Lattice Monte Carlo for carbon nanostructures

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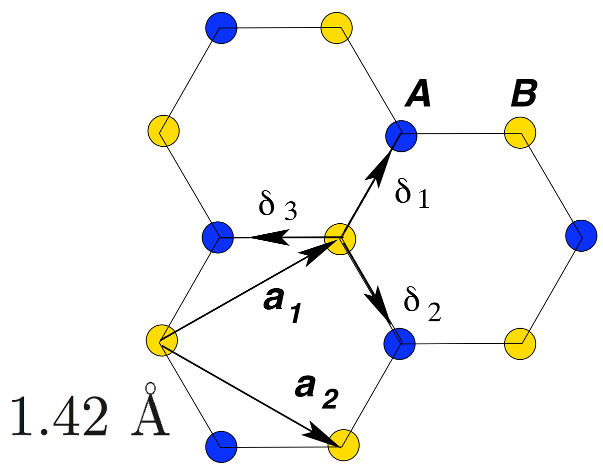
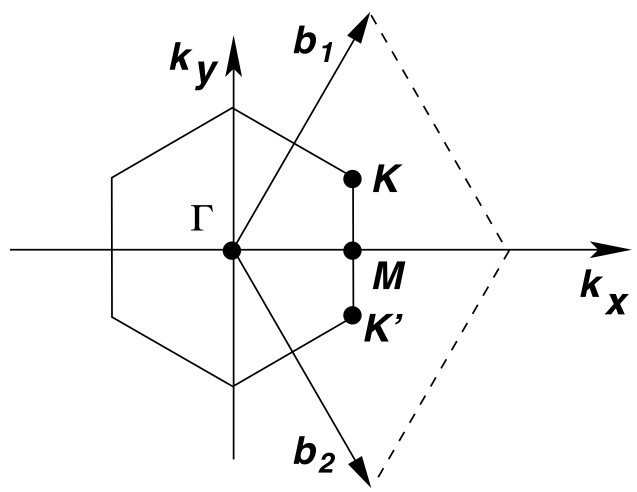
Advanced Numerical Algorithms for strongly correlated Quantum Systems
International Conference, Würzburg, Germany, February 23-26, 2015

Outline

- **Dirac theory of graphene**
  - Lattice Gauge Field Theory
  - Critical coupling for gap formation
  - Renormalization of the Fermi velocity
- **Hexagonal Hubbard theory of graphene**
  - Auxiliary-field Quantum Monte Carlo
  - Realistic electron-electron interaction in graphene
  - Extension to carbon nanotubes

Tight-binding and Dirac descriptions of graphene ...





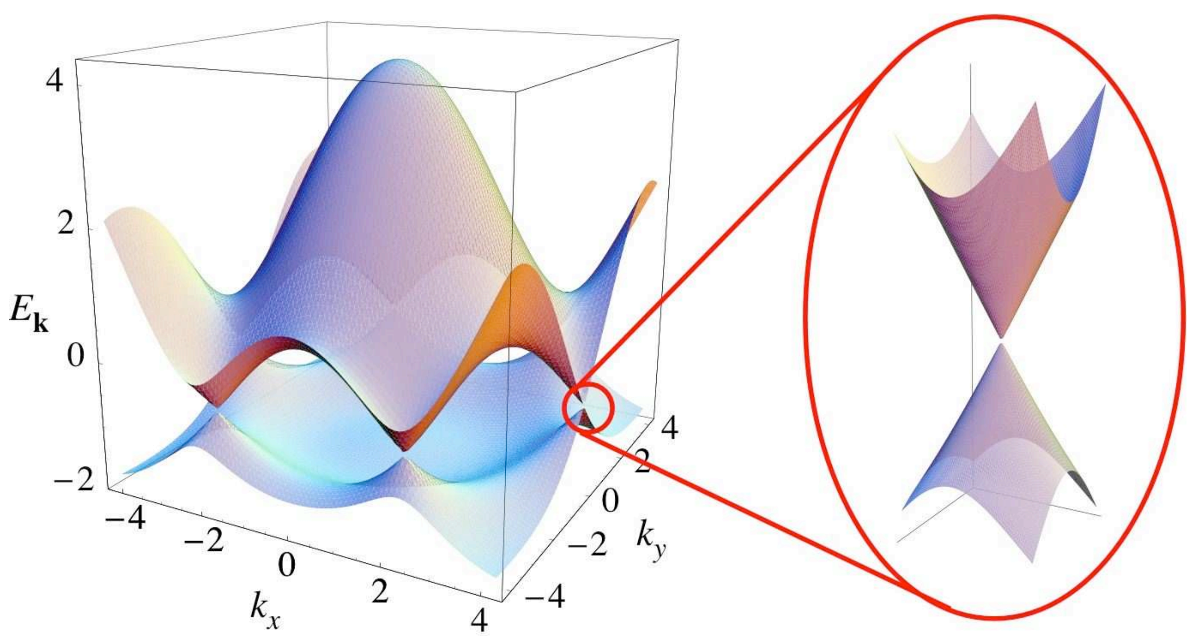
for a review,
see e.g. A. H. Castro Neto et al., …

$$-\,t \sum_{\langle x,y\rangle,s} (a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s})$$

$$t \approx 2.8\ \mathrm{eV}$$

Should we work with this?

$$E_\pm(\mathbf{k}) = \pm t\sqrt{3 + f(\mathbf{k})}$$
$$f(\mathbf{k}) = 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_x a\right)$$



$$\boldsymbol{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right) \quad \boldsymbol{K}' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right)$$

$$\mathbf{k} = \mathbf{K} + \mathbf{q}$$

$$E_\pm(\mathbf{q}) \approx \pm v_F|\mathbf{q}| + \mathcal{O}((q/K)^2)$$

$$v_F = 3ta/2 \simeq 1 \times 10^6\ \mathrm{m/s}$$

Or with the Dirac theory?

"QED for graphene"

G. Semenoff, Phys. Rev. Lett. **54**, 2449 (1984)

J. E. Drut, D. T. Son, Phys. Rev. B **77**, 075115 (2008)

$$\mathcal{Z} = \int \mathcal{D}A_0 \mathcal{D}\psi \mathcal{D}\bar{\psi} \exp(-S_E[\bar{\psi}_a, \psi_a, A_0])$$

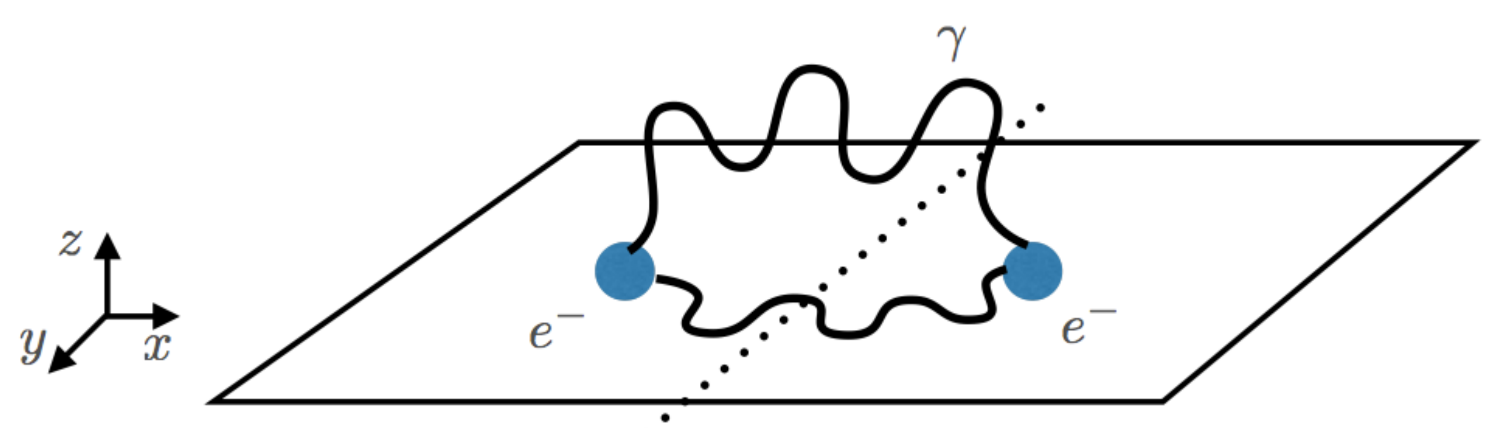
$$S_E = -\sum_{a=1}^{N_f} \int d^2x\, dt\, \bar{\psi}_a\, D[A_0]\, \psi_a + \frac{1}{2g^2} \int d^3x\, dt\, (\partial_i A_0)^2$$

$$D[A_0] = \gamma_0(\partial_0 + iA_0) + v\gamma_i\partial_i, \quad i = 1, 2$$

$$\mathcal{Z} = \int \mathcal{D}A_0 \exp(-S_{\text{eff}}[A_0])$$

$$g^2 = e^2/\epsilon_0$$

$$\alpha_g \equiv \frac{e^2}{4\pi\epsilon_0 \hbar v} \simeq 300\alpha \sim 1$$



"Lattice QCD for graphene"

J. E. Drut, T. A. Lähde,
*Phys. Rev. B **79**, (2009) 165425,*
*Phys. Rev. Lett. **102**, (2009) 026802,*
also S. Hands et al. (contact interaction, Thirring) …

Monte Carlo probability density

$$P[\theta] \equiv \exp(-S_{\mathrm{eff}}[\theta]) = \det(K[\theta])\exp(-S_E^g[\theta])$$

Non-compact gauge action (as in Lattice QED)

$$S_{E,N}^g = \frac{\beta}{2}\sum_{\mathbf{n}}\sum_{i=1}^{3}(\theta_{\mathbf{n}+\mathbf{e}_i} - \theta_{\mathbf{n}})^2 \qquad \beta \equiv v_F/g^2 = 1/(4\pi\alpha_g)$$

"Staggered" (Kogut-Susskind) fermions

$$K_{\mathbf{n},\mathbf{m}}[\theta] = \frac{1}{2}(\delta_{\mathbf{n}+\mathbf{e}_0,\mathbf{m}}U_{\mathbf{n}} - \delta_{\mathbf{n}-\mathbf{e}_0,\mathbf{m}}U_{\mathbf{m}}^{\dagger}) + \frac{v}{2}\sum_i \eta_{\mathbf{n}}^i(\delta_{\mathbf{n}+\mathbf{e}_i,\mathbf{m}} - \delta_{\mathbf{n}-\mathbf{e}_i,\mathbf{m}}) + m_0\delta_{\mathbf{n},\mathbf{m}}$$

$$U_{0,\mathbf{n}} = U_{\mathbf{n}} \equiv \exp(i\theta_{\mathbf{n}})$$

$$\eta_{\mathbf{n}}^0 = 1,$$

$$\eta_{\mathbf{n}}^1 = (-1)^{n_0},$$

$$\eta_{\mathbf{n}}^2 = (-1)^{n_0+n_1}$$

Monte Carlo calculation

$$p \equiv \frac{P[\theta']}{P[\theta]} = \exp(-\Delta S) \qquad \Delta S = S_{\mathrm{eff}}[\theta'] - S_{\mathrm{eff}}[\theta]$$

$$H = \sum_{\mathbf{n}} \frac{\pi_{\mathbf{n}}^2}{2} + S_E[\theta]$$

Hybrid Monte Carlo (HMC)
"evolution Hamiltonian"

$$\det(Q) \propto \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \, \exp(-S_E^p)$$

