\parallel} \sum_{\langle i,j\rangle,\mu,\sigma} (c^{\dagger}_{i,\mu,\sigma} c_{j,\mu,\sigma} + H.c.) \\
&+ J_{\parallel} \sum_{\langle i,j\rangle,\mu} (\mathbf{S}_{i,\mu} \cdot \mathbf{S}_{j,\mu} - \frac{1}{4} n_{i,\mu} n_{j,\mu}) \\
&- t_{\perp} \sum_{i,\sigma} (c^{\dagger}_{i,\mu=1,\sigma} c_{i,\mu=-1,\sigma} + H.c.) \\
&+ J_{\perp} \sum_{i} \mathbf{S}_{i,\mu=1} \cdot \mathbf{S}_{i,\mu=-1},
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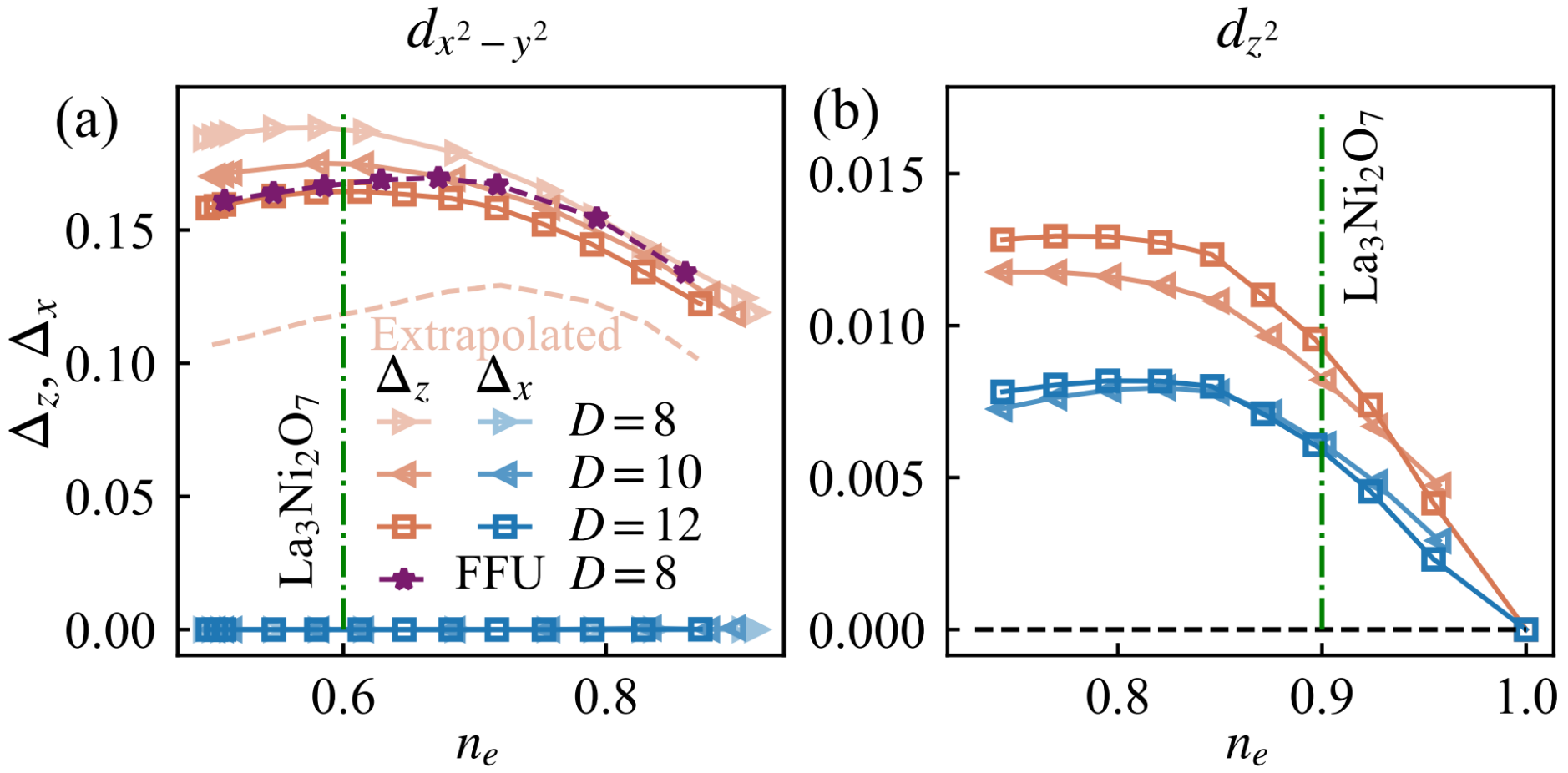
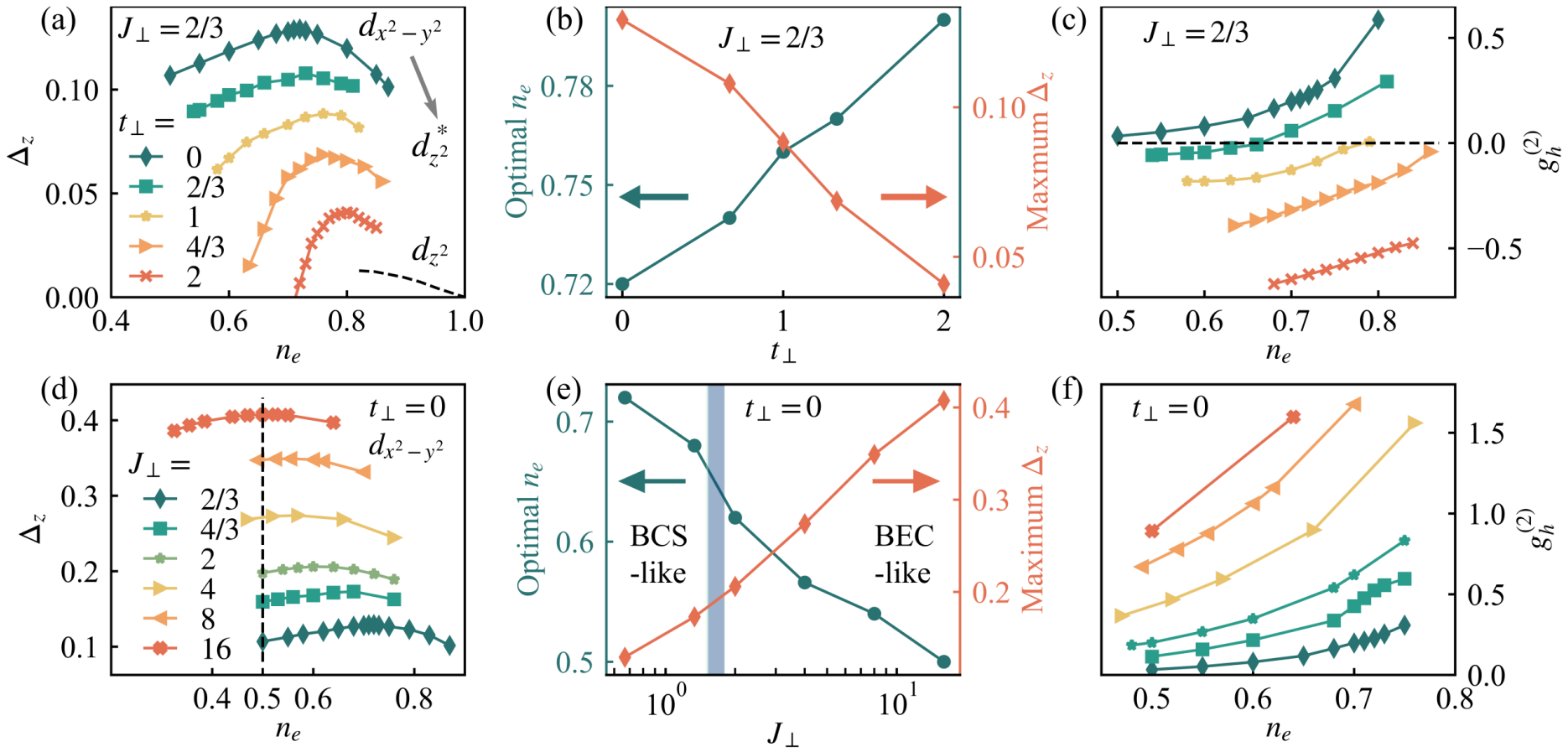
$$

