Kondo Effect and Non-Fermi Liquid Behavior in Dirac Materials

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Work supported by

Quantum and Dirac Materials for Energy Applications Conference, Santa Fe, NM. March 8–11 2015
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Kondo Effect in Dirac Materials

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Effect of Spin-orbit coupling on impurity bound states in superconductors

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Dirac Materials

2D Dirac Materials

Graphene

\[ \mathcal{H} = v_F \mathbf{p} \cdot \sigma \]

3D Dirac Materials

3D Graphene and Weyl Semimetals

\[ \mathcal{H} = v_F \mathbf{p} \cdot \sigma \]
Kondo Effect

\[ \rho(T) = \rho_0 + bT^5 - a \ln(T) \]

There is a crossover temperature, \( T_K \), below which the coupling between the conduction electrons and the dynamical magnetic impurity grows non-perturbatively.

\( T < T_K \)  Formation of a many-body singlet

For standard case

\[ T_K = D e^{-\frac{1}{JN(0)}} \]

\( N(0) \propto \epsilon^\alpha \)

Pseudogap Kondo problem


Experimental evidence

Graphene

Theoretical approach

\[ H = H_{DM} + H_{\text{imp}} \]

\[ H_{DM} = \hbar v_F \hat{c}^\dagger_{k\sigma} (k \cdot \tau_{\sigma\sigma'} - \mu) \hat{c}_{k\sigma'} \]

\[ H_{\text{imp}} = J \sum_{r,R} \hat{c}^\dagger_{r\sigma} \tau_{\sigma\sigma'} \hat{c}_{r\sigma'} \cdot S \delta(r - R) \]

Large-N expansion

\( \mathbf{S} \) is expressed in terms of auxiliary fermionic operators “f” satisfying the constrain

\[ n_f = \sum_\sigma f^\dagger_\sigma f_\sigma = 1. \]

Then

\[ H_{\text{imp}} = J \sum_{k,k',\sigma} \hat{c}^\dagger_{k\sigma} \hat{c}_{k'\sigma'} f^\dagger_{\sigma'} f_\sigma \]

The interaction is decoupled via the mean-field

\[ S \sim \sum_{k,\sigma} \langle f^\dagger_\sigma \hat{c}_{k\sigma} \rangle \]

And the constrain on \( n_f \) is enforced via a Lagrange multiplier \( \mu_f \)
**Determination of $T_K$**

The field “s” and the Lagrange multiplier are obtained via the self-consistent equations:

\[
\int_{-D-\mu}^{D-\mu} d\varepsilon \frac{n_F(\varepsilon)(\varepsilon - \mu_f)N(\varepsilon + \mu)}{(\varepsilon - \mu_f)^2 + (\pi |s|^2 N(\varepsilon + \mu)/2)^2} = -\frac{1}{J}
\]

\[
\int_{-D-\mu}^{D-\mu} d\varepsilon \frac{n_F(\varepsilon) |s|^2 N(\varepsilon + \mu)}{(\varepsilon - \mu_f)^2 + (\pi |s|^2 N(\varepsilon + \mu)/2)^2} = 1
\]

We identify $T_K$ as the highest $T$ for which the two self-consistent equations admit a solution.
Scalings for $T_K$

**At the Dirac point $\mu = 0$**

**3D**

$$T_K = D \frac{\sqrt{3}}{\pi} \sqrt{1 - \frac{2}{N(D)J}}$$

$$J_{cr} = \frac{2}{N(D)}$$

**2D**

$$T_K = \frac{D}{\ln(4)} \left[ 1 - \frac{1}{N(D)J} \right]$$

$$J_{cr} = \frac{1}{N(D)}$$

**Away from Dirac point $\mu \neq 0$**

In the limit $k_B T_K \ll \mu \ll D$ and $J \lesssim J_c$

**3D**

$$T_K = D \exp \left[ \frac{1 - 2/(JN(D))}{2\mu^2/D^2} \right]$$

**2D**

$$T_K = \kappa(\mu) \exp \left[ \frac{1 - 1/(N(D)J)}{[\mu/D]} \right]$$

where $\kappa(\mu) = \mu^2/D$ [$\kappa(\mu) = D$] for $\mu > 0$ [$\mu < 0$].