"Pseudofermion" action:
(optional) stochastic treatment
of det(Q)

$$S_E^p = \sum_{\mathbf{n},\mathbf{m}} \phi_{\mathbf{n}}^\dagger Q_{\mathbf{n},\mathbf{m}}^{-1}[\theta] \phi_{\mathbf{m}} = \sum_{\mathbf{n}} \xi_{\mathbf{n}}^\dagger \xi_{\mathbf{n}} \qquad Q \equiv K^\dagger K$$

$$\phi = K^\dagger \xi$$

$$K = \begin{pmatrix} m_0 & K_{oe} \\ K_{eo} & m_0 \end{pmatrix} \qquad Q = \begin{pmatrix} K_{eo}^\dagger K_{oe} + m_0^2 & 0 \\ 0 & K_{oe}^\dagger K_{eo} + m_0^2 \end{pmatrix}$$

Putting all the pieces together:

Hybrid Monte Carlo "equations of motion" ...

$$H = \sum_{\mathbf{n}} \frac{\pi_{\mathbf{n}}^2}{2} + S_E^g + S_E^p$$

$$\dot{\theta}_{\mathbf{n}} = \frac{\delta H}{\delta \pi_{\mathbf{n}}} = \pi_{\mathbf{n}}$$

$$\dot{\pi}_{\mathbf{n}} = -\frac{\delta H}{\delta \theta_{\mathbf{n}}} \equiv F_{\mathbf{n}}^g + F_{\mathbf{n}}^p$$

$$F_{\mathbf{n}}^g \equiv -\frac{\delta S_E^g}{\delta \theta_{\mathbf{n}}} = -\frac{1}{g^2} \sum_{j=1}^{3} \Im(U_{\mathbf{n}} U_{\mathbf{n}+\mathbf{e}_j}^\dagger - U_{\mathbf{n}-\mathbf{e}_j} U_{\mathbf{n}}^\dagger)$$

$$= -\frac{1}{g^2} \left[6\theta_{\mathbf{n}} - \sum_{j=1}^{3} (\theta_{\mathbf{n}+\mathbf{e}_j} + \theta_{\mathbf{n}-\mathbf{e}_j}) \right] + \cdots$$

$$F_{\mathbf{n}}^p = -\frac{\delta S_E^p}{\delta \theta_{\mathbf{n}}} = \phi^\dagger Q^{-1} \frac{\delta Q}{\delta \theta_{\mathbf{n}}} Q^{-1} \phi$$

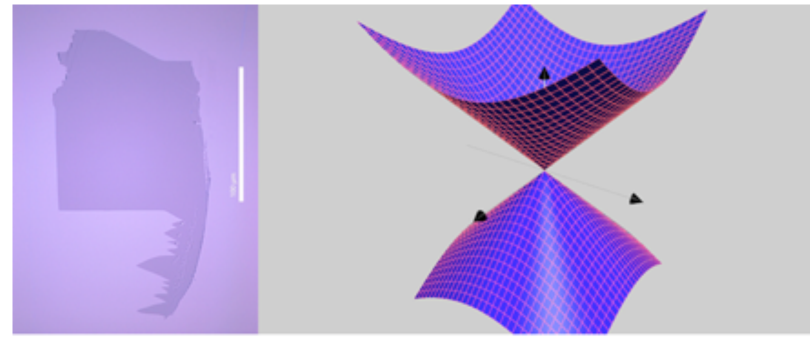
Most of the CPU time
is used here

Interaction-induced gap (semimetal-insulator transition)?

Coulomb interaction is stronger in suspended graphene ...

On a SiO_2 substrate

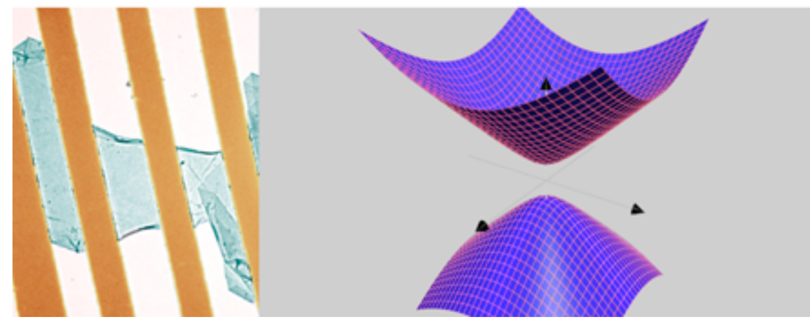
$\alpha_g \sim 0.80$



Semimetallic
(conducting) phase

Suspended graphene

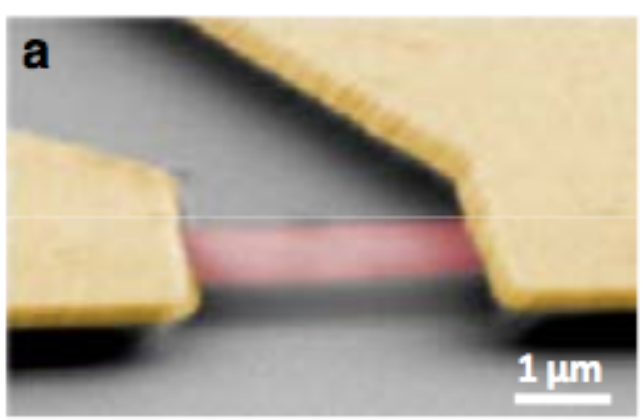
$\alpha_g \sim 2.16$

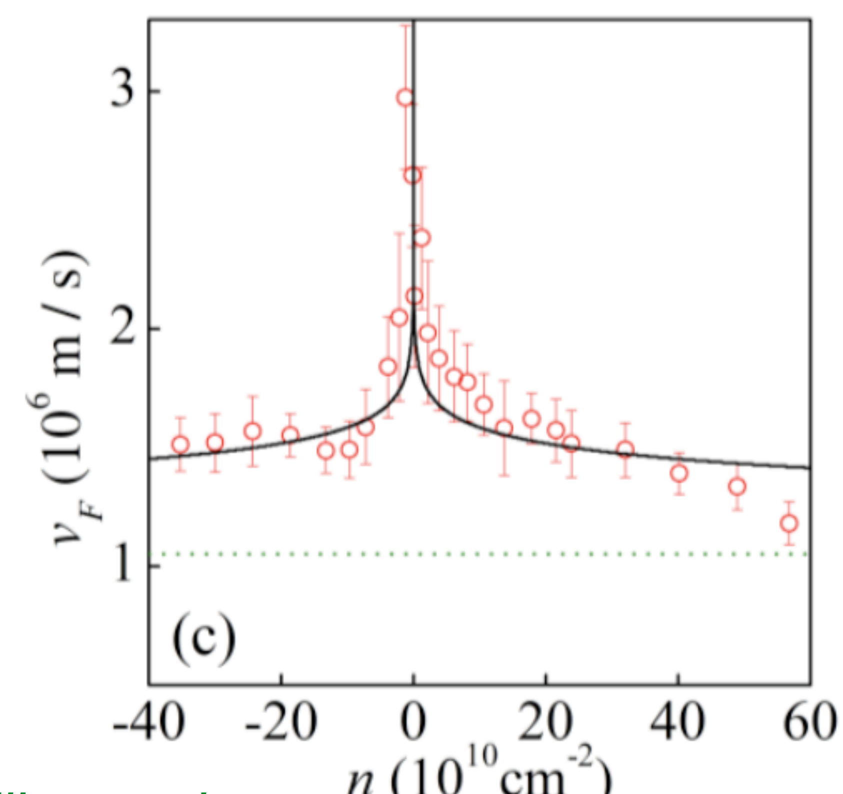


Gapped
(insulating) phase

Interaction-induced velocity renormalization?

Observed especially in suspended graphene ...





D. C. Elias et al.,
Nature Phys. ***7****, (2011) 701*

Lattice Monte Carlo calculation of the critical coupling

Chiral condensate and susceptibility ...

$$\sigma \equiv \langle \bar{\psi}_b \psi_b \rangle$$

Order parameter for spontaneous gap generation

$$\sigma = \frac{1}{V\mathcal{Z}} \int \mathcal{D}A_0 \mathcal{D}\psi \mathcal{D}\bar{\psi} \int dx \bar{\psi}_b(x) \psi_b(x) \exp(-S_E) = \frac{1}{V} \frac{\partial \ln \mathcal{Z}}{\partial m_0}$$

$$\sigma = \frac{1}{V\mathcal{Z}} \int \mathcal{D}A_0 \mathrm{Tr}(D^{-1}[A_0]) \exp(-S_{\mathrm{eff}}[A_0]) = \frac{1}{V} \langle \mathrm{Tr}(D^{-1}[A_0]) \rangle$$

$$\chi_l \equiv \frac{\partial \sigma}{\partial m_0} = \frac{1}{V} [\langle \mathrm{Tr}^2(D^{-1}) \rangle - \langle \mathrm{Tr}(D^{-2}) \rangle - \langle \mathrm{Tr}(D^{-1}) \rangle^2]$$

