Mott transition in the Hubbard model on anisotropic honeycomb lattice with implications for strained graphene

G. Rut[1,2], M. Fidrysiak[1], D. Goc-Jagło[1], and A. Rycerz[1]

[1]Institute for Theoretical Physics, Jagiellonian University, Łojasiewicza 11, PL–30348 Kraków, Poland

[2]Verisk Analytics Sp. z o.o., Rakowicka 7, PL–31511 Kraków, Poland

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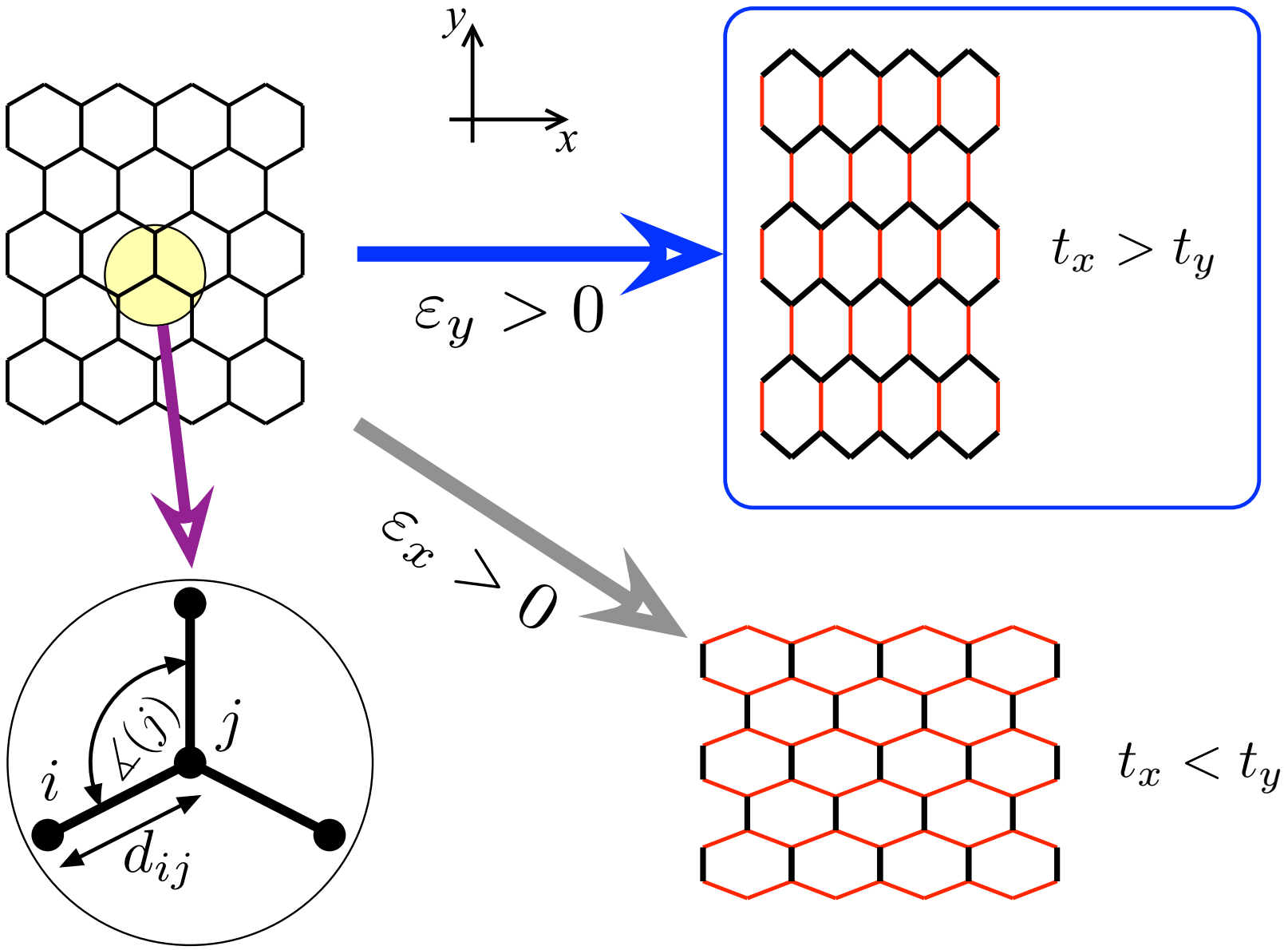
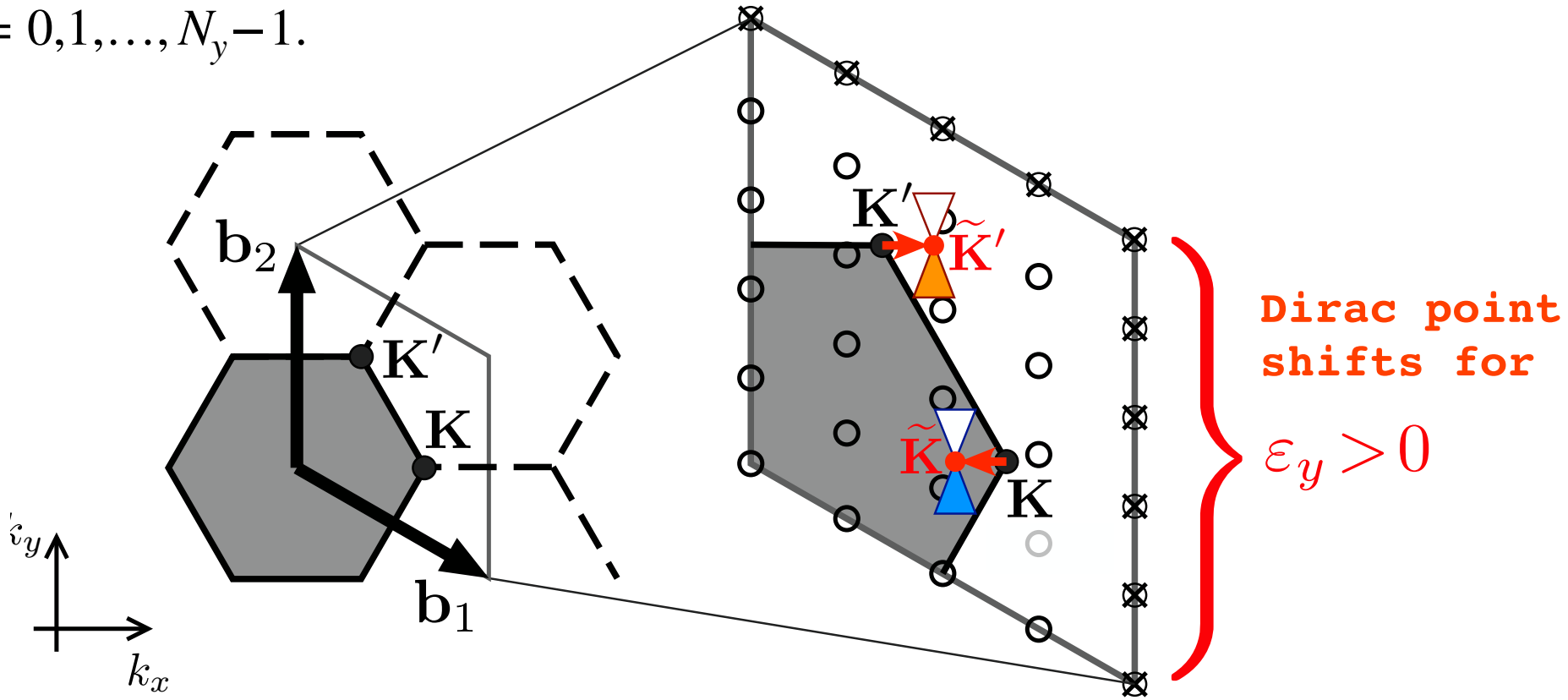
JAGIELLONIAN UNIVERSITY IN KRAKÓW

