Monte Carlo Methods for Graphene and Carbon Nanotubes

Timo A. Lähde

Institute for Advanced Simulation (IAS-4) / Institut für Kernphysik (IKP-3)
Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

**Progress in Diagrammatic Monte Carlo Methods (DIMOCA 2017)
for Quantum Field Theories in Particle, Nuclear
and Condensed Matter Physics**

Mainz Institute for Theoretical Physics (MITP),
Johannes-Gutenberg Universität Mainz, Germany, September 26, 2017

Outline

- Attempt at a pedagogical introduction to Monte Carlo simulations of graphene (and carbon nanomaterials)

- 2008: Low-energy Dirac theories of graphene
  Monte Carlo simulations with staggered fermions

  Phys. Rev. B79, 165425 (2009), arXiv:0901.0584 [cond.mat-str.el]

- Monte Carlo simulations of the hexagonal Hubbard theory, graphene and carbon nanotubes

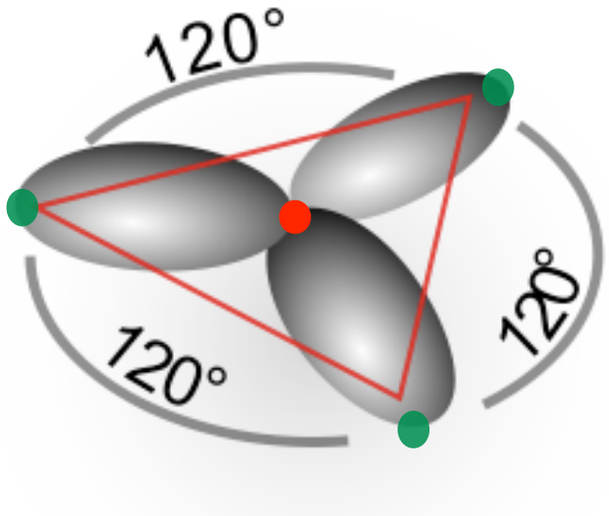
  Phys. Rev. B93, 155106 (2016), arXiv:1511.04918 [cond.mat-str.el]

- 2017: Graphene as an infinite-radius nanotube?
  Insulating state (due to interactions) observed

  Collaboration with Evan Berkowitz, Christopher Körber,
  Stefan Krieg, Peter Labus, Thomas Luu

Graphene-like carbon nano-materials:

Carbon nanotubes, graphite, fullerenes …



$1s^2$ $2s^2\ 2p^2$

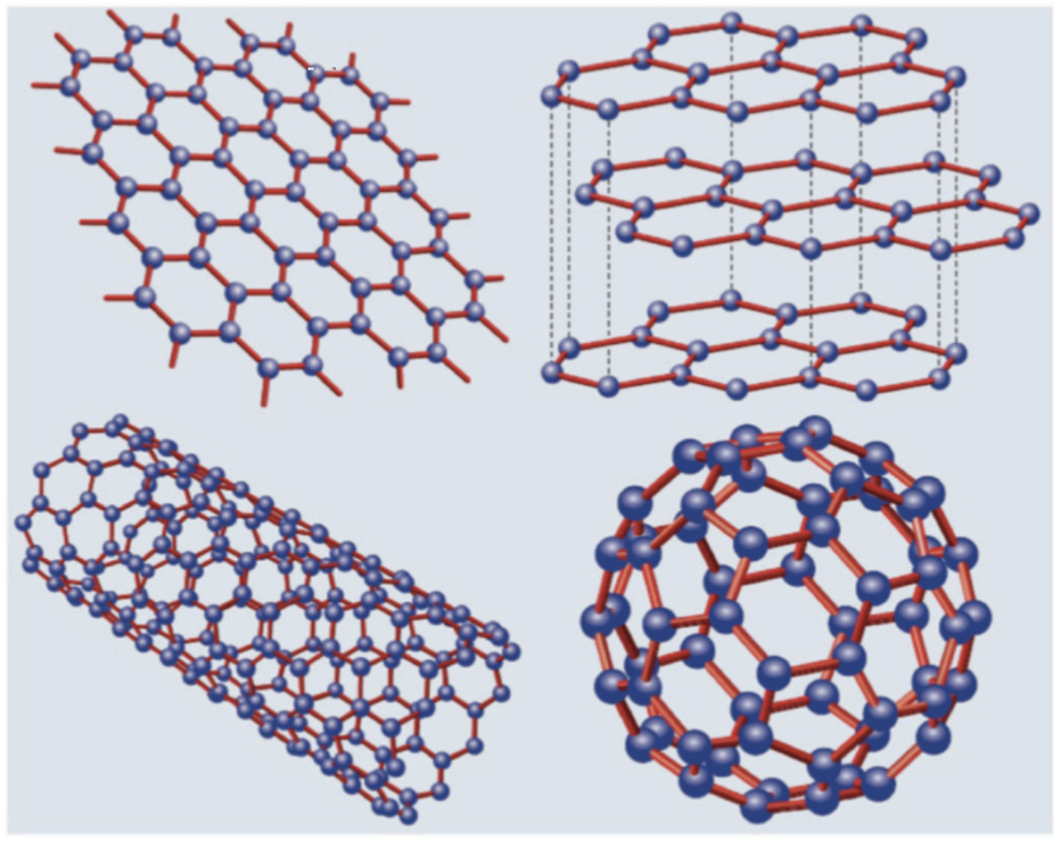
⇩

$3\ sp^2 + p$

⇩ ⇩

bonding hopping

graphene
single graphite layer



graphite
stacked graphene

nanotube
rolled graphene

fullerene
wrapped graphene

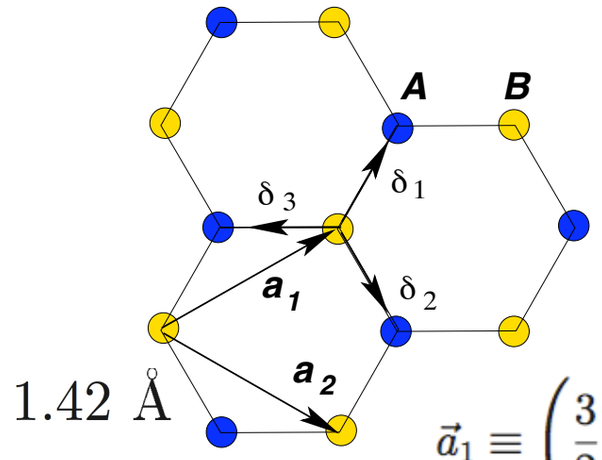
Electronic structure of graphene: Tight-binding (TB) description …

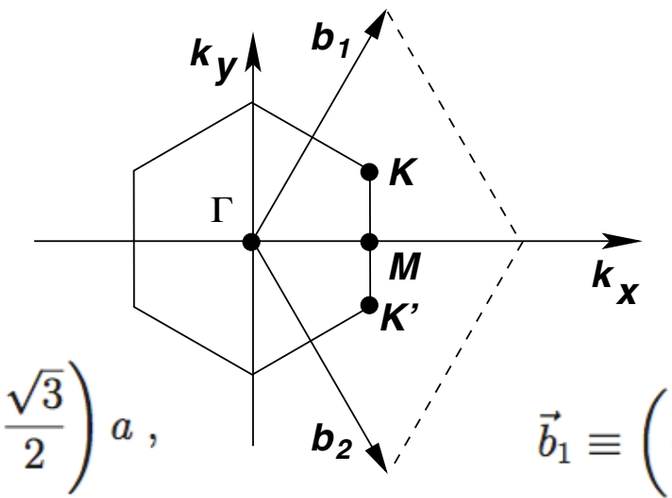
*P. R. Wallace, Phys. Rev. **71**, 622 (1947)*

*A. H. Castro Neto et al., Rev. Mod. Phys. 8**1**, 109 (2009)*

$$H \equiv H_{tb}$$

$$\equiv -\kappa \sum_{\langle x,y\rangle,s} a^{\dagger}_{x,s} a_{y,s}$$





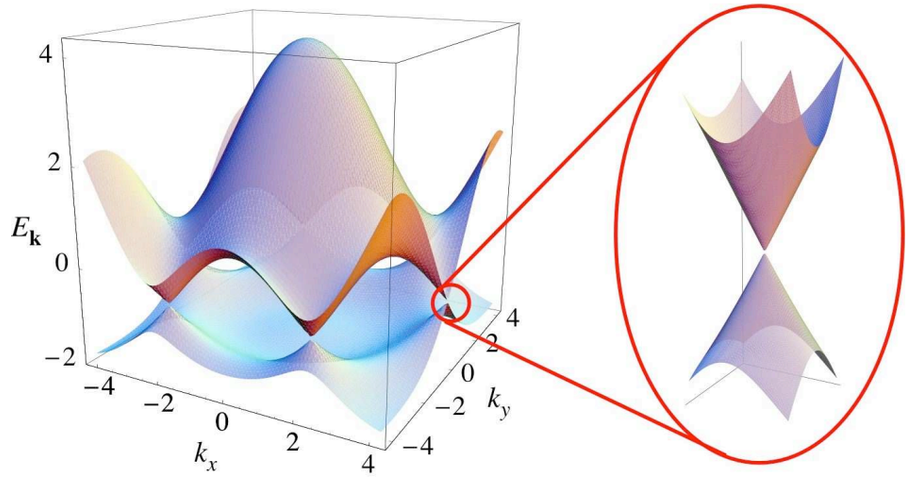
$$\vec{a}_1 \equiv \left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right) a \,, \qquad \vec{b}_1 \equiv \left(\frac{1}{3}, \frac{1}{\sqrt{3}}\right) \frac{2\pi}{a} \,,$$

$$\vec{a}_2 \equiv \left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right) a \qquad \vec{b}_2 \equiv \left(\frac{1}{3}, -\frac{1}{\sqrt{3}}\right) \frac{2\pi}{a}$$

\Kappa describes the overlap of the π-orbitals of neighboring ions

$$E(\vec{k}) = i\omega(\vec{k}) = \pm\kappa |f(\vec{k})|$$

$$f(\vec{k}) = e^{iak_x/\sqrt{3}} + 2e^{-iak_x/(2\sqrt{3})} \cos(ak_y/2)$$



\Kappa = 2.7 eV can be determined e.g. from the measured Fermi velocity

$$v_f = \frac{\sqrt{3}}{2}\kappa a \simeq \frac{c}{300}$$

Graphene with electron-electron interactions, hexagonal Hubbard theory …

NB: APPLIED GRAPHENE PHYSICS
USUALLY STOPS HERE
—> We continue …

$$H \equiv H_{tb} + H_I$$
$$\equiv -\kappa \sum_{\langle x,y\rangle,s} a^\dagger_{x,s} a_{y,s} + \frac{1}{2}\sum_{x,y} V_{x,y}\, q_x q_y$$

System is neutral at "half-filling" (i.e. one electron per lattice site)

$$q_i \equiv a^\dagger_{i,\uparrow} a_{i,\uparrow} + a^\dagger_{i,\downarrow} a_{i,\downarrow} - 1$$

In practice:
Interaction parameterized
in terms of (U_{00}, \alpha)
or (U_{00}, U_{01}, … , U_{0n}, \alpha)

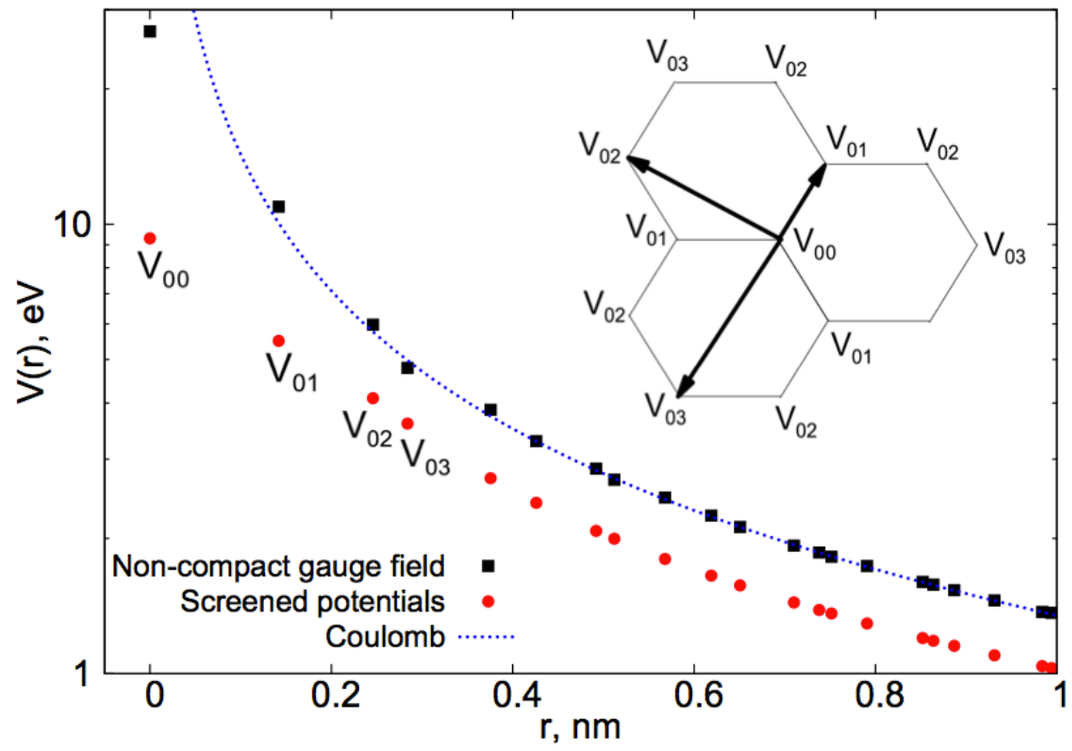
T. Paiva et al.,
*Phys. Rev. B **72**, (2005) 085123*