A. Principi, G. Vignale, ER, arXiv 1410.8532

Scalings for $T_K$: general case

3D

2D

A. Principi, G. Vignale, ER, arXiv 1410.8532
**Kondo resistivity: \( \rho_K \)**

**In the limit \( T = 0 \)**

**3D**

\[
\rho_K(T = 0) = \frac{\hbar}{e^2} \left( \frac{32 g_s}{3 \pi^2 N_w^2} \right)^{1/3} \frac{n_{\text{imp}}}{n^{4/3}}
\]

Same scaling as for the case of non magnetic long-range scatterers

AA Burkov, MD Hook, L. Balents PRB (2011)

**2D**

\[
\rho_K = \frac{\hbar}{e^2} \frac{4}{\pi N_w} \frac{n_{\text{imp}}}{n}
\]

P.S. Cornaglia et al, PRL (2009)

**At finite \( T \)**

\[
\rho(T) \simeq -\rho_0 \frac{\pi^2}{2} [J \nu(\mu)]^3 S(S + 1) \ln \left( \frac{k_B T}{D} \right)
\]

A. Principi, G. Vignale, ER, arXiv 1410.8532
Interplay of scalar and magnetic potential

\[ H_{\text{imp}} = U \sum_{r,R} \hat{c}_{r\sigma}^\dagger \hat{c}_{r\sigma} \delta(r-R) + J \sum_{r,R} \hat{c}_{r\sigma} \tau_{\sigma\sigma'} \hat{c}_{r\sigma'} \cdot S \delta(r-R) \]

d-wave superconductors

The scalar part of the impurity potential modifies the LDOS.

It modifies \( T_K \) uniformly across the sample.

\( T_K \) is uniform across the sample and well defined.

If the short range scalar potential is due to *other* impurities removed from the magnetic impurity it has little consequence.

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**Long-range disorder**

Charge impurities are a common source of disorder. However they can often be treated as short range disorder. Things are different in most Dirac materials

- Linear dispersion $\Rightarrow$ vanishing DOS close to Dirac points  
  $\Rightarrow$ poor screening of the disorder due to charge impurities

  The disorder is renormalized but retains its long-range character

- Charge impurities therefore cause strong, long-range, *density* inhomogeneities close to Dirac point

- Linear dispersion
  - Strong, long-range, *density inhomogeneities*

  Strong, long-range, inhomogeneities of the DOS
Interplay of scalar and magnetic potential: long-range scalar potential

Charge impurities

Not important in superconductors: well screened

In non-superconducting Dirac materials, due to vanishing DOS they induce strong, long-range, carrier density inhomogeneities

Experiment

Theory

Shifts bottom of the band
Fermi energy

2D
LDOS $\sim n$

3D
LDOS $\sim n^{2/3}$

Fluctuations of $n$ imply fluctuations of LDOS

ER, S. Das Sarma, PRL. (2008)


Effect of long-range scalar disorder

For simplicity we assume a Gaussian distribution for the density probability

\[ P_n(n) = \exp \left[ -\frac{(n - \bar{n})^2}{2\sigma_n^2} \right] / \sqrt{2\pi\sigma_n}. \]

Using the relation between \( T_K \) and \( \mu \) and the fact that

in 3D: \( \mu \sim n^{1/3} \) 

in 2D: \( |\mu| \sim n^{1/2} \)

