Nagaoka ferromagnetism in moiré triangular superlattice complexes

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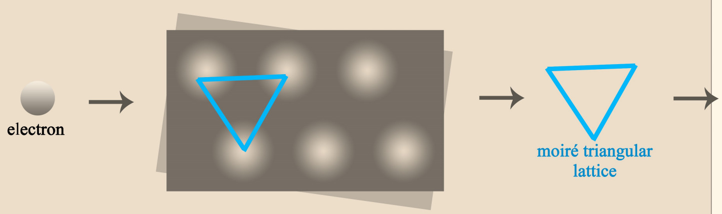
INTRODUCTION

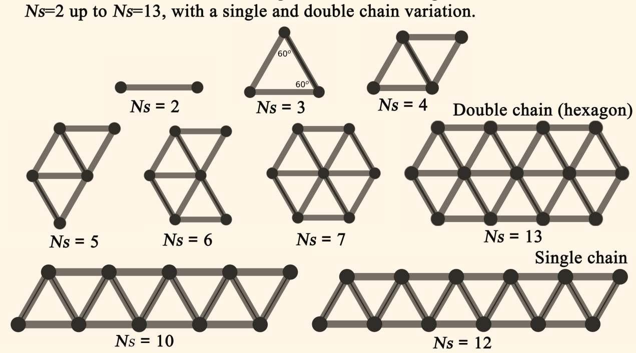
We construct different finite size fragments of moiré triangular lattice and analyze its magnetic properties when doped away from the half-filling. In such a case one can expect a transition from a nonmagnetic state to Nagaoka ferromagnetism. This type of magnetism comes from correlations effects, or in other words, is due to constructive interference between different many-body configurations.



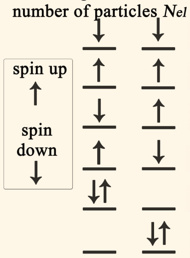
The illustration above displays how stacking and twisting monolayers result in localized potentials. Particles such as electrons tend to stay in this potential.

METHODOLOGY

1. Construct the finite moire triangular lattices, starting from the number of sites *Ns*=2 up to *Ns*=13, with a single and double chain variation.



2. Configuration of lattice *Ns* = 2 with number of particles *Nel* = 2.



$|1\rangle = c^\dagger_{1\downarrow}c^\dagger_{2\downarrow}|0\rangle$

$|2\rangle = c^\dagger_{1\uparrow}c^\dagger_{2\uparrow}|0\rangle$

$|3\rangle = c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}|0\rangle$

$|4\rangle = c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}|0\rangle$

$|5\rangle = c^\dagger_{1\downarrow}c^\dagger_{1\uparrow}|0\rangle$

$|6\rangle = c^\dagger_{2\downarrow}c^\dagger_{2\uparrow}|0\rangle$

3. Construct the Hamiltonian equation with tight-binding and extended Hubbard model. This example only calculates the on-site Coulomb interaction *U* = <ii|v|ii>.

$$\hat{H} = \sum_{ij\sigma} t_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma} + \sum_{ijkl}\langle ij|v|kl\rangle \hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{k\sigma'}\hat{c}_{l\sigma}$$

where, the Coulomb interaction defined by

$$\langle ij|v|kl\rangle = \iint d\vec{r}d\vec{r}\prime \frac{\phi^*_i(\vec{r})\phi^*_j(\vec{r}\prime)\phi_k(\vec{r})\phi_l(\vec{r}\prime)}{|\vec{r}-\vec{r}\prime|}$$

4. Using the Exact Diagonalization method, we construct the Hamiltonian matrix for *Ns* = 2 with *Nel* = 2. *t* is the nearest neighbor energy.

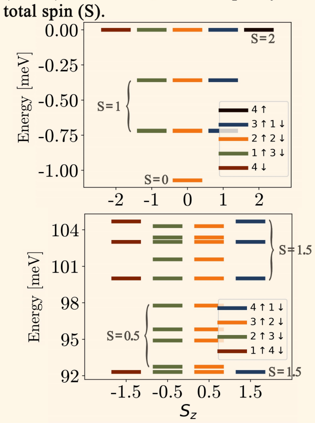
$$\hat{H} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{21} & t_{12} \\ 0 & 0 & 0 & 0 & -t_{21} & -t_{12} \\ 0 & 0 & t_{12} & -t_{12} & U & 0 \\ 0 & 0 & t_{21} & -t_{21} & 0 & U \end{pmatrix}$$

We need to calculate for all possible numbers of particles on site to get the eigen values and eigen vectors.

