[Adam Koford, 2022]

JSC END-OF-YEAR COLLOQUIUM 2023

Solar Power from Farmhand Ruperts Coal

December 5, 2023 | Marcel Rodekamp | Jülich Supercomputing Center, Forschungszentrum Jülich

- $C_{20}H_{12}$ Perylene [Donaldson et al., 1953]
    - Organic Molecule sp^2-hybridized [Golshan et al., 2021]
    - Organic Semiconductor
    - Fluorescent

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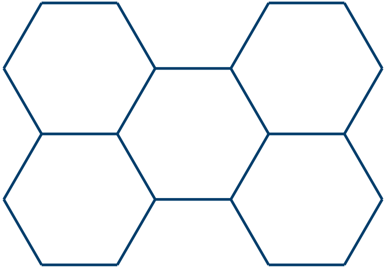
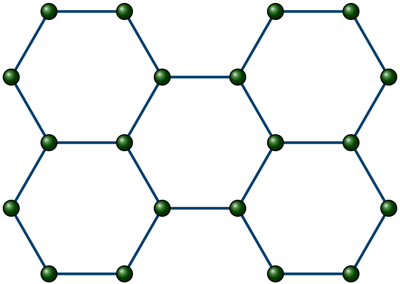


$$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{x,y}\left\{\hat{p}_x^\dagger \kappa_{xy}\hat{p}_y - \hat{h}_y^\dagger \kappa_{xy}\hat{h}_x\right\} \tag{1}$$

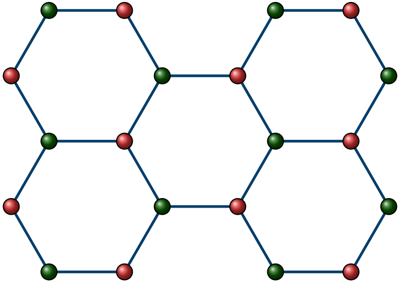
[Hubbard, 1959] [Wynen et al., 2019] [Ostmeyer et al., 2020]

JÜLICH Forschungszentrum



$$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{x,y}\left\{\hat{p}_x^\dagger \kappa_{xy}\hat{p}_y - \hat{h}_y^\dagger \kappa_{xy}\hat{h}_x\right\} + \frac{U}{2}\sum_x \hat{q}_x^2 \quad (1)$$

[Hubbard, 1959] [Wynen et al., 2019] [Ostmeyer et al., 2020]



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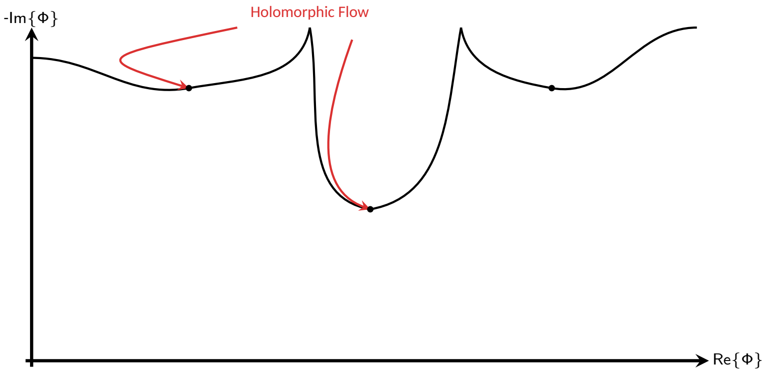
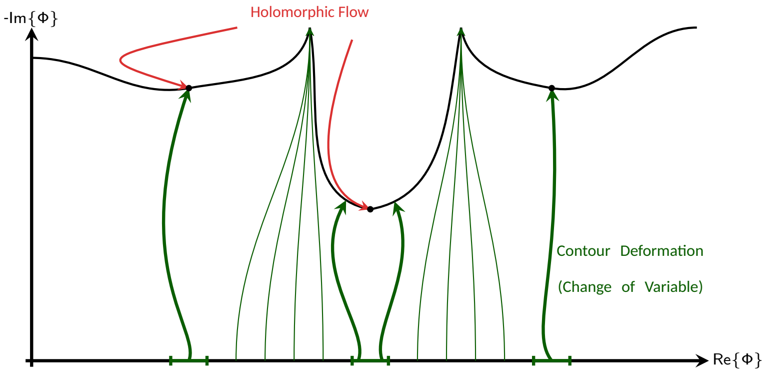
[Hubbard, 1959] [Wynen et al., 2019] [Ostmeyer et al., 2020]