Z. Y. Meng et al.,
*Nature **464**, (2010) 847*

S. Sorella et al.,
*Sci. Rep. **2**, (2012) 992*

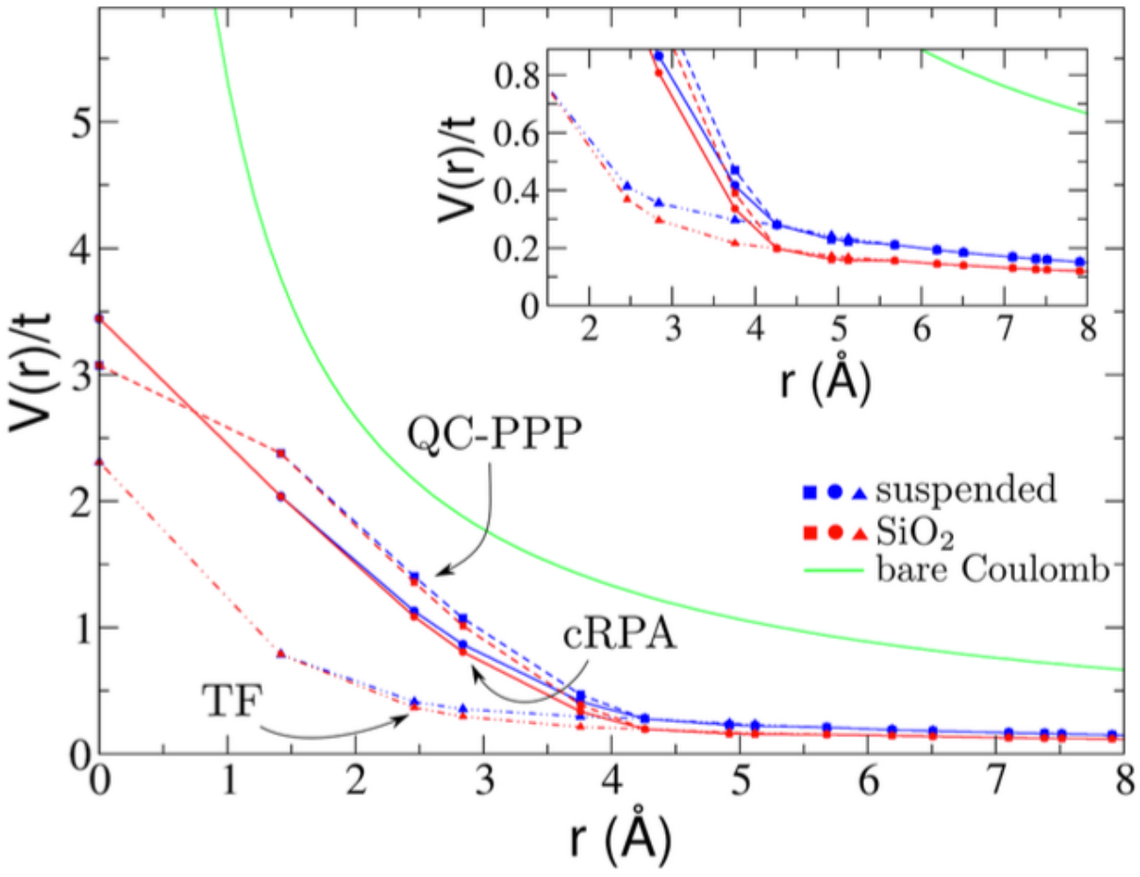
P. V. Buividovich et al.,
*Phys. Rev. B **86**, (2012) 245117*

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



How do we obtain the constants (U, alpha)?

At present, mostly theoretical input (DFT etc.) …



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

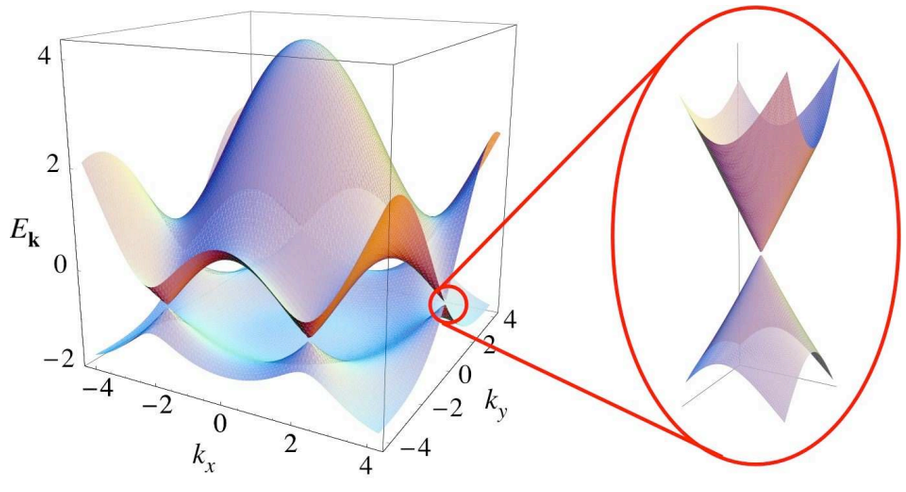
Ho-Kin Tang et al.,
Phys. Rev. Lett. ***115****, (2015) 186602*

1) Short-range screening due to electrons in sp^2 (\sigma) orbitals
2) Coulomb "tail" suppressed by dielectric constant of medium (substrate)

Dirac theory for graphene:
Linearized low-energy description …

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

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



The couplings inside the unit cell (U_{00} and U_{01}) are captured by the contact terms:

$$g_d = -2\tilde{g}_d = \frac{(U_{00}+U_{01})a^2}{8}$$

$$g_c = -2\tilde{g}_c = \frac{(U_{00}-U_{01})a^2}{8}$$

$$g_f = g_a = -2\tilde{g}_f = -2\tilde{g}_a = -\frac{U_{00}a^2}{8}$$

I. F. Herbut,
Phys. Rev. Lett. ***97****, 146401 (2006)*

Almost QED in 2+1 dimensions (A_0 in 3+1d):

$$\mathcal{L} = \sum_{\sigma=\pm1} \bar{\psi}_\sigma(\gamma_0\partial_0 + iA_0 + v_f\gamma_i\partial_i)\psi_\sigma + \frac{\varepsilon_0}{2e^2}(\partial_i A_0)^2$$

$$+ g_c \sum_{\sigma=\pm1} (\bar{\psi}_\sigma\psi_\sigma)^2 + g_d \sum_{\sigma=\pm1} (\bar{\psi}_\sigma\gamma_0\psi_\sigma)^2$$

$$+ g_f \sum_{\sigma=\pm1} (\sigma\bar{\psi}_\sigma\psi_\sigma)^2 + g_a \sum_{\sigma=\pm1} (\sigma\bar{\psi}_\sigma\gamma_0\psi_\sigma)^2$$

$$+ \tilde{g}_c \sum_{\mu=3,5}\sum_{\sigma=\pm1} (\bar{\psi}_\sigma\gamma_1\gamma_\mu\psi_\sigma)^2$$

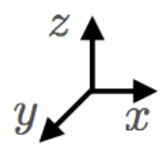
$$+ \tilde{g}_d \sum_{\mu=3,5}\sum_{\sigma=\pm1} (\bar{\psi}_\sigma\gamma_0\gamma_1\gamma_\mu\psi_\sigma)^2$$

$$+ \tilde{g}_f \sum_{\mu=3,5}\sum_{\sigma=\pm1} (\sigma\bar{\psi}_\sigma\gamma_1\gamma_\mu\psi_\sigma)^2$$

$$+ \tilde{g}_a \sum_{\mu=3,5}\sum_{\sigma=\pm1} (\sigma\bar{\psi}_\sigma\gamma_0\gamma_1\gamma_\mu\psi_\sigma)^2$$

Dirac theory + Coulomb (low energies) …

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



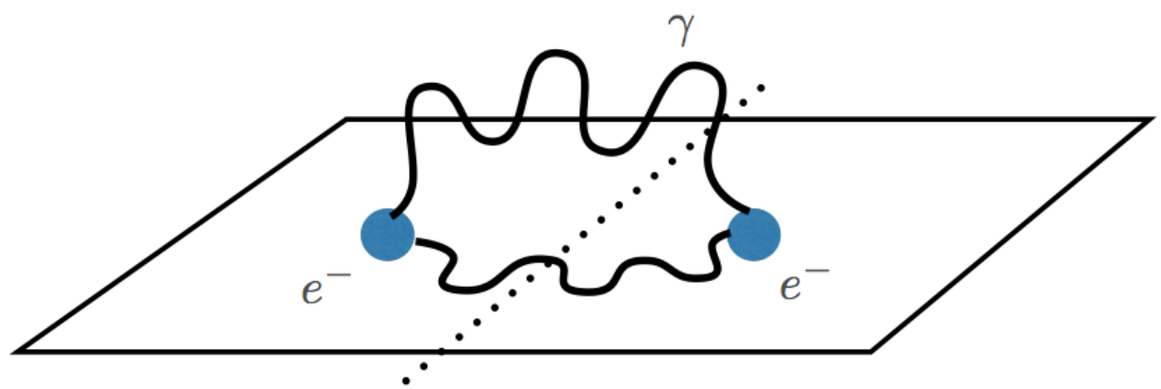


Figure by Mirco Milletari

Fermions in 2+1 dimensions
gauge field in 3+1

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

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

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

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

The U(4) chiral symmetry can spontaneously break (SSB);
NB: Earlier studies of SSB in QED3 and QED4 (Kogut, Hands, Schierholz, …)

"Lattice QCD for graphene" ...

"Staggered" or Kogut-Susskind fermions
(1 flavor = 2 spin states in graphene)
NB - no "rooting" used

$$K_{\mathbf{n},\mathbf{m}}[\theta] = \frac{1}{2}(\delta_{\mathbf{n}+\mathbf{e}_0,\mathbf{m}} U_{\mathbf{n}} - \delta_{\mathbf{n}-\mathbf{e}_0,\mathbf{m}} U^{\dagger}_{\mathbf{m}})$$

$$+ \frac{v}{2}\sum_i \eta^i_{\mathbf{n}}(\delta_{\mathbf{n}+\mathbf{e}_i,\mathbf{m}} - \delta_{\mathbf{n}-\mathbf{e}_i,\mathbf{m}}) + m_0 \delta_{\mathbf{n},\mathbf{m}} \qquad \eta^0_{\mathbf{n}} = 1\,,$$

$$U_{0,\mathbf{n}} = U_{\mathbf{n}} \equiv \exp(i\theta_{\mathbf{n}}) \qquad \eta^1_{\mathbf{n}} = (-1)^{n_0},$$

Non-compact gauge action
(as in Lattice QED)

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

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

S. Hands et al.,
*Phys. Rev. B **78**, 165423 (2008)*

J. E. Drut, T. A. Lähde,
*Phys. Rev. B **79**, (2009) 165425,*
*Phys. Rev. Lett. **102**, (2009) 026802*

P. V. Buividovich et al.,
*Phys. Rev. B **86**, (2012) 045107*

C. DeTar et al.,
*Phys. Rev. Lett. **117**, (2016) 266802*

Monte Carlo updates:

Importance sampling with Metropolis algorithm …

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

We can perform either random (local) updates or (global) Molecular Dynamics (MD) updates

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

Fermion determinant is evaluated using "pseudofermions"

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

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

$$Q \equiv K^\dagger K$$

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

Putting all the pieces together:

Hybrid Monte Carlo algorithm (with pseudofermions) …

Evolution Hamiltonian for Molecular Dynamics update

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

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

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

Numerical integration of Hamiltonian equations of motion

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

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

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

The "pseudofermion force term" uses 99% of the CPU time (iterative inversion)

Look for spontaneous chiral symmetry breaking (SSB):
Analysis of the chiral condensate …

Compute condensate and susceptibility as
a function of the lattice coupling

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

$$\sigma \equiv \langle \bar{\chi}\chi \rangle$$

$$\chi_l \equiv \frac{\partial \sigma}{\partial m_0}$$

Finite size scaling analysis in the
presence of a mass term

$$m_0 X(\beta) = Y(\beta) f_1(\sigma) + f_3(\sigma)$$

Dependence on σ:
Information on critical exponents δ, β_m !

$$f_1(\sigma) = \sigma^{\delta - 1/\beta_m}$$
$$f_3(\sigma) = \sigma^{\delta}$$

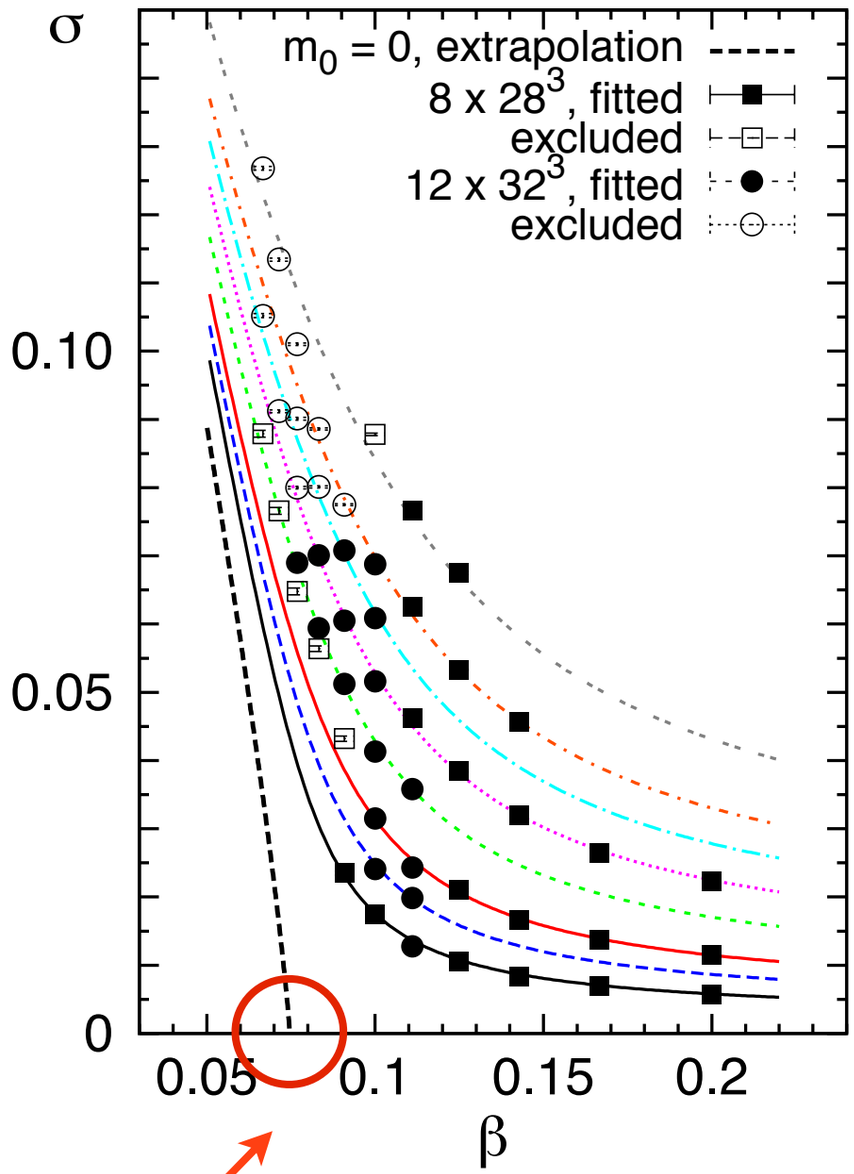
Dependence on β:
Information on critical coupling β_c!