RESULTS

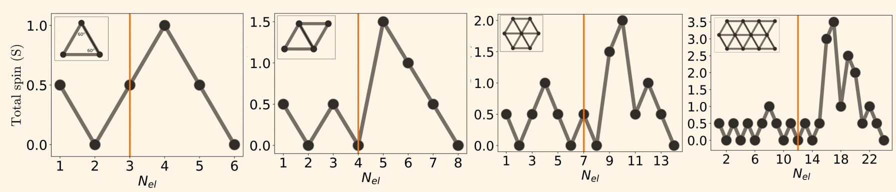
1. Spectral Energy

The spectral energy of lattice *Ns* = 4 with its quantum spin Number (*Sz*) for a number of particle *Nel* = 4 (above) and 5 (below). From here, we can specify the total spin (S).



2. Phase Diagram

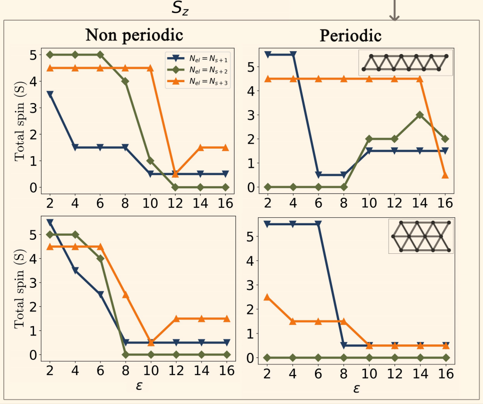
Total spin of groundstate for every possible number of particle *Nel* in the lattice site *Ns* = 3, 4, 7, 12, with ε = 10. ε is a parameter related to *t* and *U*. We can see the highest total spin appears always above half-filling. This is the sign of Nagaoka ferromagnetism.

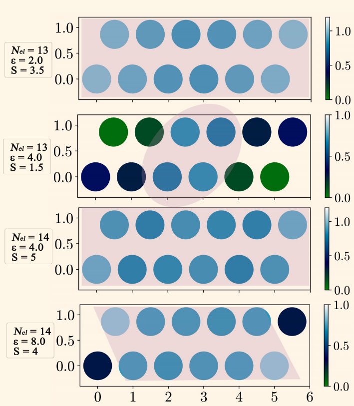


3. Spin transition

The graphs below show a spin transition happens when the total spin changes with ε.

By constructing *Ns* = 12 as single-chain and hexagon, we can see spin transition varieting with ε.





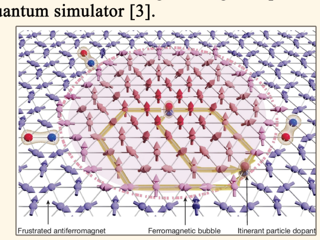
CONCLUSIONS

In summary, we observed Nagaoka ferromagnetism and Nagaoka polaron in our finite-size moiré triangular lattice when it was above half-filling.

We were able to adjust the size of the ferromagnetic bubble on the site by selecting an appropriate number of particles and a parameter ε.

4. Spin density

Experimental result on observing the Nagaoka polarons in a Fermi-Hubbard quantum simulator [3].



The graphs on the left display the spin density of a single-chain lattice *Ns* = 12, with *Nel* = 13 and *Nel* = 14. When the total spin is high, the particles tend to polarize on all sites. We can observe parts of the edge of the ferromagnetic bubble at a lower total spin.

REFERENCES

[1] F. Wu, T. Lovorn, E. Tutuc, and A.H. MacDonald, *Phys. Rev. Lett.* 121, 026402 (2018).
[2] Yosuke Nagaoka, *Phy.Rev.* 147, 392 (1966).
[3] M.Lebrat, M. Xu, L. H. Kendrick, A.Kale, Y. Gang, P. Seetharaman, I. Morera, E. Khatami, E. Demler, & M. Greiner, *Nature.* 629, (8011), 317-322 (2024).

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