NARODOWE CENTRUM NAUKI


y
x
$\varepsilon_y > 0$
$t_x > t_y$
$\varepsilon_x > 0$
$t_x < t_y$
i
j
ϕ_{ij}
d_{ij}

Discrete FBZ: $k_x = \frac{2\pi}{N_x} n_x, \quad k_y = \frac{4\pi}{\sqrt{3}} \left(\frac{n_y}{N_y} - \frac{n_x}{2N_x} \right), \quad n_x = 0,1,\ldots,N_x-1,$

$n_y = 0,1,\ldots,N_y-1.$



Dirac point ≠ high symmetry points (!)

The Hamiltonian: $H = \sum_{\langle ij \rangle, s} t_{ij} \left(c^{\dagger}_{i,s} c_{j,s} + \text{H.c.} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow},$

where $t_{ij} = \begin{cases} -t_x & \text{if i,j belongs to same zigzag line,} \\ -t_y & \text{otherwise .} \end{cases}$

[$c^{\dagger}_{i,s}/c_{i,s}$– creation/annihilation operator, $s = \uparrow, \downarrow$, $n_{is} = c^{\dagger}_{i,s} c_{i,s}$.]

The Hartree-Fock approximation:

$$U\hat{D} \approx U \sum_{i} \left(\langle n_{i\uparrow} \rangle n_{i\downarrow} + n_{i\uparrow} \langle n_{i\downarrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right),$$

where $\hat{D} = \sum_j n_{j\uparrow} n_{j\downarrow}$, $\langle n_{i\uparrow} \rangle = \frac{\overline{n} + \lambda_i m}{2}$, $\langle n_{i\downarrow} \rangle = \frac{\overline{n} - \lambda_i m}{2}$, and

$\lambda_i = \pm 1$ alternates between the sublattices on *bipartite lattice*.

For the half filling ($\overline{n} = 1$) **the HF ground-state energy**:

$$\frac{E_G^{(\mathrm{HF})}}{N} = -\frac{2}{N}\sum_{\mathbf{k}}\sqrt{E_{\mathbf{k}}^2 + \left(\frac{Um}{2}\right)^2} + \frac{U(1+m^2)}{4},$$

with the factor 2 accounting for $s = \uparrow, \downarrow$ and

$\mathbf{k} \equiv (k_x, k_y) \in$ FBZ. [**No. of lattice sites** $N = 2N_xN_y$.]

The band energy: $E_{\mathbf{k}} = t_x\sqrt{a_{\mathbf{k}}^2 + b_{\mathbf{k}}^2},$

where $$a_{\mathbf{k}} = -\cos\left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right) - \cos\left(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2}\right) - \frac{t_y}{t_x},$$

$$b_{\mathbf{k}} = \sin\left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right) - \sin\left(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2}\right).$$

The density of states:

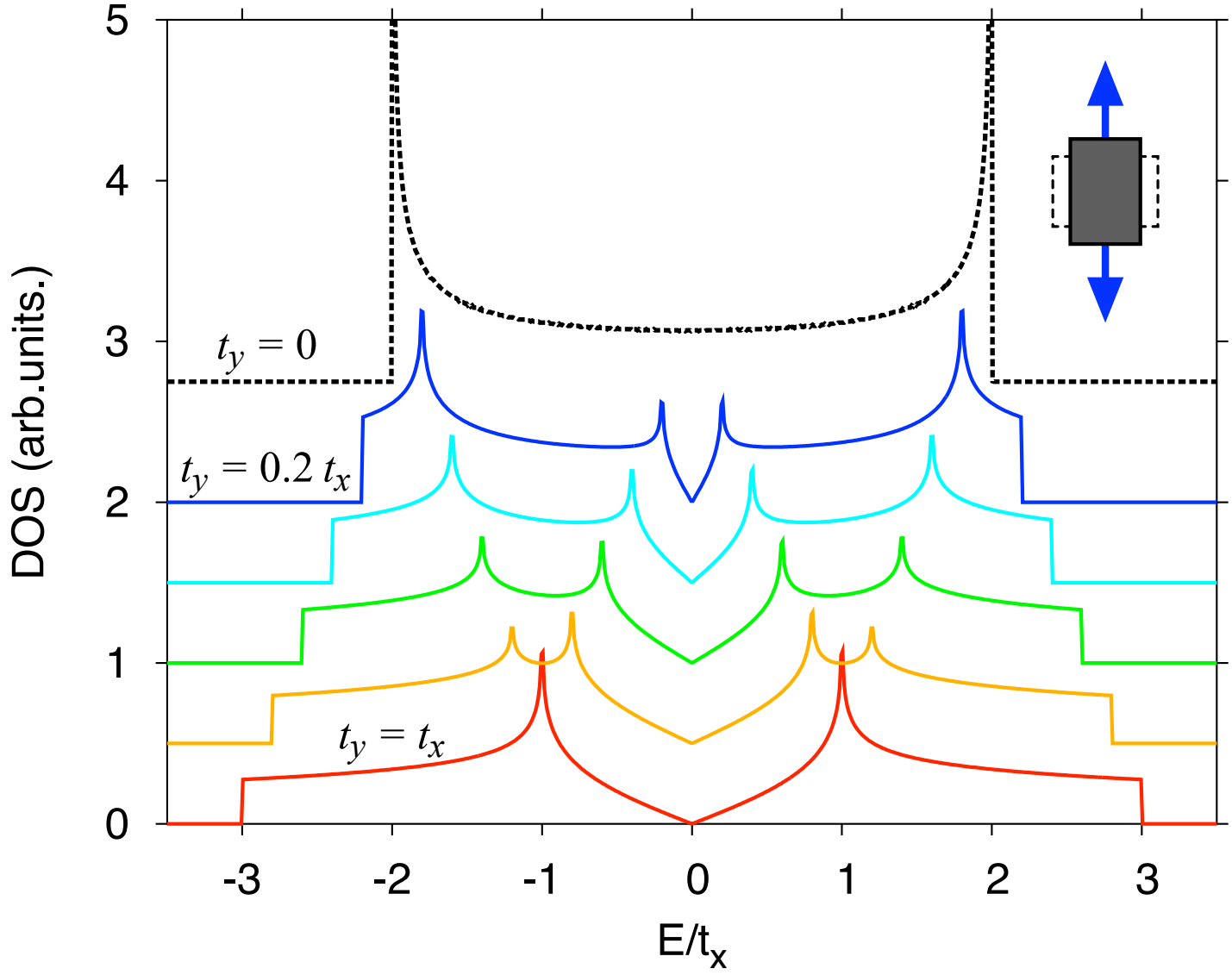
$$\rho(E) = 2N^{-1} \sum_{\mathbf{k}} \left[\delta\left(E - E_{\mathbf{k}}\right) + \delta\left(E + E_{\mathbf{k}}\right) \right],$$

where the two parts correspond to the conduction (E>0) and valence (E<0) band.

The gap equation: $1 = \int_{E<0} dE\, \rho(E) \frac{U/2}{\sqrt{E^2 + (Um/2)^2}}$.

Unlike for square lattice, for which one gets $m \neq 0$ for any $U > 0$ [see Hirsch, 1985], on a honeycomb lattice the minimization gives $m = 0$ for $U \leqslant U_c^{(\mathrm{HF})}$ and $m \neq 0$ for $U > U_c^{(\mathrm{HF})}$ [see Martelo *et al.*, 1997]. **This is because** $\rho(E) \to 0$ [$\rho(E) \propto |E|$] for $E \to 0$.

