Singularity of density of states in the pi-flux lattice

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Outline

1. Motivation
   - Interactions vs disorder
   - π-flux model
   - Lattice deformations and ripples
2. Random hopping in π-flux model
   - Singularity of DOS
   - $k-$dependent self-energy and minimal conductivity
3. Summary

disorder in semimetals

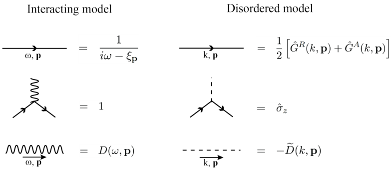
Why disorder?

1. inherently present in all solid-states systems
2. determine/dominate properties
   localization, symmetry broken, new phase...
3. adjustable
   doping, impurities, vacancies, absorption, strain...

Interactions-disorder duality and critical phenomena

non-Anderson transition

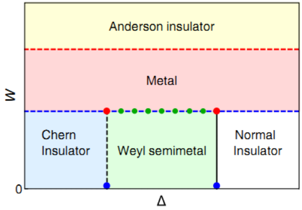
$$H = \int \Psi^\dagger(r)\xi_p\Psi(r)d^d r - \frac{1}{2}\int \Psi^\dagger(r)\Psi^\dagger(r')\xi_p\Psi(r')\Psi(r)d^d r d^d r'$$



	Interacting model	Disordered model
Coordinates	$(\tau,\mathbf{r})$	$(\mathrm{r}_{d+1},\mathbf{r})$
Temperature/size	T	$1/\ell_{d+1}$
Coupling to interactions/disorder	$\hat{\Psi}^\dagger\hat{\Psi}\phi$	$\hat{\psi}^\dagger\hat{\sigma}_z\hat{\psi}u$
Observables	$\hat{n}$ (density)	ρ_s, Eq. (5)

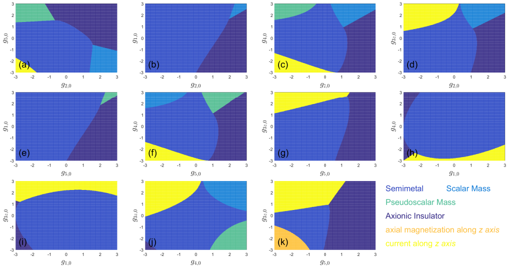
Syzranov, Sergey V.,etc al, Annu. Rev. Condens. Matter Phys. 9, 1 (2018); Sun, Shijun, and Sergey Syzranov. Phys. Rev. B 108 195132 (2023)

disorder-driven transition in semimetals



W: strength of disorder
$\Delta = t_z - m_z$: QPT parameter of SM-IN transition

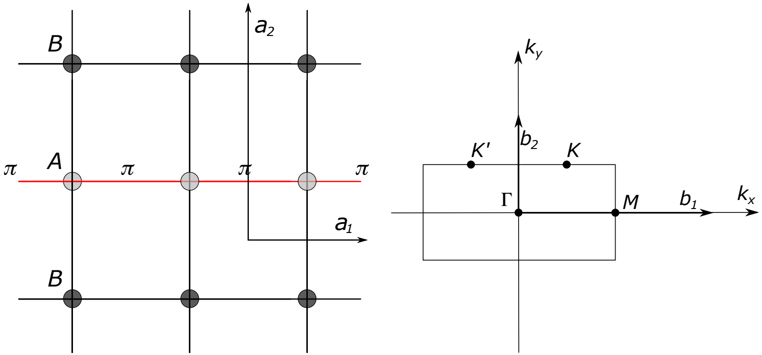
global phase diagram of semi-Dirac semimetals



Physical Review B, 102, 085132 (2020); **Journal of Physics: Condensed Matter**, 33, 125601 (2021); **Physical Review B**, 107, 155125 (2023).

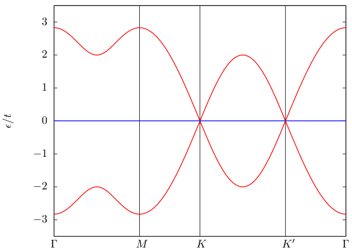
$\pi-$flux model

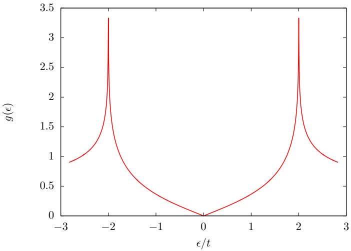
$$t_{j+\hat{x},j} = (-1)^{j_x},\ t_{j+\hat{y},j} = 1, \quad \epsilon_{\pm}(k) = \pm 2t\sqrt{\cos^2 k_x + \cos^2 k_y}$$



$\pi-$flux model

$$\epsilon_{\pm}(k) = \pm t\sqrt{1 + 4\cos(\frac{k_x}{2})\cos(\frac{\sqrt{3}k_y}{2}) + 4\cos^2(\frac{k_x}{2})}$$





Random hopping Dirac fermions on $\pi-$flux lattice

Gade's Model: $P[\delta t] \propto [-W, \; W]$,

$\rho(E) = \frac{1}{E} exp(-cln|E|^{1/x}), \quad x = \frac{3}{2}$ or 2?