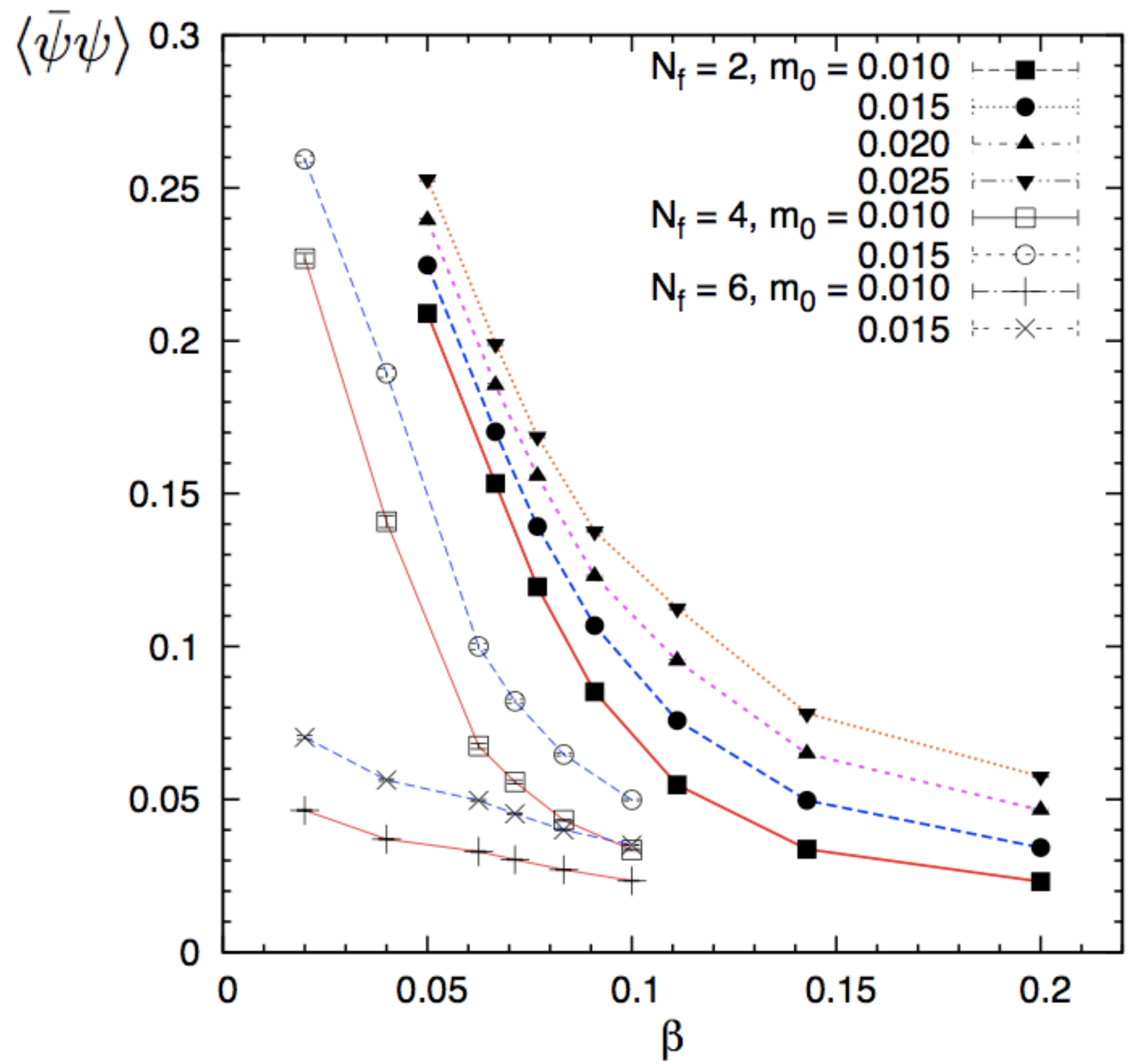
Stochastic calculation using gauge field configurations generated by HMC

Chiral condensate (Metropolis algorithm)

First results on small lattices (L = 16 cube)

- $N_f = 2$
  Possible transition below $\beta \sim 0.10$
- $N_f = 4$
  Possible transition below $\beta \sim 0.05$
- $N_f = 6$
  No transition observed

$4 < N_{crit} < 6$

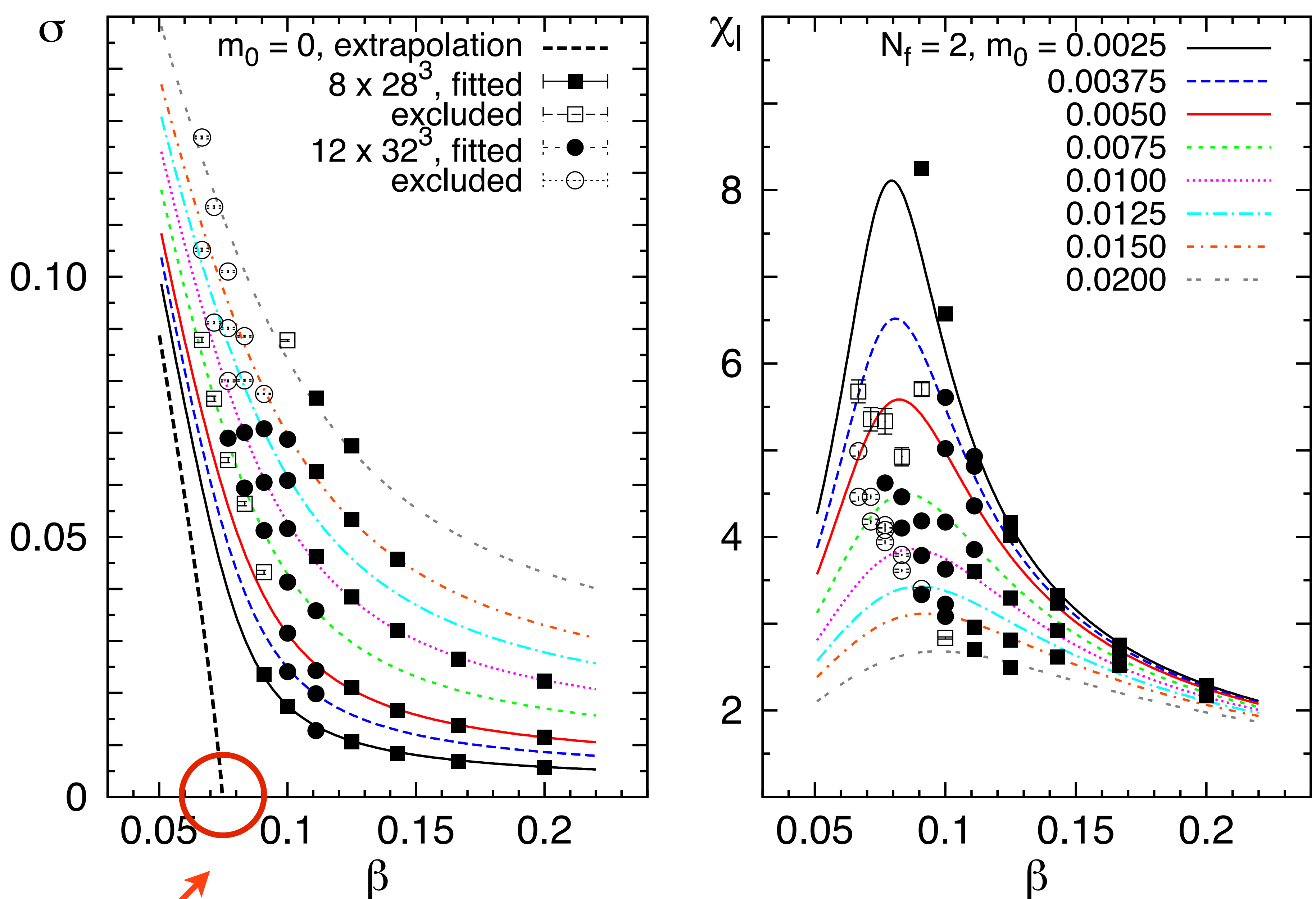


J. E. Drut, T. A. Lähde, Phys. Rev. Lett. **102**, (2009) 026802

Lattice Monte Carlo data using the HMC algorithm

Note that $\beta \equiv v_F/g^2 = 1/(4\pi\alpha_g)$

J. E. Drut, T. A. Lähde,
*Phys. Rev. B **79**, (2009) 241405(R)*



$\beta_c \sim 0.073$

$\alpha_c \sim 1.1$

Analytical calculation (preliminary)
Milletari and Adam, arXiv:1406.6113
suggests critical coupling of 4/pi?

Lattice calculation (attempt :) of the Fermi velocity

Temporal and spatial fermion correlators ...

W. Armour et al.,
*Phys. Rev. B **84**, (2011) 075123*

J. E. Drut, T. A. Lähde,
PoS (Lattice 2013) 498

$$C_f(x,y,t) \equiv \langle \chi(x,y,t)\bar{\chi}(x_0,y_0,t_0)\rangle$$

$$C_{ft}(p_1,p_2,t) \equiv \sum_{x,y} \exp(-ip\cdot x)\, C_f(x,y,t)$$

$$C_{fx}(p_0,p_2,t) \equiv \sum_{t,y} \exp(-ip\cdot x)\, C_f(x,y,t)$$

$$p_0 = \frac{2\pi(n-1/2)}{N_t}, \quad n = 0,\ldots,N_t/4$$

$$p_1 = \frac{2\pi n}{N_x}, \quad p_2 = \frac{2\pi n}{N_x}, \quad n = 0,\ldots,N_x/4$$

Problems:
I) Correlators not gauge invariant
II) Correlators are complex-valued

$$K_{\mathbf{n},\mathbf{m}}[\theta_0] = \frac{1}{2a}(\delta_{\mathbf{n}+\mathbf{e}_0,\mathbf{m}} U_{0,\mathbf{n}} - \delta_{\mathbf{n}-\mathbf{e}_0,\mathbf{m}} U^\dagger_{0,\mathbf{m}}) + \frac{\lambda}{2a}\sum_i \eta^i_{\mathbf{n}}(\delta_{\mathbf{n}+\mathbf{e}_i,\mathbf{m}} - \delta_{\mathbf{n}-\mathbf{e}_i,\mathbf{m}}) + m_0\,\delta_{\mathbf{n},\mathbf{m}}$$

For U = I, (no interaction)
the correlators can be computed analytically

Analysis of Monte Carlo data at strong coupling ...

J. E. Drut, T. A. Lähde, PoS (Lattice 2013) 498, Schierholz et al., …

$$t = 0, 2, \ldots, N_t - 2$$

$$C^R_{ft}(t, p_1, p_2) = Z_R G_t(p_1, p_2)$$

Staggered fermion "sawtooth" correlator

$$t = 1, 3, \ldots, N_t - 1$$

$$C^R_{ft}(t, p_1, p_2) = -\frac{Z_R}{2m_R}\left[\exp(iB_0)\, G_{t+1}(p_1, p_2) - \exp(-iB_0)\, G_{t-1}(p_1, p_2)\right]$$

$$G_t(p_1, p_2) \equiv \frac{N}{C^2(\mu_t) - B^2(B_0)}$$
$$\times \Big[A(B_0)C(\mu_t)\cos(B_0 t^\star)\sinh(\mu_t t^\star) + B(B_0)D(\mu_t)\sin(B_0 t^\star)\cosh(\mu_t t^\star)$$
$$+ iA(B_0)C(\mu_t)\sin(B_0 t^\star)\sinh(\mu_t t^\star) - iB(B_0)D(\mu_t)\cos(B_0 t^\star)\cosh(\mu_t t^\star)\Big]$$

