How Experience from Lattice QCD can help in Condensed Matter

Johann Ostmeyer

Helmholtz-Institut für Strahlen- und Kernphysik

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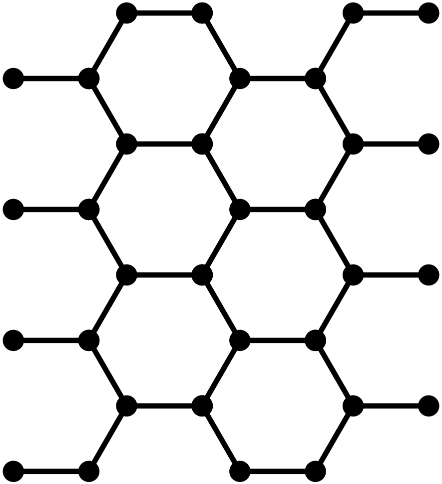
Graphene [Lee *et al.* 2008; Lin *et al.* 2010; Novoselov *et al.* 2004]



- Carbon atoms
- 2-dimensional hexagonal lattice

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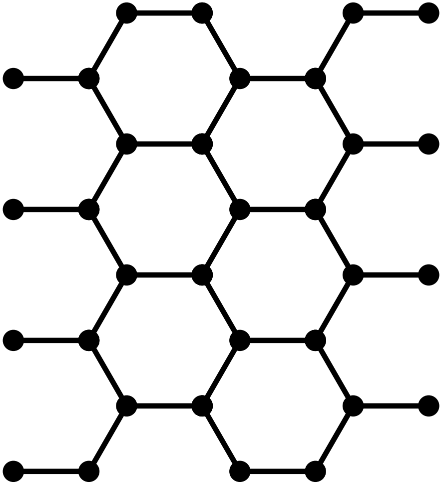

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- ≈125 times stronger than steel

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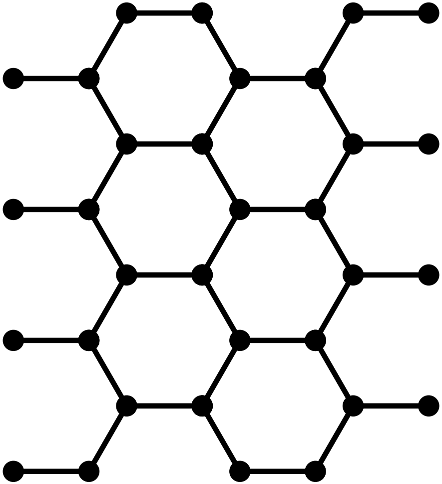
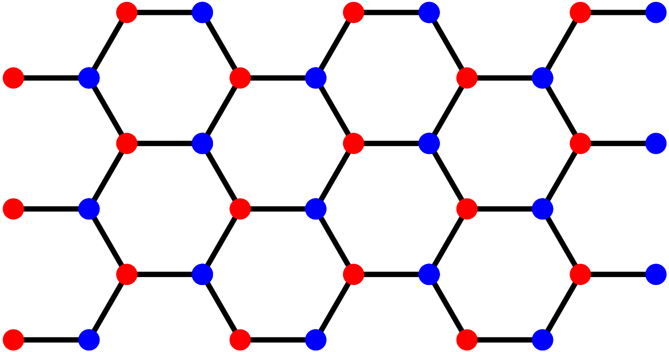


- Carbon atoms
- 2-dimensional hexagonal lattice
- $\approx$125 times stronger than steel
- Might be the transistor material of the future

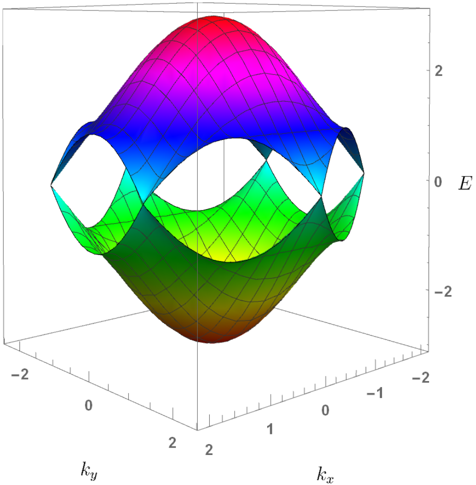
Tight binding model [Bloch 1929]

$$H = -\sum_{\langle x,y \rangle} c_x^\dagger c_y$$

$\langle x,y \rangle$ denotes nearest neighbours



$$E_k^0 = \pm\sqrt{3 + 2\left(\cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) + \cos\left(\sqrt{3}k_y\right)\right)}$$



Band structure [Wallace 1947]

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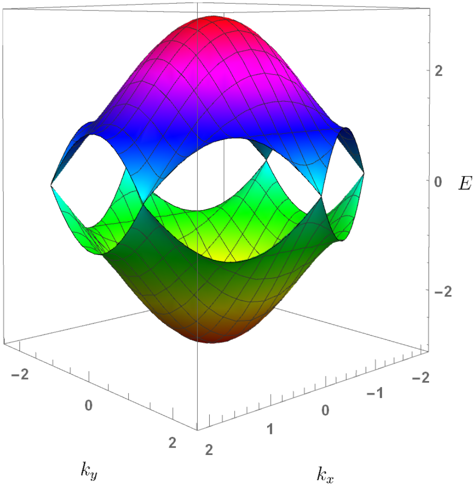