Instead of a single value of \( T_K \) we have a distribution of \( T_K \)

\[ P^{(3D)}(T_K) = \frac{3D^3}{8\sqrt{\pi} \sigma^3 \mu T_K} \left[ \frac{(1 - J_c/J)^3}{\ln^5(k_B T_K/D)} \right]^{1/2} e^{-\frac{(\mu^3 - \bar{\mu}^3)^2}{2\sigma^6 \mu}} + e^{-\frac{(\mu^3 + \bar{\mu}^3)^2}{2\sigma^6 \mu}} \]

\[ P^{(3D)} \propto \frac{1}{T_K[\ln(T_K)]^{5/2}} \]

\[ P^{(2D)}(T_K) = \frac{\sqrt{2}D^2}{\sqrt{\pi} \sigma^2 \mu T_K} \left[ \frac{(1 - J_c/J)^2}{\ln^3(k_B T_K/D)} \right] e^{-\frac{(\mu^2 - \bar{\mu}^2)^2}{2\sigma^4 \mu}} + e^{-\frac{(\mu^2 + \bar{\mu}^2)^2}{2\sigma^4 \mu}} \]

\[ P^{(2D)} \propto \frac{1}{T_K[\ln(T_K)]^3} \]

Agrees with scaling obtained from numerical results by V.G. Miranda et al PRB (2014)

A. Principi, G. Vignale, ER, arXiv 1410.8532
For low $T_K$ the scaling

$$\frac{1}{[T_K \ln^3(T_K)]}$$

very similar to

$$\frac{1}{(T_K^{0.8})}$$

obtained by fitting numerical results by V.G. Miranda et al. PRB (2014)

A. Principi, G. Vignale, ER, arXiv 1410.8532
**LDOS fluctuations close to MIT**

Typically in materials other than Dirac materials is difficult to obtain strong, long-range fluctuations of the LDOS. A similar situation can be obtained close to a metal-insulator transition. In this case the probability distribution for the LDOS $\rho$ is log-normal

$$P(\rho) = \frac{1}{\sqrt{4\pi u}} \frac{1}{\rho} \exp \left\{ - \frac{1}{4u} \ln^2 \left( \frac{\rho}{\rho_0} e^u \right) \right\}.$$  

In this case we also get a singular distribution for $T_K$

$$P(T_K) = (4\pi u)^{-1/2} \frac{1}{T_K \ln(\epsilon_F/T_K)} \exp \left\{ - \frac{1}{4u} \ln^2 [\rho_0 I e^{-u} \ln(\epsilon_F/T_K)] \right\}$$


V. Dobrosavlyevic, T.R. Kirkpatrick, G. Kotliar

PRL (1992)

However:

- **The conditions are difficult to achieve**

- **The effects are weaker than in Dirac Materials**
Free carriers even for $T \rightarrow 0$

Considering that

$$P^{(3D)} \propto \frac{1}{TK[\ln(TK)]^{5/2}}$$

$$P^{(2D)} \propto \frac{1}{TK[\ln(TK)]^{3}}$$

We see that at any is a considerable fraction of the sample for which $T_k$ is very small.

At any $T$, no matter how low, there is a significant fraction, $n_{fr}$, of carriers not bound to the impurities.

We can obtain such fraction at temperature $T$ by calculating the integral

$$n_{fr}(T) = \int_{0}^{T} dT_k P(T_k)$$

And we find, for $T \rightarrow 0$

$$n_{fr}(T) \propto |\ln(T)|^{-3/2} e^{-\bar{n}^2/(2\sigma_n^2)}$$

Even for $T \rightarrow 0$ $n_{fr}$ is significant.
Non-Fermi liquid behavior

Consider the magnetic susceptibility. We have

\[ \chi_m \propto \frac{n_{fr}(T)}{T} \]

And therefore we find:

3D

\[ \chi_m \propto \frac{1}{T|\ln(T)|^{3/2}} \]

2D

\[ \chi_m \propto \frac{1}{T|\ln(T)|^{2}} \]

\( \chi_m \) diverges for for \( T \to 0 \)

Strong Non-Fermi-Liquid Behavior

\( \chi_m \) also does not follow the Curie-Weiss law \((1/T)\) it diverges more slowly

P. Nozieres (1974)

A. Principi, G. Vignale, ER, arXiv 1410.8532
Impurity-bound states in SCs with SOC: motivation

A magnetic impurity can create states with energies within the gap due to the superconducting pairing. These states are spatially bound to the impurity (Yu-Shiba-Rusinov). A chain of impurities can create a band of these states.

