Magnetic impurity on the surface of a topological insulator

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Strong Topological Insulator

- Spin-orbit coupling
- Gapped bulk bands
- gapless surface mode (odd-number of Dirac cones)
- surface modes protected by a topological invariant
- examples: $\mathrm{Bi_2Se_3}, \mathrm{Bi_2Te_3}$

Warping

- By crystal symmetry, 6-fold axis
- Perturbation to the perfect Dirac cone
- weak in $\mathrm{Bi_2Se_3}$, strong in $\mathrm{Bi_2Te_3}$.

Hamiltonian

$$H_0 = \sum_{\mathbf{k},\alpha,\beta} \{ c^\dagger_{\mathbf{k},\alpha} [-i\hbar v_F \hat{\mathrm{z}} \cdot (\sigma_{\alpha\beta} \times \mathbf{k}) + \frac{\lambda}{2} [(k_x + i k_y)^3 + (k_x - i k_y)^3] \sigma^z_{\alpha\beta} - \mu \delta_{\alpha\beta}] \} c_{\mathbf{k},\beta}$$

Magnetic impurity on the surface

Kondo interaction with surface modes:

$$H_{\text{Kondo}} = \frac{J_K}{L^2} \sum_{\mathbf{k},\mathbf{k}',\alpha,\beta} \mathbf{S} \cdot c^\dagger_{\mathbf{k},\alpha} \sigma_{\alpha\beta} c_{\mathbf{k}',\beta}$$

1. Does the spin orbit interaction/anisotropy modify the Kondo effect ?
2. Friedel oscillations around the Kondo impurity ?

Mapping to one dimension (I)

Eigenstates in first quantization:

$$\psi^{\pm}_{k,\phi}(r,\theta) = \begin{pmatrix} \alpha_\pm \\ -i\beta_\pm e^{i\phi} \end{pmatrix} e^{ik\rho\cos(\theta-\phi)}$$

Define $(|\phi| < 2\pi/3, \ell = 0, \pm 1)$:

$$\begin{aligned} \psi_{k,\phi,\ell}(r,\theta) &= \frac{1}{\sqrt{3}} \sum_{n=0,1,2} e^{i\frac{2\pi}{3}\ell n} \psi_{k,\phi+\frac{2n\pi}{3}}(r,\theta) \\ \psi_{k,\phi,+1}(0,\theta) &= 0 \end{aligned}$$

$$\Psi(\mathbf{r}) = \sum_{\ell,s=\pm} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \psi^{(s)}_{\mathbf{k},\ell}(\mathbf{r}) c_{\ell,s}(\mathbf{k})$$

Mapping to one dimension (II): Kondo interaction

$$\Psi(\mathbf{0}) = \sqrt{3}\int \frac{d^2\mathbf{k}}{(2\pi)^2} \begin{pmatrix} \alpha c_{0,+} - \beta c_{0,-} \\ -i(\beta c_{-1,+} + \alpha c_{-1,-}) \end{pmatrix} (\mathbf{k})$$

$$\begin{aligned} H &= \sum_{\ell,s} \int \frac{d^2\mathbf{k}}{(2\pi)^2} (sE(\mathbf{k}) - \mu) c^\dagger_{\ell,s}(\mathbf{k}) c_{\ell,s}(\mathbf{k}) + J_K \mathbf{S} \cdot \Psi^\dagger(\mathbf{0}) \sigma \Psi(\mathbf{0}) \\ E(k,\phi) &= \sqrt{(\hbar v k)^2 + \lambda^2 k^6 \cos^2(3\phi)}; \frac{\alpha + i\beta}{\alpha - i\beta} = \frac{i\hbar v k + \lambda k^3 \cos 3\phi}{E(k,\phi)} \end{aligned}$$

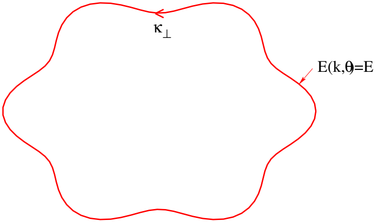
$\ell = 1$ decouples, $\ell = -1 \leftrightarrow \downarrow, \ell = 0 \leftrightarrow \uparrow$