- Two energy bands
- Touching at single points

Hubbard model [Hubbard 1963]

$$H = -\kappa \sum_{\langle x,y \rangle, s} c^{\dagger}_{x,s} c_{y,s}$$

Hubbard model [Hubbard 1963]

$$H = -\kappa \sum_{\langle x,y \rangle, s} c^\dagger_{x,s} c_{y,s} + \frac{1}{2} U \sum_x q_x^2$$

$$q_x = n_{x,\uparrow} + n_{x,\downarrow} - 1$$

$$n_{x,s} = c^\dagger_{x,s} c_{x,s}$$

- U is a repulsive coupling

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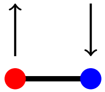
- Expect a phase transition at critical U_c
- Staggered mass m_s introduces bias between sublattices



Path integral formalism [Duane *et al.* 1987; Luu & Lähde 2016]

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- Discretise time into N_t slices of length $\delta = \frac{\beta}{N_t}$

$$Z = \int \prod_{t=0}^{N_t-1} \mathcal{D}\left[\psi_t^*, \psi_t, \eta_t^*, \eta_t\right] \mathrm{e}^{-\sum_\alpha \left(\psi_{\alpha,t+1}^* \psi_{\alpha,t+1} + \eta_{\alpha,t+1}^* \eta_{\alpha,t+1}\right)}$$

$$\times \left\langle \psi_{t+1}, \eta_{t+1} \left| \mathrm{e}^{-\delta H} \right| \psi_t, \eta_t \right\rangle$$

Path integral formalism [Duane *et al.* 1987; Luu & Lähde 2016]

- Wick rotation
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- Hubbard-Stratonovich transformation

$$\mathrm{e}^{-\frac{1}{2}U\sum_x q_x^2} \propto \int \mathcal{D}\phi_t \, \mathrm{e}^{-\frac{1}{2U}\sum_x \phi_{x,t}^2 + \mathrm{i}\sum_x \phi_{x,t} q_x}$$

Path integral formalism [Duane *et al.* 1987; Luu & Lähde 2016]

- Wick rotation
- Discretise time into N_t slices of length $\delta = \frac{\beta}{N_t}$
- Hubbard-Stratonovich transformation
- Hybrid Monte Carlo simulation

$$\mathcal{H} = \frac{\delta}{2U}\phi^2 + \chi^\dagger \left(MM^\dagger\right)^{-1} \chi + \frac{1}{2}\pi^2$$

$$M_{(x,t)(y,t')} = \delta_{xy} \left(\delta_{tt'} - \delta_{t-1,t'} \left(\mathrm{e}^{-\mathrm{i}\,\delta\cdot\phi_{x,t}} - \delta \cdot m_s\right)\right) - \delta \cdot \kappa \delta_{\langle x,y \rangle} \delta_{tt'}$$

Integrator [Forest & Ruth 1990; Omelyan *et al.* 2002; Ostmeyer *et al.* 2018; Yin & Mawhinney 2011]

- Equations of motion $\dot{\phi} = \pi \, , \, \dot{\pi} = -F(\phi)$

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- Symplectic integrator

$$\phi_i = \phi_{i-1} + c_i \Delta t \, \pi_{i-1}$$
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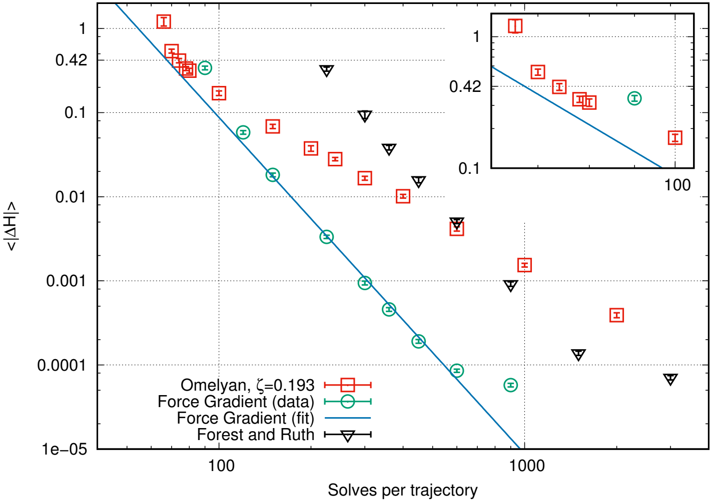
- Example: 2nd order Omelyan integrator

$$c_1 = c_3 = \zeta$$
$$c_2 = 1 - 2\zeta$$
$$d_1 = d_2 = \frac{1}{2}$$
$$d_3 = 0$$

Integrator [Forest & Ruth 1990; Omelyan *et al.* 2002; Ostmeyer *et al.* 2018; Yin & Mawhinney 2011]