$d_{x^2-y^2}$ responsible for SC order

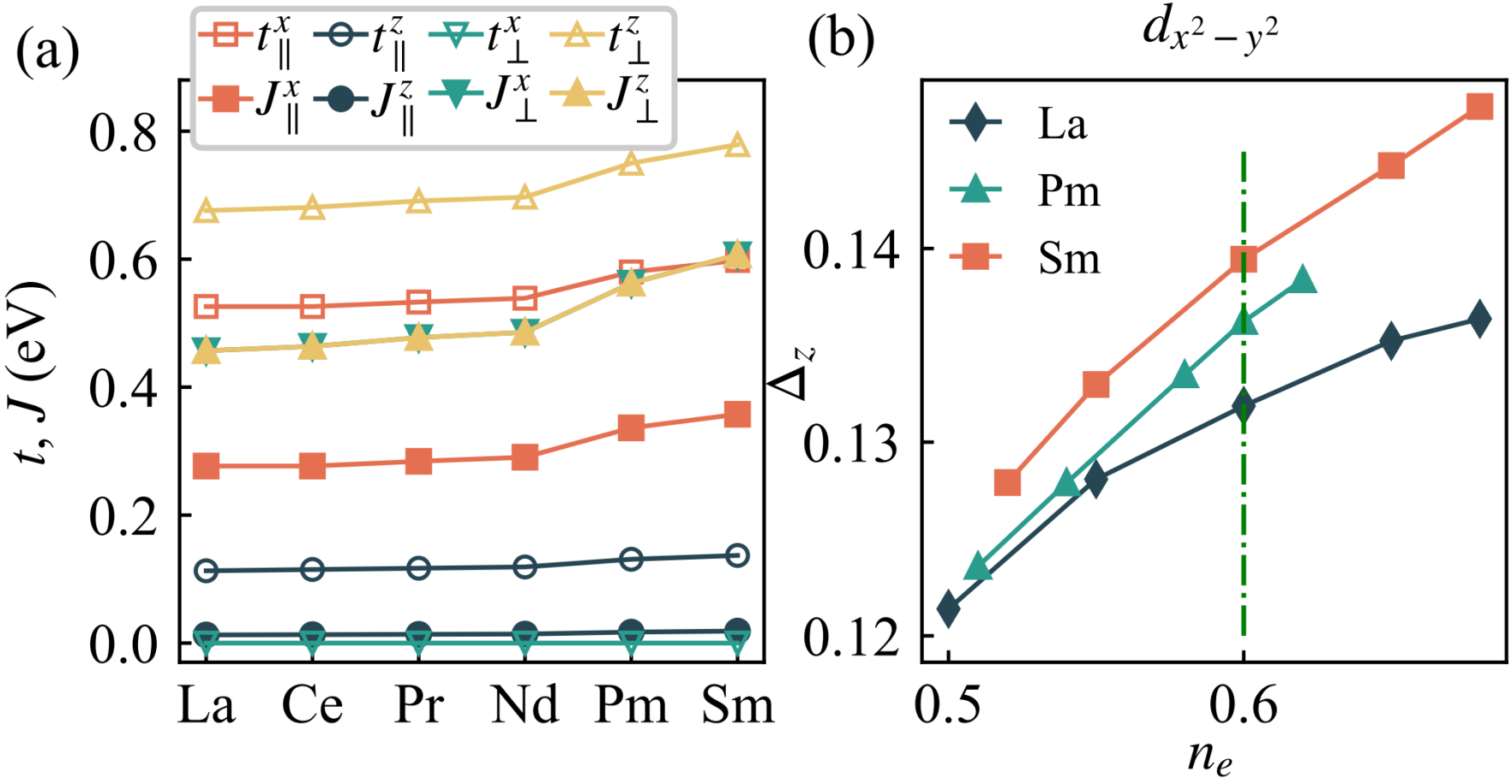


SC order parameter $\Delta_z = \frac{1}{\sqrt{2}}\langle \sum_{\mu=\pm 1} c^{\dagger}_{i,\mu,\uparrow} c^{\dagger}_{i,-\mu,\downarrow} \rangle$

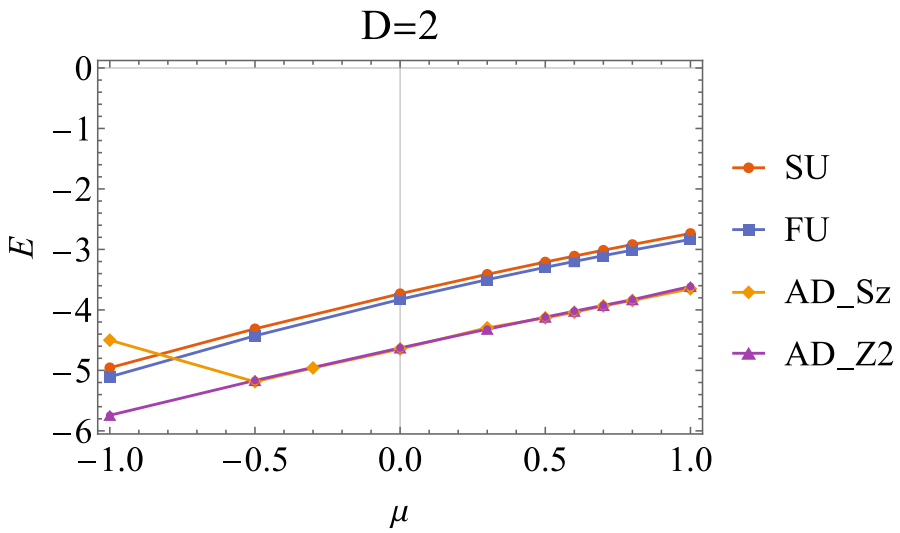
Tuning parameters



$R_3Ni_2O_7$

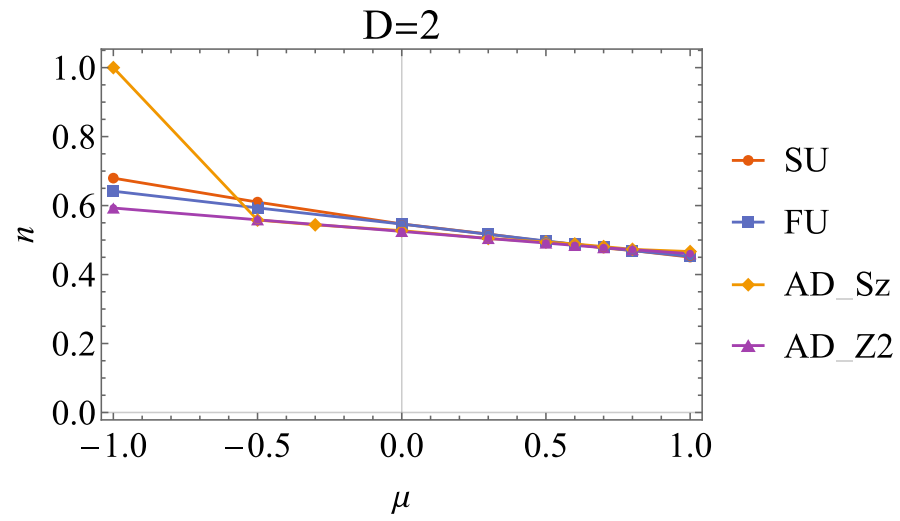

(a)
$t_{\parallel}^{x}$ $t_{\parallel}^{z}$ $t_{\perp}^{x}$ $t_{\perp}^{z}$
$J_{\parallel}^{x}$ $J_{\parallel}^{z}$ $J_{\perp}^{x}$ $J_{\perp}^{z}$
t, J (eV)
0.0
0.2
0.4
0.6
0.8
La Ce Pr Nd Pm Sm
(b)
$d_{x^2-y^2}$
La
Pm
Sm
Δ_z
0.12
0.13
0.14
0.5
0.6
n_e