Mapping to one dimension (III): curvilinear coordinates

$$a_{\ell,s}(E,\kappa_\perp) = \frac{c_{\ell,s}(\mathbf{k})}{\sqrt{||\nabla_{\mathbf{k}} E(\mathbf{k})||}}; \frac{1}{w(E)} = \int \frac{d\kappa_\perp}{2||\nabla_{\mathbf{k}} E(\mathbf{k})||}$$

$$H_0 = \sum_{\ell,s} \int \frac{dE d\kappa_\perp}{(2\pi)^2} (sE-\mu) a^\dagger(E,\kappa_\perp) a(E,\kappa_\perp)$$

$$\{a_{l,s}(E,\kappa_\perp), a^\dagger_{l,s}(E',\kappa'_\perp)\} = (2\pi)^2 \delta(E-E')\delta(\kappa_\perp - \kappa'_\perp)$$



Mapping to one dimension (IV): projection of Hilbert space

$$\Psi(\mathbf{0}) = \int_0^{+\infty} \frac{dE}{(2\pi)^2} \int \frac{\sqrt{3} d\kappa_\perp}{\sqrt{||\nabla_{\mathbf{k}} E(\mathbf{k})||}} \begin{pmatrix} \alpha a_{0,+} - \beta a_{0,-} \\ -i(\beta a_{-1,+} + \alpha a_{-1,-}) \end{pmatrix} (E, \kappa_\perp)$$

$$a_{\uparrow,+}(E) = \int \frac{d\kappa_\perp \alpha(E,\kappa_\perp) a_{0,+}(E,\kappa_\perp)}{\sqrt{w(E)||\nabla_{\mathbf{k}} E(\mathbf{k})||}}$$

$$a_{\uparrow,-}(E) = \int \frac{d\kappa_\perp \beta(E,\kappa_\perp) a_{0,-}(E,\kappa_\perp)}{\sqrt{w(E)||\nabla_{\mathbf{k}} E(\mathbf{k})||}}$$

$$a_{\downarrow,+}(E) = \int \frac{d\kappa_\perp \beta(E,\kappa_\perp) a_{-1,+}(E,\kappa_\perp)}{\sqrt{w(E)||\nabla_{\mathbf{k}} E(\mathbf{k})||}}$$

$$a_{\downarrow,-}(E) = \int \frac{d\kappa_\perp \alpha(E,\kappa_\perp) a_{-1,-}(E,\kappa_\perp)}{\sqrt{w(E)||\nabla_{\mathbf{k}} E(\mathbf{k})||}}$$

Mapping to one dimension (V)

$$a_\sigma(E) = (-i)^{1/2-\sigma} \sum_{s=\pm} \theta(sE) s^{1/2+\sigma} a_{\sigma,s}(E)$$

$$\psi_\sigma(0) = \sqrt{3} \int_{-\infty}^{\infty} \frac{dE\sqrt{w(|E|)}}{(2\pi)^2} a_\sigma(E)$$

$$H_0 = \int_{-\infty}^{+\infty} \frac{dE}{(2\pi)^2} \sum_\sigma (E-\mu) a^\dagger_\sigma(E) a_\sigma(E) + \dots$$

$$H_K = J_K \sum_{\sigma,\sigma'} \mathbf{S} \cdot \psi^\dagger_\sigma(0) \sigma_{\sigma,\sigma'} \psi_{\sigma'}(0)$$

large doping $w(E) \simeq w(\mu) = 2\pi^2\rho(\mu)$

$$\Rightarrow T_K = De^{\gamma_E - 1/4} \exp\left(\frac{-1}{3J_K\rho(\mu)}\right)$$

small doping $w(E) \propto |E|$

$$T_K = 0.$$

E. M. Fradkin and D. Withoff Phys. Rev. Lett. **64** 1835 (1990)

Abrikosov fermions representation

$$S^+ = f_\uparrow^\dagger f_\downarrow; S^z = \frac{1}{2}(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow)$$

$$1 = f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow$$

Mean field theory

$$J_K \mathbf{S} \cdot \psi_\sigma^\dagger(0)\sigma_{\sigma\sigma'}\psi_{\sigma'}(0) \rightarrow \Delta \sum_\sigma (f_\sigma^\dagger \psi_\sigma(0) + \mathrm{H.c.})$$

$$\Delta = J_K \langle \psi_\sigma^\dagger(0) f_\sigma \rangle$$

T-matrix

$$
\begin{aligned}
G(\mathbf{r},\mathbf{r}',\omega_n) &= G_0(\mathbf{r}-\mathbf{r}',\omega_n) + G_0(\mathbf{r},\omega_n)T(\omega_n)G_0(-\mathbf{r}',\omega_n) \\
T(\omega_n) &= \frac{\Delta^2}{i(\omega_n + \Gamma \mathrm{sign}(\omega_n))}; \Gamma = \frac{\pi}{2}\Delta^2\rho(\mu)
\end{aligned}
$$