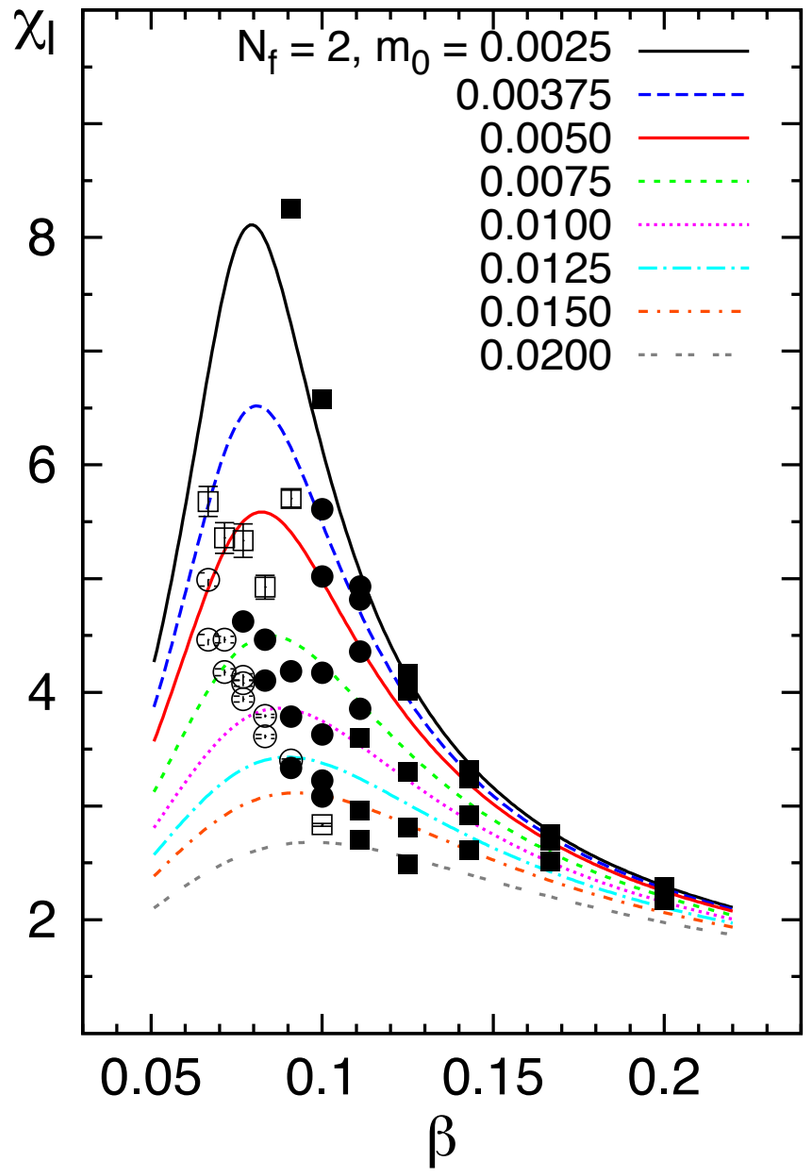
$$X(\beta) = X_0 + X_1(1 - \beta/\beta_c)$$
$$Y(\beta) = Y_1(1 - \beta/\beta_c)$$

Spontaneous Chiral Symmetry breaking …

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

J. E. Drut, T. A. Lähde,
*Phys. Rev. Lett. **102**, (2009) 026802*
*Phys. Rev. B **79**, (2009) 241405(R)*





$\beta_c \sim 0.073$
$\alpha_c \sim 1.1$

NB: bosonization calculation suggests critical coupling of 4/pi?

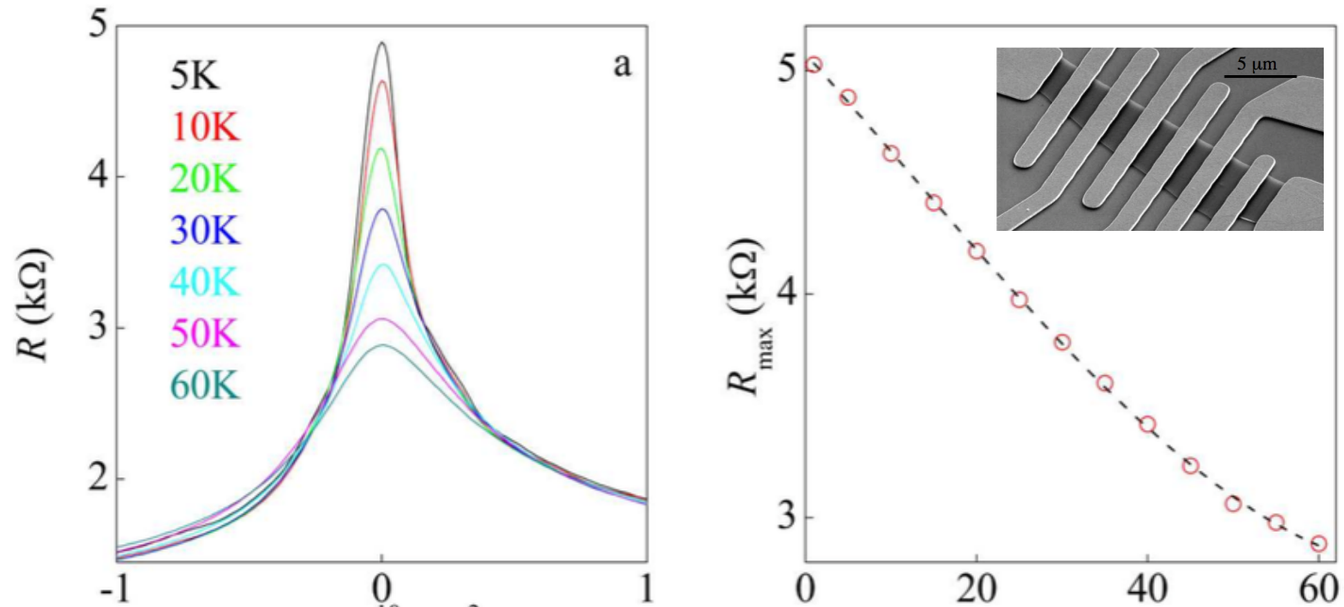
M. Milletari, S. Adam, arXiv:1406.6113

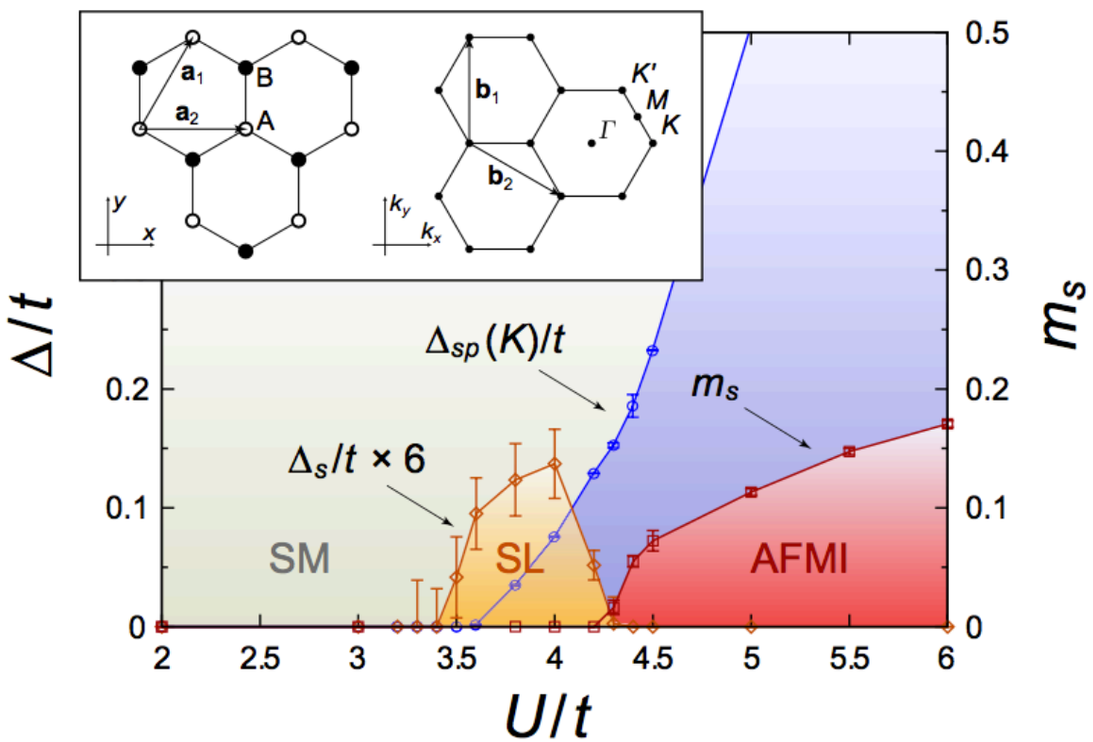
However …

How should we interpret these results?

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

No insulating phase detected in suspended graphene at low T (conductivity measurements)





In hexagonal Hubbard theory: Transition to AFMI (Anti-ferromagnetic Mott Insulator) phase at U_{00}/kappa = 3.8

Z. Y. Meng et al.,
*Nature **464**, (2010) 847*

S. Sorella et al.,
*Sci. Rep. **2**, (2012) 992*

"Lattice QCD" formulation for the hexagonal Hubbard theory …

$$H \equiv H_{tb} + H_I$$

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

$$q_i \equiv a^\dagger_{i,\uparrow} a_{i,\uparrow} + a^\dagger_{i,\downarrow} a_{i,\downarrow} - 1$$

Move to a description in terms of particle and hole operators

$$b^\dagger_{x,\downarrow} \equiv a_{x,\downarrow}, \qquad b_{x,\downarrow} \equiv a^\dagger_{x,\downarrow}$$

$$H = -\kappa \sum_{\langle x,y\rangle} \left(a^\dagger_{x,\uparrow} a_{y,\uparrow} - b^\dagger_{x,\downarrow} b_{y,\downarrow} \right) + \frac{1}{2}\sum_{x,y} V_{x,y}\, q_x q_y$$

$$q_i = a^\dagger_{i,\uparrow} a_{i,\uparrow} - b^\dagger_{i,\downarrow} b_{i,\downarrow}$$

Flip the sign of the b (hole) operators on one sublattice

$$H = -\kappa \sum_{\langle x,y\rangle} \left(a^\dagger_x a_y + b^\dagger_x b_y \right) + \frac{1}{2}\sum_{x,y} V_{x,y}\, q_x q_y$$

NB! Many other formulations possible: See e.g. S. Beyl et al., arXiv:1708.03661

*R. Brower et al., PoS **LATTICE2011**, (2011) 056*

*P. V. Buividovich et al., Phys. Rev. B **86**, (2012) 245117*

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

*T. Luu and T. A. Lähde, Phys. Rev. B **93**, (2016) 155106*

Lattice Monte Carlo for the hexagonal Hubbard theory:

Grassmann path integral formulation …

Computation of operator expectation values in terms of Grassmann fields (for particles and holes)

$$\langle O(t) \rangle \equiv \frac{1}{Z} \mathrm{Tr}\left[O(t) e^{-\beta H} \right]$$

$$= \frac{1}{Z} \int \left[\prod_{\alpha} d\psi^*_{\alpha} d\psi_{\alpha} d\eta^*_{\alpha} d\eta_{\alpha} \right] e^{-\sum_{\alpha} (\psi^*_{\alpha} \psi_{\alpha} + \eta^*_{\alpha} \eta_{\alpha})} \langle -\psi, -\eta | O(t) e^{-\beta H} | \psi, \eta \rangle$$

Subdivide Euclidean time into N_t "slices"

\delta = \beta / N_t

$$e^{-\beta H} \equiv e^{-\delta H} e^{-\delta H} \cdots e^{-\delta H}$$

$$Z = \mathrm{Tr}\left[e^{-\beta H} \right] =$$

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

Product of time slices,
anti-periodic boundary conditions in time

Hubbard-Stratonovich (HS) transformation …

$$\langle \psi_{t+1}, \eta_{t+1} | e^{-\delta H} | \psi_t, \eta_t \rangle = \langle \psi_{t+1}, \eta_{t+1} | e^{\delta\kappa \sum_{\langle x,y \rangle} \left(a_x^\dagger a_y + b_x^\dagger b_y \right) - \frac{1}{2} \sum_{x,y} \delta V_{x,y} q_x q_y} | \psi_t, \eta_t \rangle$$

$$\propto \int \prod_x d\tilde{\phi}_x \langle \psi_{t+1}, \eta_{t+1} | e^{\tilde{\kappa} \sum_{\langle x,y \rangle} \left(a_x^\dagger a_y + b_x^\dagger b_y \right) - \frac{1}{2} \sum_{x,y} [\tilde{V}]^{-1}_{x,y} \tilde{\phi}_x \tilde{\phi}_y + \sum_x i \tilde{\phi}_x q_x} | \psi_t, \eta_t \rangle$$

$$\tilde{\kappa} \equiv \delta\kappa, \quad \tilde{V} \equiv \delta V, \quad \tilde{\phi} \equiv \delta\phi$$

If we assume that exp(-\delta*H) is normal-ordered:

$$\langle \psi_{t+1}, \eta_{t+1} | e^{-\delta H} | \psi_t, \eta_t \rangle = \int \prod_x d\tilde{\phi}_{x,t} \, e^{-\frac{1}{2} \sum_{x,y} [\tilde{V}]^{-1}_{x,y} \tilde{\phi}_{x,t} \tilde{\phi}_{y,t}}$$

$$\times \exp \left\{ \tilde{\kappa} \sum_{\langle x,y \rangle} \left(\psi^*_{x,t+1} \psi_{y,t} + \eta^*_{x,t+1} \eta_{y,t} \right) + \sum_x \left(e^{i\tilde{\phi}_{x,t}} \psi^*_{x,t+1} \psi_{x,t} + e^{-i\tilde{\phi}_{x,t}} \eta^*_{x,t+1} \eta_{x,t} \right) \right\} + \mathcal{O}(\delta^2)$$

For the \phi_x*q_x term, we used the following identity:

$$\langle \psi | \exp \left\{ \sum_{x,y} a_x^\dagger A_{x,y} a_y \right\} | \psi' \rangle \equiv \exp \left\{ \sum_{x,y} \psi^*_x [e^A]_{x,y} \psi'_y \right\}$$

Similarly to Lattice QCD,
integrate out Grassmann fields ...

$$Z = \int \mathcal{D}\tilde{\phi}\mathcal{D}\psi^*\mathcal{D}\psi\mathcal{D}\eta^*\mathcal{D}\eta\, e^{-\frac{1}{2}\sum_{x,y,t}[\tilde{V}]^{-1}_{x,y}\tilde{\phi}_{x,t}\tilde{\phi}_{y,t}} \exp\left\{\tilde{\kappa}\sum_{\langle x,y\rangle,t}\left(\psi^*_{x,t+1}\psi_{y,t} + \eta^*_{x,t+1}\eta_{y,t}\right)\right.$$
$$\left. - \sum_{x,t}\left(\psi^*_{x,t+1}(\psi_{x,t+1} - e^{i\tilde{\phi}_{x,t}}\psi_{x,t}) + \eta^*_{x,t+1}(\eta_{x,t+1} - e^{-i\tilde{\phi}_{x,t}}\eta_{x,t})\right)\right\}$$