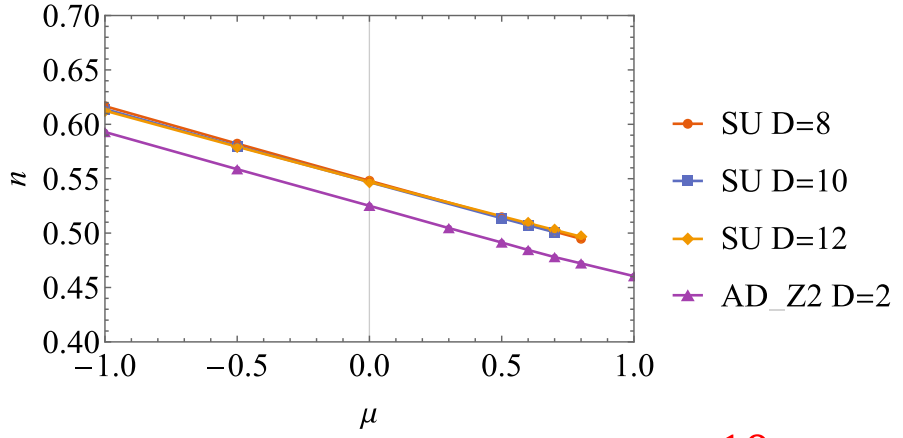
$d_{x^2-y^2}$ $t_{\parallel} = 3, J_{\parallel} = 1, t_{\perp} = 0, J_{\perp} = 2$



Problems:

1. VUMPS doesn't converge
2. Up and down environment converges but the energy is not good
3. Local minimum when n approach to 1





Thank you for listening!

Q&A?

Recent progress in bilayer t-J model with iPEPS calculation

Xing-Yu Zhang

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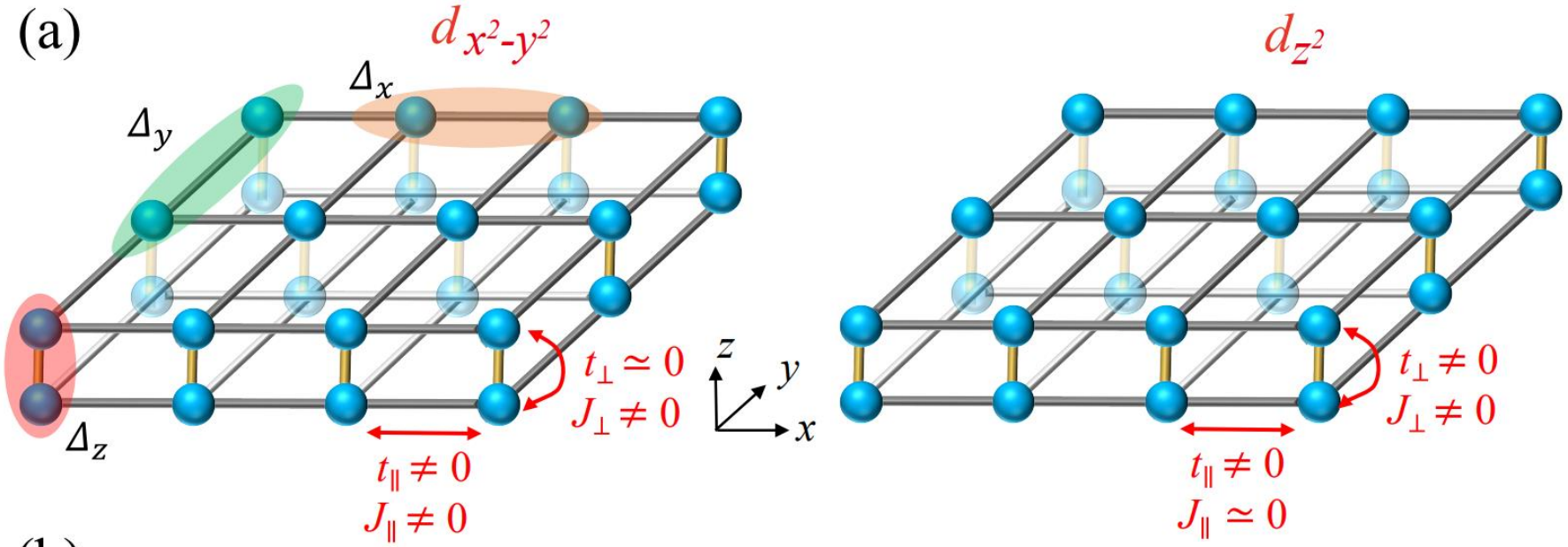