- Want acceptance ≈ 0.66 $\Rightarrow \Delta\mathcal{H} \approx 0.42$
- Chose 2nd order Omelyan integrator

Solver [Hestenes & Stiefel 1952; Saad 1993]

- Have to solve $\left(MM^{\dagger}\right)\eta = \chi$

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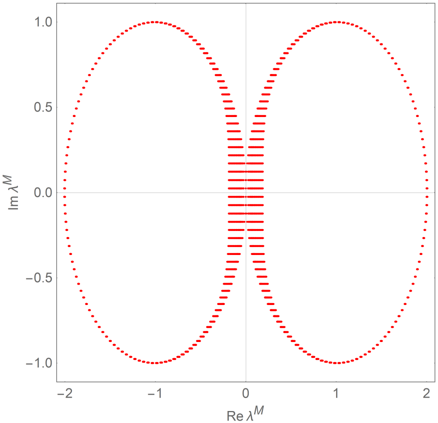
$$\boxed{\approx 2.2 \times \text{ faster}}$$

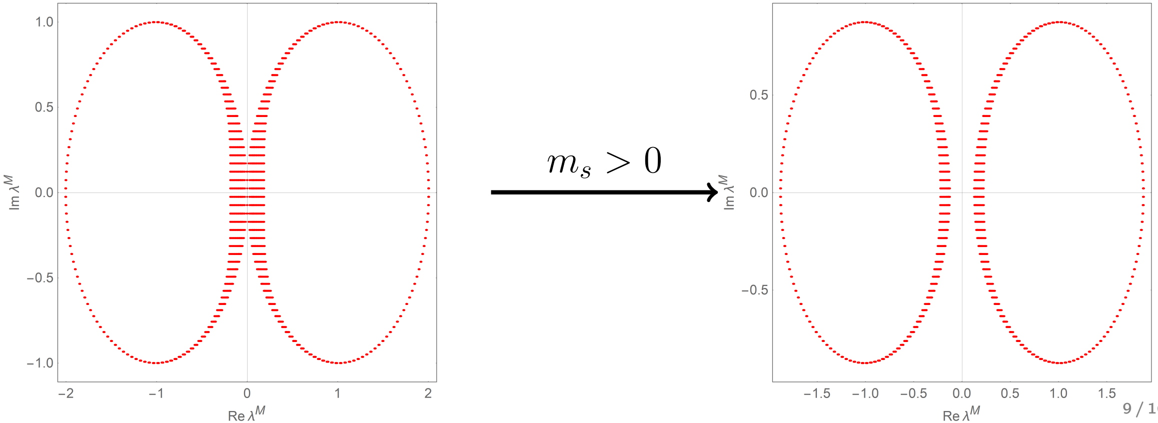
Hasenbusch trick [Hasenbusch 2001]

- Inversion of $MM^\dagger$ has runtime $\propto \left|\frac{\lambda^M_{\text{max}}}{\lambda^M_{\text{min}}}\right|^2$



Hasenbusch trick [Hasenbusch 2001]

- Inversion of $MM^\dagger$ has runtime $\propto \left|\frac{\lambda^M_{\text{max}}}{\lambda^M_{\text{min}}}\right|^2$
- $\left|\lambda^M_{\text{min}}\right| \geq \delta \cdot m_s$



Hasenbusch trick [Hasenbusch 2001]

Sample from probability distribution

$$\det\left(MM^\dagger\right) = \int \mathcal{D}\chi\mathcal{D}\chi^\dagger\, \mathrm{e}^{-\chi^\dagger\left(MM^\dagger\right)^{-1}\chi}$$

$$= \int \mathcal{D}\chi_1\mathcal{D}\chi_1^\dagger\mathcal{D}\chi_2\mathcal{D}\chi_2^\dagger\, \mathrm{e}^{-\chi_1^\dagger\left(M_{ms}M_{ms}^\dagger\right)^{-1}\chi_1-\chi_2^\dagger\left(\frac{MM^\dagger}{M_{ms}M_{ms}^\dagger}\right)^{-1}\chi_2}$$

Sample from probability distribution

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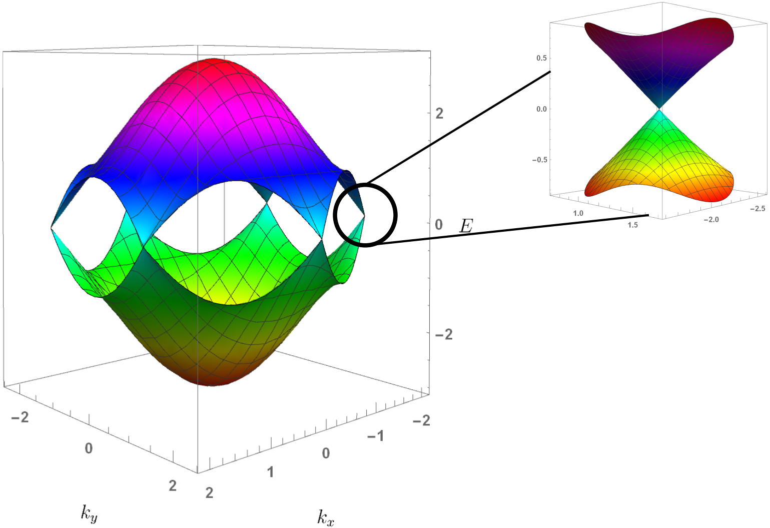
$$= \int \mathcal{D}\chi_1\mathcal{D}\chi_1^\dagger\mathcal{D}\chi_2\mathcal{D}\chi_2^\dagger\, \mathrm{e}^{-\chi_1^\dagger\left(M_{m_s}M_{m_s}^\dagger\right)^{-1}\chi_1-\chi_2^\dagger\left(\frac{MM^\dagger}{M_{m_s}M_{m_s}^\dagger}\right)^{-1}\chi_2}$$