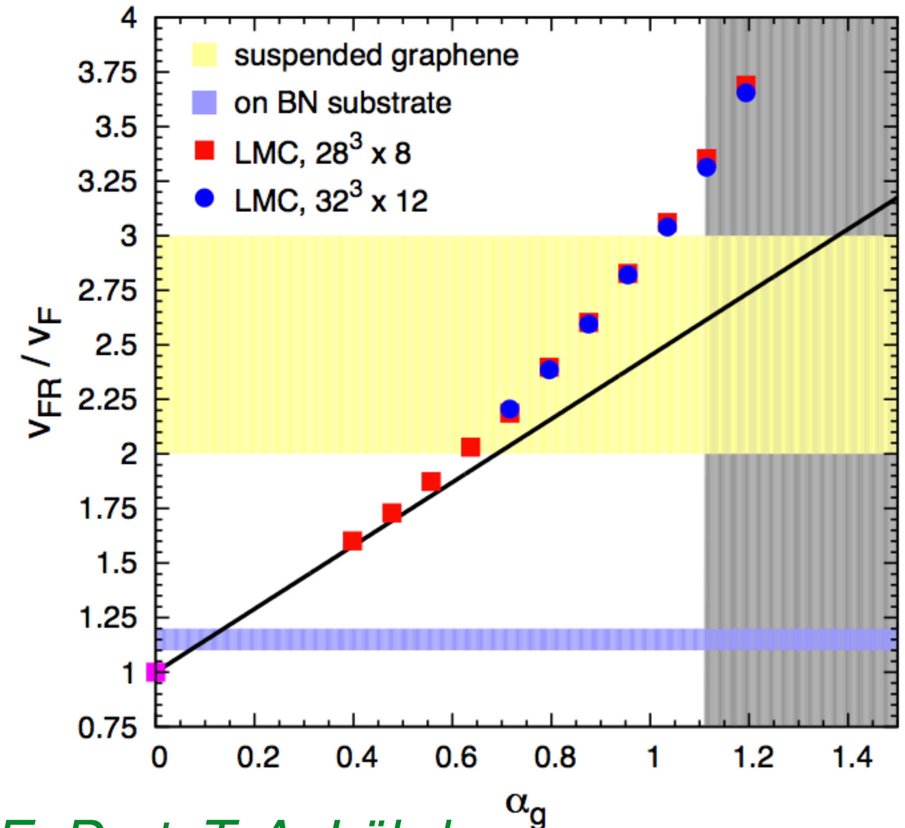
$$\sinh^2(\mu_t) \equiv m_R^2 + \lambda_R^2 \sin^2(p_1) + \lambda_R^2 \sin^2(p_2)$$

"Renormalized" dispersion relation

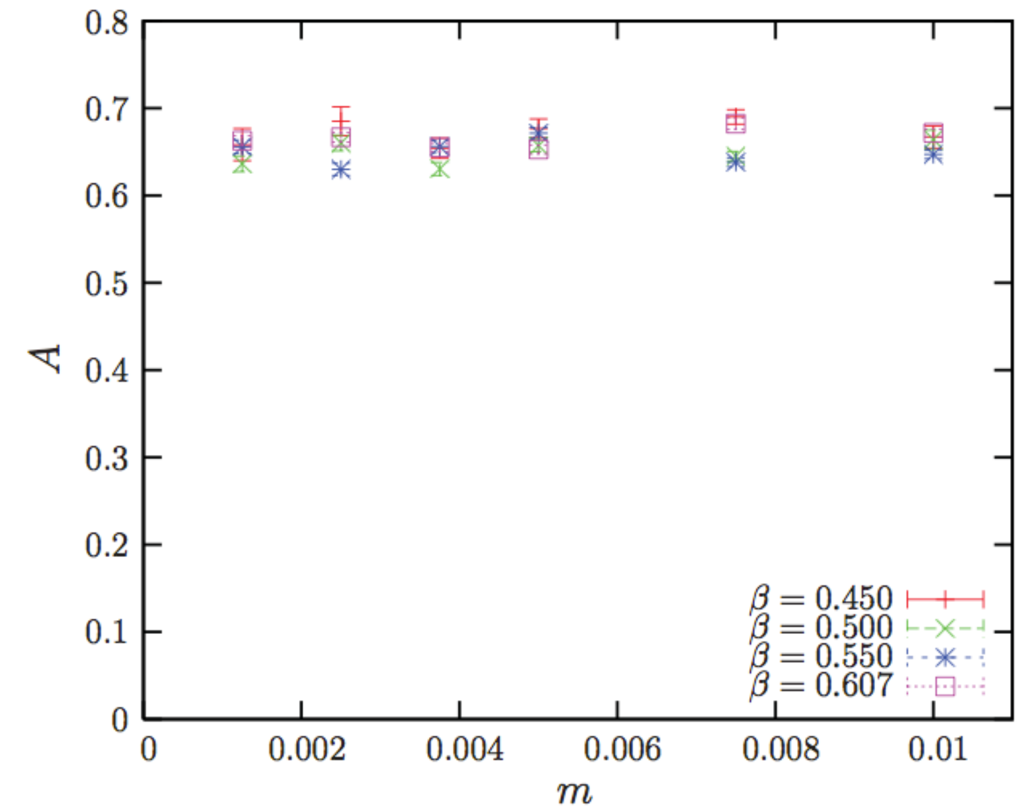
$$\lambda_R \equiv v_{FR}(a/a_x)_R$$

Unfortunately: Lattice spacing anisotropy mixed in!

Still need to separate the lattice spacing anisotropy ...



J. E. Drut, T. A. Lähde,
PoS (Lattice 2013) 498



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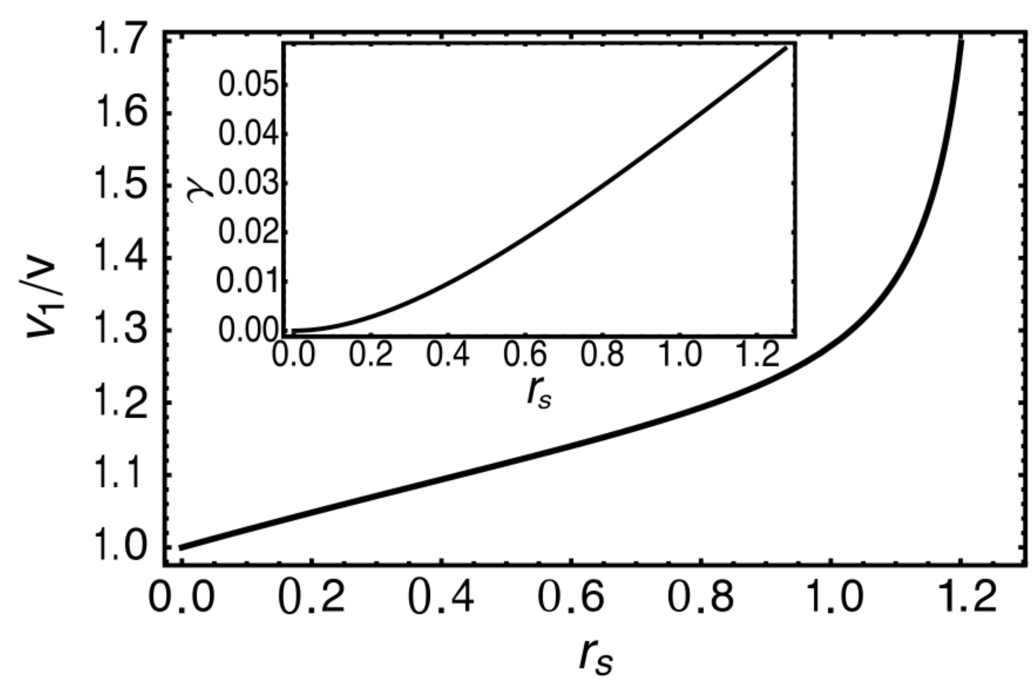


Alternative:

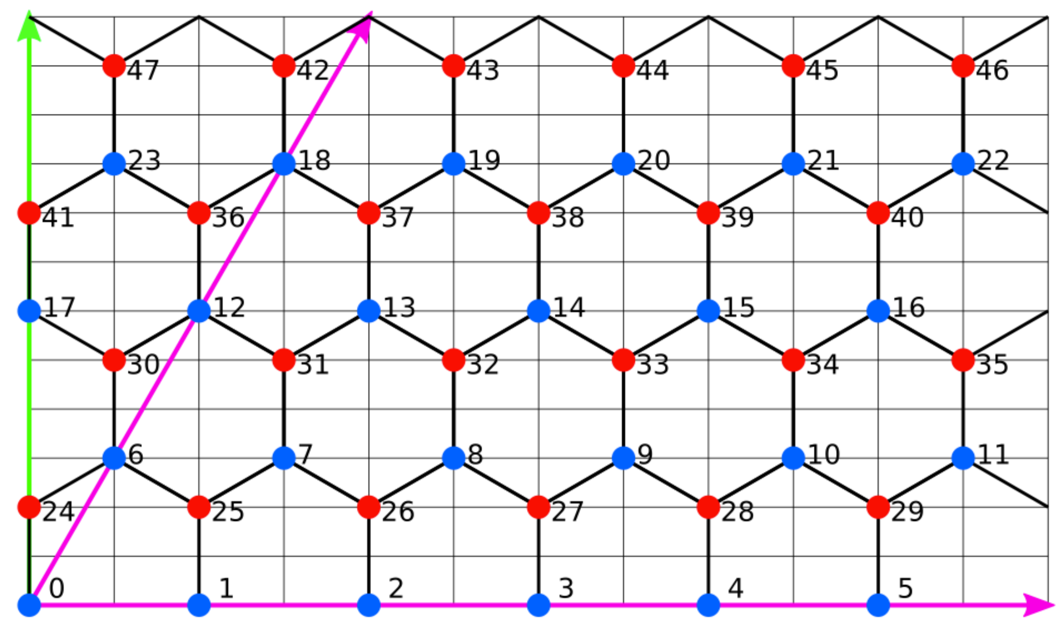
Hexagonal Hubbard Model for graphene …

Paiva et al., Assaad et al., Sorella et al., Brower et al., Buividovich et al., von Smekal et al., …

$$-\kappa \sum_{\langle x,y\rangle,s} (a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s}) + \frac{1}{2}\sum_{x,y} q_x V_{xy} q_y + \sum_x m_s (a^\dagger_{x,+1} a_{x,+1} + a_{x,-1} a^\dagger_{x,-1})$$

$$q_x = a^\dagger_{x,1} a_{x,1} + a^\dagger_{x,-1} a_{x,-1} - 1$$

$$m_s = \begin{cases} +m\,, & x \in A \\ -m\,, & x \in B \end{cases}$$



$$a_x = a_{x,1}, a^\dagger_x = a^\dagger_{x,1}, b^\dagger_x = a_{x,-1}, b_x = a^\dagger_{x,-1} \qquad q_x = a^\dagger_x a_x - b^\dagger_x b_x$$

$$b_x, b^\dagger_x \longrightarrow -b_x, -b^\dagger_x \quad \forall x \in B$$

$$H = \sum_{\langle x,y\rangle} (-\kappa)(a^\dagger_x a_y - b^\dagger_x b_y + \text{h.c.}) + \frac{1}{2}\sum_{x,y} q_x V_{xy} q_y + \sum_x m_s (a^\dagger_x a_x + b^\dagger_x b_x)$$

Again, very similar to Lattice QCD ...

$$Z = \mathrm{Tr}\, e^{-\beta H} \qquad \beta = 1/k_B T$$

$$e^{-\beta H} = e^{-\delta H}\, e^{-\delta H} \ldots e^{-\delta H} \quad (\delta = \beta/N_t)$$

Discrete Euclidean time evolution

$$\exp\left(-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y} Q_{x,t+1,t} V_{xy} Q_{y,t+1,t}\right) \propto$$

$$\int \mathcal{D}\phi\, \exp\left(-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t} V_{xy}^{-1}\phi_{y,t} - i\,\delta\sum_{t=0}^{N_t-1}\sum_{x}\phi_{x,t} Q_{x,t+1,t}\right)$$

Hubbard-Stratonovich auxiliary field

$$\mathrm{Tr}\, e^{-\beta H} = \int \mathcal{D}\phi\, \det\left[M(\phi)M^{\dagger}(\phi)\right]\exp\left(-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}V_{xy}^{-1}\phi_{y,t}\right)$$

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - e^{-i\frac{\beta}{N_t}\phi_{x,t}}\delta_{t-1,t'}) - \kappa\frac{\beta}{N_t}\sum_{\vec{n}}\delta_{y,x+\vec{n}}\delta_{t-1,t'} + m_s\frac{\beta}{N_t}\delta_{xy}\delta_{t-1,t'}$$

"non-compact gauge action" + fermion determinant with "gauge links"

What options do we have for the potential?