[Alexandru et al., 2017]
[Wynen et al., 2021]
[Rodekamp et al., 2022]
[Gäntgen et al., 2023]



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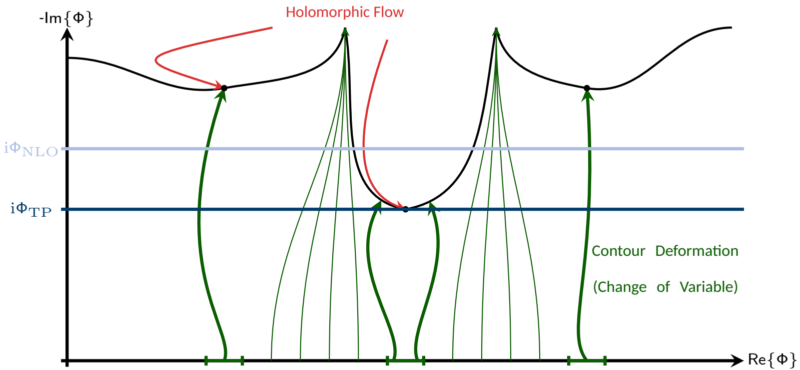

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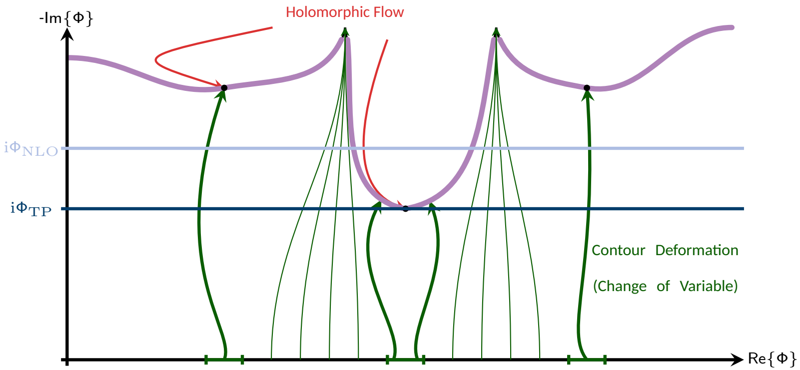

[Alexandru et al., 2017]
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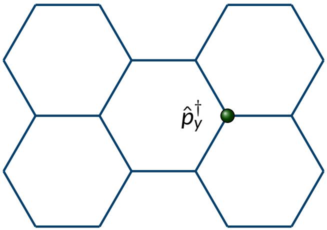
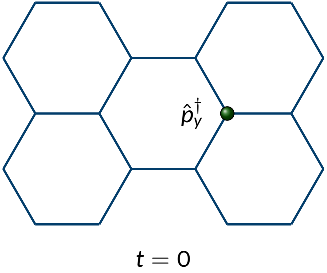
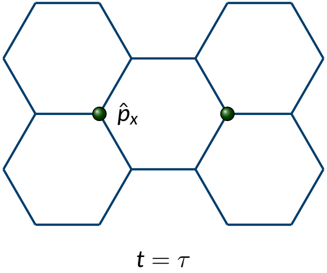
$$\langle \mathcal{O} \rangle \equiv \mathrm{C} \quad (\tau) = \Big\langle \qquad\qquad \Big\rangle \tag{2}$$



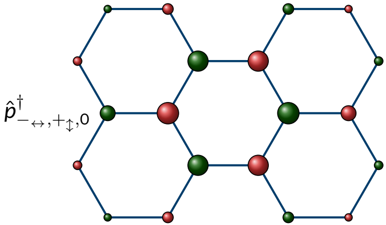
$t = 0$

$$\langle \mathcal{O} \rangle \equiv \mathrm{C} \quad _y(\tau) = \Big\langle \qquad \hat{p}_y^\dagger(0) \Big\rangle \tag{2}$$





$$\langle \mathcal{O} \rangle \equiv \mathrm{C}_{x,y}(\tau) = \left\langle \hat{p}_x(\tau)\hat{p}_y^\dagger(0) \right\rangle \tag{2}$$



$$C_k(\tau) \equiv \left\langle u_k \cdot \hat{p}(\tau)\hat{p}^{\dagger}(0) \cdot u_k^{\dagger} \right\rangle \quad (3)$$