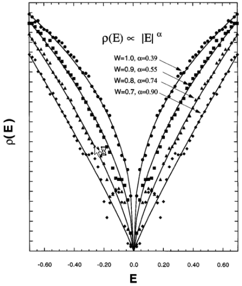


FIG. 1. The density of states $\rho(E)$ (with small imaginary part $\delta = 0.02$), where $L = 50$ and $W = 0.7, 0.8, 0.9$, and 1.0. We have fitted the data by the power-law form $\rho(E) = CE^{\alpha(W)}$, where $\alpha(W) = 0.90, 0.74, 0.55$, and 0.39 for $W = 0.7, 0.8, 0.9$, and 1.0, respectively.

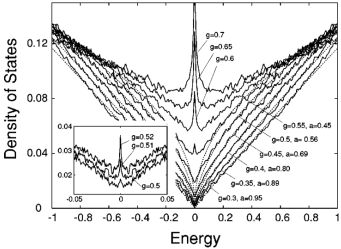


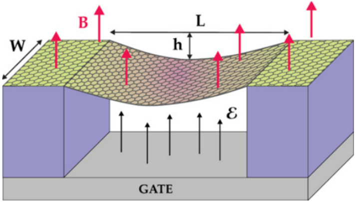
FIG. 4. Same as Fig. 3 on a 100×100 lattice for $g=0.3$–0.7, and $\delta=0.005$, averaged over 50 samples. Away from zero energy ($E>0.1$) and for sufficiently weak randomness, data are fitted to a power law $\rho(E)\propto|E|^a$. Inset: same as Fig. 3 on a 250×250 lattice for $g=0.5, 0.51, 0.52$, and $\delta=0.0005$, averaged over 70 samples.

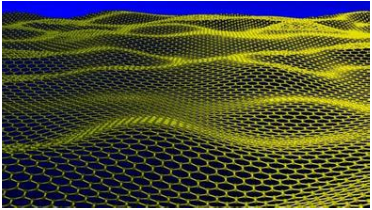
NPB 398, 499 (1993), PRL, 79 (19) (1997), PRB, 58 (11) (1998), PRB 65, 064206(2002), PRB 67, 064202 (2003);

PRL 113, 5, 186802 (2014), PRL 117, 5, 116806 (2016)

Lattice deformations

$$\Delta h \sim 1 - 4Å, \;\; u \sim 0.1 - 1\%, \;\; L \sim 100nm$$

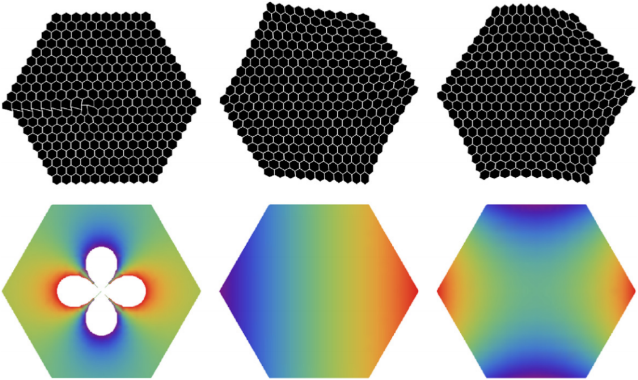




1. hybridized orbitals and "topological" defects.
2. modulate the on-site energies (ϵ_{ij}) and the hopping parameter (γ_{ij}) .
3. pseudo magnetic field (gauge field)