- $M_{m_s}M_{m_s}^\dagger$ easy to invert
- $\frac{MM^\dagger}{M_{m_s}M_{m_s}^\dagger}$ has small influence, allows coarser time steps

Expected phase transition



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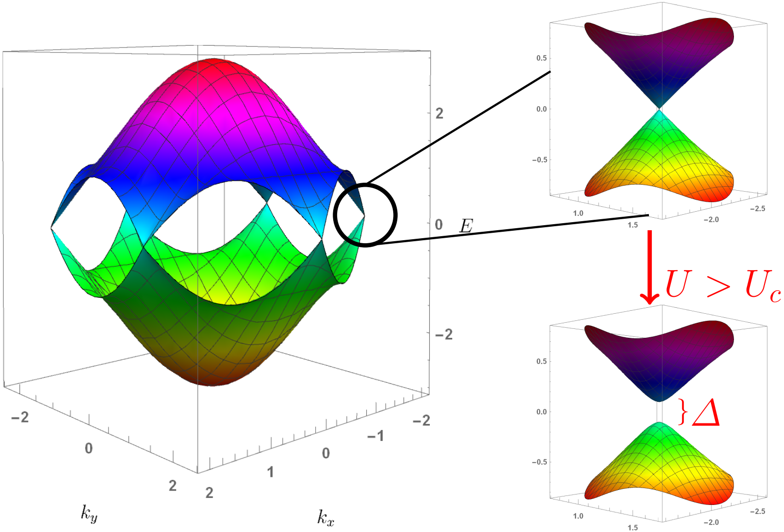

Previous works

- Mostly usage of algorithms scaling with volume cubed [Blankenbecler *et al.* 1981; Ulybyshev *et al.* 2018]

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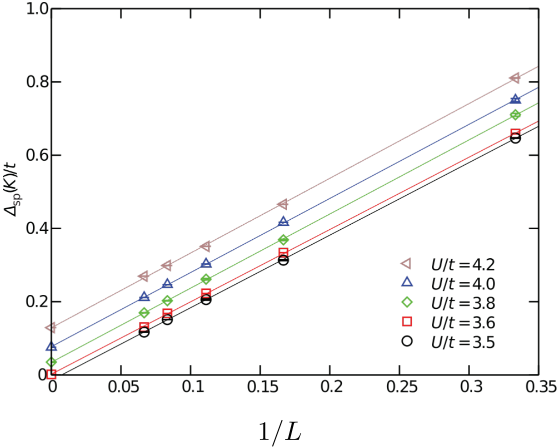

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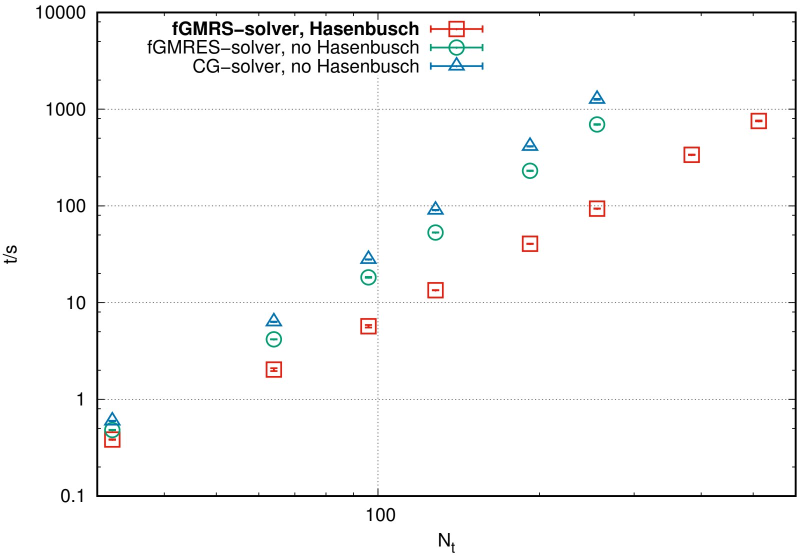
- Mostly usage of algorithms scaling with volume cubed [Blankenbecler *et al.* 1981; Ulybyshev *et al.* 2018]
- Poor thermodynamic limit extrapolation [Meng *et al.* 2010]
- To our knowledge no continuum limit extrapolation
- Largest systems simulated to date $2 \times 48^2 \times 80$ [Stauber *et al.* 2017]

Speedup [Ostmeyer *et al.* 2018]



