In memoriam

Prof. Malek Zareyan (1971-2014)

- Quantum Transport
- Graphene
- Superconductivity

Kondo effect graphene

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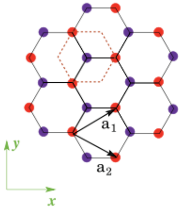
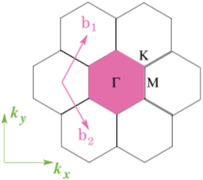
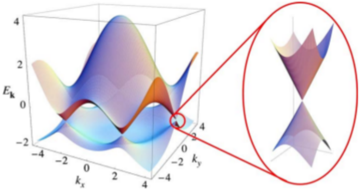
Table of contents

Energy dispersion over the whole BZ



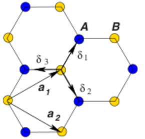


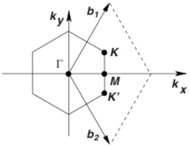
Castro Neto et al, Rev. Mod. Phys. (2009)



$$
\begin{aligned}
H\psi_A &= -t\left(\psi_{B1}+\psi_{B2}+\psi_{B3}\right)\\
H\psi_B &= -t\left(\psi_{A1}+\psi_{A2}+\psi_{A3}\right)\\
H\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix} &= \begin{pmatrix}0 & \Phi^*(\vec{k})\\ \Phi(\vec{k}) & 0\end{pmatrix}\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}\\
\Phi(\vec{k}) &= -t\left(e^{i\vec{k}.\vec{\delta}_1}+e^{i\vec{k}.\vec{\delta}_2}+e^{i\vec{k}.\vec{\delta}_3}\right)
\end{aligned}
$$

Massless Dirac cones in graphene and graphite





$$H = \begin{pmatrix} 0 & \Phi^*(\vec{k}) \\ \Phi(\vec{k}) & 0 \end{pmatrix}, \qquad \Phi(\vec{k}) = -t \sum_{n=1}^{3} e^{i\vec{k}.\vec{\delta}_n}$$

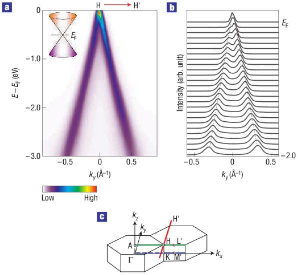
Near K : $\vec{k} = K + \vec{p} \Rightarrow \Phi(\vec{p}) \propto p_x + ip_y$

$$\Rightarrow H_K = \hbar v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = \hbar v_F \vec{\sigma}.\vec{p}$$

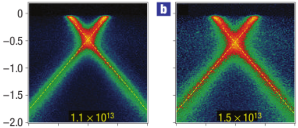
$K \to \bar{K} \equiv p_y \to -p_y$

Near $\bar{K}$: $H_{\bar{K}} = \hbar v_F \vec{\sigma}^*.\vec{p}$

S.Y. Zhou, et al, Nature Phys. (2006)



A. Bostwick, et al, Nature Phys. (2007)



Anderson model

P. Coleman, arxiv:0206003 (2002)

$$H = H_{\rm host} + H_{\rm local} + H_{\rm hyb}$$

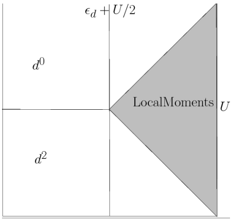
$$H_{\rm host} = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}}\, c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}$$

$$H_{\rm local} = \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

$$H_{\rm hyb} = \sum_{\vec{k}\sigma} V_{\vec{k}} d^\dagger_\sigma c_{\vec{k}\sigma} + h.c.$$

$$E|d^0\rangle \to (d^0) = 0$$
$$E|d^1_\sigma\rangle \to (d^1) = \varepsilon_d$$
$$E|d^2\rangle \to (d^2) = 2\varepsilon_d + U$$
$$E(d^2) - E(d^1) > 0 \to \varepsilon_d + U/2 > -U/2$$
$$E(d^0) - E(d^1) > 0 \to \varepsilon_d + U/2 > U/2$$