- Total Charge

$$Q = \sum_x \left[\left\langle \hat{p}_x(0)\hat{p}_x^\dagger(0) \right\rangle - \left\langle \hat{h}_x(0)\hat{h}_x^\dagger(0) \right\rangle \right] \tag{4}$$

- Total Charge

$$Q = \sum_x \left[\left\langle \hat{p}_x(0)\hat{p}_x^\dagger(0) \right\rangle - \left\langle \hat{h}_x(0)\hat{h}_x^\dagger(0) \right\rangle \right] \tag{4}$$

- Excitation Energy

$$\mathrm{C}_k(\tau) = \sum_{n=0}^{\infty} A_n e^{-\tau E_n^k} \tag{5}$$

- Total Charge

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- Particle-Hole Excitation

$$\left\langle \hat{h}_x(\tau)\hat{p}_x(\tau)\hat{h}_y^\dagger(0)\hat{p}_y^\dagger(0) \right\rangle \tag{6}$$

- Total Charge

$$Q = \sum_x \left[\left\langle \hat{p}_x(0)\hat{p}_x^\dagger(0) \right\rangle - \left\langle \hat{h}_x(0)\hat{h}_x^\dagger(0) \right\rangle \right] \tag{4}$$

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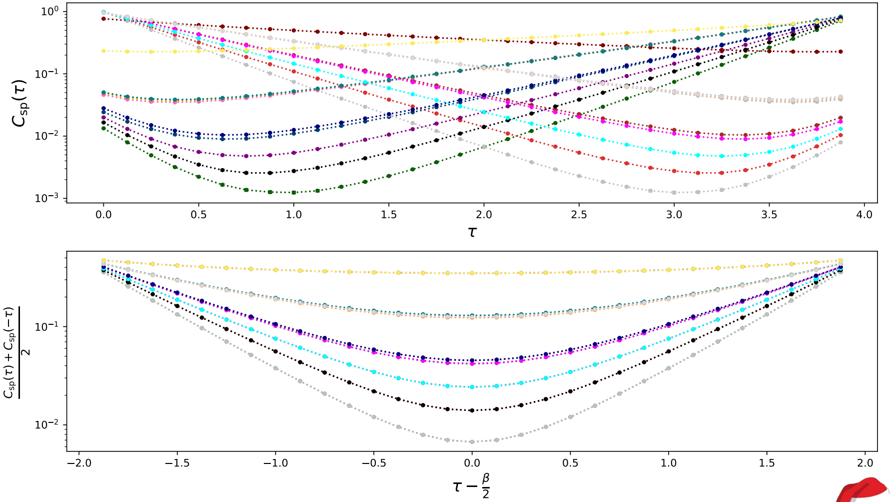
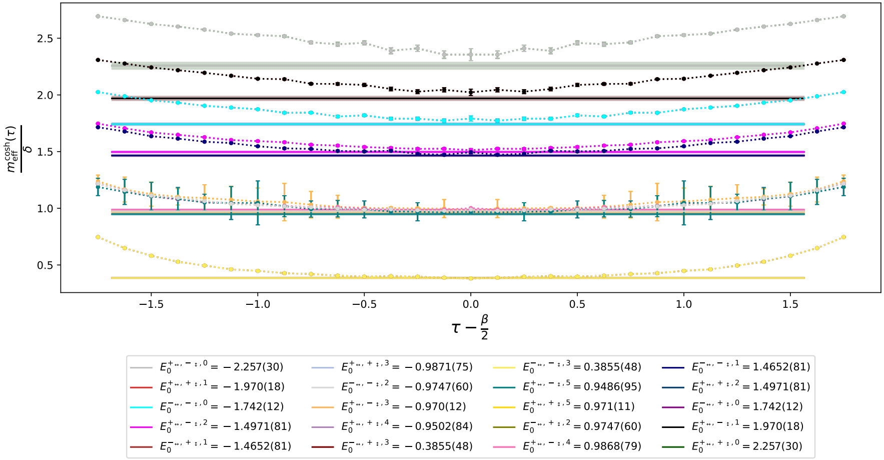
$$\left\langle \hat{h}_x(\tau)\hat{p}_x(\tau)\hat{h}_y^\dagger(0)\hat{p}_y^\dagger(0) \right\rangle \tag{6}$$