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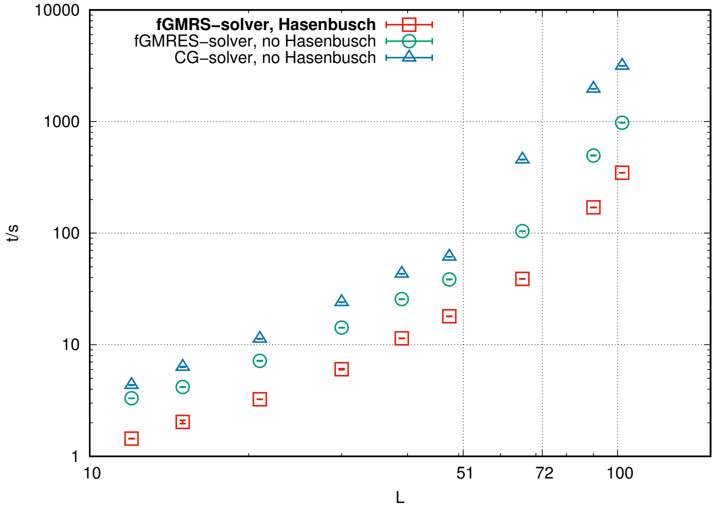
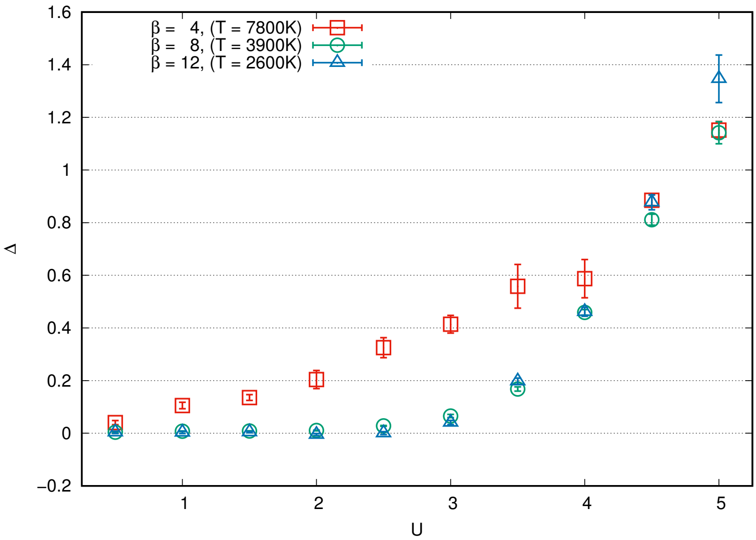
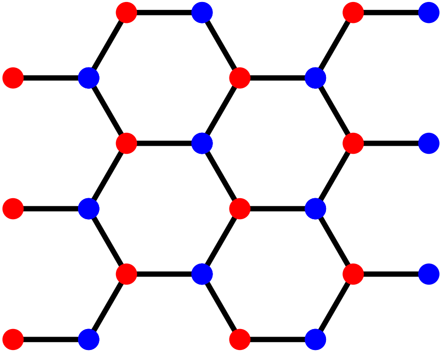


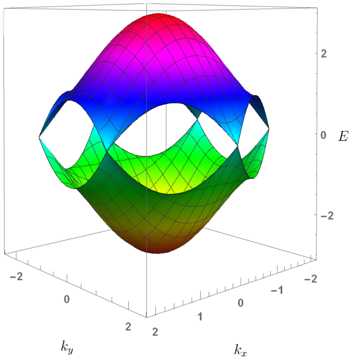
Linear volume scaling → largest lattices $2 \times 102^2 \times 64$

Preliminary results



Summary





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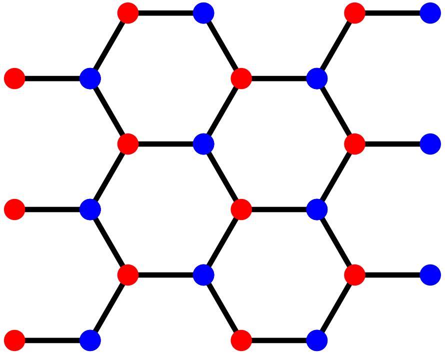

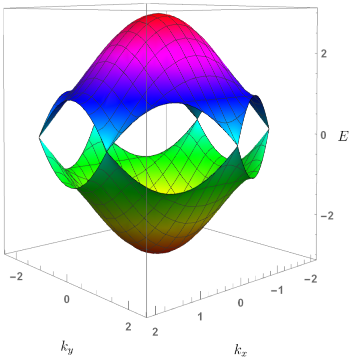

- Hubbard model: Hopping + onsite interaction

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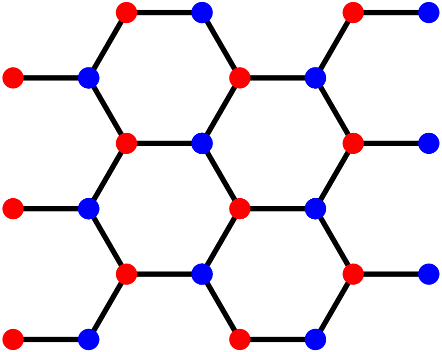

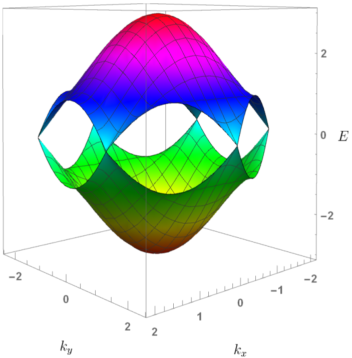

- Hubbard model: Hopping + onsite interaction
- Field approach to graphene very similar to QCD

Outlook

- Port the code to GPU

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- Try out the nth root trick
- Other interactions, chemical potential, several layers...