Fermion determinants for particles and holes, potential contained in the "gauge action" term

$$Z = \int \mathcal{D}\tilde{\phi}\,\det[M(\tilde{\phi})]\,\det[M^*(\tilde{\phi})]\exp\left\{-\frac{1}{2}\sum_{x,y,t=0}^{N_t-1}[\tilde{V}]^{-1}_{x,y}\tilde{\phi}_{x,t}\tilde{\phi}_{y,t}\right\}$$

$$M(x,t;y,t';\tilde{\phi}) \equiv \delta_{x,y}\left(\delta_{t,t'} - e^{i\tilde{\phi}_{x,t'}}\delta_{t-1,t'}\right) - \tilde{\kappa}\,\delta_{\langle x,y\rangle}\delta_{t-1,t'}$$

Compact form of fermion operator "link variables" \exp(\pm i\phi)

Monte Carlo probability weight,
should be positive definite …

$$P(\tilde{\phi}) \equiv \frac{1}{Z} \det[M(\tilde{\phi})] \det[M^*(\tilde{\phi})] \exp\left\{ -\frac{1}{2} \sum_{x,y,t=0}^{N_t-1} [\tilde{V}]^{-1}_{x,y} \tilde{\phi}_{x,t} \tilde{\phi}_{y,t} \right\}$$

$$= \frac{1}{Z} \det[M(\tilde{\phi}) M^\dagger(\tilde{\phi})] \exp\left\{ -\frac{1}{2} \sum_{x,y,t=0}^{N_t-1} [\tilde{V}]^{-1}_{x,y} \tilde{\phi}_{x,t} \tilde{\phi}_{y,t} \right\},$$

Generate "ensembles" of configurations with your favorite Monte Carlo algorithm!
Here: –> Hybrid Monte Carlo (HMC)

$$\langle O \rangle \approx \frac{1}{N_{\rm cf}} \sum_{i=1}^{N_{\rm cf}} O[\tilde{\phi}_i]$$

$$\langle a_x(\tau) a_y^\dagger(0) \rangle = \langle M^{-1}(x,\tau;y,0) \rangle \approx \frac{1}{N_{\rm cf}} \sum_{i=1}^{N_{\rm cf}} M^{-1}(x,\tau;y,0;\tilde{\phi}_i)$$

For instance:
Single quasiparticle propagator
–> quasiparticle spectrum

Computing the single-particle correlator, dispersion relation with interactions …

Block notation makes the A/B sublattice structure explicit

$$M(x,t';y,t)\Psi(y,t) =$$

$$\begin{pmatrix} \delta_{x,y}\left(\delta_{t',t} - e^{i\Phi_A(x,t')}\delta_{t-1,t'}\right) & -\tilde{\kappa}\ \delta_{\langle x,y\rangle}\delta_{t-1,t'} \\ -\tilde{\kappa}\ \delta_{\langle x,y\rangle}\delta_{t-1,t'} & \delta_{x,y}\left(\delta_{t',t} - e^{i\Phi_B(x,t')}\delta_{t-1,t'}\right) \end{pmatrix} \begin{pmatrix} \Psi_A(y,t) \\ \Psi_B(y,t) \end{pmatrix}$$

$$\Psi(x,t) = \begin{pmatrix} \Psi_A(x,t) \\ \Psi_B(x,t) \end{pmatrix} = \begin{pmatrix} \psi_{x,t} \\ \psi_{x+\vec{a},t} \end{pmatrix} \qquad \Phi(x,t) = \begin{pmatrix} \Phi_A(x,t) \\ \Phi_B(x,t) \end{pmatrix} = \begin{pmatrix} \tilde{\phi}_{x,t} \\ \tilde{\phi}_{x+\vec{a},t} \end{pmatrix}$$

Momentum projection for a given lattice momentum mode

$$G_\pm(\vec{k}_i,\tau) \equiv \langle a_\pm(\vec{k}_i,\tau)a_\pm^\dagger(\vec{k}_i,0)\rangle = \frac{1}{N^2}\sum_{\vec{x}_j,\vec{x}_k\in\{\vec{X}\}} e^{i\vec{k}_i\cdot(\vec{x}_j-\vec{x}_k)}\langle a_\pm(\vec{x}_j,\tau)a_\pm^\dagger(\vec{x}_k,0)\rangle$$

$$a_\pm^\dagger(\vec{x}) \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} a_A^\dagger(\vec{x}) \\ \pm a_B^\dagger(\vec{x}) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} a_{\vec{x}}^\dagger \\ \pm a_{\vec{x}+\vec{a}}^\dagger \end{pmatrix}$$

Large-time behavior of correlators …

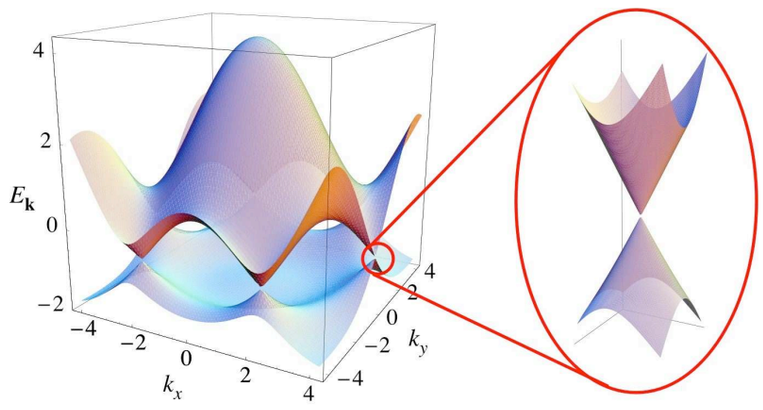
$$G_{\pm}(\vec{k}_i,\tau) = \frac{1}{2N^2}\sum_{\vec{x}_j,\vec{x}_k\in\{\vec{X}\}} e^{i\vec{k}_i\cdot(\vec{x}_j-\vec{x}_k)}\Big\{\langle M^{-1}_{AA}(\vec{x}_j,\vec{x}_k;\tau)\rangle + \langle M^{-1}_{BB}(\vec{x}_j,\vec{x}_k;\tau)\rangle$$
$$\pm\left(\langle M^{-1}_{AB}(\vec{x}_j,\vec{x}_k;\tau)\rangle + \langle M^{-1}_{BA}(\vec{x}_j,\vec{x}_k;\tau)\rangle\right)\Big\}$$

Compare with TB (non-interacting) correlator:

$$G_{\pm}(\vec{k}_i,\tau) \equiv \frac{1}{2}\left[G_{AA}(\vec{k}_i,\tau) + G_{BB}(\vec{k}_i,\tau) \pm (G_{AB}(\vec{k}_i,\tau) + G_{BA}(\vec{k}_i,\tau))\right]$$
$$= \frac{1}{2\cosh(\omega(\vec{k}_i)\beta/2)}\left[\cosh(\omega(\vec{k}_i)(t-\beta/2)) \pm \cos(\theta_{k_i})\sinh(\omega(\vec{k}_i)(t-\beta/2))\right]$$

At large Euclidean projection time:

$$G_{\pm}(\vec{k}_i,\tau) \propto e^{\pm\omega(\vec{k}_i)\tau}$$



$$E(\vec{k}) = i\omega(\vec{k}) = \pm\kappa|f(\vec{k})|$$

$$f(\vec{k}) = e^{iak_x/\sqrt{3}} + 2e^{-iak_x/(2\sqrt{3})}\cos(ak_y/2)$$

$$\theta_{k_i} \equiv \tan^{-1}(\mathrm{Im}f(\vec{k}_i)/\mathrm{Re}f(\vec{k}_i))$$

Advantages (and disadvantages) of the hexagonal formulation ...

1) Hexagonal Hubbard theory allows for easy contact with the cond-mat (and applied physics) communities

2) Lattice artifacts are now actual physical effects, no need for extrapolation in the (spatial) lattice spacing

3) Spatial lattice dimensions can also be physical (for instance the length of a nanotube) especially in applied physics

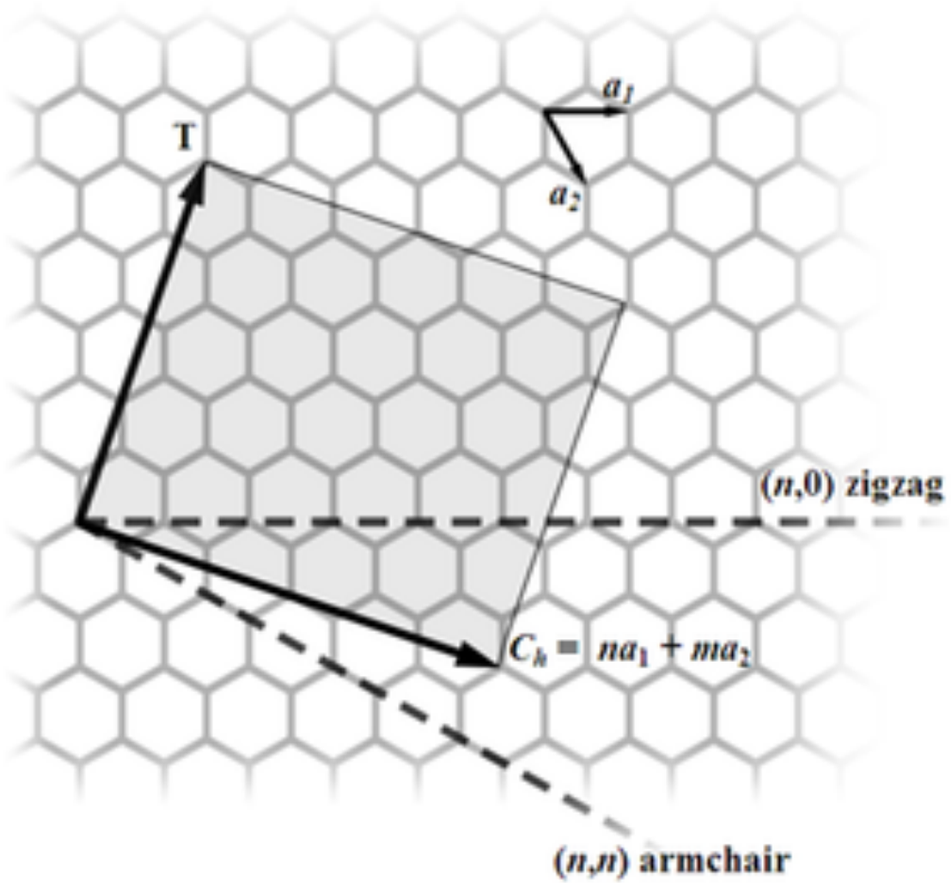
4) Possible disadvantage: Tight-binding approach not considered ab initio, cannot be systematically improved?

5) However: Still considered "sufficiently ab initio" in most cond-mat and applied settings

Carbon nanotubes:

Definitions, basic concepts ...

Saito, Dresselhaus & Dresselhaus,
"Physical properties of carbon nanotubes"



Chiral vector:

$$\vec{C}_h \equiv n\vec{a}_1 + m\vec{a}_2$$

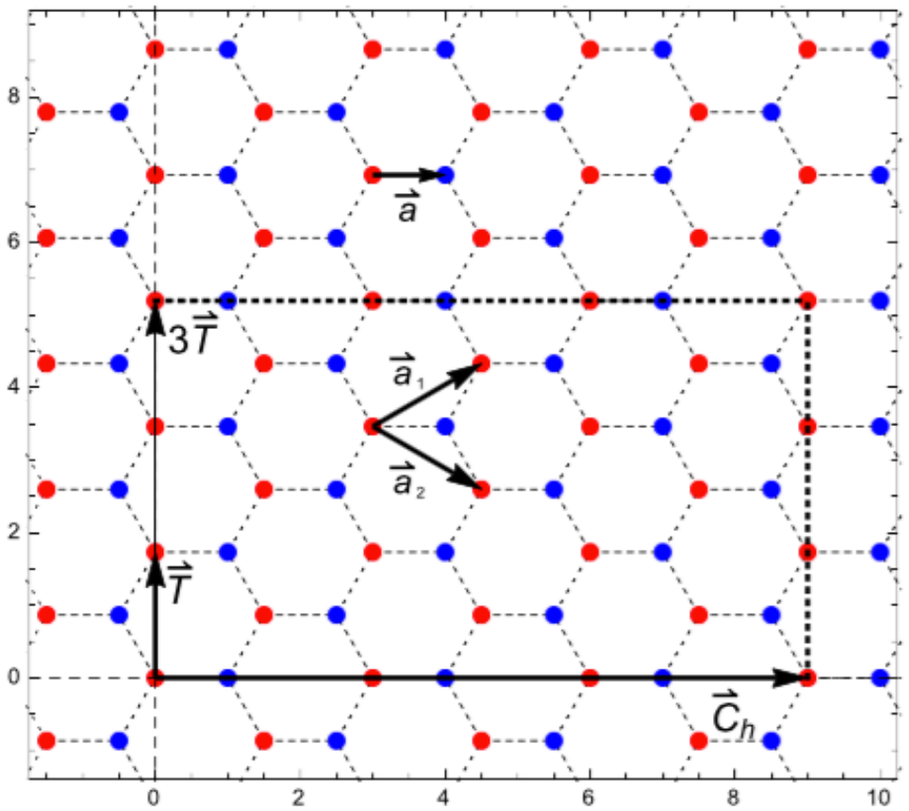
Translation vector:

$$\vec{T} \equiv t_1\vec{a}_1 + t_2\vec{a}_2$$

$$t_1 \equiv \frac{2m+n}{d_R}$$

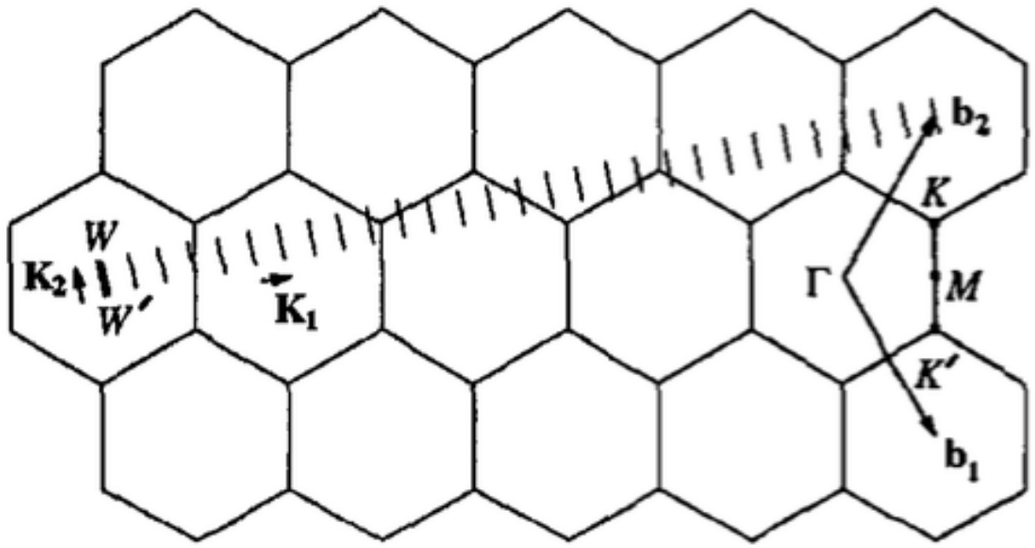
$$t_2 \equiv -\frac{2n+m}{d_R}$$

$$d_R \equiv \gcd(2m+n, 2n+m)$$



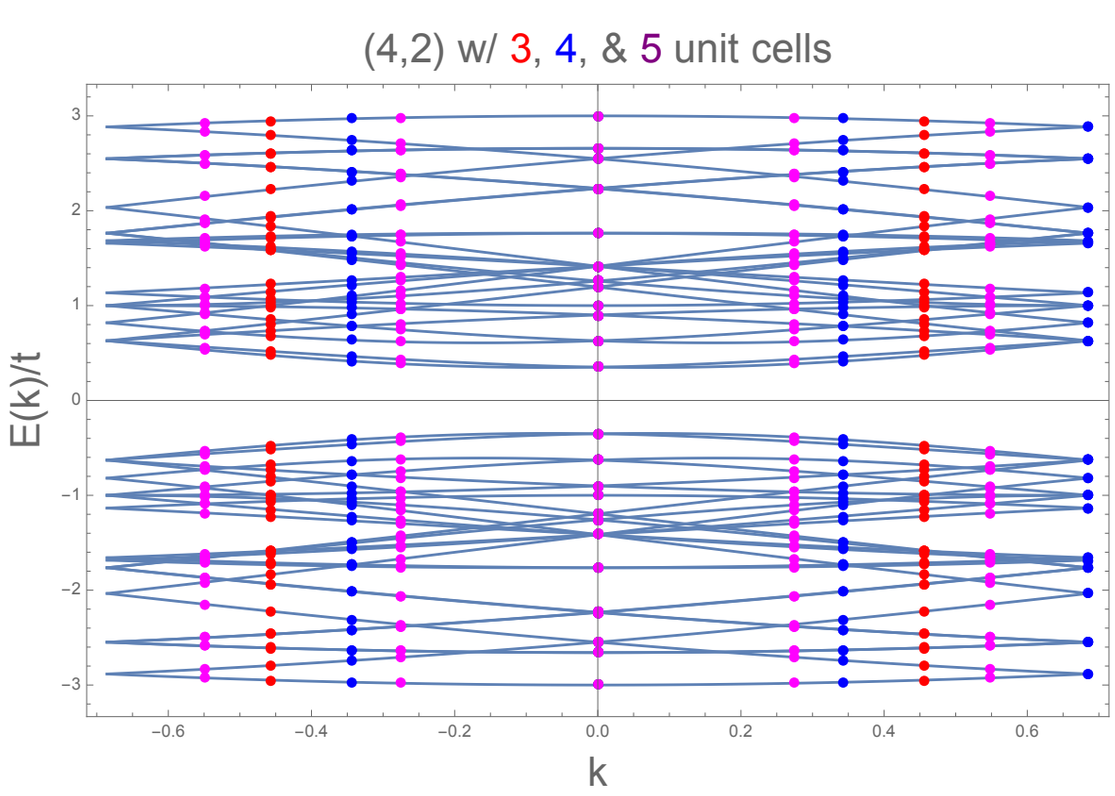
Chiral (4,2) nanotube - semiconducting …

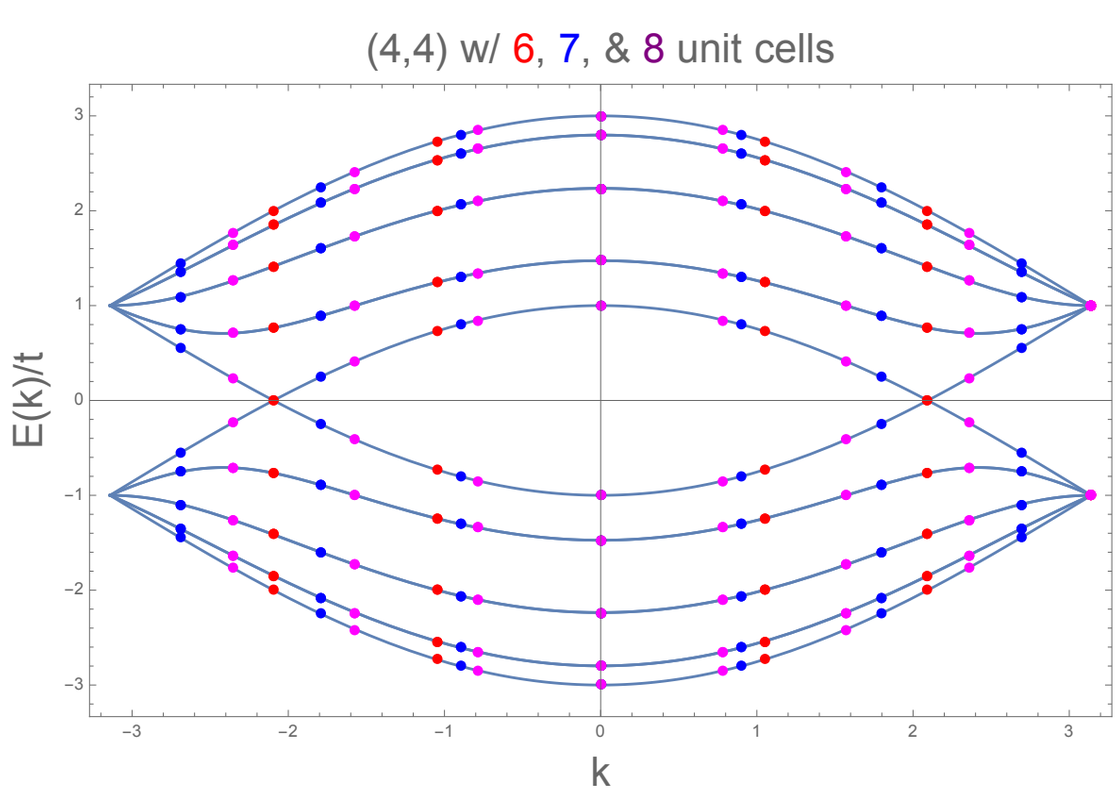
Saito, Dresselhaus & Dresselhaus,
"Physical properties of carbon nanotubes"



$$N_U = \frac{|\vec{C}_h \times \vec{T}|}{|\vec{a}_1 \times \vec{a}_2|}$$

$$\boldsymbol{K}_1 = \frac{1}{N}(-t_2\boldsymbol{b}_1 + t_1\boldsymbol{b}_2), \quad \boldsymbol{K}_2 = \frac{1}{N}(m\boldsymbol{b}_1 - n\boldsymbol{b}_2)$$

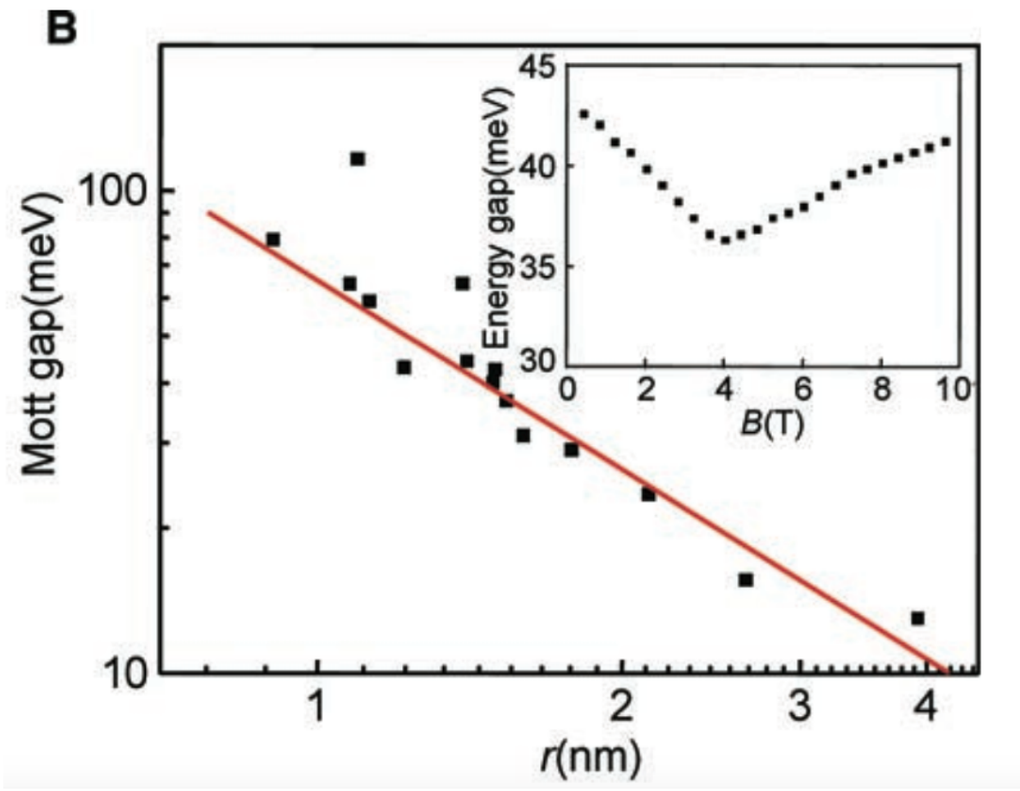




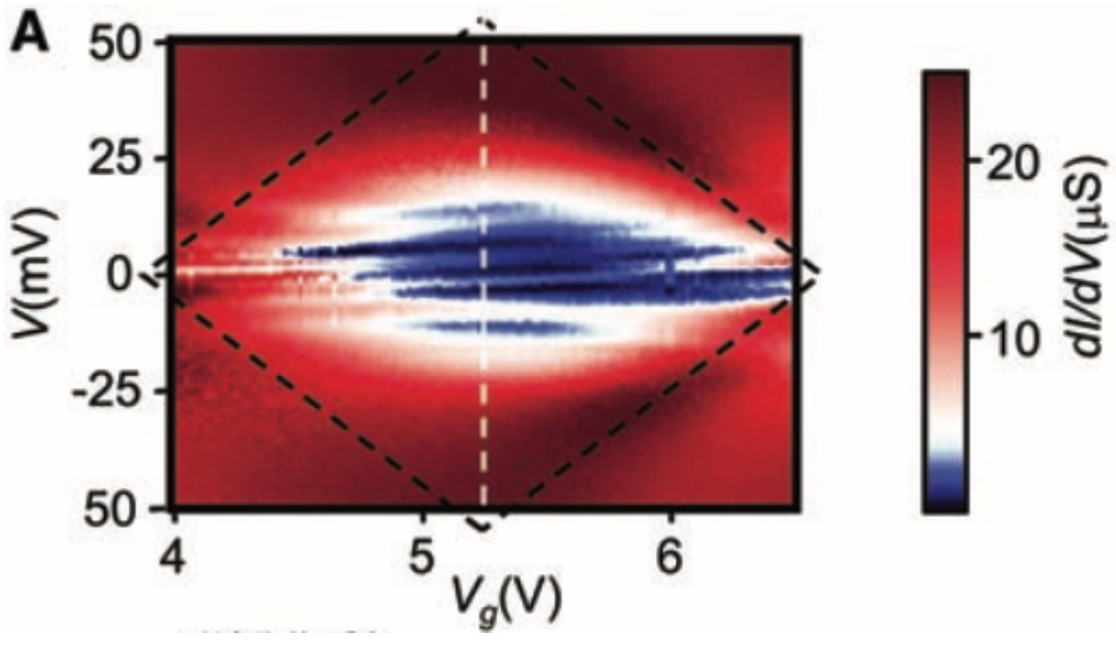
Figures by Thomas Luu

Advantage of studying carbon nanotubes:
Extant experimental data …

V. V. Deshpande et al.,
*Science **323**, (2009) 106*



Interaction-induced energy gap measured in (n,n) nanotubes of radii 1-4 nm



Purely "geometric" effects (bandgap) carefully ruled out, also: observation of excitons

Current status of nanotube calculations ...

1) No curvature effects accounted for (most relevant for high-energy spectrum), also important only for r < 1 nm?

2) Only contact interaction U_{00} used, what is the effect from including \alpha (long-range interactions) as well?

3) Extrapolation in temporal lattice spacing \delta (very important effect!)

4) Extrapolation in # of nanotube unit cells (length of nanotube) appears to be less important (we use 15-25 unit cells)

5) Monte Carlo simulations at low T (algorithmic challenge, is HMC the most efficient choice?)