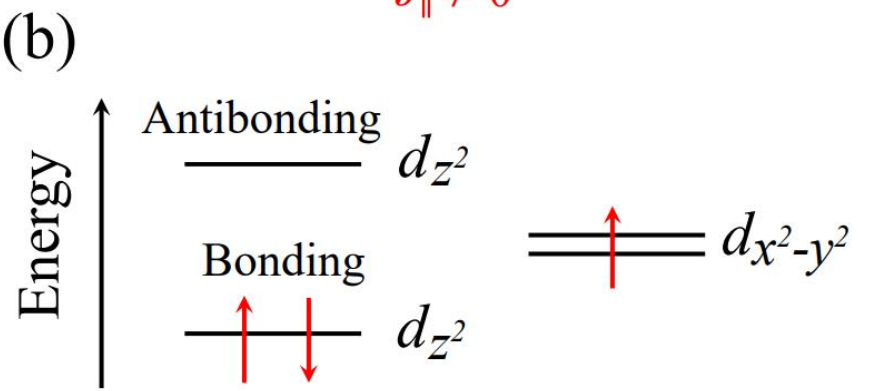

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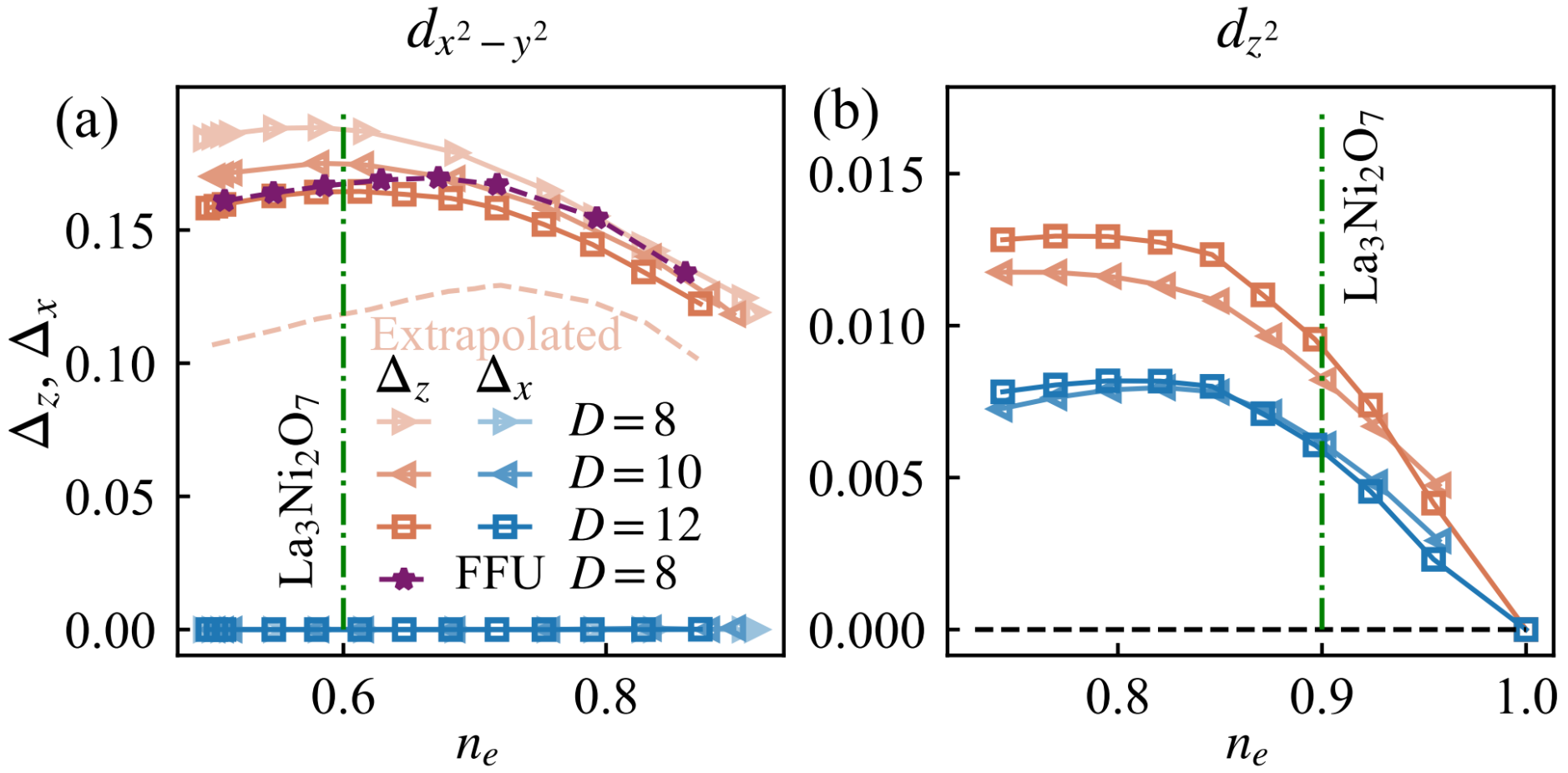

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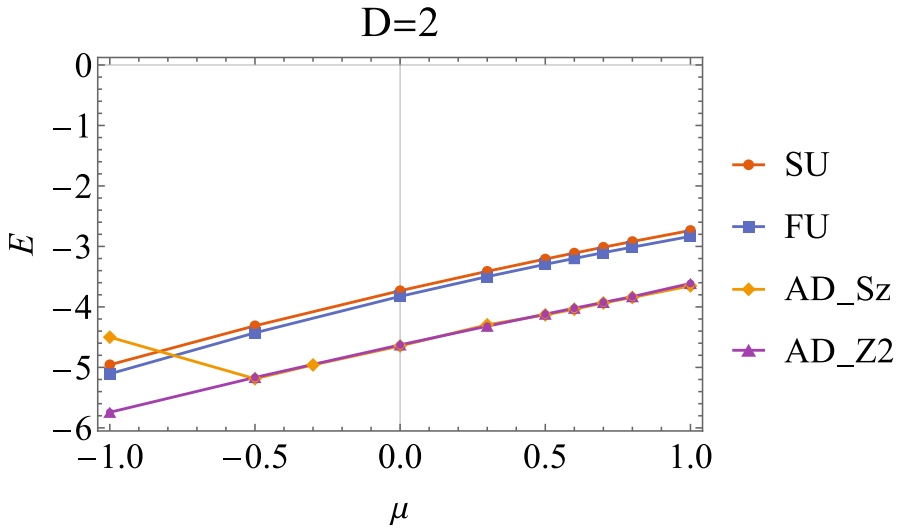

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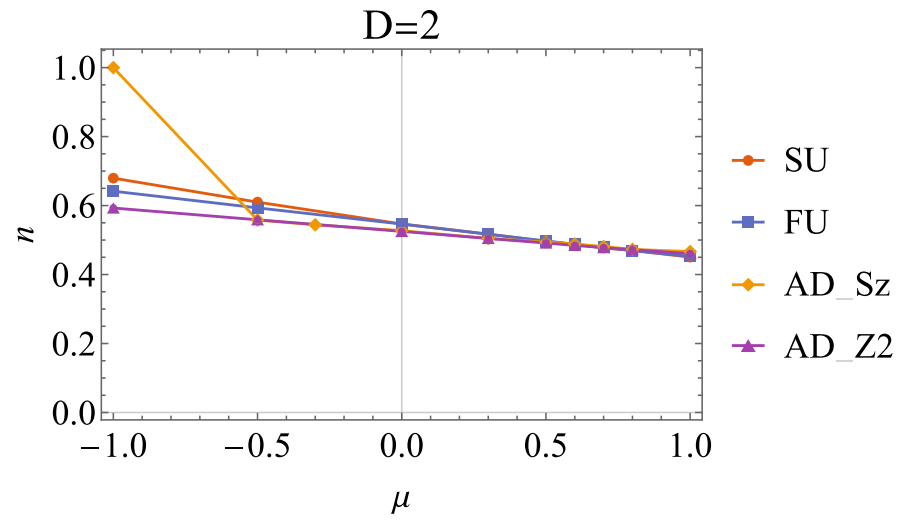