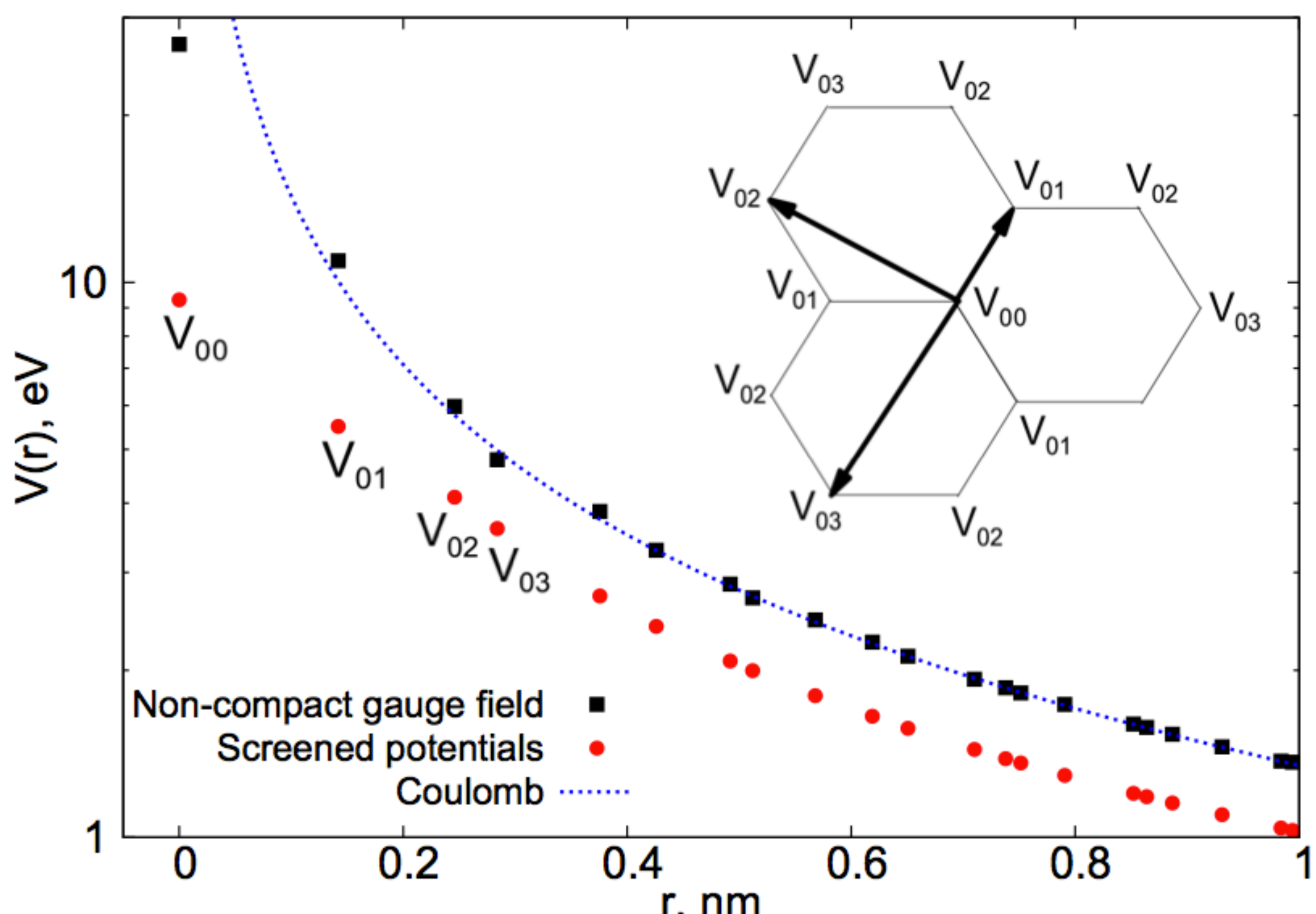
T. O. Wehling et al., Phys. Rev. Lett. ***106****, (2011) 236805*

$$\hat{H}_0 = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} - t' \sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle,\sigma} c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + U_{00} \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} + \frac{1}{2} \sum_{\mathbf{i}\neq\mathbf{j},\sigma,\sigma'} U_{\mathbf{i}\mathbf{j}} n_{\mathbf{i},\sigma} n_{\mathbf{j},\sigma'},$$

Microscopic *ab initio* (DFT) calculation of the interaction coefficients

Potential from the non-compact gauge field
(can be integrated out!)

"Screened" potential
matched to
the coefficients of Wehling *et al.*



M. V. Ulybyshev et al., Phys. Rev. Lett. ***111****, (2013) 056801*

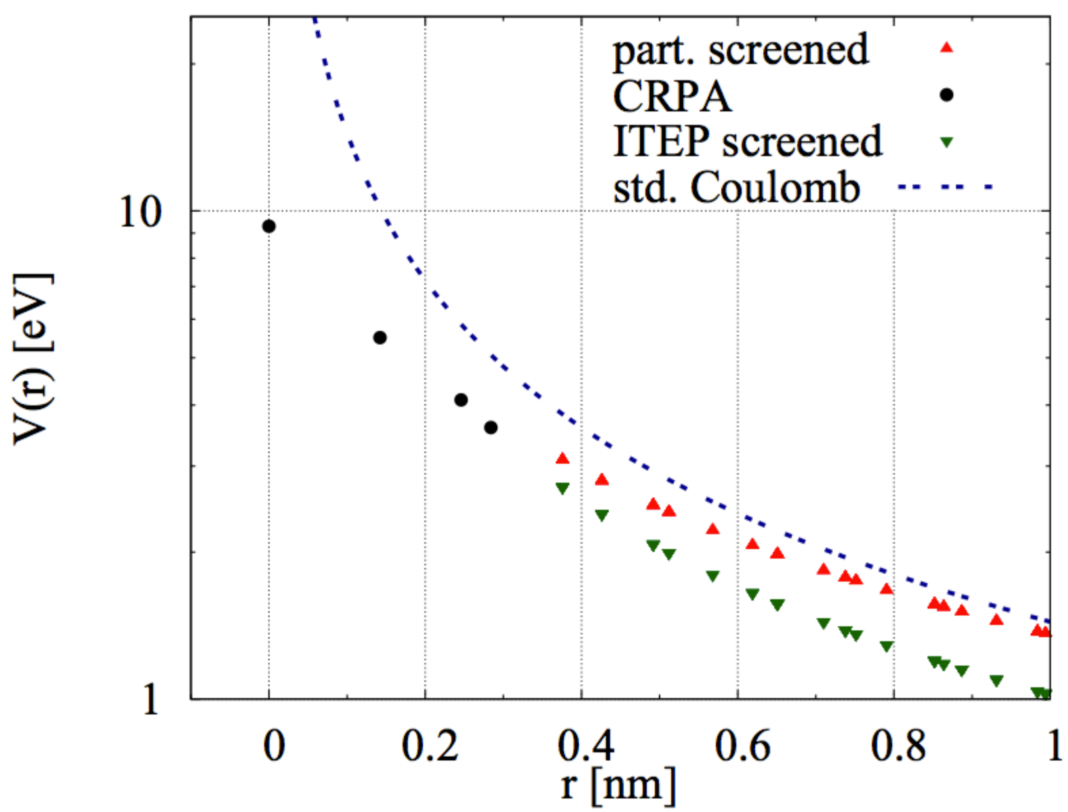
What happens to the semimetal-insulator transition?

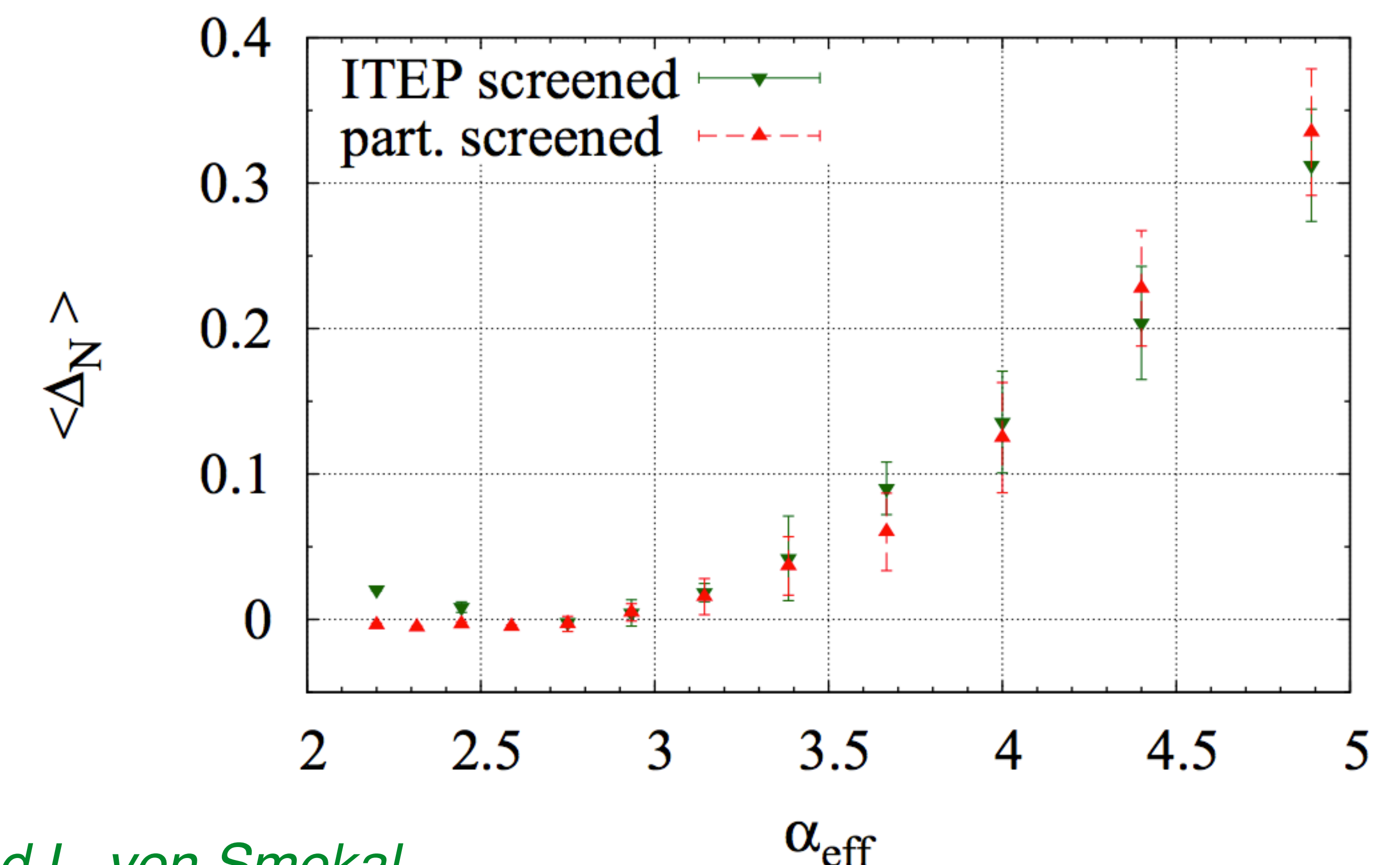
$$\Delta_N = n_A - n_B$$
$$= \frac{1}{L_x L_y}\left[\sum_{x\in X_A}(a_x^\dagger a_x + b_x^\dagger b_x) - \sum_{x\in X_B}(a_x^\dagger a_x + b_x^\dagger b_x)\right]$$