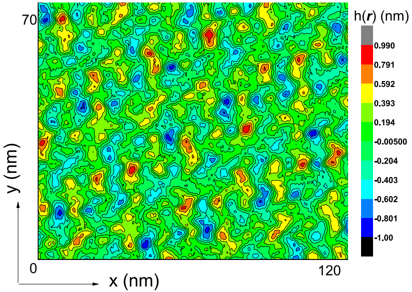
F. Guinea, Solid State Commun., 152 (15) (2012)

effective magnetic fields induced by the deformations



F. Guinea, Strain engineering in graphene, Solid State Commun., 152 (15) (2012)

Model of Ripples



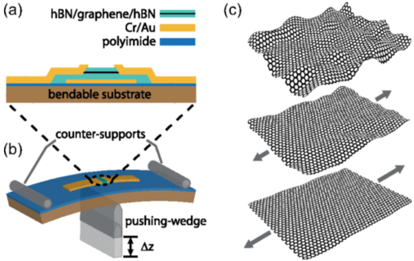
$$h(\mathbf{r}) = C \sum_i^{N_r} C_{\mathbf{q}_i} \sin(\mathbf{q}_i \cdot \mathbf{r} + \delta_i),\ \ \delta_i\ \in [0, 2\pi],\ \ \mathbf{q}_i\ \in [2\pi/L, 2\pi/3a]$$

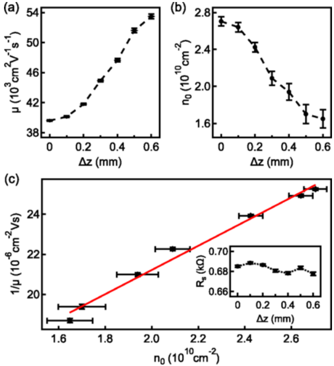
$$C_{q_i} = \begin{cases} \sqrt{2}/q_i^2, & q_i > q_{ripple},\ \ q_{ripple} = 2\pi/\lambda_{ripple} \\ \sqrt{2}/q_{ripple}^2, & otherwise,\ \ \lambda_{ripple} \approx 8nm \end{cases}$$

$$\delta t_{ij} = t\alpha\Delta a/a,\ \ \Delta a = \sqrt{a^2 + (h(\mathbf{r}) - h(\mathbf{r}'))^2} - a,\ \ \alpha = -2$$

Effects of Random Strain Fluctuations on mobility

$$\text{Drude model:}\quad G = \frac{1}{\frac{\alpha}{\epsilon\mu\sqrt{n^2+n_0^2}}+R_s},\quad \Delta z = 0.6nm \ \sim\ \bar{\sigma} \approx 0.2\%$$





Wang, L. et al, Phys. Rev. Lett. 124, 157701 (2020); Wang, L., et al. Commun. Phys. 4, 147 (2021)

Random hopping model

A graphene or $\pi-$flux model with bond disorder belongs to the **chiral orthogonal symmetry** class since time-reversal symmetry is preserved

$$\mathcal{H} = \mathcal{H}_0 + V = \sum_{<ij>} c_i^\dagger t_{ij} c_j + V + h.c.$$

$$V = \sum_{<ij>} \delta t_{ij} |i><j| + h.c., \;\; P[\delta t] \propto exp[-\delta t^2/2g_b]$$

LMTB (Lanczos method on Tight-binding)

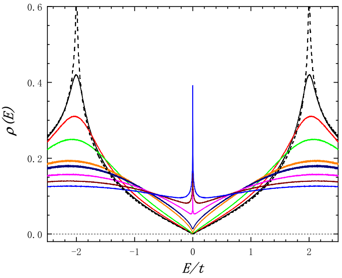
- large-scale accurate simulation in real/momentum space
- strong disorder (non-purtubative, beyond SCBA)

Physical Review B, 85 073407 (2012)

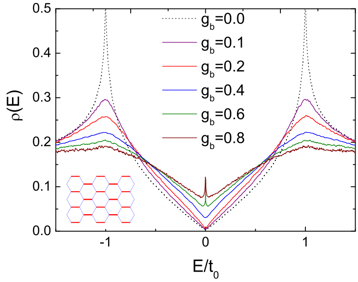
Average density of states

$$\rho(E) = -\frac{1}{\pi}\overline{<\psi|\frac{1}{E-H+i\gamma}|\psi>}, \quad \gamma \sim 1/L$$

π−flux model

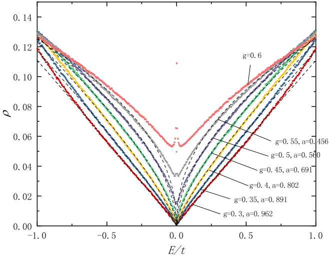


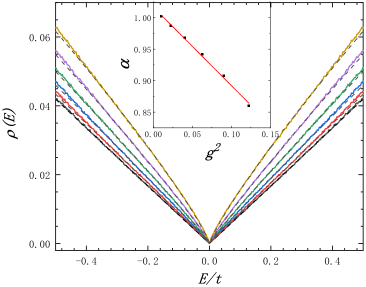
graphene



Low energy DOS for weak disorder: Power Law

- $g_b = 0, \quad \rho(E) = |E|$
- $g_b < g_b^c, \quad \rho(E) = \rho_1 |E|^{\alpha}, \ \alpha = 1.05 - 1.24 g_b$