That's all Folks!

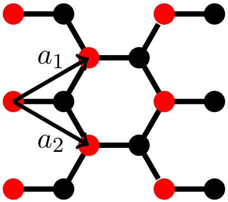
Hubbard model Hamiltonian

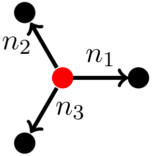
$$
\begin{aligned}
H &\equiv H_{\mathsf{tb}} + H_{\mathsf{I}} + H_{\mathsf{m}} \\
&= -\kappa \sum_{\langle x,y\rangle,s} c^{\dagger}_{x,s} c_{y,s} + \frac{1}{2} \sum_{x,y} V_{xy} q_x q_y + m_s \sum_x \mathrm{sgn}(x) \left(c^{\dagger}_{x,\uparrow} c_{x,\uparrow} + c_{x,\downarrow} c^{\dagger}_{x,\downarrow} \right) \\
&= -\kappa \sum_{\langle x,y\rangle} \left(p^{\dagger}_x p_y + h^{\dagger}_x h_y \right) + \frac{U}{2} \sum_x q_x^2 + m_s \sum_x \mathrm{sgn}(x) \left(p^{\dagger}_x p_x + h^{\dagger}_x h_x \right)
\end{aligned}
$$

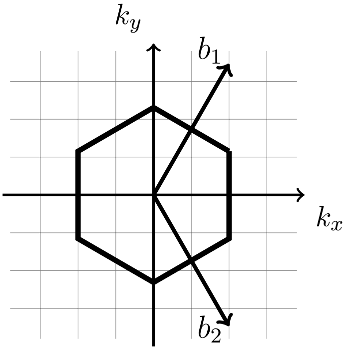
$$
\mathrm{sgn}(x) = \begin{cases} -1 & x \in A \\ 1 & x \in B \end{cases}
$$

Particle-hole transformation:

$$
p^{\dagger}_x \equiv c^{\dagger}_{x,\uparrow} \, , \, p_x \equiv c_{x,\uparrow} \, , \, h^{\dagger}_x \equiv c_{x,\downarrow} \, , \, h_x \equiv c^{\dagger}_{x,\downarrow}
$$







$$k_{\mathsf{D}} \equiv \frac{2\pi}{9a} \begin{pmatrix} 3 \\ \pm\sqrt{3} \end{pmatrix}$$

Band structure (Fourier trafo)

$$
\begin{aligned}
H =& -\kappa \sum_{\langle x,y\rangle} c_x^\dagger c_y \;+\; m_s \sum_x \operatorname{sgn}(x) \left(c_x^\dagger c_x\right) \\
=& -\kappa \sum_{x\in A,n} \left(a_x^\dagger b_{x+n} + b_{x+n}^\dagger a_x\right) \;+\; m_s \sum_{x\in A} \left(a_x^\dagger a_x - b_{x+n_1}^\dagger b_{x+n_1}\right) \\
=& \frac{1}{N} \sum_{k,k'} \sum_{x\in A} \mathrm{e}^{\mathrm{i}(k'-k)x} \left(-\kappa \sum_n \left(\mathrm{e}^{\mathrm{i}\,k'n} a_k^\dagger b_{k'} + \mathrm{e}^{-\mathrm{i}\,kn} b_k^\dagger a_{k'}\right)\right. \\
& \left. \;+\; m_s \left(a_k^\dagger a_{k'} - \mathrm{e}^{\mathrm{i}(k'-k)n_1} b_k^\dagger b_{k'}\right)\right) \\
=& \sum_k \left(-\kappa \sum_n \left(\mathrm{e}^{\mathrm{i}\,kn} a_k^\dagger b_k + \mathrm{e}^{-\mathrm{i}\,kn} b_k^\dagger a_k\right) \;+\; m_s \left(a_k^\dagger a_k - b_k^\dagger b_k\right)\right) \\
=& \sum_k \left(a_k^\dagger, b_k^\dagger\right) \begin{pmatrix} m_s & -\kappa \sum_n \mathrm{e}^{\mathrm{i}\,kn} \\ -\kappa \sum_n \mathrm{e}^{-\mathrm{i}\,kn} & -m_s \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}
\end{aligned}
$$