Preliminary results for carbon nanotubes with radii up to 1 nm …

*V. V. Deshpande et al., Science **323**, (2009) 106*

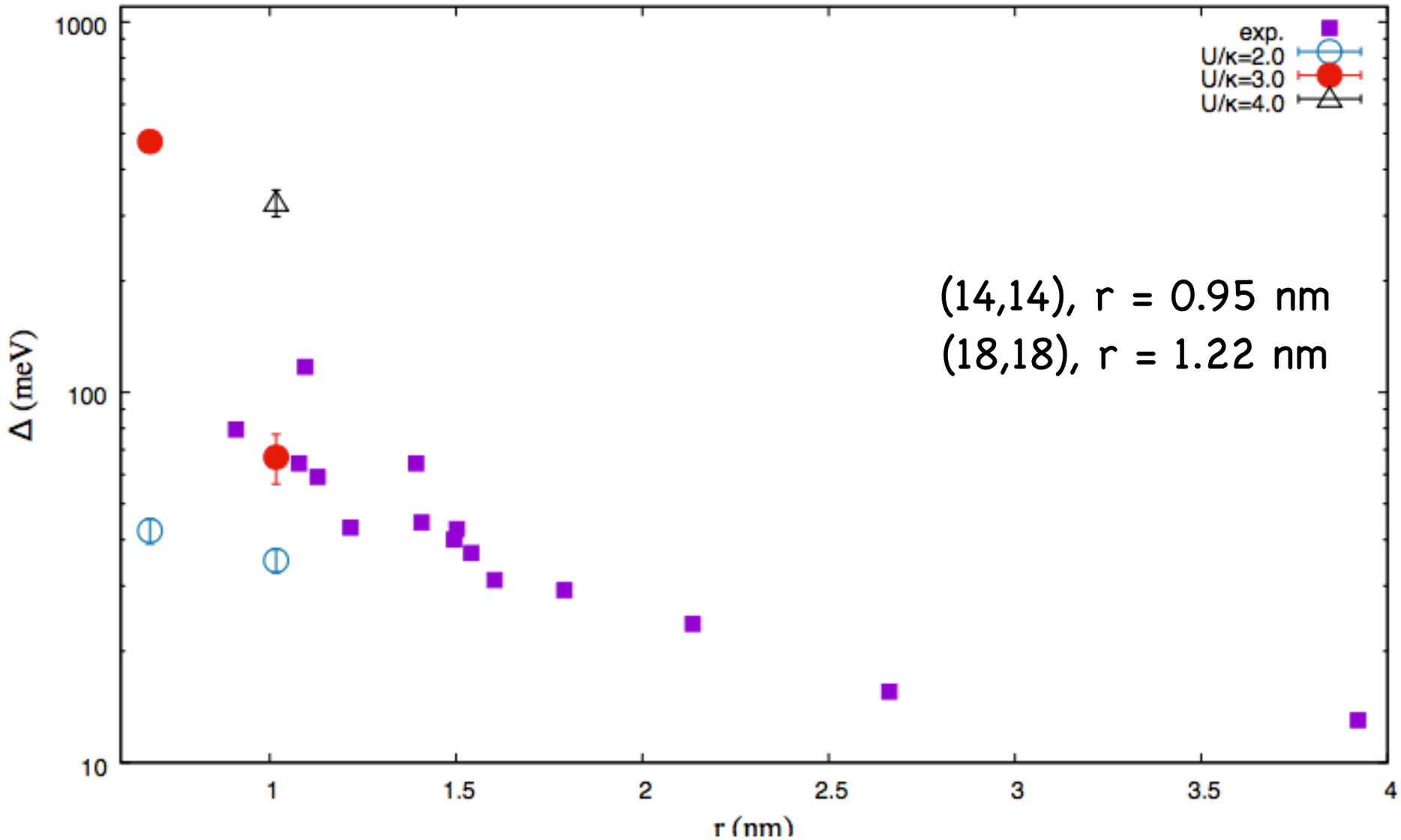


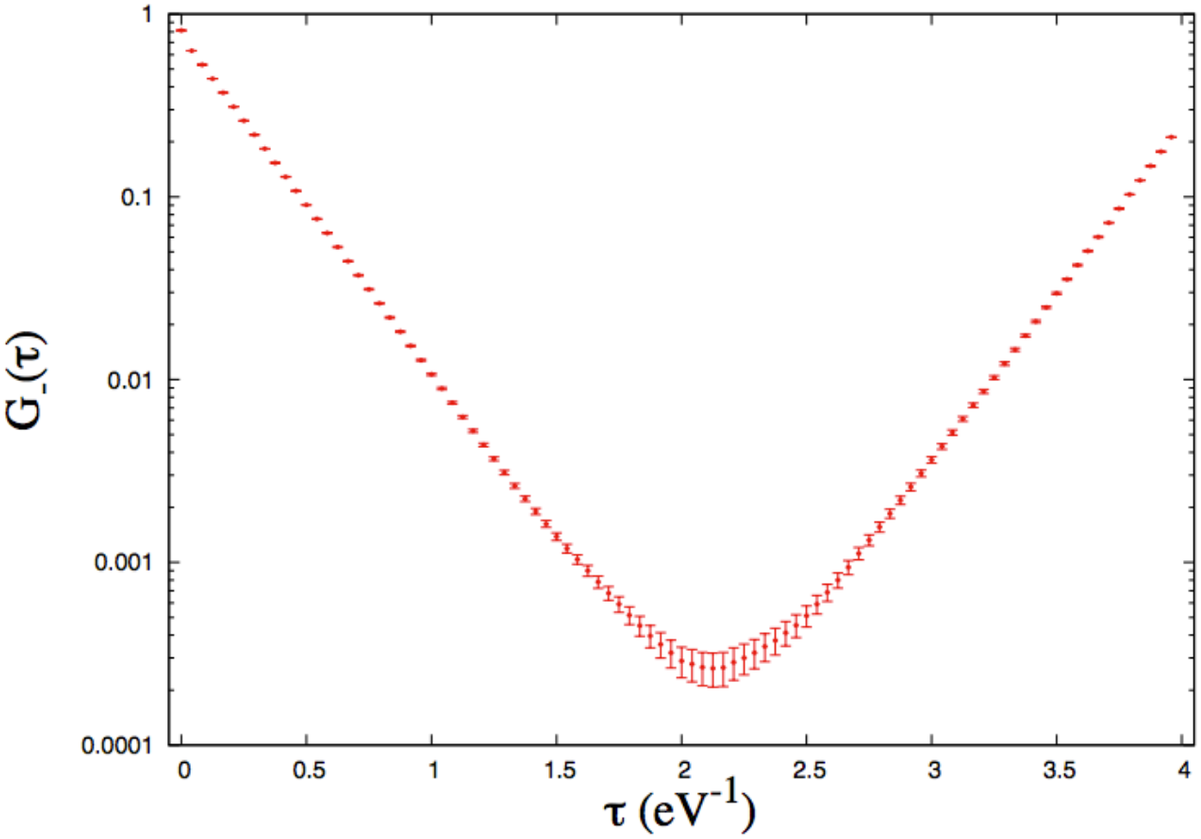
Figure by Thomas Luu

These nanotubes appear to be very close to the critical U/kappa = 3.8

Spare slides

Determination of the single-particle gap:

(3,3) armchair nanotube, actual Monte Carlo data …

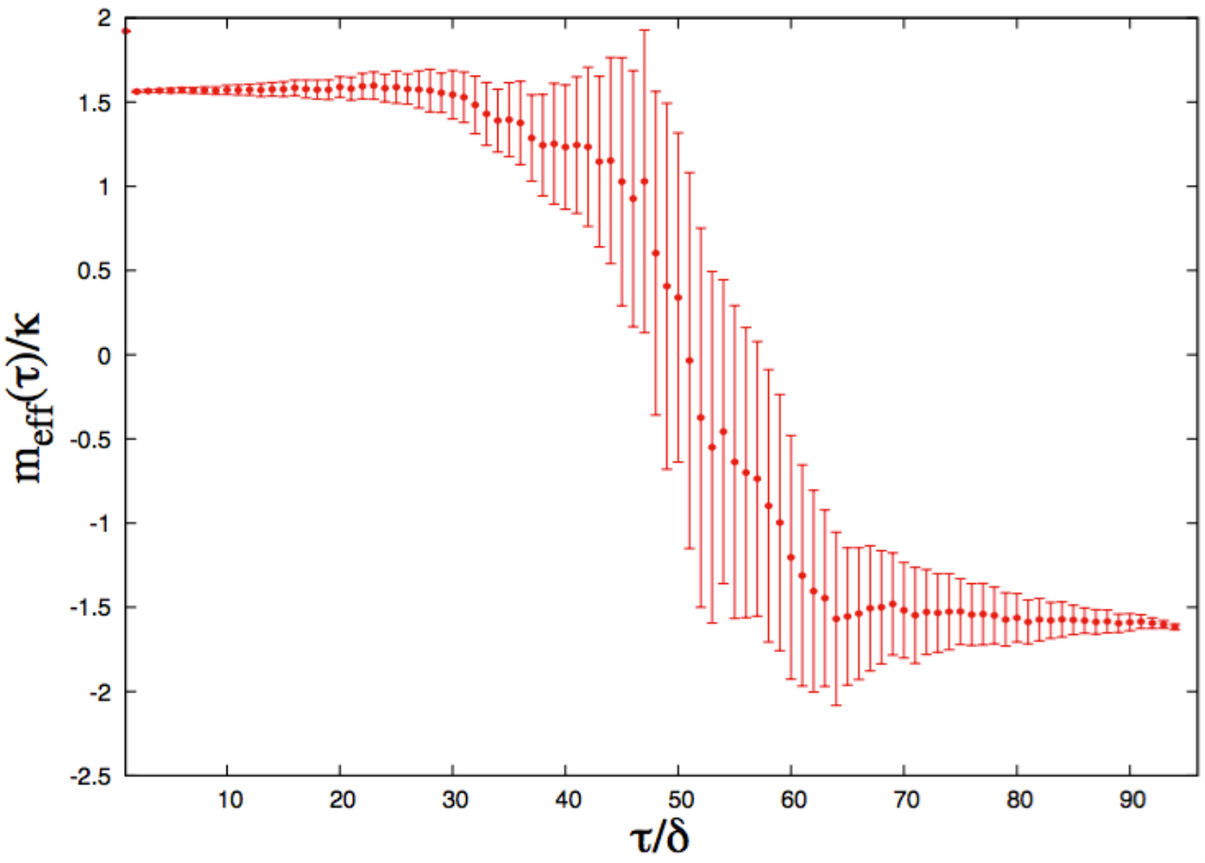


Projected onto a specific momentum mode in the spectrum

$$|\vec{T}|(|k_\perp|, |k_{||,i}|) = \left(\frac{2\pi}{3}, \frac{4\pi}{3\sqrt{3}}\right)$$

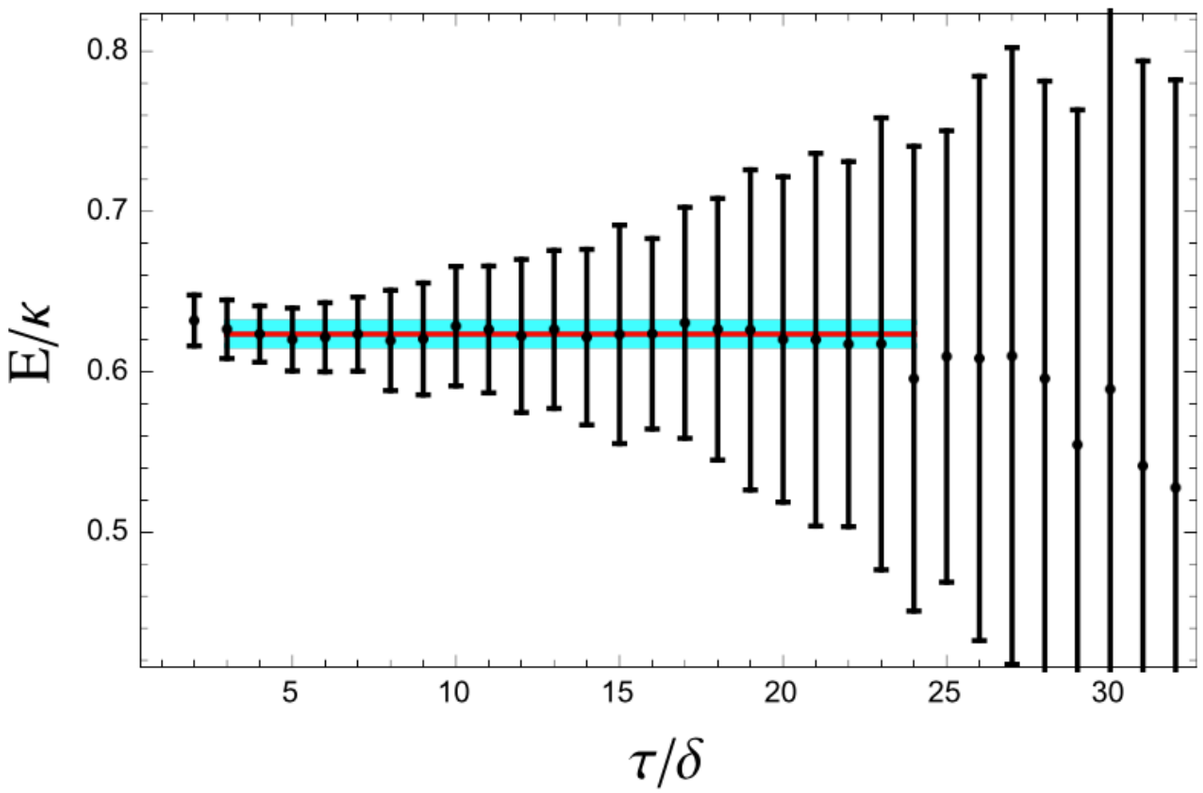
$$m_{\text{eff}}((\tau/\delta + \Delta)/2) = -\frac{1}{\Delta}\frac{\ln(G_-(\tau/\delta + \Delta))}{\ln(G_-(\tau/\delta))}$$