- Atomic limit local moments: $|\varepsilon_d + U/2| < U/2$



Turning on the hybridization: Hartree mean field

Splitting and broadening of the impurity level:

$$\rho_{d\sigma}(\omega) = \frac{\Delta}{(\omega - \varepsilon_{d\sigma})^2 + \Delta^2}$$

$$\varepsilon_{d\sigma} = \varepsilon_d + U n_{d\bar{\sigma}} \quad \text{Hartree shift}$$

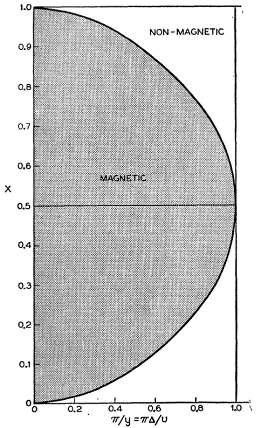
$$\Delta(\omega) = \pi \sum_{\vec{k}} |V_{\vec{k}}|^2 \delta(\omega - \varepsilon_{\vec{k}}) \approx \pi V^2 \rho_0$$

$$n_{d\sigma} = \int_{-\infty}^{0} d\omega \rho_{d\sigma}(\omega) = \frac{1}{\pi} \cot^{-1}\left(\frac{\varepsilon_d + U n_{d\bar{\sigma}}}{\Delta}\right)$$

In terms of total charge $n_d = n_{d\uparrow} + n_{d\downarrow}$ and magnetic moment $m = n_{d\uparrow} - n_{d\downarrow}$

$$n_d = \frac{1}{\pi} \sum_{\sigma=\pm 1} \cot^{-1}\left(\frac{\varepsilon_d + U/2(n_d - \sigma m)}{\Delta}\right)$$

$$m = \frac{1}{\pi} \sum_{\sigma=\pm 1} \sigma \cot^{-1}\left(\frac{\varepsilon_d + U/2(n_d - \sigma m)}{\Delta}\right)$$



P. W. Anderson, Phys. Rev. (1961)

Hybridization function in graphene

K. Sengupta, G. Baskarna, PRB, 2008

C_3 symmetry and spinorial nature of Dirac wave function $\rightarrow$

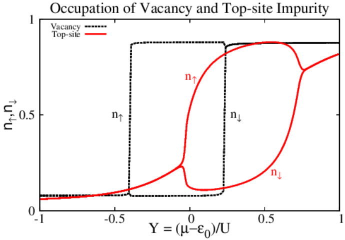
- s-wave $V(\vec{k}) = V$
  Top-site ad-atom
- p-wave $V(\vec{k}) = (k_x + ik_y)V$
  Vacancy, Subsitutional ad-atom, Hollow-site ad-atom

$$\Sigma^{\mathrm{p}}(\omega) = -\frac{\omega\Delta}{\pi t^2}\left[D^2 + \omega^2 \ln(\frac{|\omega^2 - D^2|}{\omega^2}) + i\pi\omega|\omega|\theta(D - |\omega|)\right]$$

$$\Sigma^{\mathrm{s}}(\omega) = -V^2\frac{\omega}{D^2}\ln\left(\frac{|\omega^2 - D^2|}{\omega^2}\right) - iV^2\frac{\pi|\omega|}{D^2}\theta(D - |\omega|)$$

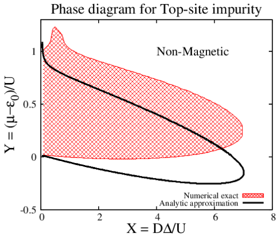
Local moments in p-wave channel

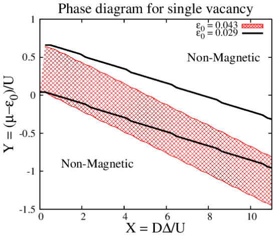
M. Mashkoori, SAJ, arxiv:1401.1637



Local moments in s-wave and p-wave channels.