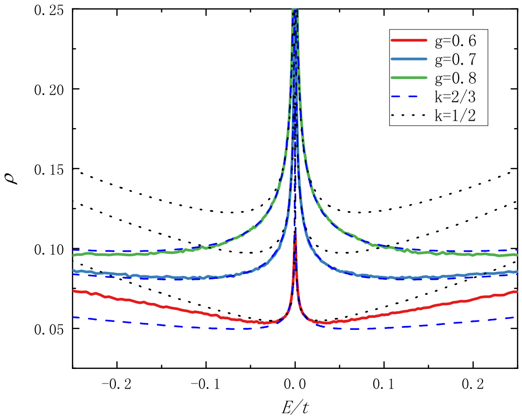


Born Approximation:

$$\rho(E) = -\frac{1}{\pi}\mathrm{Im}\langle G_{rr}\rangle = \frac{A_c\lambda}{2\pi v^2}\left(\frac{E}{\lambda}\right)^{1-(2gA_c/\pi v^2)} .$$

Low energy DOS for strong disorder: Singularity

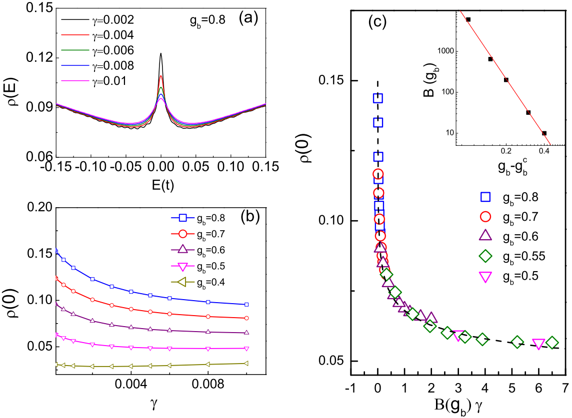
Gade's Model: $\rho(E) = \frac{1}{E} exp(-c ln|E|^{1/x}), \quad x = \frac{3}{2}$ or 2? $\quad x = \frac{3}{2}$



Gade, et al, Nucl. Phys. B 398, 499 (1993); Mudry, et al, Phys. Rev. B 67, 064202 (2003)

Low energy DOS for strong disorder

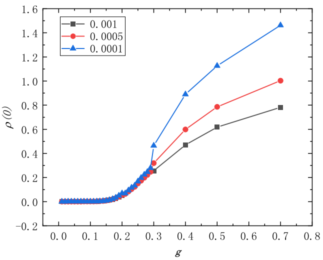
- $g_b > g_b^c, \quad \rho(0) = \frac{A}{(B\gamma)^\nu}, \; B(g_b) = \frac{1}{(g_b - g_b^c)^\kappa}$
  with critical exponent $\nu = 0.12$ and $A = 0.07$



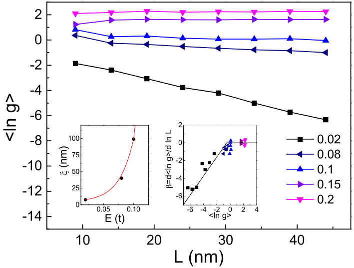
Crossover: semi-metal to diffusion metal

power-law behavior $\rightarrow$ singular behavior

$\rho(0)$ vs g
for different γ

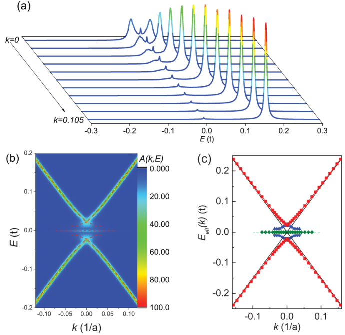


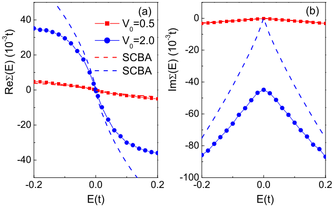
one-parameter scaling theory
at $g = 0.7$