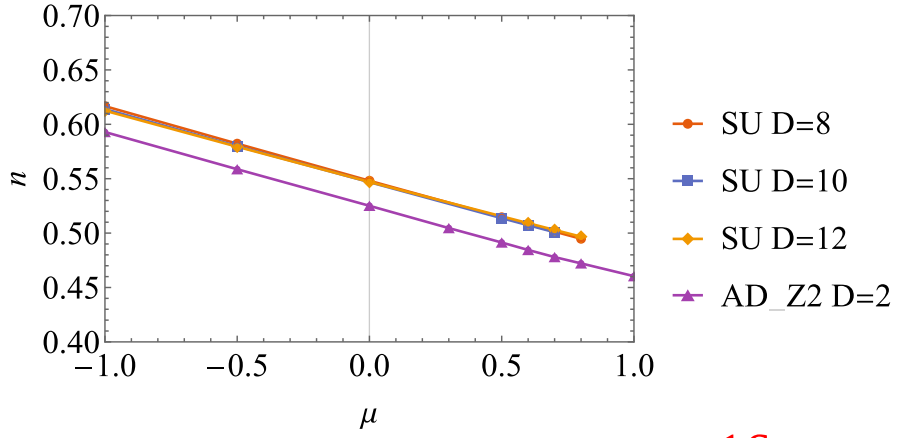

Observables during optimization

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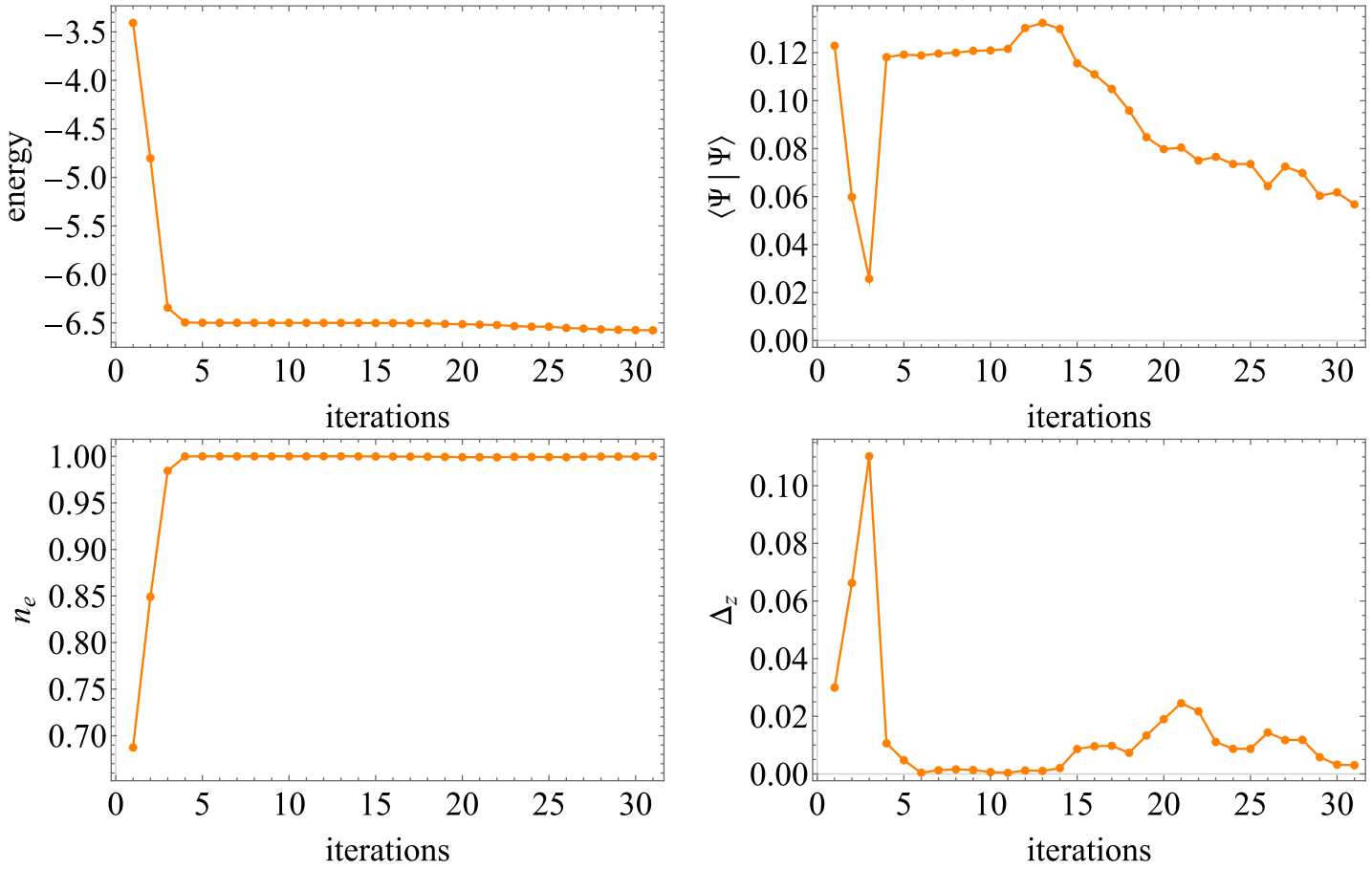
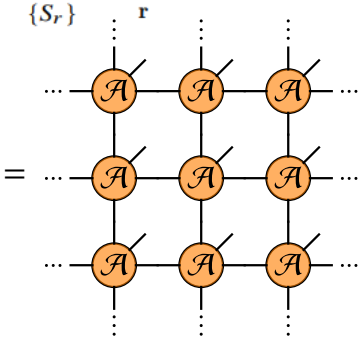
- VUMPS with Z2-symmetry 1×1 unit cell



Method to 2D infinite systems

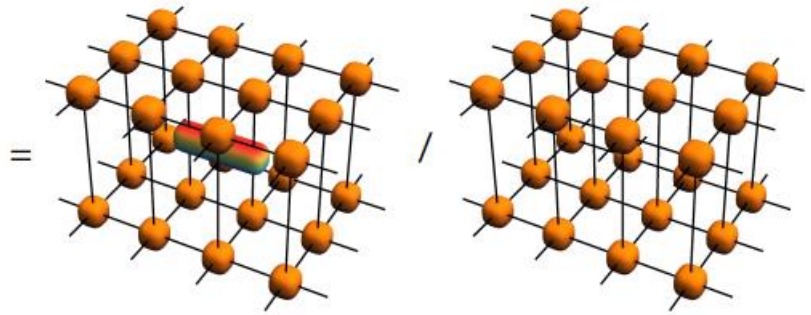
- 2D ansatz

$$|\Psi(\mathcal{A})\rangle = \sum_{\{S_r\}} \mathrm{Tr} \prod_{\mathbf{r}} \mathcal{A}^{S_r}[\mathbf{r}] \, |\{S_r\}\rangle$$



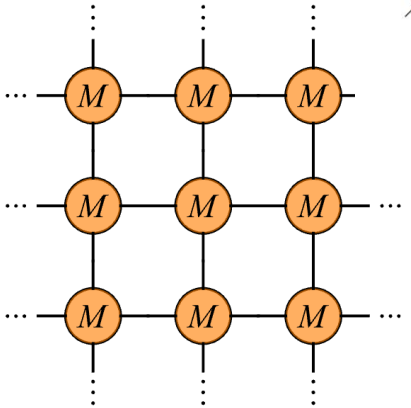
- Energy

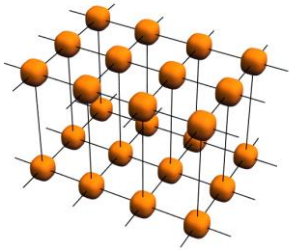
$$E(\mathcal{A}) = \langle\Psi(\bar{\mathcal{A}})|H|\Psi(\mathcal{A})\rangle / \langle\Psi(\bar{\mathcal{A}}) \mid \Psi(\mathcal{A})\rangle$$