"Effective mass plot"
à la Lattice QCD →

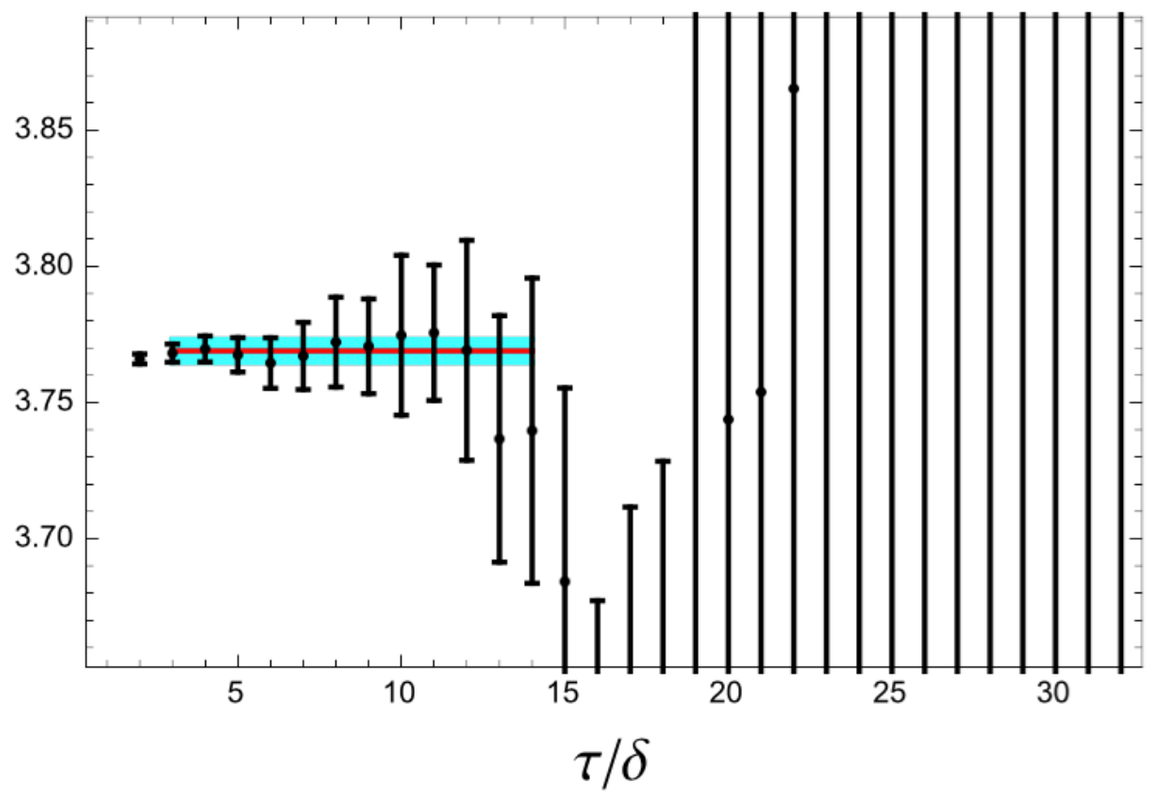


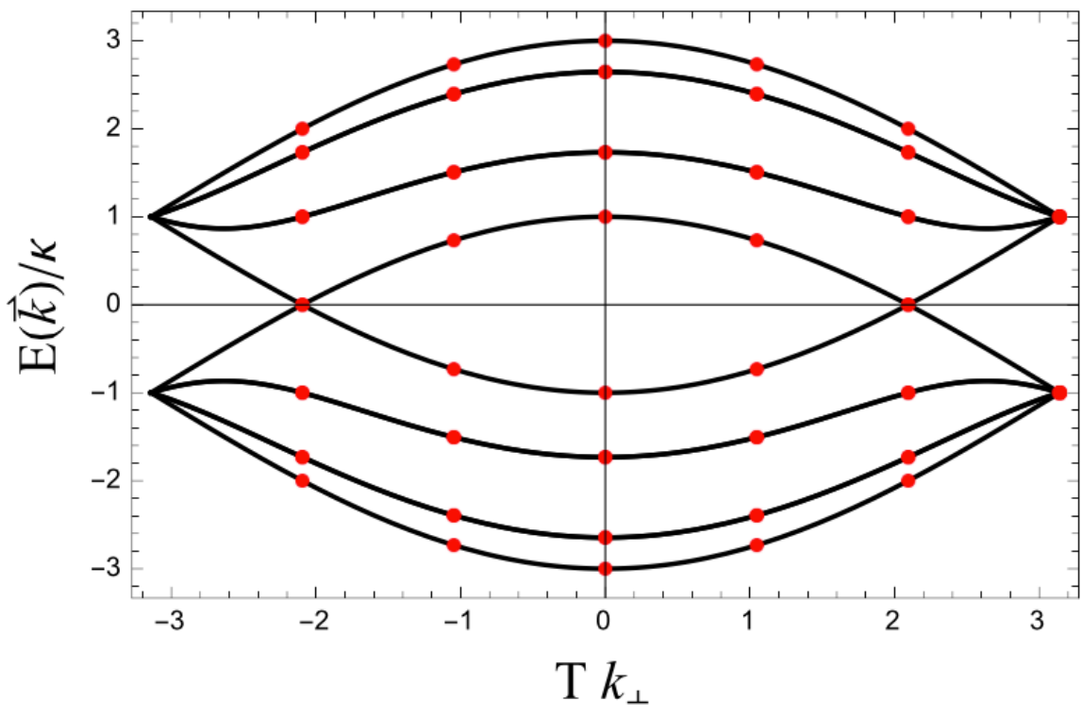
Colored bands —> fit to asymptotic correlator
Points with errorbars —> effective mass (illustration only)

K (Dirac) point



Gamma point (highest energy)