- More stable local moments in p-channel.
- Local moments in negative Y in p-channel

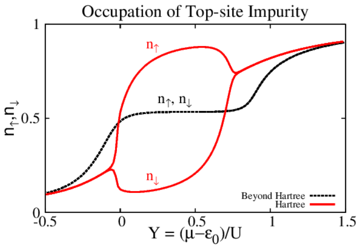


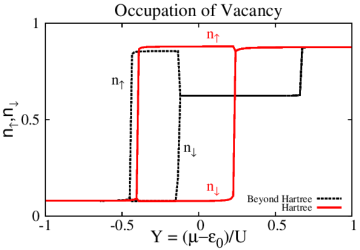


First step beyond Hartree

M. Mashkoori, SAJ, arxiv:1401.1637

$$\langle\langle f_\sigma | f_\sigma^\dagger \rangle\rangle = \left[\omega - \varepsilon_0 - \Sigma^{s,p}(\omega) - \Sigma'(\omega)\right]^{-1}, \quad \Sigma'(\omega) \equiv \frac{U(\omega - \varepsilon_0)\langle n_{\bar\sigma}\rangle}{\omega - \varepsilon_0 - U(1 - \langle n_{\bar\sigma}\rangle)}.$$





p-channel offers robust local moments agains quantum fluctuations

Fluctuations of local moments: Kondo screening

- One impurity is not macroscopic $\rightarrow$ Strong fluctuations of the moments

$$t_K \leftrightarrow \frac{\hbar}{k_B T_K}$$

- For observation time $t \gg t_K$ or $T \ll T_K$ the average magnetic moment is zero
- "Screening of moments" $\leftrightarrow$ Singlet state between d-electron and conduction electrons

- **Variational approach:**

$$|\Psi\rangle = \sum_{\vec{k}} a(\vec{k}) \left(d_\uparrow^\dagger c_{\vec{k}\uparrow} + d_\downarrow^\dagger c_{\vec{k}\downarrow} \right) |FS\rangle_{N+1}$$

Schrodinger eq.

$$E\ a(\vec{k}) = \left(E_{FS} + \varepsilon_d - \varepsilon)\vec{k} \right) a(\vec{k}) - \frac{3J}{L} \sum_{\vec{q}} a(\vec{q})$$

$$1 = -\frac{3J}{4L} \sum_{\vec{k}} \frac{1}{E - E_{FS} + \varepsilon_{\vec{k}} - \varepsilon_d}$$

Binding energy scale:

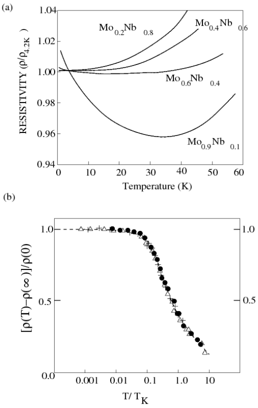
$$\Delta E = -\varepsilon_F e^{-\frac{4}{3K\rho_0}} \sim k_B T_K$$

Strong vs. Weak Coupling

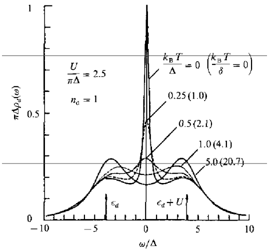
- T_K separates hight temperature "magnetic moment" regime from low-temperature "Fermi liquid" regime.
- In low-temperature (strong coupling regime) the only energy scale is T_K
- Universal dependence of transport and thermal quantities on (log) T/T_K

$$\chi(T) \sim \frac{1}{T} F(T/T_K)$$
$$\frac{1}{\tau} = \frac{1}{\tau_0} \mathcal{G}(T/T_K)$$

A. C. Hewson, "The Kondo problem ..." (1997)



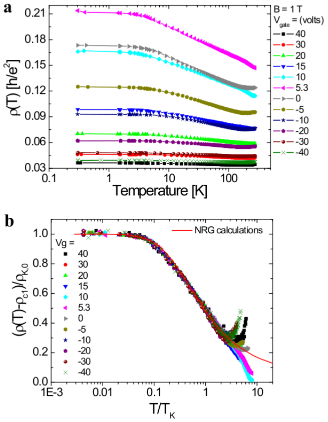
P. Coleman, arxiv:0206003 (2002)