In the presence of SOC a FM chain on SC with SOC appears to have Majorana states at the ends.


Measured using STM for isolated impurities

Shuai-Hua Ji et al. PRL (2008)
Impurity-bound states in SCs with SOC: model

\[ H = H_{SC} + H_{imp} \]

\[ H_{SC} = \sum_{\mathbf{p}} \psi_{\mathbf{p}}^\dagger [\tau_z \otimes (\xi_{\mathbf{p}} + \alpha l_{\mathbf{p}} \cdot \mathbf{\sigma}) + \tau_x \otimes (\Delta_0(\mathbf{p})\sigma_0 + \Delta_1 \cdot \mathbf{\sigma})] \psi_{\mathbf{p}} \]

\[ H_{imp} = \hat{U}(|\mathbf{r} - \mathbf{R}|)\tau_z \otimes \sigma_0 + \hat{J}(|\mathbf{r} - \mathbf{R}|)\tau_0 \otimes \mathbf{S} \cdot \mathbf{\sigma} \]

Let

\[ G_{SC} \equiv [E - H_{SC}]^{-1} \]

Then the Schrödinger equation for the Hamiltonian \( H \) can be rewritten as (F. Pientka, L. I. Glazman, and F. von Oppen, PRB (2013))

\[ \psi(\mathbf{p}) - G_{SC}(E, \mathbf{p}) \int_{\mathbf{p}'} H_{imp}(|\mathbf{p} - \mathbf{p}'|)\psi(\mathbf{p}') = 0. \]

This equation admits nontrivial solutions for values of \( E \) such that

\[ \det[1 - G_{SC}(E, \mathbf{p})H_{imp}(|\mathbf{p} - \mathbf{p}'|)] = 0. \]

For values of \(|E| < \Delta\) we have bound states (Shiba states)
Impurity-bound states in SCs with SOC: results

s-wave superconductor

\[
\frac{|E_{l=0,1}|}{\Delta_s} = \frac{\gamma^2 - J_0^2 J_1^2 \pm \gamma^{\frac{3}{2}} \sqrt{(J_0^2 - J_1^2)^2 + (\gamma - 1)(J_0 - J_1)^4}}{\gamma^2(1 + (J_0 - J_1)^2) + 2\gamma J_0 J_1 + J_0^2 J_1^2}
\]

\[
\gamma = 1 + \tilde{\alpha}^2
\]

\[
\frac{|E_{l=-1}|}{\Delta_s} = \frac{1 - J_1^2}{1 + J_1^2}
\]

As expected SOC mixes states with different \( l \). It also causes an interplay of \( U \) and \( J \)

Y. Kim, J. Zhang, ER, R. Lutchyn
Impurity-bound states in SCs with SOC: results

Dependence on $\theta$

**s-wave**

**p-wave**

SOC induces strong $\theta$ dependence that can be used to tune the fermion parity of the bound state
Conclusions

• Obtained scaling of $T_K$ and Kondo resistivity in 3D Dirac materials

$$\rho_K(T = 0) \propto \frac{n_{\text{imp}}}{n^{4/3}}$$

• Interplay of long-range disorder and Kondo effect in Dirac materials gives rise to a distribution of Kondo temperatures. Close to Dirac point:

$$P^{(3D)} \propto \frac{1}{T_K [\ln(T_K)]^{5/2}}$$

$$P^{(2D)} \propto \frac{1}{T_K [\ln(T_K)]^{3}}$$

• Low T tail of $P(T_K)$ induces NFL

$$\chi_m \propto \frac{1}{T |\ln(T)|^{3/2}}$$

$$\chi_m \propto \frac{1}{T |\ln(T)|^{2}}$$

• Study effect of SOC on impurity bound states in 2D superconductors

SOC strongly affects the bound states created by isolated impurities in superconductors

Can change parity of Shiba state
References

• A. Principi, G. Vignale, ER, arXiv 1410.8532 (2014)


For more see:

http://physics.wm.edu/~erossi/publications.html