Band structure (diagonalization)

$$H_k = \begin{pmatrix} m_s & -\kappa \sum_n \mathrm{e}^{\mathrm{i}\,kn} \\ -\kappa \sum_n \mathrm{e}^{-\mathrm{i}\,kn} & -m_s \end{pmatrix}$$

$$\begin{aligned} \det\left(H_k - E_k\right) =& \left(m_s - E_k\right)\left(-m_s - E_k\right) - K \\ =& E_k^2 - m_s^2 - K \end{aligned}$$

$$K = \left(\kappa \sum_n \mathrm{e}^{\mathrm{i}\,kn}\right)\left(\kappa \sum_n \mathrm{e}^{-\mathrm{i}\,kn}\right)$$

Partition function $Z \equiv \mathrm{Tr}\left[\mathrm{e}^{-\beta H}\right] = \mathrm{Tr}\left[\prod_{t=0}^{N_t-1} \mathrm{e}^{-\delta \cdot H}\right]$.

$$Z = \int \prod_{t=0}^{N_t-1} \mathcal{D}\left[\psi_t^*,\psi_t,\eta_t^*,\eta_t\right] \mathrm{e}^{-\sum\limits_{\alpha}\left(\psi^*_{\alpha,t+1}\psi_{\alpha,t+1}+\eta^*_{\alpha,t+1}\eta_{\alpha,t+1}\right)} \left\langle \psi_{t+1},\eta_{t+1} \left| \mathrm{e}^{-\delta H} \right| \psi_t,\eta_t \right\rangle$$

Hubbard-Stratonovich transformation:

$$\mathrm{e}^{-\frac{1}{2}\delta\sum_{x,y} V_{x,y} q_x q_y} \propto \int \mathcal{D}\phi_t \, \mathrm{e}^{-\frac{1}{2}\sum_{x,y} \tilde{V}^{-1}_{x,y} \tilde{\phi}_{x,t}\tilde{\phi}_{y,t} + \mathrm{i}\sum_x \tilde{\phi}_{x,t} q_x}$$

$$\tilde{\kappa} := \delta \cdot \kappa \,, \quad \tilde{V} := \delta \cdot V \,, \quad \tilde{\phi} := \delta \cdot \phi \,, \quad \tilde{m}_s := \delta \cdot m_s \,.$$

Sketch of the derivation of the path integral formalism II

$$\left\langle \psi_{t+1},\eta_{t+1} \middle| \mathrm{e}^{-\delta H} \middle| \psi_t,\eta_t \right\rangle = \int \mathcal{D}\phi_t \, \exp\Bigg\{ -\frac{1}{2}\sum_{x,y} \tilde{V}^{-1}_{x,y}\tilde{\phi}_{x,t}\tilde{\phi}_{y,t} + \sum_x \left(\mathrm{e}^{\mathrm{i}\,\tilde{\phi}_{x,t}} \psi^*_{x,t+1}\psi_{x,t} + \mathrm{e}^{-\mathrm{i}\,\tilde{\phi}_{x,t}} \eta^*_{x,t+1}\eta_{x,t} \right) + \tilde{\kappa} \sum_{\langle x,y \rangle} \left(\psi^*_{x,t+1}\psi_{y,t} + \eta^*_{x,t+1}\eta_{y,t} \right) - \tilde{m}_s \sum_x \mathrm{sgn}(x) \left(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t} \right) \Bigg\} + \mathcal{O}(\delta^2)$$

Fermion matrix:

$$M_{(x,t)(y,t')} \equiv \delta_{xy}\delta_{tt'} - \mathrm{e}^{-\mathrm{i}\,\tilde{\phi}_{x,t}}\delta_{xy}\delta_{t-1,t'} - \tilde{\kappa}\delta_{\langle x,y \rangle}\delta_{t-1,t'} + \mathrm{sgn}(x)\tilde{m}_s\delta_{xy}\delta_{t-1,t'}$$

Sketch of the derivation of the path integral formalism III

$$
\begin{aligned}
Z &= \int \mathcal{D}\psi^* \mathcal{D}\psi \mathcal{D}\eta^* \mathcal{D}\eta \mathcal{D}\phi \, \mathrm{e}^{-\frac{1}{2}\tilde{\phi}^t \tilde{V}^{-1}\tilde{\phi} - \psi^\dagger M^* \psi - \eta^\dagger M \eta} \\
&= \int \mathcal{D}\phi \; \det M^* \det M \, \mathrm{e}^{-\frac{1}{2}\tilde{\phi}^t \tilde{V}^{-1}\tilde{\phi}} \\
&= \int \mathcal{D}\phi \; \det\left(M M^\dagger\right) \, \mathrm{e}^{-\frac{1}{2}\tilde{\phi}^t \tilde{V}^{-1}\tilde{\phi}} \\
&= \int \mathcal{D}\phi \mathcal{D}\chi^* \mathcal{D}\chi \, \mathrm{e}^{-\frac{1}{2}\tilde{\phi}^t \tilde{V}^{-1}\tilde{\phi} - \chi^\dagger \left(M M^\dagger\right)^{-1} \chi} \\
&= \int \mathcal{D}\phi \mathcal{D}\chi^* \mathcal{D}\chi \mathcal{D}\pi \, \mathrm{e}^{-\frac{1}{2}\tilde{\phi}^t \tilde{V}^{-1}\tilde{\phi} - \chi^\dagger \left(M M^\dagger\right)^{-1} \chi - \frac{1}{2}\pi^t \pi}
\end{aligned}
$$