I) Potential from the non-compact gauge field (agrees with Dirac calculation)

$$\alpha_c = 0.9 \pm 0.2$$

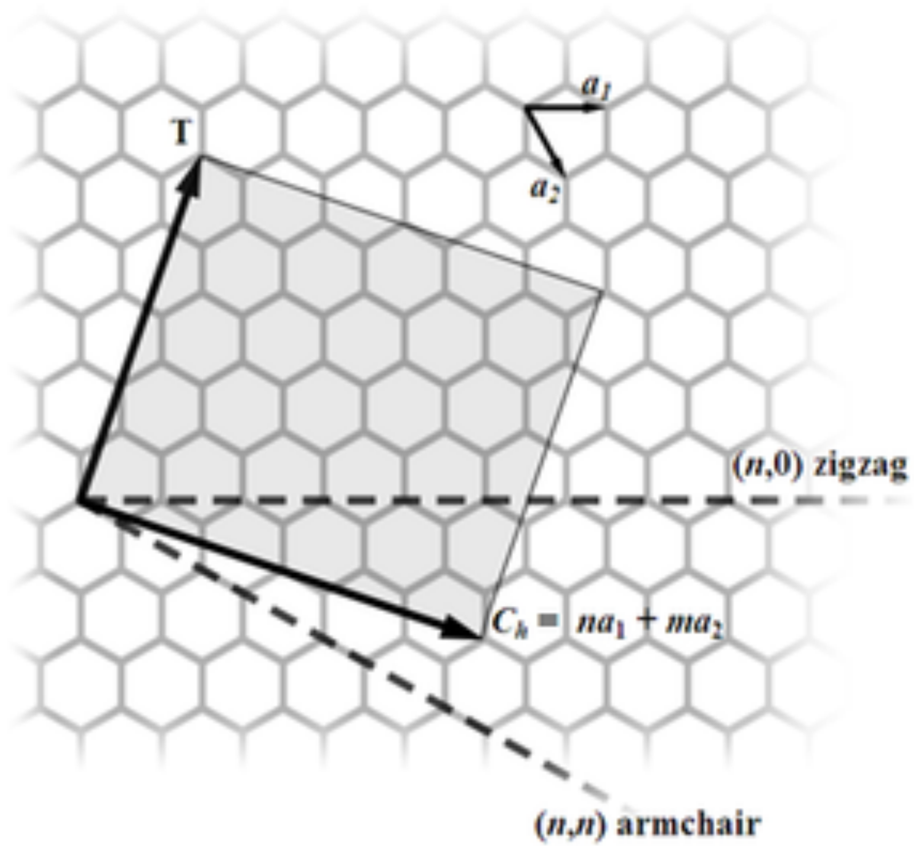
II) Using the Wehling *et al.* potential the transition is shifted to $\alpha_c = 3$

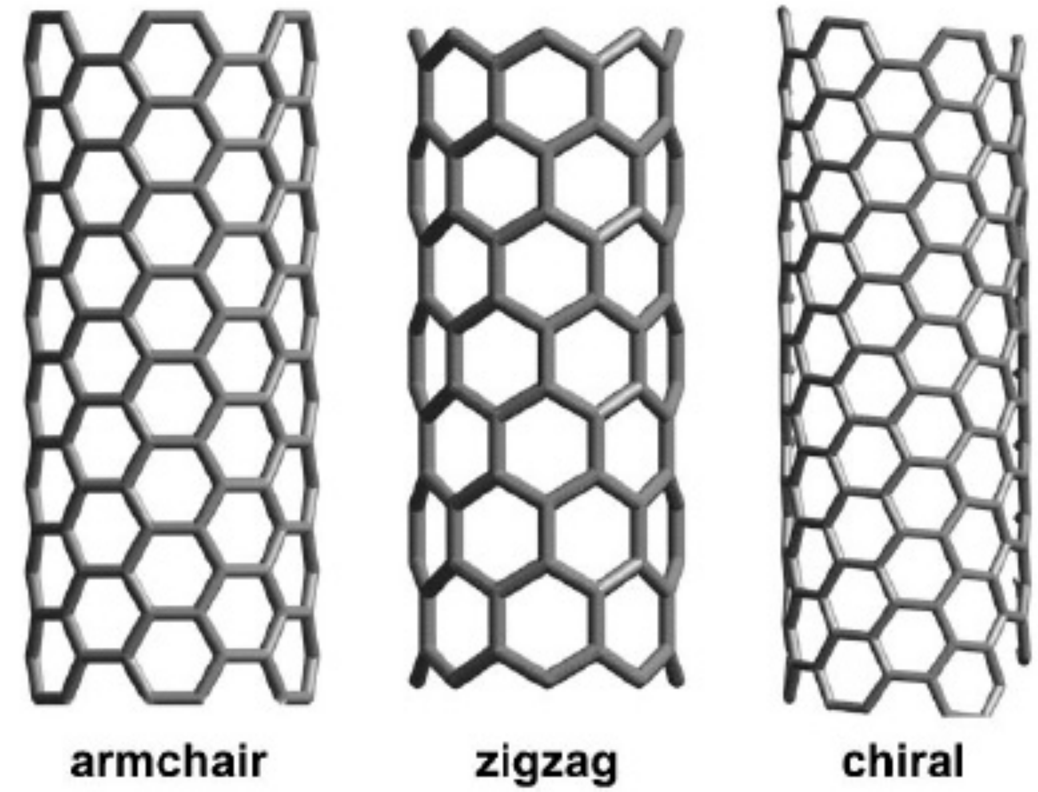




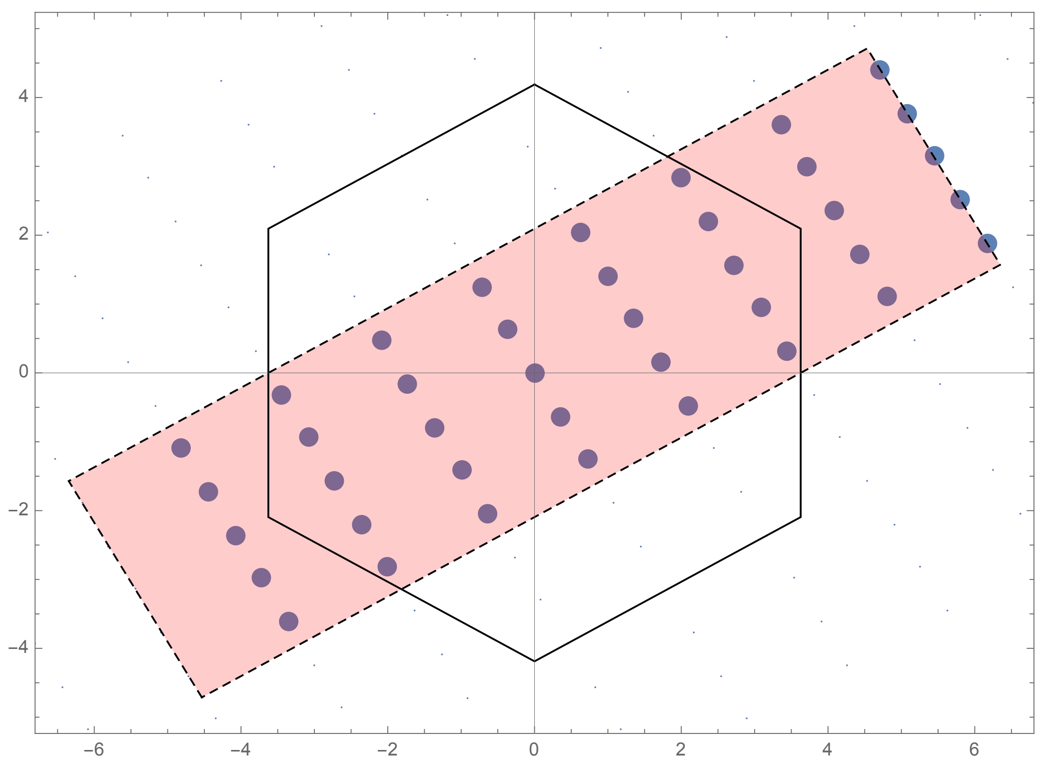
*D. Smith and L. von Smekal, Phys. Rev. B **89**, (2014) 195429*

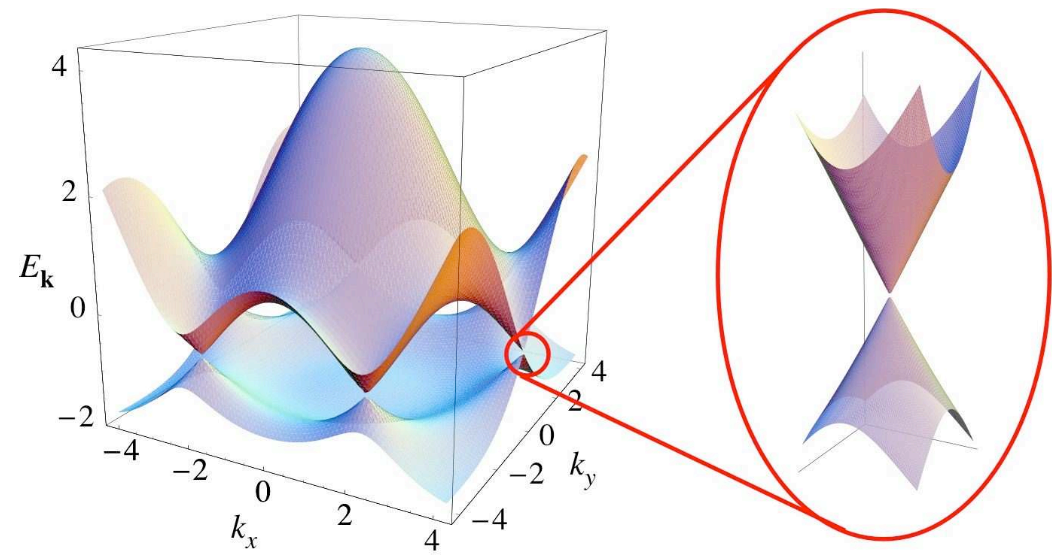
Let's apply this to Carbon Nanotubes!