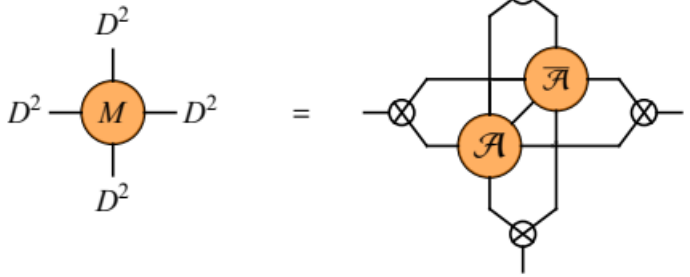


- Contraction

$$\langle\Psi(\bar{\mathcal{A}}) \mid \Psi(\mathcal{A})\rangle =$$

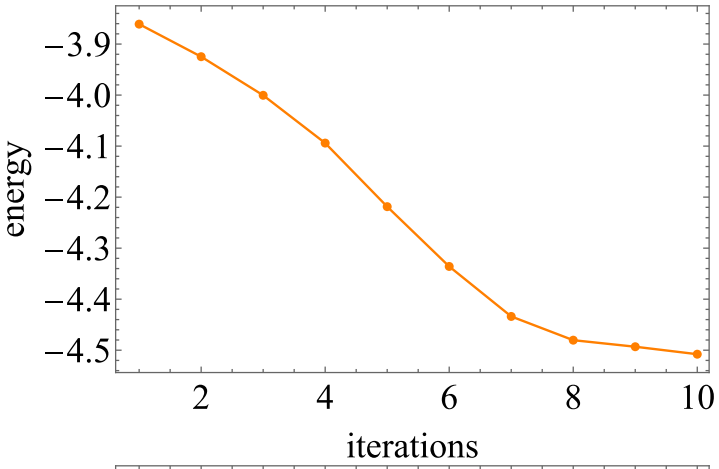


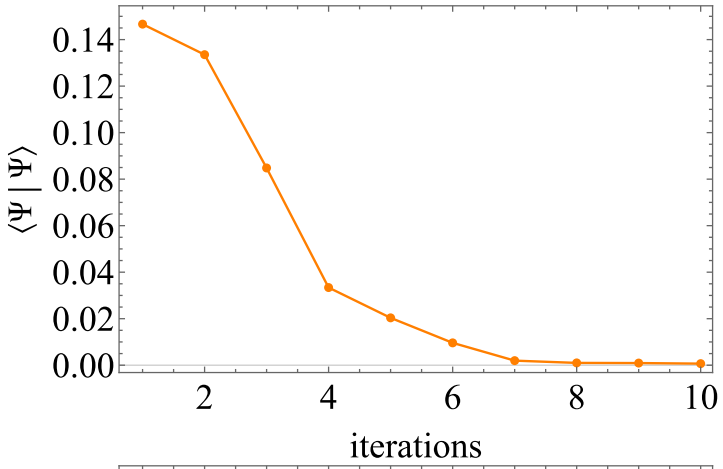


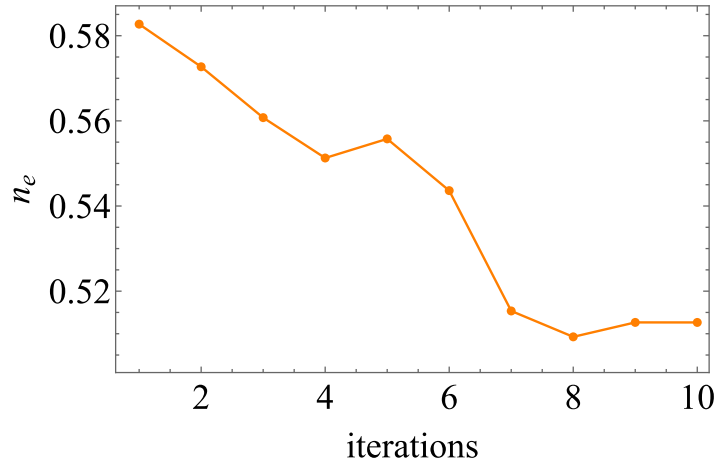


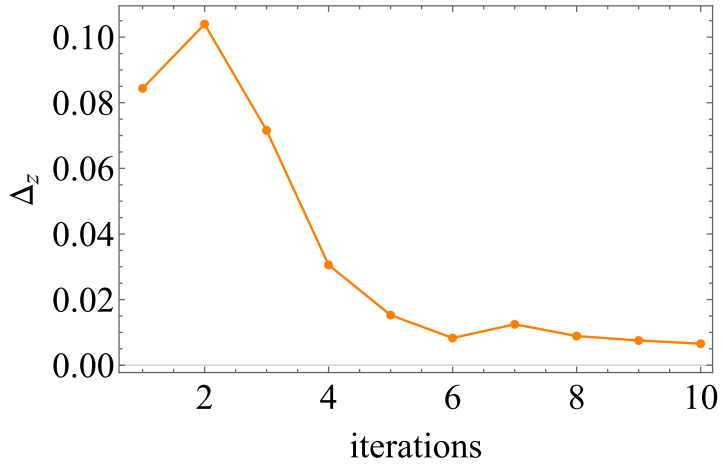
Observables during optimization

- Initial from SU, $d_{x^2-y^2}, \mu = 0$
- VUMPS with Z2-symmetry 1×1 unit cell



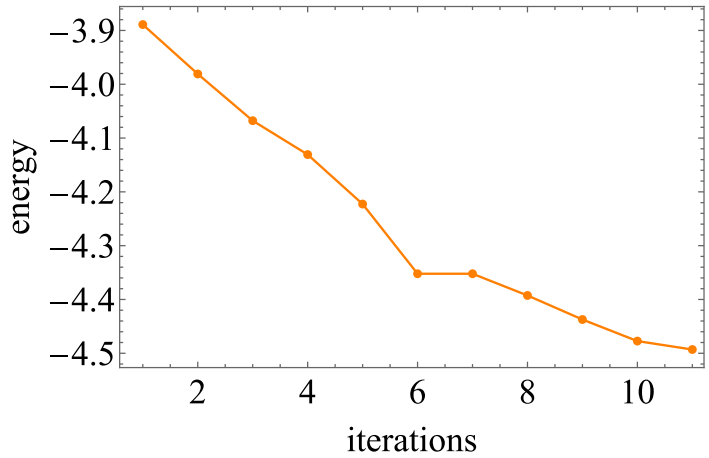