Effective Hamiltonian:

$$
\mathcal{H} = \frac{1}{2}\tilde{\phi}^t \tilde{V}^{-1}\tilde{\phi} + \chi^\dagger \left(M M^\dagger\right)^{-1} \chi + \frac{1}{2}\pi^t \pi
$$

Exact form of M

Pure backward differencing:

$$M_{(x,t)(y,t')} = \delta_{xy}\left(\delta_{tt'} - \delta_{t-1,t'}\left(\mathrm{e}^{-\mathrm{i}\,\tilde{\phi}_{x,t}} - \tilde{m}_s\right)\right) - \tilde{\kappa}\delta_{\langle x,y\rangle}\delta_{tt'}$$

Mixed differencing:

$$\begin{aligned} M^{AA}_{(x,t)(y,t')} &= \delta_{xy}\left(\delta_{t+1,t'} - \delta_{tt'}\left(\mathrm{e}^{-\mathrm{i}\,\tilde{\phi}_{x,t}} + \tilde{m}_s\right)\right) \\ M^{BB}_{(x,t)(y,t')} &= \delta_{xy}\left(\delta_{tt'} - \delta_{t-1,t'}\left(\mathrm{e}^{-\mathrm{i}\,\tilde{\phi}_{x,t}} - \tilde{m}_s\right)\right) \\ M^{AB}_{(x,t)(y,t')} = M^{BA}_{(x,t)(y,t')} &= -\tilde{\kappa}\delta_{\langle x,y\rangle}\delta_{tt'}\ , \end{aligned}$$

$$\tilde{a} := \delta \cdot a$$

Equations of motion

$$\dot{\phi}^T = \frac{\partial \mathcal{H}}{\partial \pi} = \pi^T$$
$$\dot{\pi}^T = -\frac{\partial \mathcal{H}}{\partial \phi} = -\phi^T \frac{1}{\delta U} + 2\,\mathrm{Re}\left(\eta^\dagger \frac{\partial M}{\partial \phi} \xi\right)$$

with the two complex vector fields

$$\eta = \left(M M^\dagger\right)^{-1} \chi\,, \quad \xi = M^\dagger \eta$$

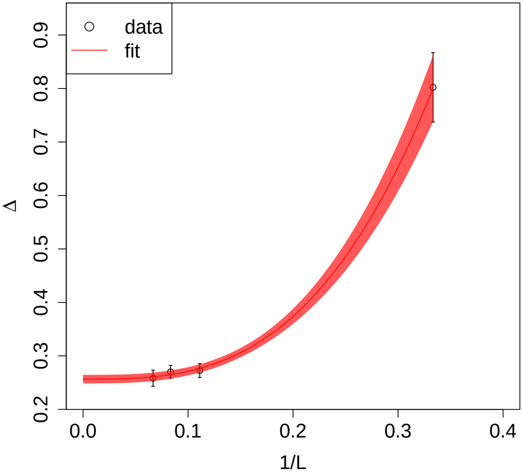
Forces with n staggered masses

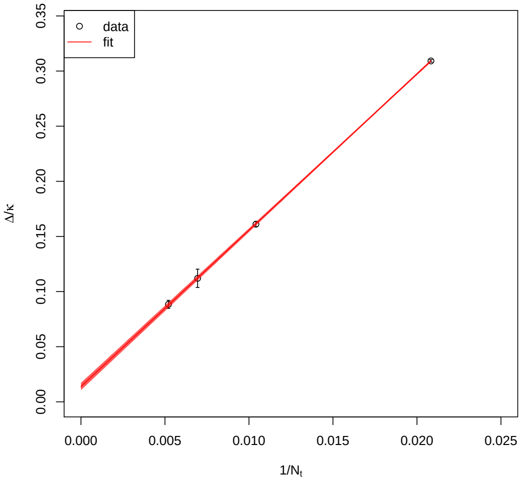
$$\begin{aligned}
\dot{\pi}^T &= F_\phi + \sum_{i=0}^{n} F_{\chi_i} \\
F_\phi &= -\delta\phi^T V^{-1} \\
F_{\chi_n} &= 2\,\mathrm{Re}\left(\eta_n^\dagger \frac{\partial M}{\partial \phi} \xi_n\right) \\
F_{\chi_i} &= 2\,\mathrm{Re}\left(\eta_i^\dagger \frac{\partial M}{\partial \phi} \left(\xi_i - \chi_i\right)\right) \quad \text{for } i < n
\end{aligned}$$

with

$$\begin{aligned}
\eta_i &= \left(M_{\mu_{i-1}} M_{\mu_{i-1}}^\dagger\right)^{-1} M_{\mu_i} \chi_i \\
\xi_i &= M_{\mu_{i-1}}^\dagger \eta_i = M_{\mu_{i-1}}^{-1} M_{\mu_i} \chi_i
\end{aligned}$$

Thermodynamic and continuum limits





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