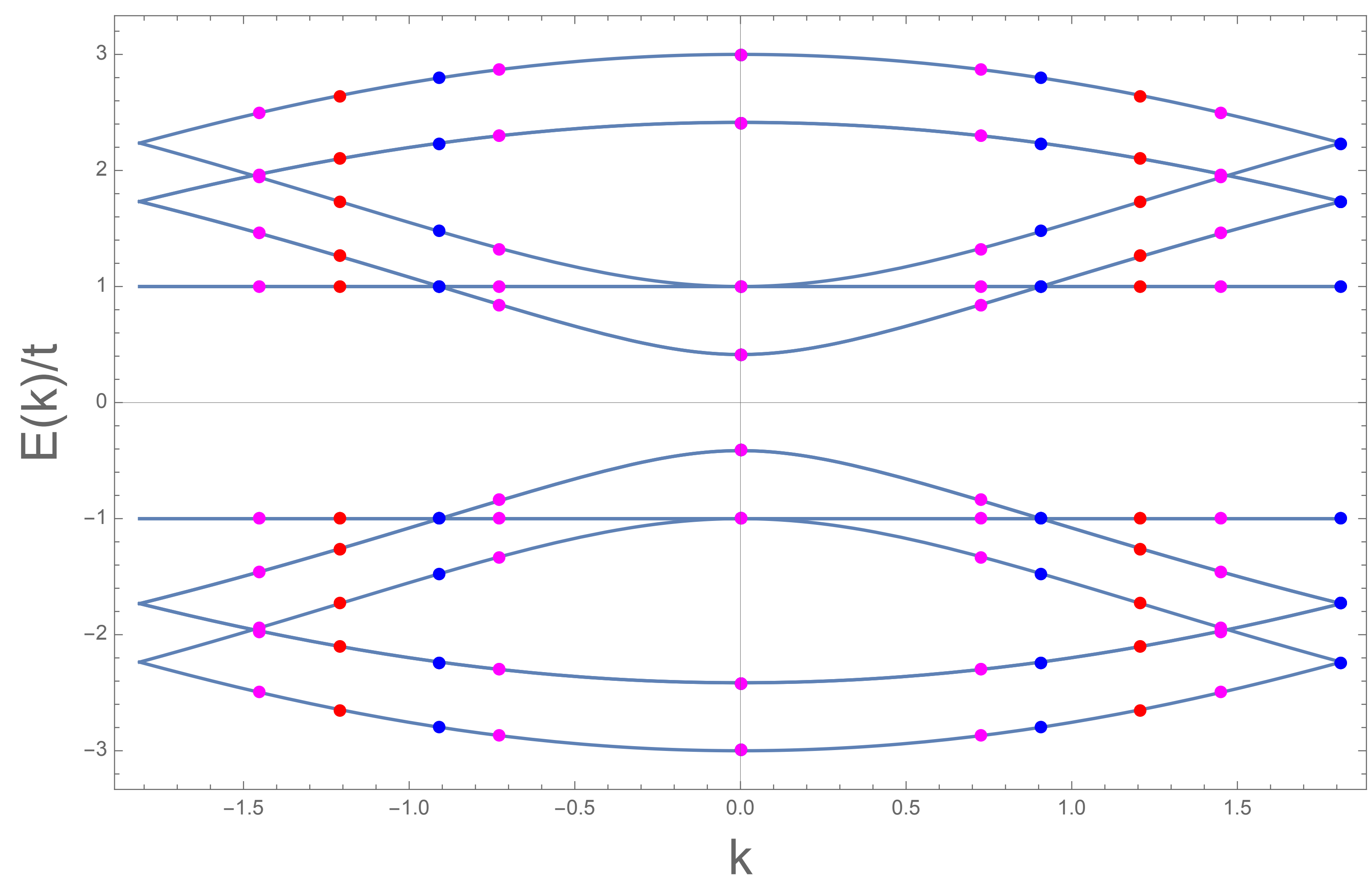


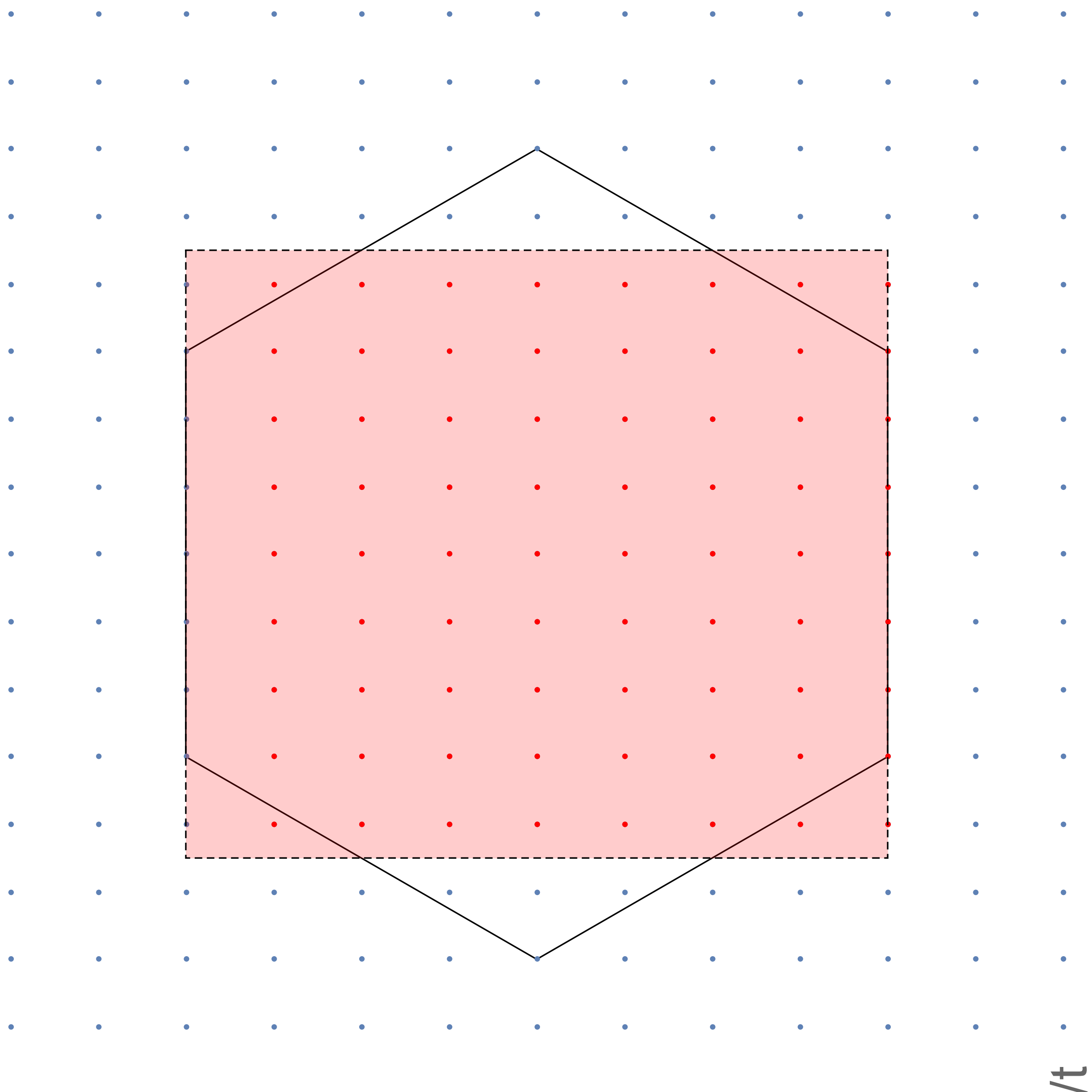
I) Many different types of nanotubes
II) Modifications to long-range potential
III) Different boundary conditions