Kondo resonance at low $T \ll T_K$

Fermi liquid $\rightarrow$ low-energy QP

Anomalous Kondo behavior in graphene



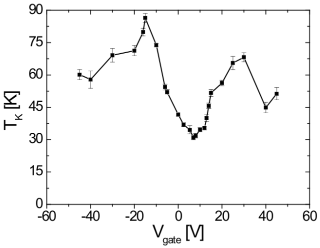
NATURE PHYSICS | LETTER

Tunable Kondo effect in graphene with defects

Jian-Hao Chen, Liang Li, William G. Cullen, Ellen D. Williams & Michael S. Fuhrer

Affiliations | Contributions | Corresponding author

Nature Physics 7, 535–538 (2011) | doi:10.1038/nphys1962



$$T_K = ?\exp\left[-\frac{1}{\rho_0 J}\right]$$

Modified perturbation theory

M. Potthoff, et al, Phys. Rev. B. (1997)

$$g_{\sigma}^{-1}(\omega) = g_{0\sigma}^{-1}(\omega) - (\Sigma_{\sigma} + \mu_{x\sigma} -$$

$$\Sigma_{\sigma}^{\rm int}(\omega) = Un_{d\bar{\sigma}} + \frac{A_{\sigma}\Sigma_{\sigma}^{(2)}(\omega)}{1 - B_{\sigma}\Sigma_{\sigma}^{(2)}(\omega)}$$

$$\Sigma_{\sigma}^{(2)}(t) = -U^2 g_{0\sigma}(t) g_{0\sigma}(t) g_{0\sigma}(-t$$

$$A_{\sigma} = \frac{n_{d\bar{\sigma}}(1 - n_{d\bar{\sigma}})}{n_{0d\bar{\sigma}}(1 - n_{0d\bar{\sigma}})}$$

$$B = \frac{(1 - n_{d\bar{\sigma}})U + \mu_{x\sigma} - \mu}{n_{0d\bar{\sigma}}(1 - n_{0d\bar{\sigma}})U^2}$$

SAJ, T. Tohyama, unpublished

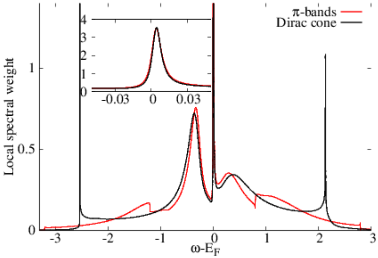


FIG. 4. (Color online) Local spectral weight for the typical values of $V = 0.82, U = 1.74, \varepsilon_d = -0.53, E_F = 0.2$. The black and red lines correspond to Dirac cone and the whole tight-binding band structure for the graphene host. Energies are in units of the hopping amplitude t. Inset shows the details of the Kondo resonance.

MPT at $E_F = 0$

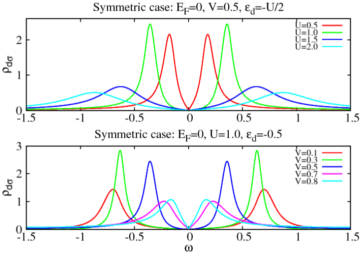


FIG. 2. (Color online) The Dirac model pseudogap Anderson model at the symmetric point with $E_F = 0$ and $\varepsilon_d = -U/2$. In the upper panel $V = 0.5$ is fixed and U is variable, while in the second panel $U = 1.0$ is fixed and V is variable as indicated in the legend.

SAJ, T. Tohyama, unpublished

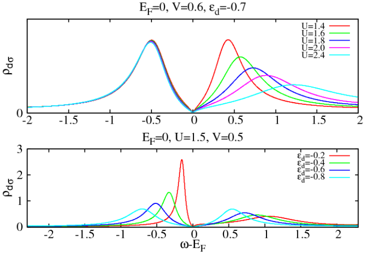
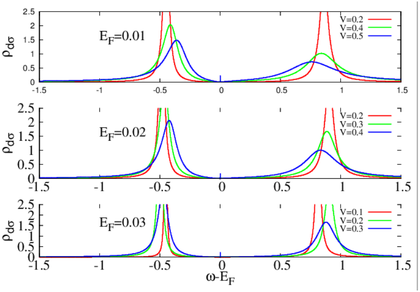


FIG. 3. (Color online) Local spectral weight using the Dirac cone model for the graphene host. Energies are in units of the hopping amplitude t. At $E_F = 0$ variations in the parameters does not give rise to Kondo resonance.