I. Affleck *et al.* Phys. Rev. B **77**, 180404 (2008)

Local density

$$
\rho(\mathbf{r}) = \rho_0 + \frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\left[\frac{G_0(\mathbf{r}, i\omega_n)G_0(-\mathbf{r}, i\omega_n)}{i(\omega_n + \Gamma \mathrm{sign}(\omega_n))}\right]
$$

Approximate Green's function

$$
\begin{aligned}
G_0(\mathbf{r}, i\omega_n) &= \frac{i\omega_n + \mu}{2\pi v^2}\left[K_0(\zeta) + \mathrm{sign}(\omega_n)\hat{\mathbf{z}}\cdot(\sigma\times\hat{\mathbf{r}})K_1(\zeta)\right. \\
&\quad \left. +\lambda \cos 3\varphi (i\omega_n + \mu)^2 \mathrm{sign}(\omega_n) K_3(\zeta)/v^3\right] + O(\lambda^2) \\
\zeta &= \frac{|\omega_n| - i\mu\,\mathrm{sign}(\omega_n)}{v} r
\end{aligned}
$$

$$\ln \frac{T_K}{T} + \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{\beta\Gamma}{2\pi}\right) = 0$$

No warping, $T = 0$

$$\delta\rho(\mathbf{r}) = -\frac{v}{2\pi\mu r^3}\cos\left(\frac{2\mu r}{v}\right) G\left(\frac{2\Gamma r}{v}\right)$$

$$G(u) = u e^u E_1(u); G(u \to +\infty) \to 1$$

M.-T. Tran, K.-S. Kim Phys. Rev. B **82**, 155142 (2010)

No warping, $T > 0$

$$\delta\rho(\mathbf{r}) = -\frac{\Delta^2}{4\pi^2 v^2 r^2}\frac{e^{-\frac{2\pi r}{\beta v}}}{\frac{1}{2}+\frac{\beta\Gamma}{2\pi}}\,{}_2F_1\left(1, \frac{1}{2}+\frac{\beta\Gamma}{2\pi}; \frac{3}{2}+\frac{\beta\Gamma}{2\pi}; e^{-\frac{4\pi r}{\beta v}}\right)\cos\left(\frac{2\mu r}{v}\right)$$

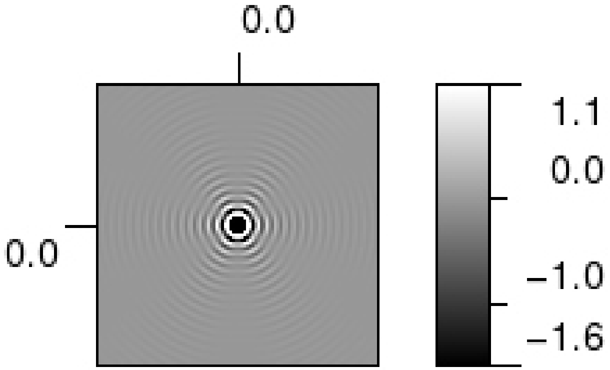
With warping, $T = 0$

$$\begin{aligned} \Gamma r/v &\gg 1 \\ \delta\rho(\mathbf{r}) &= \delta\rho(\mathbf{r})|_{\lambda=0} - \frac{\lambda^2\mu^5\cos^2 3\varphi}{4\pi^3 v^8 \rho(\mu) r^2}\cos(2\mu r/v) \end{aligned}$$

$\Rightarrow$ 6-fold symmetry of Friedel oscillations.

$\Rightarrow$ dominates the isotropic term at long distances

With warping, $T > 0$



Conclusion

1. Conventional Kondo effect for magnetic impurities on the surface of a topological insulator (spin-orbit coupling does not modify the Kondo effect)
2. Pseudogap at the Dirac point $\Rightarrow T_K = 0$.
3. with warping, Friedel oscillation have a 6-fold symmetry.

Perspectives

1. Friedel oscillations for any λ.
2. Use of form factor expansion to derive Friedel oscillations

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