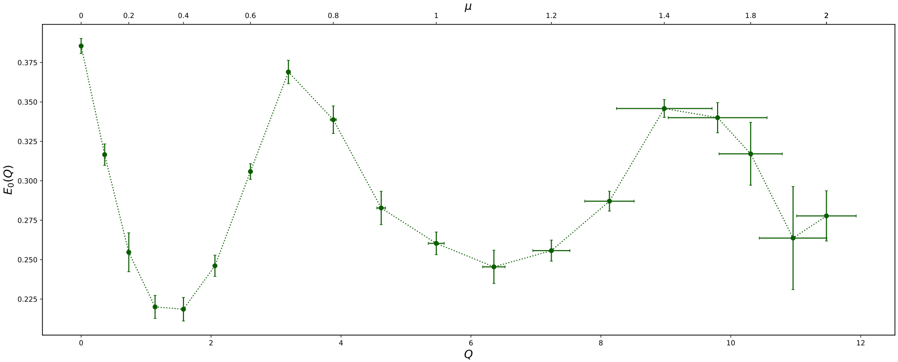
Santa's Wish List

Single Particle Correlator: Perylene$(N_t = 32,\ \beta = 4,\ U = 2,\ \mu = 0 \,|\, N_{\mathrm{conf}} = 10000)$





$\frac{m_{\mathrm{eff}}^{\cosh}(\tau)}{\delta}$
2.5
2.0
1.5
1.0
0.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
$\tau - \frac{\beta}{2}$
$E_0^{+\leftrightarrow, -\updownarrow, 0} = -2.257(30)$
$E_0^{+\leftrightarrow, +\updownarrow, 1} = -1.970(18)$
$E_0^{-\leftrightarrow, -\updownarrow, 0} = -1.742(12)$
$E_0^{+\leftrightarrow, -\updownarrow, 2} = -1.4971(81)$
$E_0^{-\leftrightarrow, +\updownarrow, 1} = -1.4652(81)$
$E_0^{+\leftrightarrow, +\updownarrow, 3} = -0.9871(75)$
$E_0^{-\leftrightarrow, -\updownarrow, 2} = -0.9747(60)$
$E_0^{+\leftrightarrow, -\updownarrow, 3} = -0.970(12)$
$E_0^{+\leftrightarrow, +\updownarrow, 4} = -0.9502(84)$
$E_0^{-\leftrightarrow, +\updownarrow, 3} = -0.3855(48)$
$E_0^{-\leftrightarrow, -\updownarrow, 3} = 0.3855(48)$
$E_0^{+\leftrightarrow, -\updownarrow, 5} = 0.9486(95)$
$E_0^{+\leftrightarrow, +\updownarrow, 5} = 0.971(11)$
$E_0^{-\leftrightarrow, +\updownarrow, 2} = 0.9747(60)$
$E_0^{+\leftrightarrow, -\updownarrow, 4} = 0.9868(79)$
$E_0^{-\leftrightarrow, -\updownarrow, 1} = 1.4652(81)$
$E_0^{+\leftrightarrow, +\updownarrow, 2} = 1.4971(81)$
$E_0^{-\leftrightarrow, +\updownarrow, 0} = 1.742(12)$
$E_0^{+\leftrightarrow, -\updownarrow, 1} = 1.970(18)$
$E_0^{+\leftrightarrow, +\updownarrow, 0} = 2.257(30)$



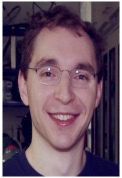
μ
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.8
2
$E_0(Q)$
0.375
0.350
0.325
0.300
0.275
0.250
0.225
0
2
4
6
8
10
12
Q


Evan Berkowitz

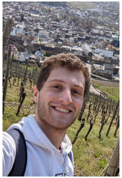

Christoph Gäntgen


Stefan Krieg


Tom Luu

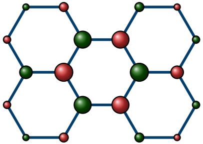

Johann Ostmeyer


Giovanni Pederiva


Lado Razmadze


Aleena Sibi


Petar Sinilkov



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$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \operatorname{Tr}\left\{ \hat{\mathcal{O}} e^{-\beta \hat{\mathcal{H}}} \right\} \tag{7}$$

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$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left\{ \mathcal{O} e^{-\beta \hat{\mathcal{H}}} \right\} \rightarrow \frac{1}{\mathcal{Z}} \int \mathcal{D}[\Phi]\, \mathcal{O}[\Phi]\, e^{-S[\Phi]} \tag{7}$$

$$S[\Phi] = \frac{1}{\delta U} \Phi^2 + \log\det\left\{ M^p[\Phi] \cdot M^h[\Phi] \right\} \tag{8}$$