MPT for $F_F \to 0$

SAJ, T. Tohyama, unpublished



- For s-wave hybridization, a $V_{\rm min}$ dependent on E_F is needed.
- $V_{\rm min}$ increases by approaching the Dirac node.
- At Dirac node, infinitely large $V_{\rm min}$ is needed to get Kondo.

  L. Fritz, M. Vojta, Rep. Prog. Phys. 2013
- How can we understand Kondo resonance in graphene with finite $V_{\rm min}$?

Slave rotor mean field

Formulation:

$$H_{\rm local} = \sum_\sigma (\varepsilon - \mu) d_\sigma^\dagger d_\sigma + \frac{U}{2}\left[\sum_\sigma d_\sigma^\dagger d_\sigma - \frac{N}{2}\right]^2$$

$\varepsilon = \varepsilon_d + U/2,$ $\quad SU(N) \rightarrow SU(2)$

$d_\sigma^\dagger = f_\sigma^\dagger e^{i\theta}$ $\quad$ spinor $\times$ rotor

$\hat{L} = \sum_\sigma \left[f_\sigma^\dagger f_\sigma - \frac{1}{2}\right]$ $\quad$ rotor-spinon constraint

Self-consistency:

$$\tilde{V}_{\vec{k}} = V_{\vec{k}} \langle \cos\theta \rangle_\theta$$

$$K = \sum_{\vec{k}\sigma} V_{\vec{k}}^* \langle a_{\vec{k}\sigma} f_\sigma^\dagger \rangle_f$$

$V_{\vec{k}} = (k_x + ik_y)V$ $\quad$ p-wave

$$\langle \hat{L} \rangle_\theta = 2\left[n_F(\xi - h) - \frac{1}{2}\right]$$

$\xi = h \leftrightarrow L = 0 \leftrightarrow N = 1$

Decoupling of rotor and spinor parts

$$H_f = (\xi - h)\sum_\sigma f_\sigma^\dagger f_\sigma + \sum_{\vec{k}\sigma} \Phi_{\vec{k}} a_{\vec{k}\sigma}^\dagger b_{\vec{k}\sigma} + h.c. + \sum_{\vec{k}\sigma} \tilde{V}_{\vec{k}} a_{\vec{k}\sigma}^\dagger f_\sigma + \tilde{V}_{\vec{k}}^* f_\sigma^\dagger a_{\vec{k}\sigma} - \mu \sum_{\vec{k}} \left(a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} + b_{\vec{k}\sigma}^\dagger b_{\vec{k}\sigma}\right)$$

$H_\theta = \frac{U}{2}\hat{L}^2 + h\hat{L} + K\cos\theta$ $\quad$ h : Lagrange multiplier, $\quad \xi = \varepsilon - \mu$

Slave rotor equations in p-wave channel

SAJ, T. Tohyama, arxiv:1308.4173

$$\frac{\tilde{V}^2}{V^2}\frac{4\xi^2-U^2}{2U} = \sum_{\vec{k}\sigma} \tilde{V}^*_{\vec{k}} \langle a_{\vec{k}\sigma} f^\dagger_\sigma \rangle_f$$

$$\langle\langle a_{\vec{k}\sigma} | f^\dagger_\sigma \rangle\rangle = \frac{\tilde{V}}{v_F}\frac{z\Phi_{\vec{k}}}{z^2-|\Phi_{\vec{k}}|^2}\frac{1}{z-\mu-\Delta_{\rm p}(z)}$$

$$z=\omega+\mu$$

$$\Delta_{\rm p}(z) = \frac{\tilde{V}^2}{v_F^2}\sum_{\vec{p}}\frac{z|\Phi_{\vec{p}}|^2}{z^2-|\Phi_{\vec{p}}|^2} =$$

$$-\frac{\pi|\tilde{V}|^2 z}{D^4}\left[D^2+z^2\ln\frac{D^2-z^2}{z^2}\right] - i\frac{\pi^2|\tilde{V}|^2 z^2|z|}{D^4}$$