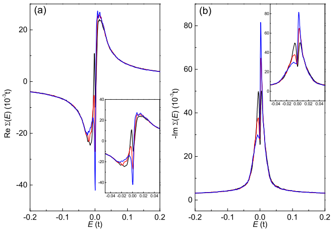


Accurate calculation of self-energy of Dirac fermions

spectral function and self-energy of strong disorder

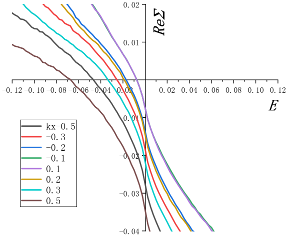


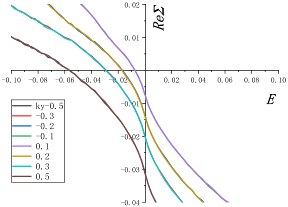


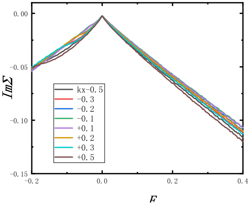


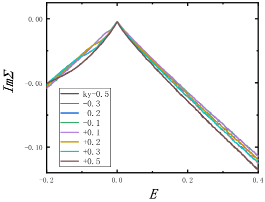
Zhu et al.,Phys. Rev. B 85 .073407 (2012)

k-dependent of self-energy









Born approximation of self-energy

self-energy function $\Sigma(\mathbf{k}, E) = G_0^{-1}(\mathbf{k}, E) - G^{-1}(\mathbf{k}, E)$
Random hopping disorder

$$\Re e\Sigma(k, E) = \gamma \left[-\frac{6E}{\pi} \ln \frac{\omega_c}{|E|} - \frac{3sa^2}{4\pi\hbar v_F} \left(\omega_c^2 + 2E^2 \ln \frac{\omega_c}{|E|} \right) k \right]$$

$$\Im m\Sigma(k, E) = -\gamma \left(3|E| + \frac{3sa^2}{4\pi\hbar v_F} E^2 k \right)$$

$$\gamma = \frac{A_c n_i}{4\pi^2\hbar v_F} \frac{\pi}{\hbar^2 v_F^2} \frac{w^2}{12}$$

lattice disorder

$$\Sigma(k, E) = \gamma \left[-\frac{2E}{\pi} \ln \frac{\omega_c}{|E|} - i|E| \right]$$

Minimal conductivity

Sample-dependent minimal conductivity $\sigma_{min} = \frac{1}{1-\alpha^2}\frac{4e^2}{\pi h}$

$$\Sigma(\mathbf{k}s, E) = \Sigma_1(E) - \alpha s \hbar v_F k + i\Sigma_2(E) = E - a - \alpha s \hbar v_F k + i\eta$$

$$\sigma_{xx}^0(E) = \sigma_{xx}^{0,RA}(E) - \Re e[\sigma_{xx}^{0,RR}(E)]$$
$$= \frac{2e^2}{\pi h}\frac{1}{1-\alpha^2}\left[1 + \left(\frac{a}{\eta} + \frac{\eta}{a}\right)\arctan\frac{a}{\eta}\right] = \frac{4e^2}{\pi h}\frac{1}{1-\alpha(g_b)^2}\Big|_{E\to 0}$$

- scattering-independent value $\sigma_{min} = \frac{4e^2}{\pi h}$
- universal value $\sigma_{min} = \frac{4e^2}{h}$
- disorder-dependent value σ_{min}
- Experimental measurements : $\sigma_{min} \approx \frac{4e^2}{h} = C \times \frac{4e^2}{\pi h}$, $C = 1.7 \sim 10$

Nature 438,197 (2005), Nature 438,201 (2005), PNAS 102,10451(2005); PRL 99,216602(2007), PRL 98,076602(2007), PRL 98,256801(2007), PNAS 104,18392(2009)

Summary

Random hopping disorder in $\pi-$flux model

1. $g_b = 0, \quad \rho(E) = |E|$
2. $g_b < g_b^c, \quad \rho(E) = \rho_1 |E|^{\alpha}, \ \alpha = 1.05 - 1.24 g_b$
3. $g_b > g_b^c, \quad \rho(0) = \frac{A}{(B\gamma)^{\nu}}, \ B(g_b) = \frac{1}{(g_b - g_b^c)^{\kappa}}$
4. $g_b > g_b^c, \quad \rho(E) = \frac{1}{E} exp(-cln|E|^{2/3})$
5. Crossover: semi-metal to diffusion metal
6. $k-$dependent self-energy and sample-dependent minimal conductivity

Singularity of density of states in the pi-flux lattice, to be submitted

Criticism or suggestion welcome!