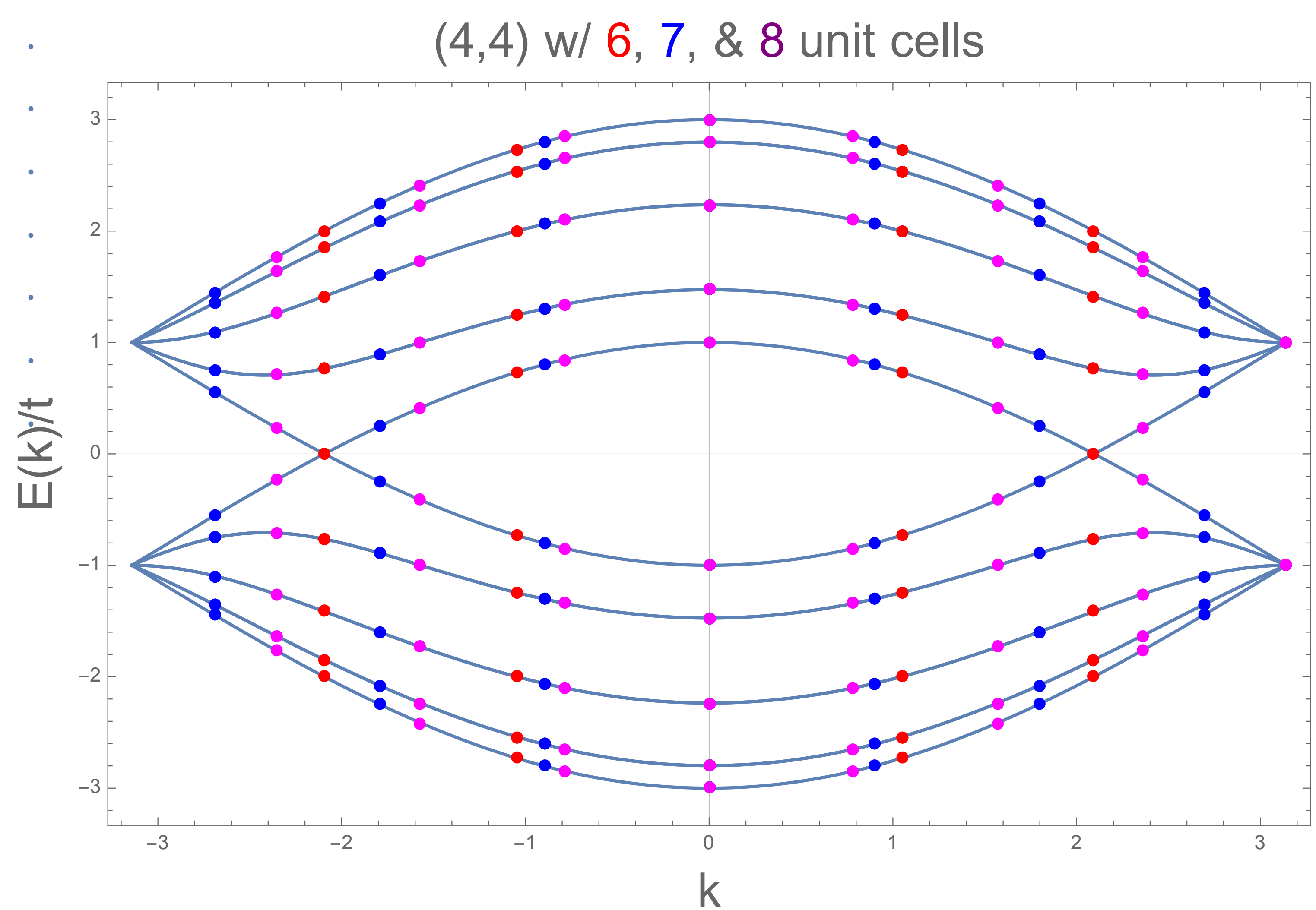




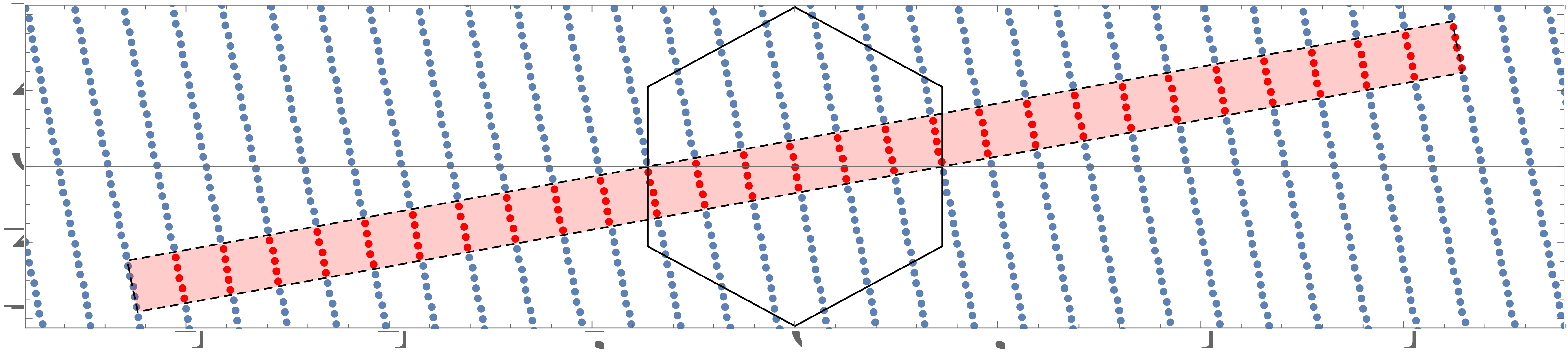
(4,0) w/ 3, 4, & 5 unit cells



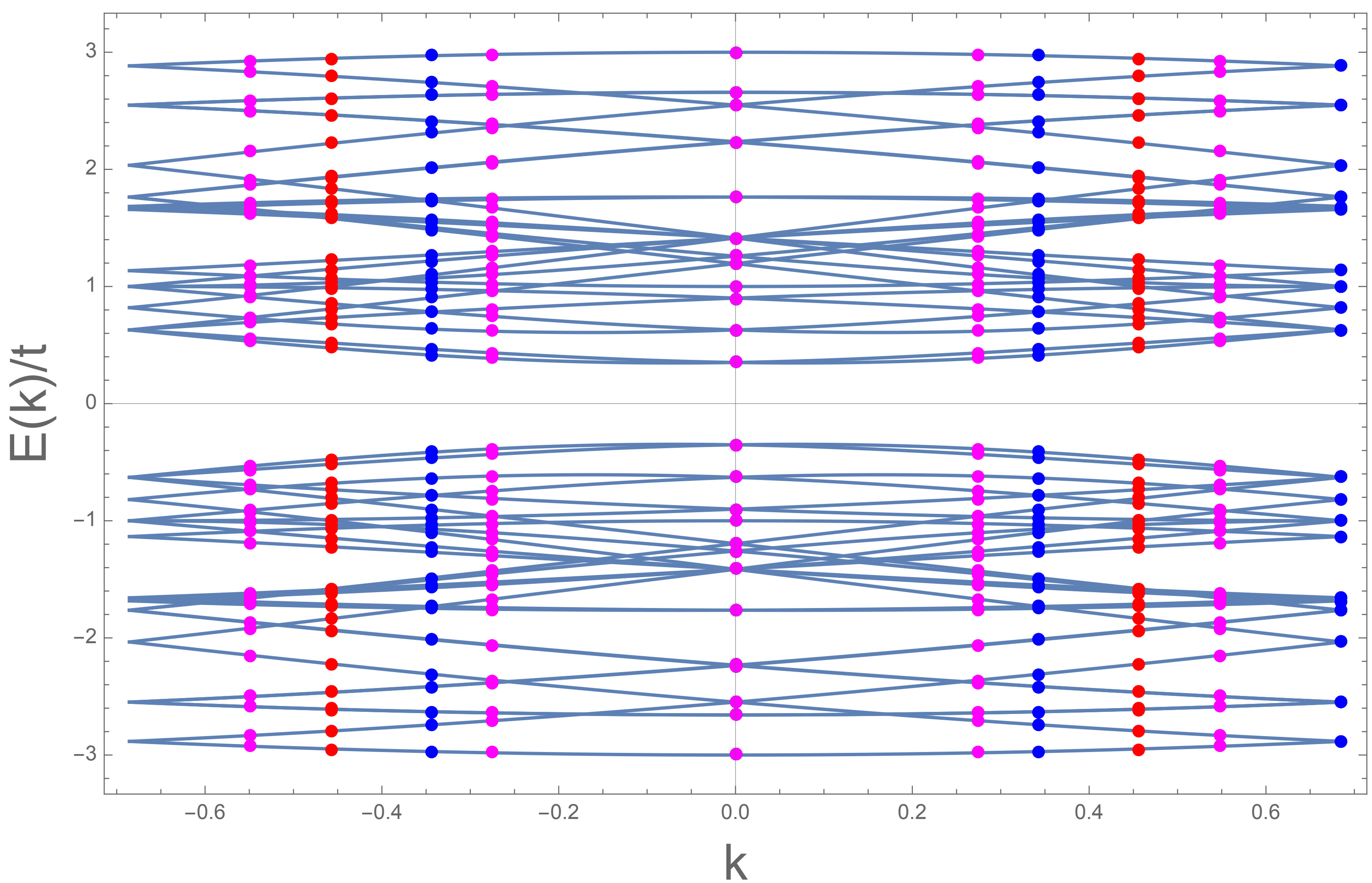




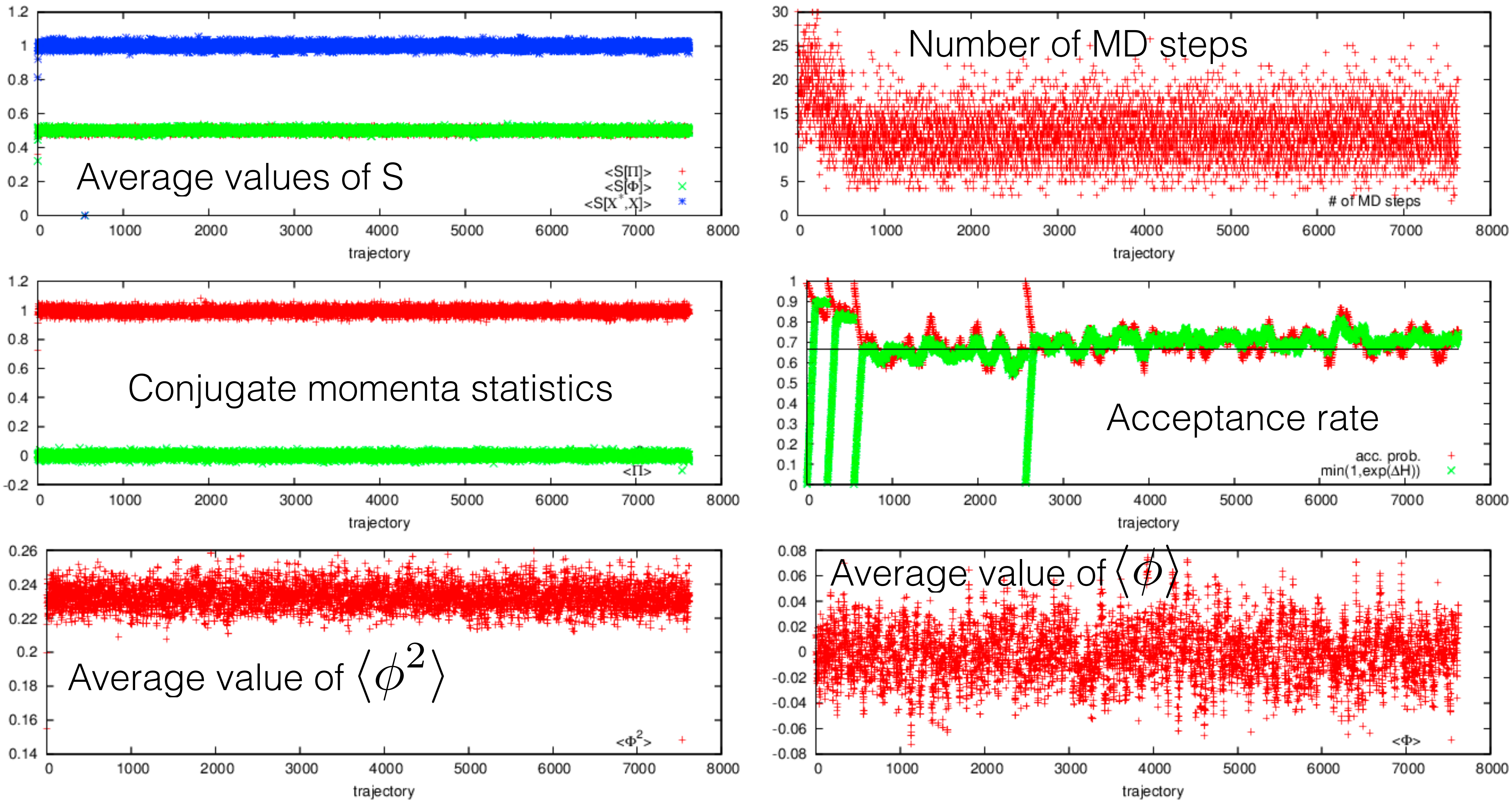
(4,4) w/ 6, 7, & 8 unit cells
E(k)/t
k
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3



(4,2) w/ 3, 4, & 5 unit cells



"Telemetry" from the Monte Carlo simulation of a nanotube ...



Allocations of supercomputing time (example for 2013-2014)
Resources provided by Forschungszentrum Jülich and RWTH Aachen

- JUQUEEN (BG/Q, Jülich), 30 Mcore-h (project) + > 100 Mcore-h (institutional)
- RWTH cluster (Intel, Aachen), 1.3 Mcore-h (project)

Figure courtesy of Jülich Supercomputer Centre (JSC)

Conclusions

Advantages and disadvantages

Dirac theory

- More model-independent approach?
- Unphysical square lattice, continuum limit needed
- Best suited to dimensionless observables?
- Connection to applied physics not obvious

Hexagonal Hubbard theory

- Based on the tight-binding approximation
- Physical lattice spacing, scales set from the start
- Direct connection to cond-mat and applied physics
- Versatile, multilayers, nanotubes, ribbons …