p-wave spectral function:

$$\rho_f(z) = \frac{1}{\pi}\frac{cz^2|z|}{(z-b)^2+c^2z^6}$$

Self-consistency condtion:

$$\frac{4\zeta^2-u^2}{4v^2u} = \int_{-D}^{\mu}(z-\mu)\rho_f(z)dz$$

$$c=\pi^2\tilde{v}^2/D^2,\quad b-\mu-\Delta_R(b)=0$$

$$\tilde{v}=\tilde{V}/D,\ v=V/D,\ u=U/D, \zeta=\xi/D$$

Kondo resonance at $\mu = 0$

Spinon spectral density at $\mu = 0$,

$$\rho_f(z) = \frac{1}{\pi}\frac{c|z|}{1+c^2z^4}, \qquad c = \pi^2\tilde{v}^2/D^2$$

- Properly renomralizable at $D \to \infty$.
- Standard deviation determines $T_K^{\rm Diran} = \sqrt{\pi/2}\tilde{v}D$.
- Same method in normal metals: $T_K^{\rm metal} = \pi\tilde{v}^2 D$
  S. Florens, et al, PRB (2004)
- $T_K^{\rm metal}/T_K^{\rm Dirac} \sim \tilde{v} \ll 1 \to$
  Under comparable conditions, a host of Dirac fermions
  gives rise to larger Kondo temperature than metals
- Self-consistency at $\mu = 0$ can be handled analytically:

SAJ, T. Tohyama, arxiv:1308.4173

- To have a solution for $\tilde{v}$ (hence for $T_K \sim \tilde{v}D$):

$$-\frac{1}{3} < \frac{4\zeta^2 - u^2}{2uv^2} < 0 \Rightarrow v^2 \geq \frac{3}{2}\frac{u^2-4\zeta^2}{u}. \qquad (1)$$

- The requirement for non-zero T_K at $\mu = 0$:

$$|V_{\rm min}| = -6\varepsilon_d D\left(1+\frac{\varepsilon_d}{U}\right)$$

- **For vacancies $\varepsilon_d \sim 10$ meV $\to V_{\rm min} \sim 0.5$ eV**

$$\frac{4\zeta^2-u^2}{2uv^2} = \int_{-D}^{0} z\rho_f(z)dz = \frac{-\sqrt{2}}{8\pi^3\tilde{v}^3}\times\left[\ln\frac{(\pi\tilde{v})^2-\sqrt{2}\pi\tilde{v}+1}{(\pi\tilde{v})^2+\sqrt{2}\pi\tilde{v}+1} - 2\tan^{-1}(1-\sqrt{2}\pi\tilde{v}) + 2\tan^{-1}(1+\sqrt{2}\pi\tilde{v})\right]$$

Doping away from Dirac point

$$\frac{4\zeta^2 - u^2}{4v^2 u} = \frac{\pi}{D^3} \sum_{m=\pm 1} \frac{z_m^3 (z_m - \mu)}{2(z_m - \mu) + 6c^2 z_m^5} \int_{-D}^{\mu} \frac{sgn(z)dz}{z - z_m}$$

$$z_m \approx \mu + icm\mu^3 \text{ with } m = \pm 1,$$

dominant poles

- The Kondo temperature for small $\mu = \tilde{\mu} D$:

$$\frac{T_K}{D} \sim \pi \tilde{v} = |\tilde{\mu}|^{x_\pm} \exp\left[-\frac{1}{2\pi|\tilde{\mu}|^3} \frac{u^2 - 4\zeta^2}{4v^2 u}\right]$$

$$x_\pm = sign(\mu)/2 - 1,$$

electron-hole asymmetry

- for non-zero doping, smallest value of V can lead to Kondo screening.

Conclusions:

Kondo screening in 2D Dirac host (graphene) with p-wave hybridization:

- **For non-zero doping, smallest value of V gives Kondo screening.**
- **For $\mu = 0$, $V_{\min} = -6\varepsilon_d D(1 + \varepsilon_d/U)$ is required.**
- **Boron and Nitrogen subsitution in graphene is expected to give reasonably small $V_{\min}$**

Thank you for your attention