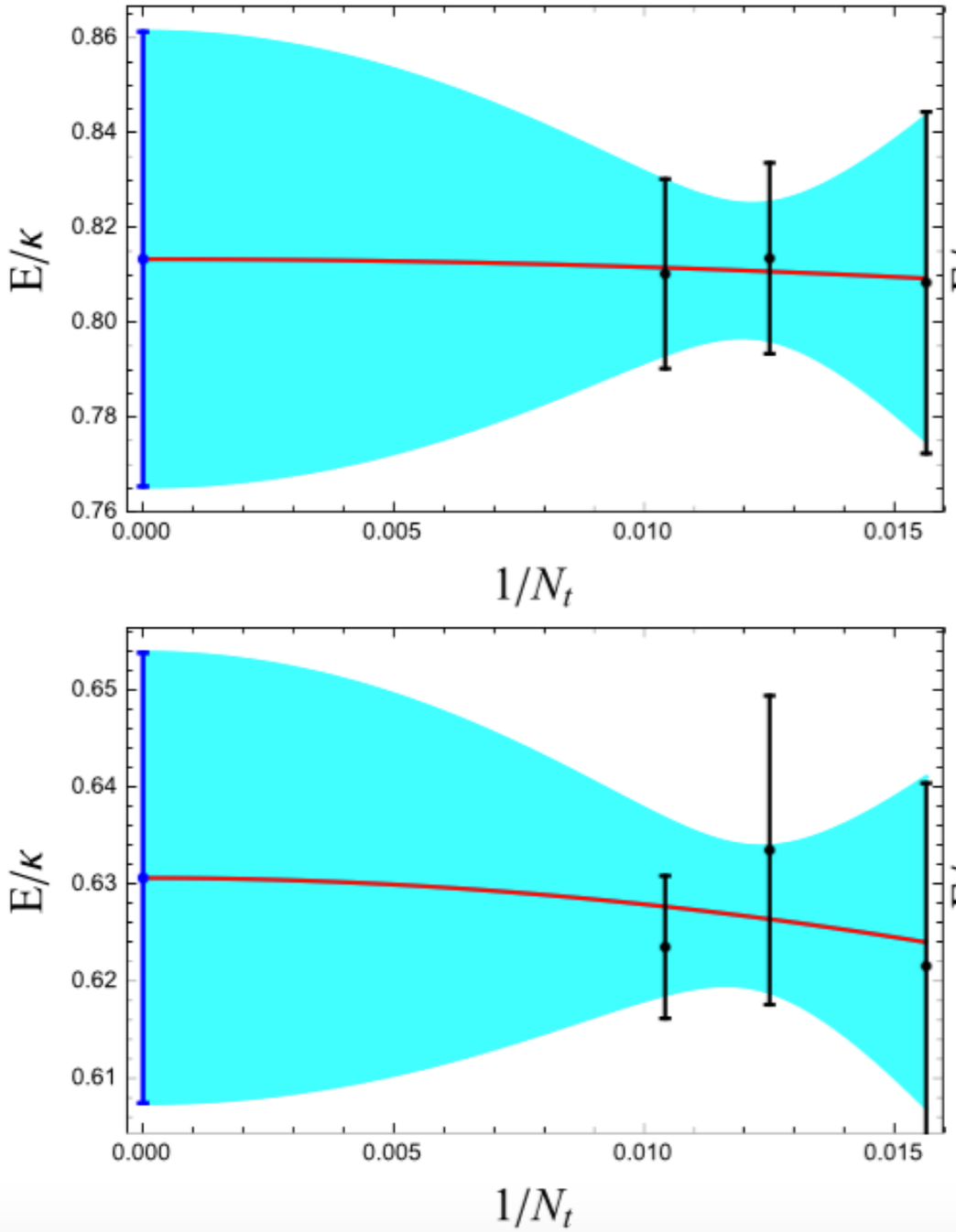


Extrapolation in Euclidean time, tube length …

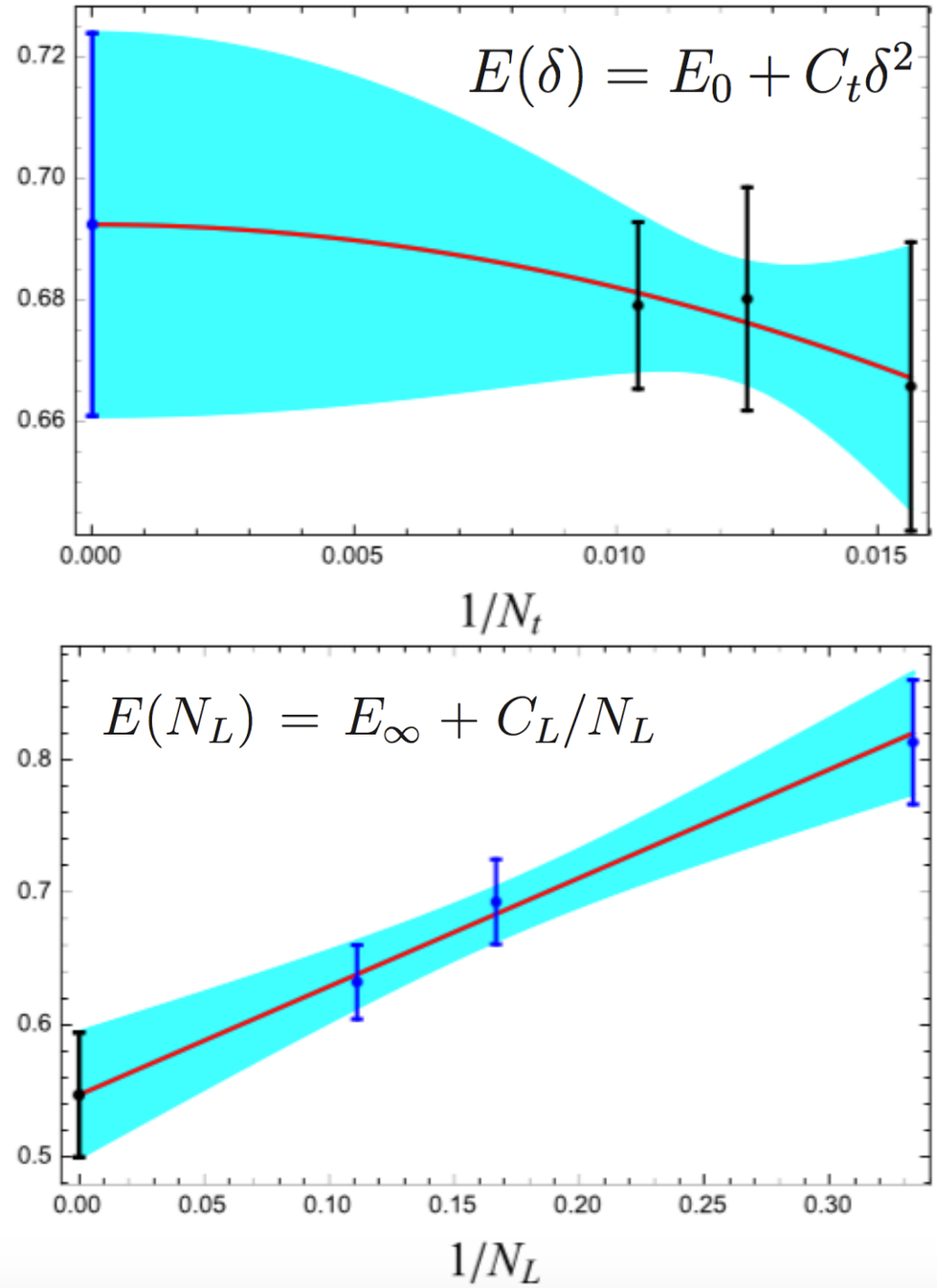
Dirac (K) point …

$$E_K/\kappa \;=\; .551(46)$$

3 unit cells



6 unit cells

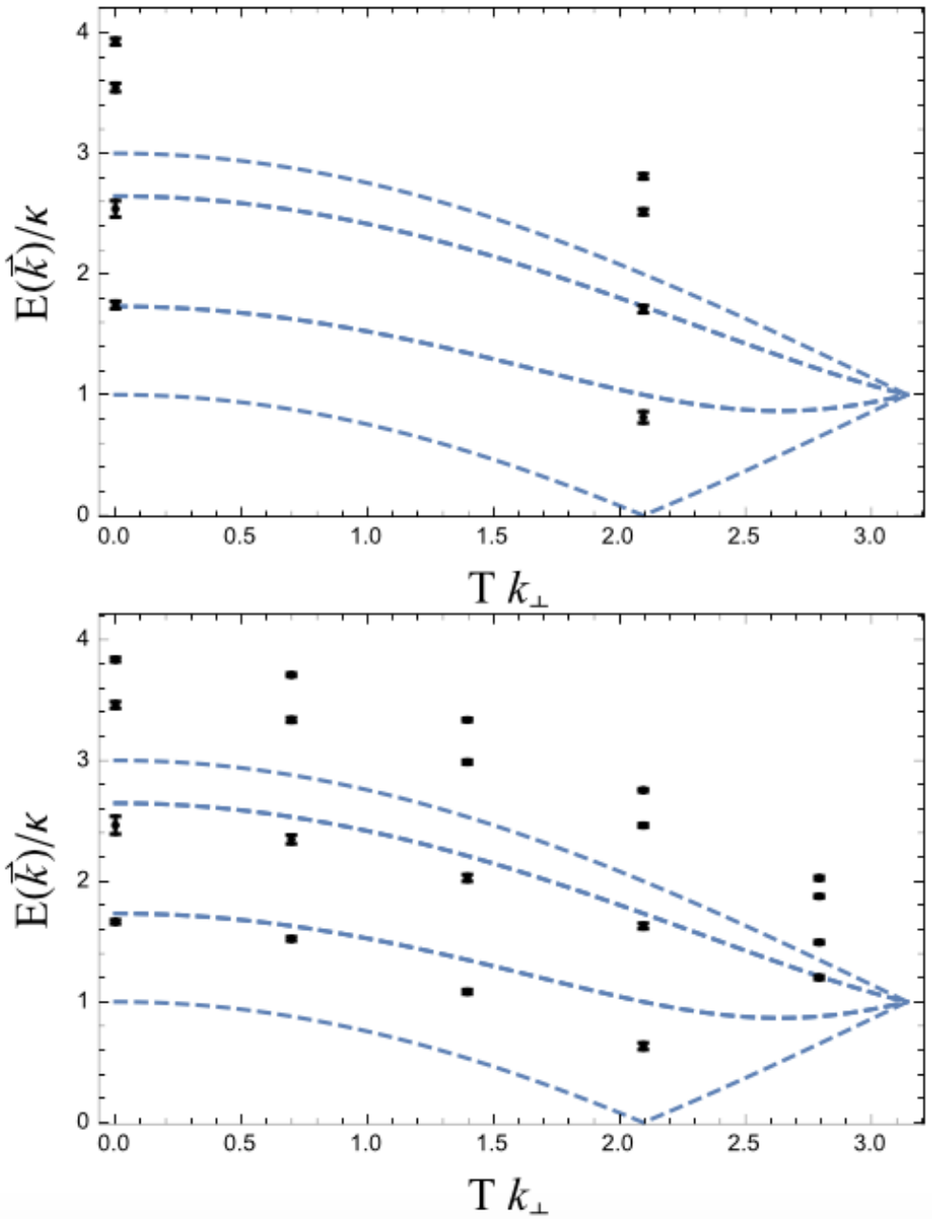


9 unit cells

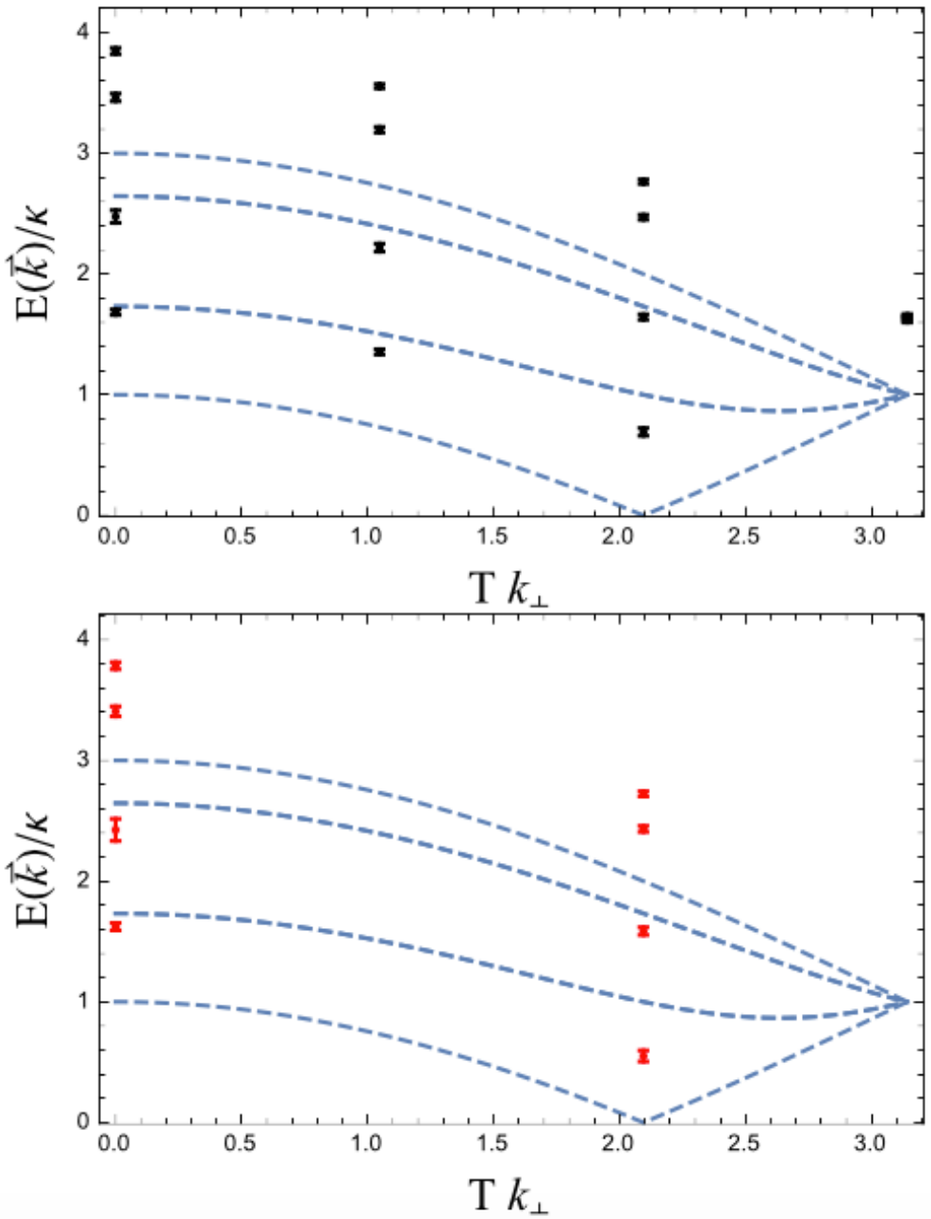
Extrapolated (but finite T) spectrum:

(3,3) nanotube ...

3 unit cells



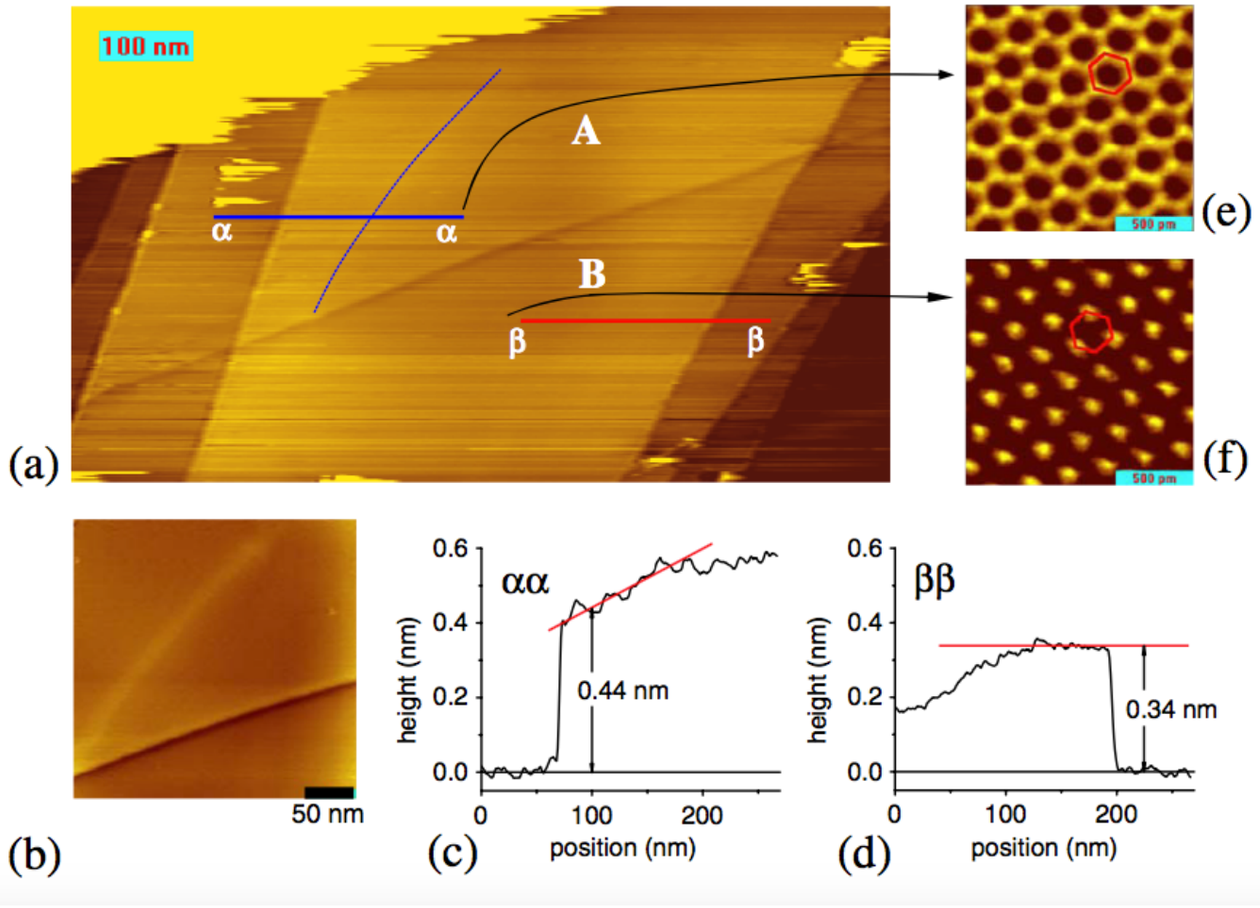
6 unit cells

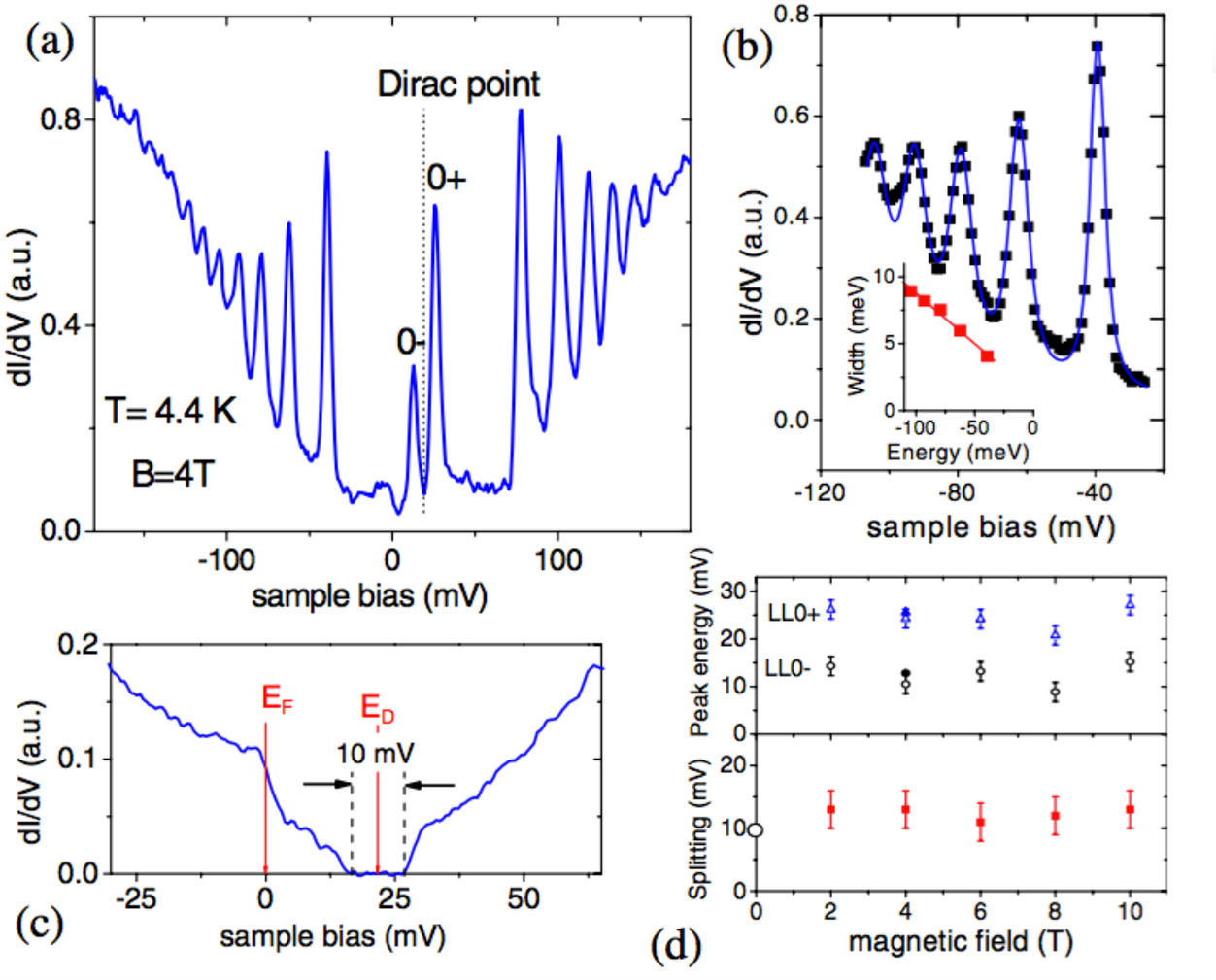


9 unit cells

Spectrum is (too?) strongly modified by interactions

STM observation of an energy gap in "quasi-suspended graphene" (controversial) ?





Guohong Li et al.,
Phys. Rev. Lett. ***112****, (2010) 176804*

Table 3.3: Parameters for Carbon Nanotubes.[a)]

symbol	name	formula	value
a	length of unit vector	$a = \sqrt{3}a_{C-C} = 2.49$ Å,	$a_{C-C} = 1.44$ Å
$\boldsymbol{a}_1$,$\boldsymbol{a}_2$	unit vectors	$\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) a$, $\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) a$	x, y coordinate
$\boldsymbol{b}_1$, $\boldsymbol{b}_2$	reciprocal lattice vectors	$\left(\frac{1}{\sqrt{3}}, 1\right) \frac{2\pi}{a}$, $\left(\frac{1}{\sqrt{3}}, -1\right) \frac{2\pi}{a}$	x, y coordinate
$\boldsymbol{C}_h$	chiral vector	$\boldsymbol{C}_h = n\boldsymbol{a}_1 + m\boldsymbol{a}_2 \equiv (n,m)$,	$(0 \le \lvert m\rvert \le n)$
L	length of $\boldsymbol{C}_h$	$L = \lvert\boldsymbol{C}_h\rvert = a\sqrt{n^2+m^2+nm}$	
d_t	diameter	$d_t = L/\pi$	
θ	chiral angle	$\sin\theta = \frac{\sqrt{3}m}{2\sqrt{n^2+m^2+nm}}$	$0 \le \lvert\theta\rvert \le \frac{\pi}{6}$
		$\cos\theta = \frac{2n+m}{2\sqrt{n^2+m^2+nm}}$, $\tan\theta = \frac{\sqrt{3}m}{2n+m}$	
d	$\gcd(n,m)$[b)]		
d_R	$\gcd(2n+m, 2m+n)$[b)]	$d_R = \begin{cases} d & \text{if } (n-m) \text{ is multiple of } 3d \\ 3d & \text{if } (n-m) \text{ is not multiple of } 3d \end{cases}$	
$\boldsymbol{T}$	translational vector	$\boldsymbol{T} = t_1\boldsymbol{a}_1 + t_2\boldsymbol{a}_2 \equiv (t_1, t_2)$	$\gcd(t_1, t_2) = 1$[b)]
		$t_1 = \frac{2m+n}{d_R}$, $t_2 = -\frac{2n+m}{d_R}$	
T	length of $\boldsymbol{T}$	$T = \lvert\boldsymbol{T}\rvert = \frac{\sqrt{3}L}{d_R}$	
N	Number of hexagons in the nanotube unit cell.	$N = \frac{2(n^2+m^2+nm)}{d_R}$	
$\boldsymbol{R}$	symmetry vector	$\boldsymbol{R} = p\boldsymbol{a}_1 + q\boldsymbol{a}_2 \equiv (p,q)$	$\gcd(p,q) = 1$[b)]
		$t_1 q - t_2 p = 1$, $(0 < mp - nq \le N)$	
τ	pitch of $\boldsymbol{R}$	$\tau = \frac{(mp-nq)T}{N} = \frac{MT}{N}$	
ψ	rotation angle of $\boldsymbol{R}$	$\psi = \frac{2\pi}{N}$	in radians
M	number of $\boldsymbol{T}$ in $N\boldsymbol{R}$.	$N\boldsymbol{R} = \boldsymbol{C}_h + M\boldsymbol{T}$	

[a)] In this table n, m, t_1, t_2, p, q are integers and d, d_R N and M are integer functions of these integers.

[b)] $\gcd(n,m)$ denotes the greatest common divisor of the two integers n and m.