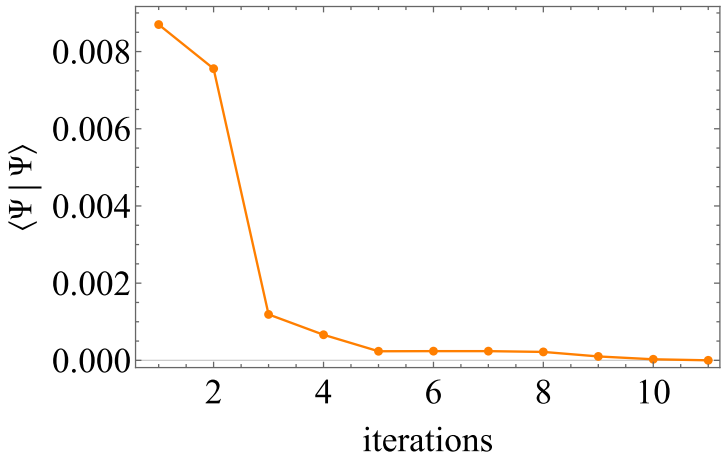


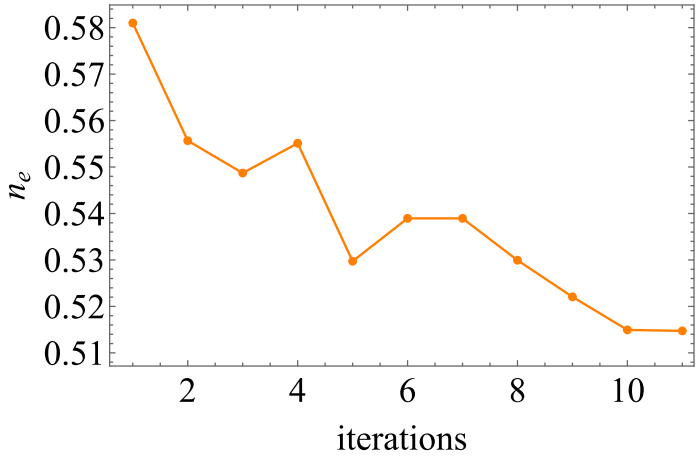


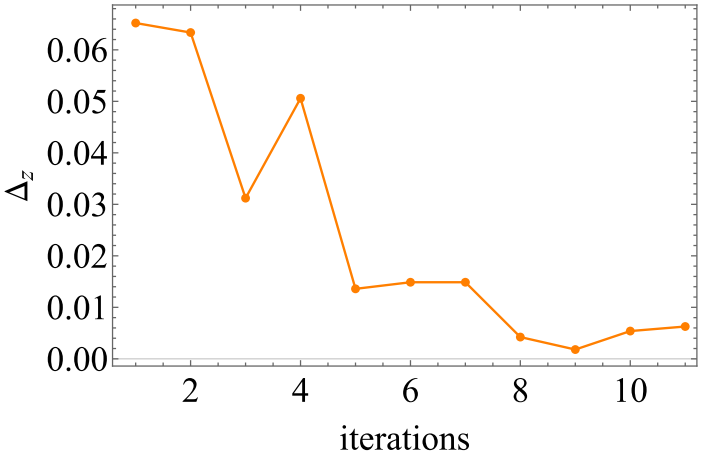
Observables during optimization

- Initial from SU, $d_{x^2-y^2}, \mu = 0$
- FPCM with Z2-symmetry 1×1 unit cell



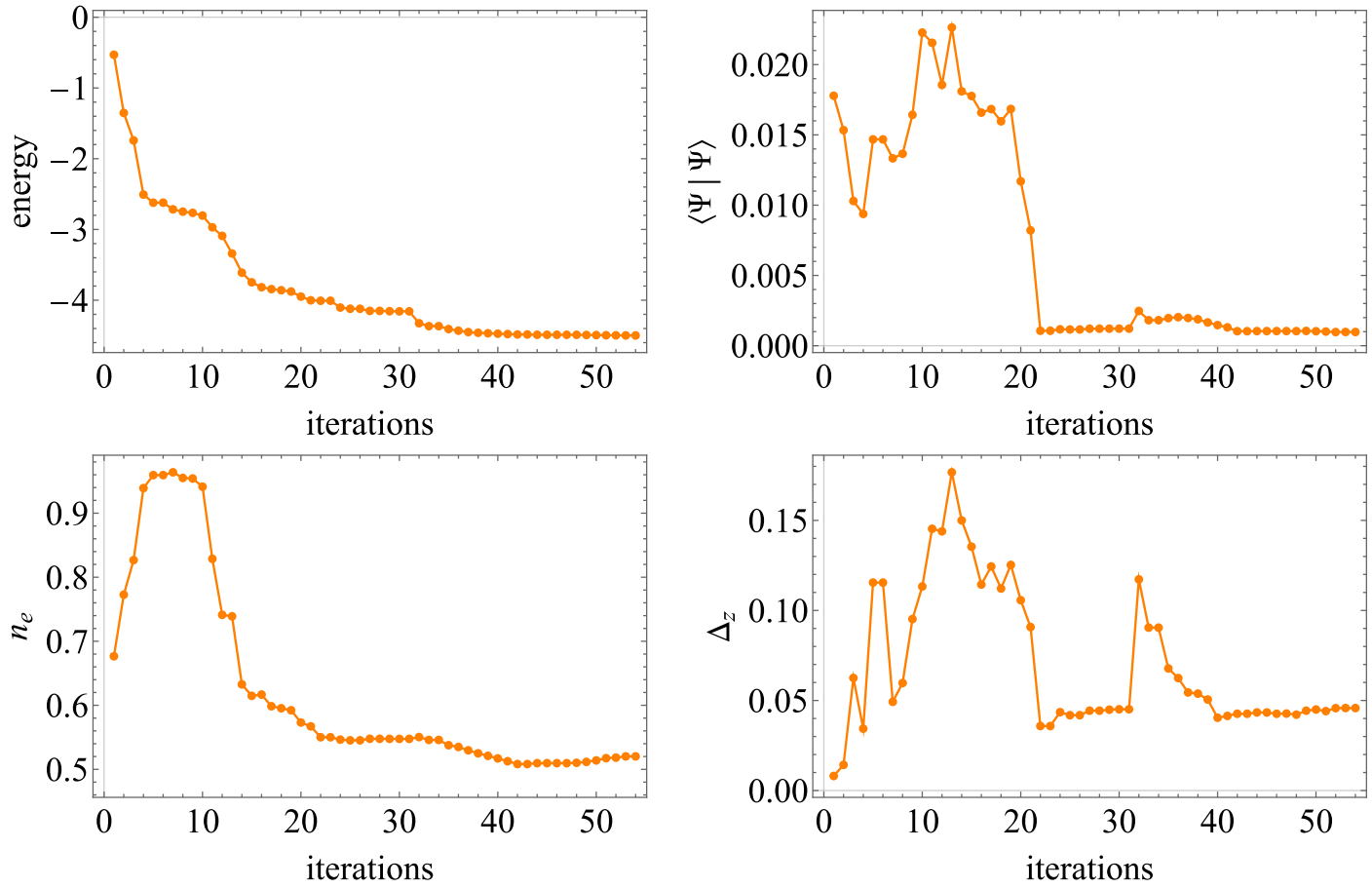






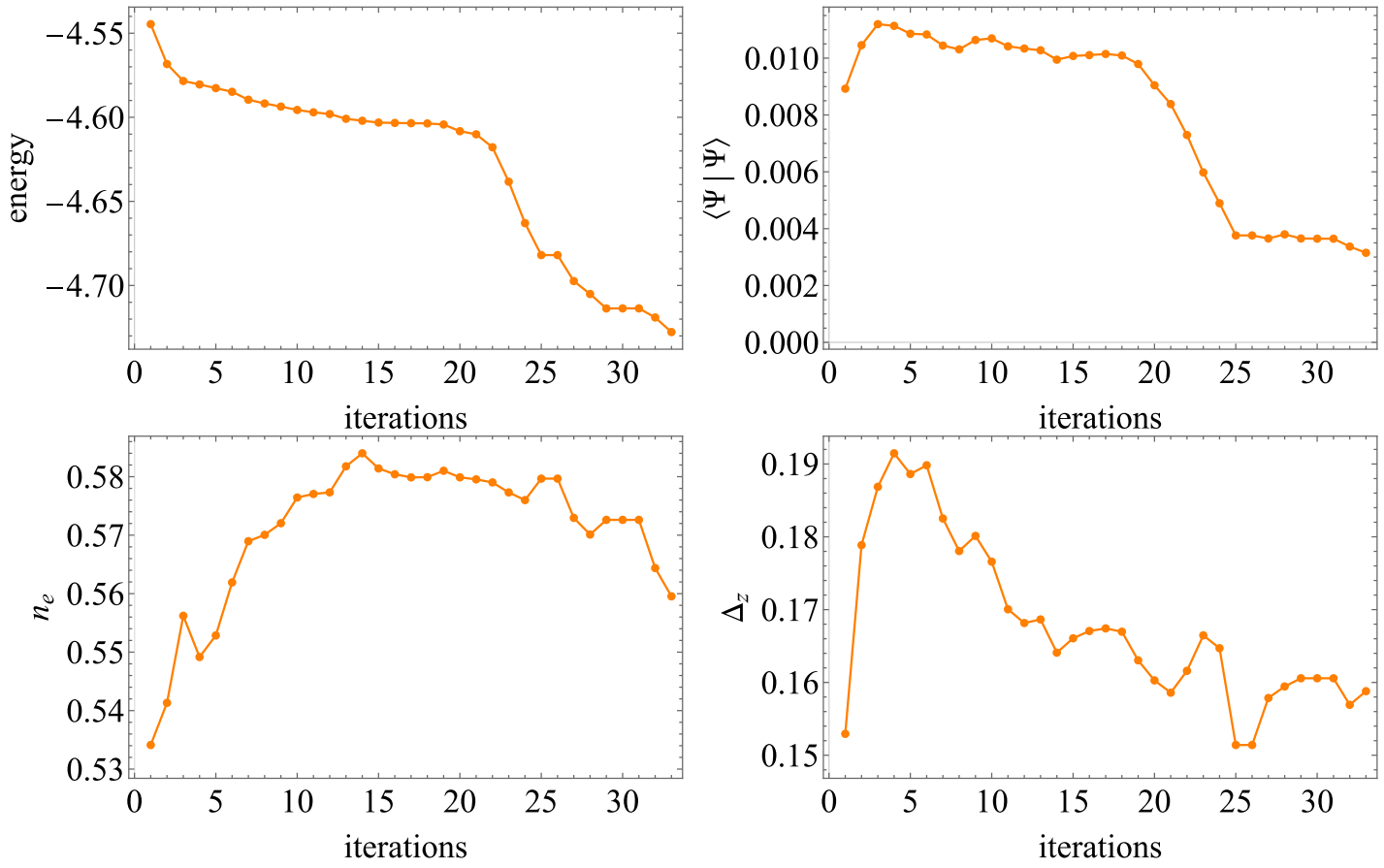
Observables during optimization

- Initial from random, $d_{x^2-y^2}, \mu = 0, D = 2$
- VUMPS with Z2-symmetry 2×2 unit cell