Density of states for $U = 0,\ \varepsilon_y > 0$:



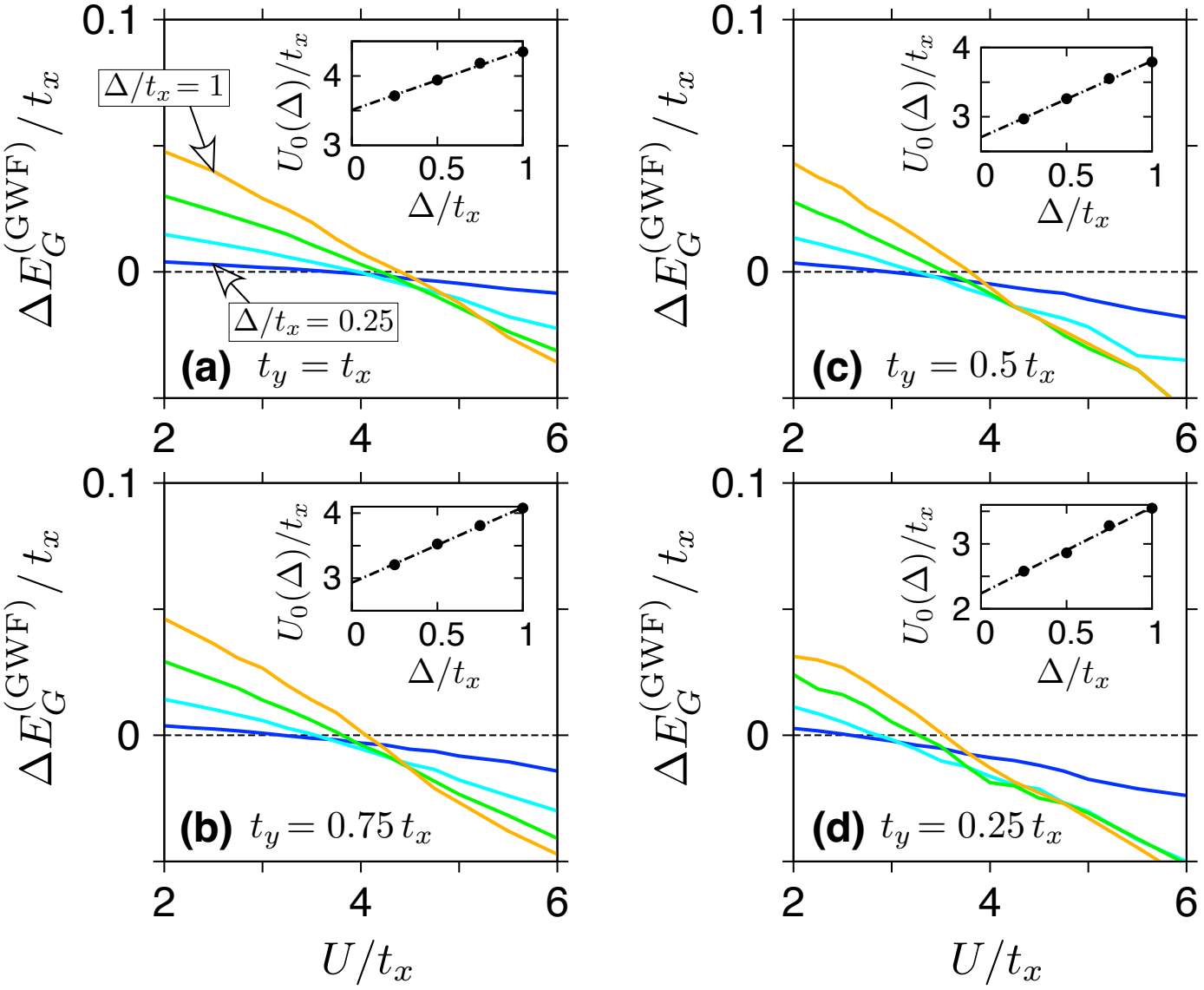
Gutzwiller wavefunction (GWF): $\left|\Psi_{\mathrm{GWF}}\right\rangle = e^{-\eta\hat{D}}\left|\psi_0(m)\right\rangle,$

where $\left|\psi_0(m)\right\rangle$ denotes a Slater determinant corresponding to a given m and η is a variational parameter (quantifying electron correlations).