Observables during optimization

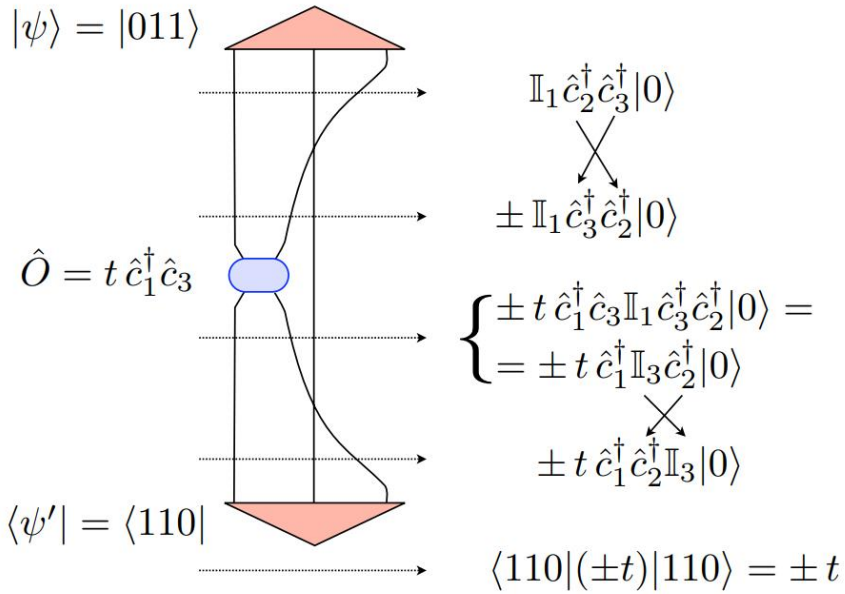
- Initial from SU, $d_{x^2-y^2}, \mu = 0, D = 4$
- VUMPS with Z2-symmetry 2×2 unit cell

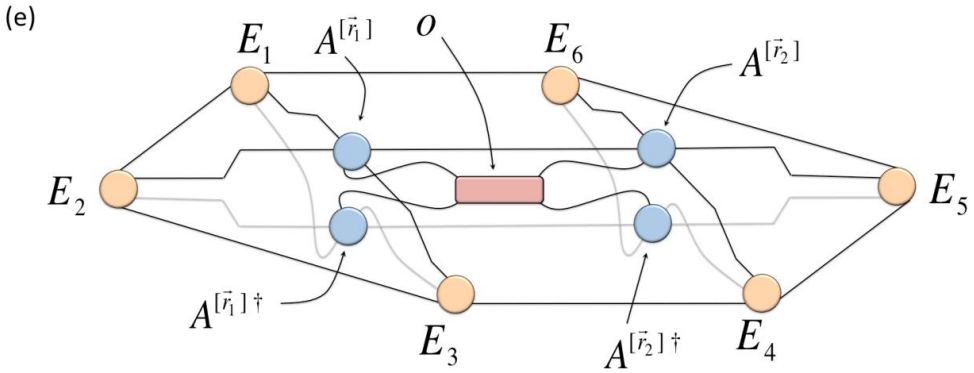


summery

- 1×1 unit cell, whether SU or random, $\Delta \to 0$
- When $D = 4$ and 2×2 unit cell， from SU get lower energy and $\Delta \neq 0$
- Outlook
  - Larger D
  - Large unit cell FPCM?
  - VUMPS with TensorKit?

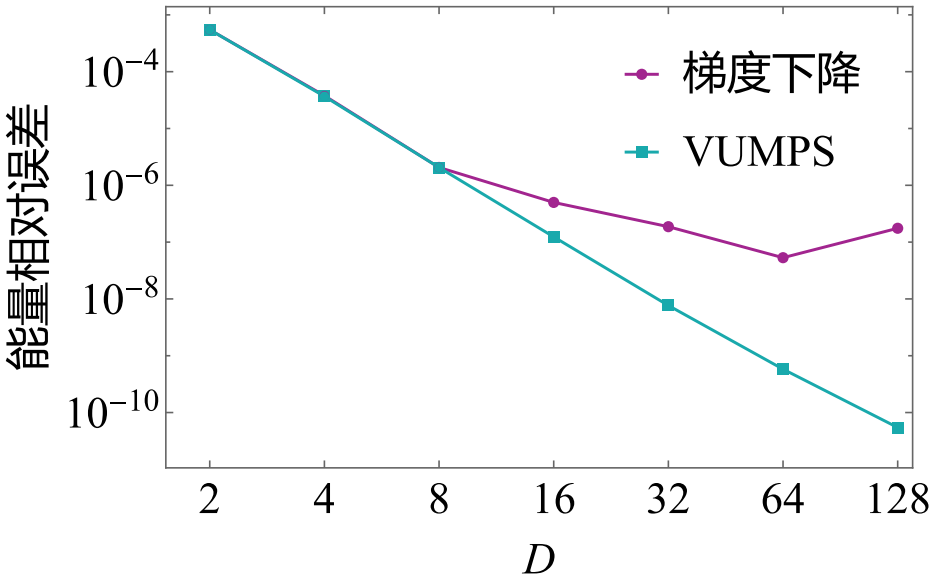
Others: swapgates behave differently in 1D and 2D?





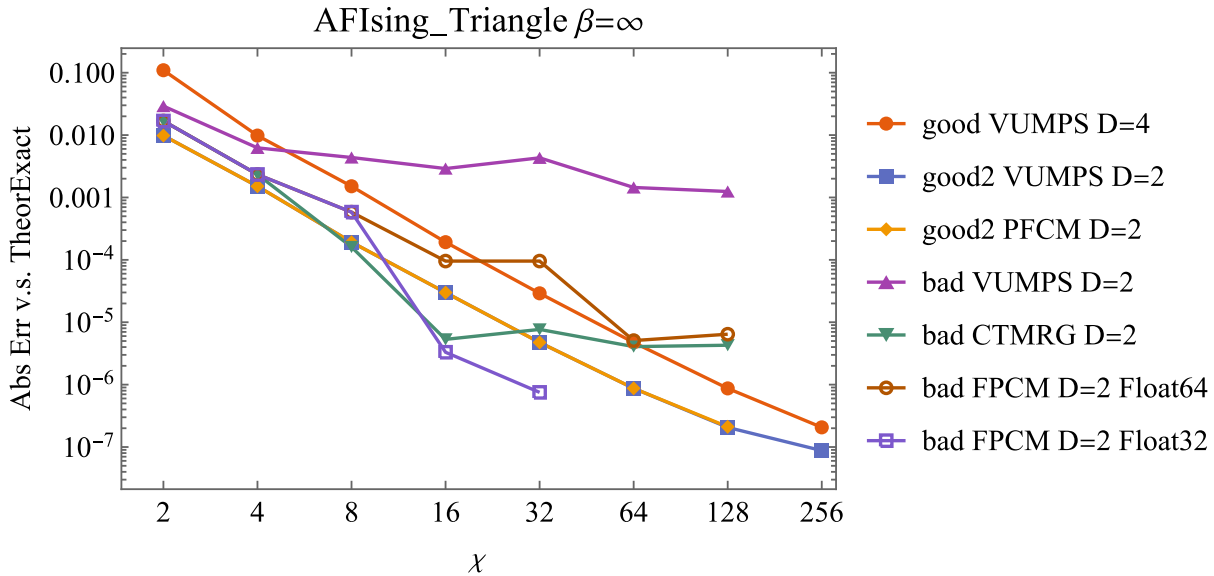
If only the nearest interaction in 1D,
there is not the swapgate.

Others: what is the manifold space of $\langle\psi_d|\psi_u\rangle = 1$?



TFIsing at critical point
Minimum error > 10^{-7}

Common point: without canonical form!



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