Variational energy (to be minimized with respect to η and m):

$$E_G^{(\mathrm{GWF})} = \frac{\left\langle\psi_0(m)\right| e^{-\eta\hat{D}} H e^{-\eta\hat{D}} \left|\psi_0(m)\right\rangle}{\left\langle\psi_0(m)\right| e^{-2\eta\hat{D}} \left|\psi_0(m)\right\rangle}.$$

In many cases, the system may prefer to reduce m (even to $m = 0$) and increase η, allowing to expect that $U_c^{(\mathrm{GWF})} \geqslant U_c^{(\mathrm{HF})}$.



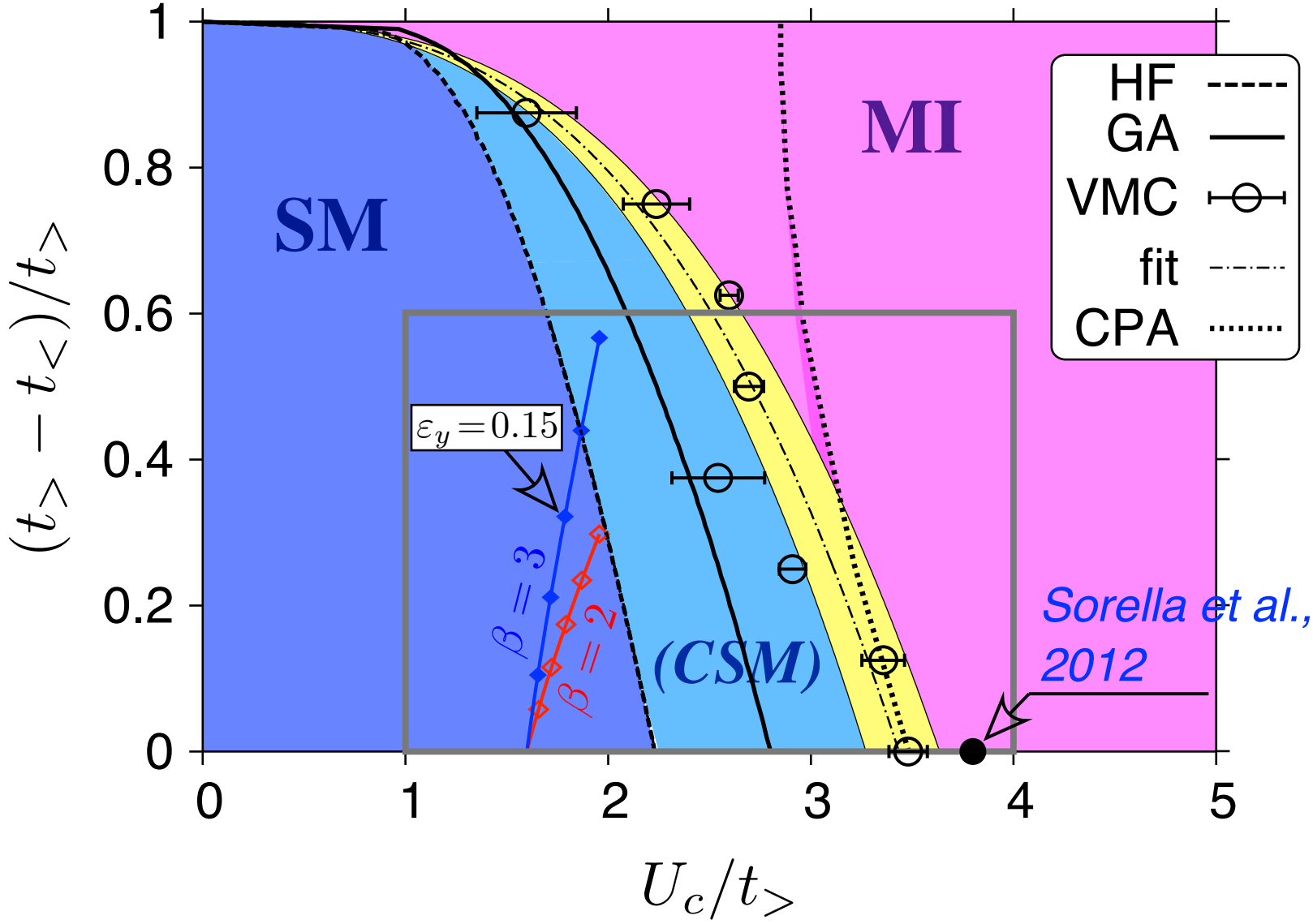
[*Definitions*: $\Delta E_G^{(\mathrm{GWF})}(\Delta) = E_G^{(\mathrm{GWF})}(\Delta) - E_G^{(\mathrm{GWF})}(0),\ \ \Delta \equiv Um.$]

Critical U_C-s obtained within different methods:

t_y/t_x	$U_c^{(\mathrm{HF})}/t_x$	$U_c^{(\mathrm{GA})}/t_x$	$U_c^{(\mathrm{GWF})}/t_x$
1.00	2.231	2.804	$3.48(1)$ *)
0.75	2.034	2.550	$2.91(1)$
0.50	1.803	2.241	$2.69(3)$
0.25	1.510	1.830	$2.24(1)$

$\Rightarrow$ Values of $U_c^{(\mathrm{HF})}$ and $U_c^{(\mathrm{GA})}$ [*GA – Gutzwiller Approximation*] correspond to $N_x, N_y \to \infty$; $U_c^{(\mathrm{GWF})}$ is obtained for $N_x = N_y = 10$ [$\Leftrightarrow N = 200$]

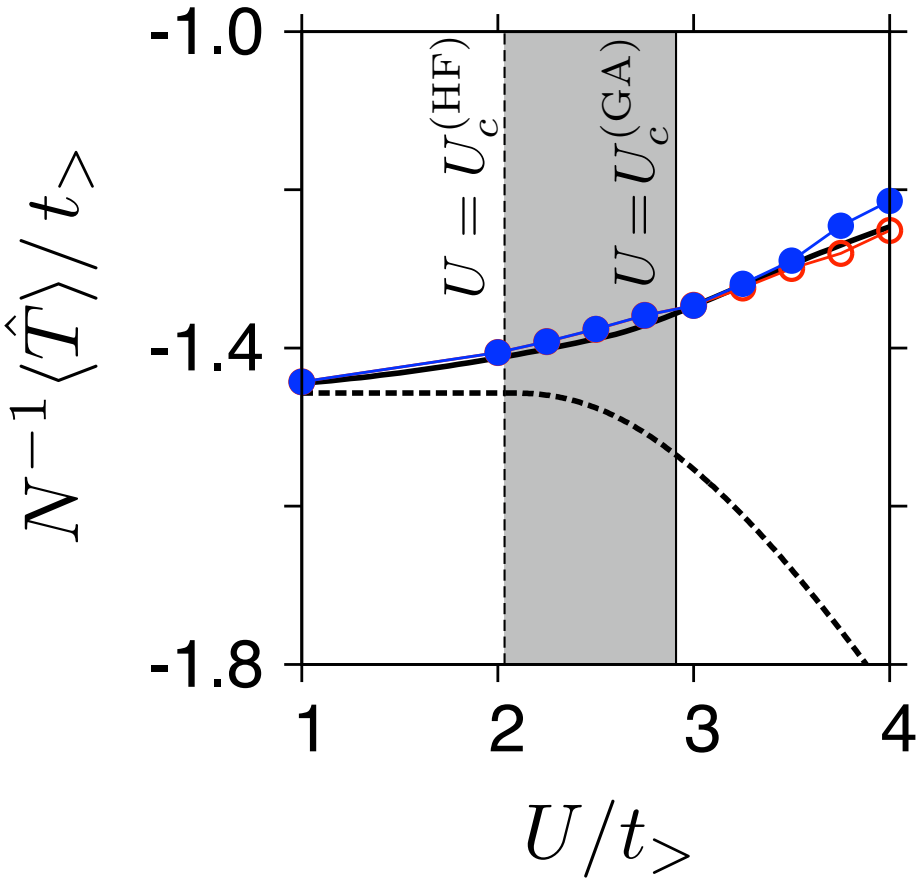
*) Value of $U_c^{(\mathrm{GWF})} = 3.48\, t_x$ [for $t_y = t_x$] can be compared with **the 'exact' QMC results**: $U_c^{(\mathrm{QMC})} = 3.86\, t_x$ [see Sorela et al., 2012]

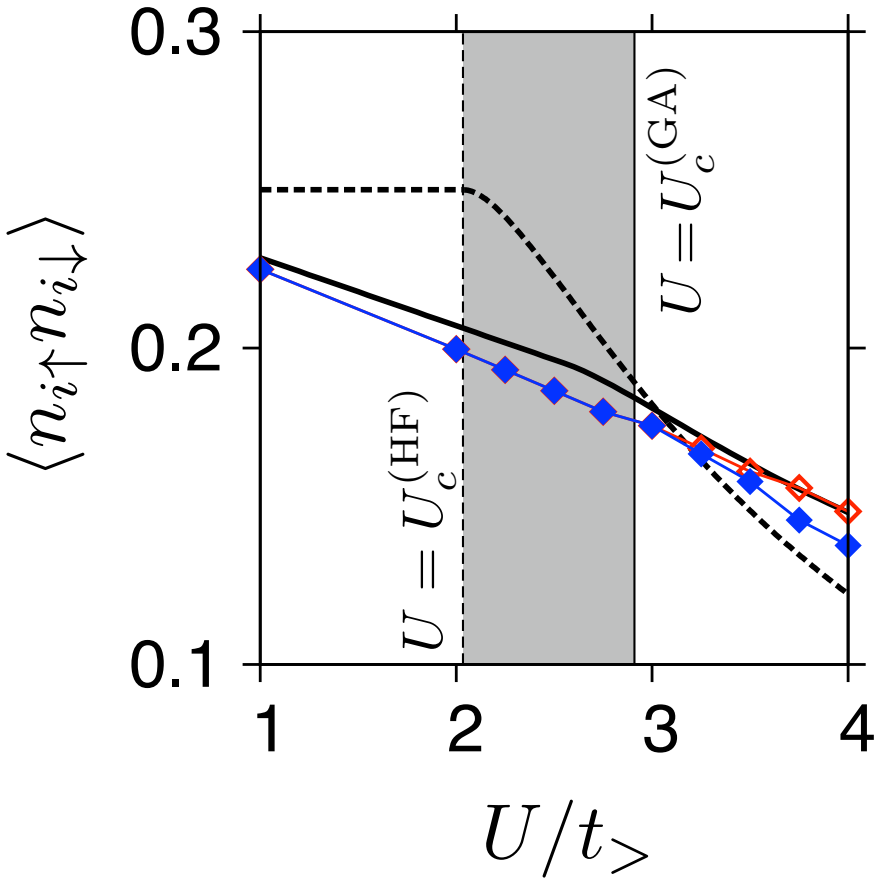


[*Notation:* $t_> \equiv t_x$, $t_< \equiv t_y$ for $\varepsilon_y > 0$; $\beta = -\partial \ln t_{ij} / \partial \ln d_{ij}$.]

Band narrowing and the reduction of double occupancies

$(\implies t_y/t_x = 0.75)$





Concluding remarks

⇒ Strain applied along armchair direction *modifies DOS without opening a gap*; possibility for Mott semimetal-insulator transition

⇒ Different numerical approaches (HF, GA, GWF, CPA…) predicts the critical U_c to *decrease* with the strain

⇒ A modified Su-Schrieffer-Heeger model for graphene predicts the parameters (U_c, t_x, t_y) stay in a semimetal range; for maximum possible strains $\varepsilon_y \approx 0.15$ the effects of electron correlations (*such as the reduced* $\langle n_{i\uparrow} n_{i\downarrow} \rangle$) are noticeable.

Key references:

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Acknowledgment

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THANK YOU!