Rotational symmetry breaking and partial Majorana corner states in a heterostructure based on high-T$_c$ superconductors

李玉轩
`yxli@m.scnu.edu.cn`

School of Phisics and
Telecommunication Engineering

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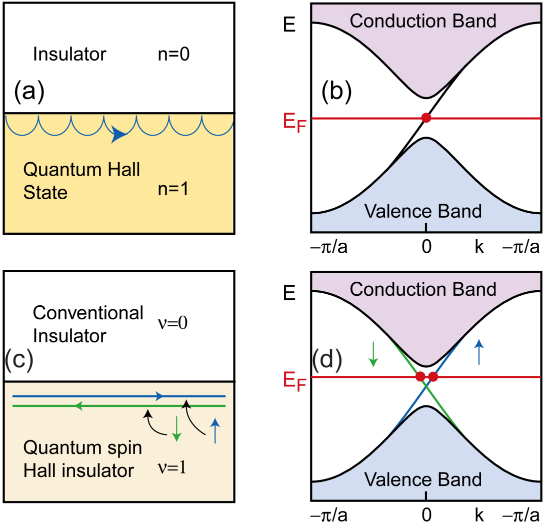
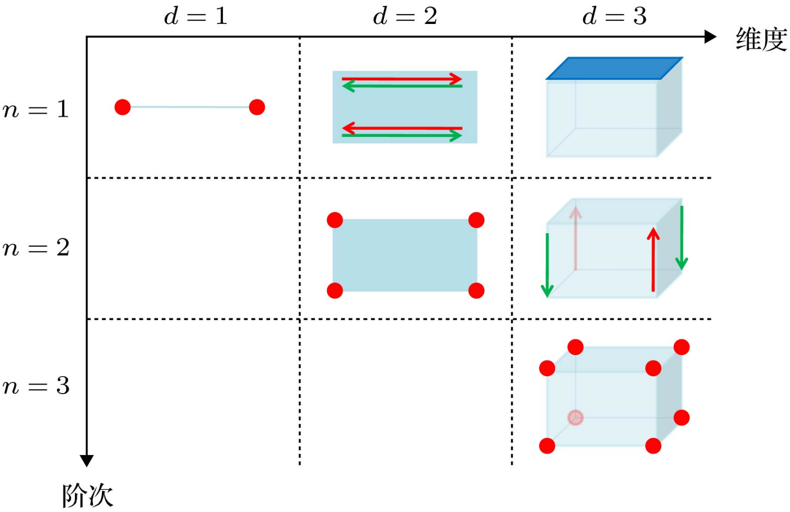
Outline

Introduction



$$n = \frac{1}{2}\int_{\mathrm{BZ}} d^2k \nabla_k \times i \sum_{l\in\mathrm{bands}} \langle \varphi_l | \nabla_k | \varphi_l \rangle \tag{1}$$

Introduction



Introduction

$$H_c(\mathbf{k}) = (M + t\sum_i \cos k_i)\tau_z\sigma_0 + \Delta_1 \sum_i \sin k_i \tau_x \sigma_i + \Delta_2(\cos k_x - \cos k_y)\tau_y\sigma_0 \quad (2)$$

$$(\hat{C}_4^z\mathcal{T})H_c(\mathbf{k})(\hat{C}_4^z\mathcal{T})^{-1} = H_c(D_{\hat{C}_4^z\mathcal{T}}\mathbf{k}), \quad D_{\hat{C}_4^z\mathcal{T}}\mathbf{k} = (k_y, -k_x, -k_z) \quad (3)$$

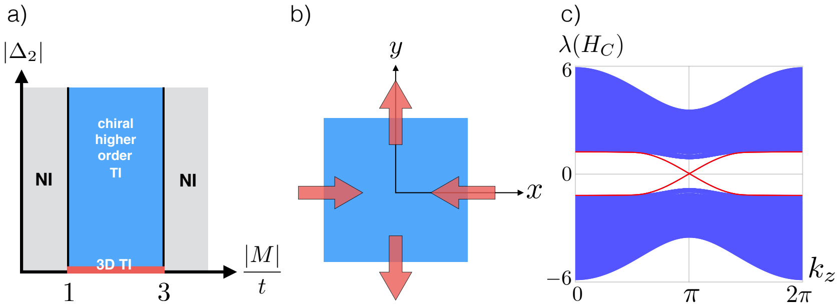


Figure: 手性高阶拓扑绝缘体；(a) 哈密顿量 (2) 的相图，(b) 一个元胞内满足 $\hat{C}_4^z\mathcal{T}$ 的非共线反铁磁，(c) 存在手性棱态 (红色) 的哈密顿量 (2) 的能谱图

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Method 1

$$H(\mathbf{k}) = M(\mathbf{k})\sigma_z\tau_z + A_x \sin k_x \sigma_x s_z + A_y \sin k_y \sigma_y \tau_z + \Delta(\mathbf{k}) s_y \tau_y - \mu\tau_z$$
$$M(\mathbf{k}) = m_0 - t_x \cos k_x - t_y \cos k_y \tag{4}$$

$$\Delta(\mathbf{k}) = \Delta_x + \Delta_x \cos k_x + \Delta_y \cos k_y \tag{5}$$

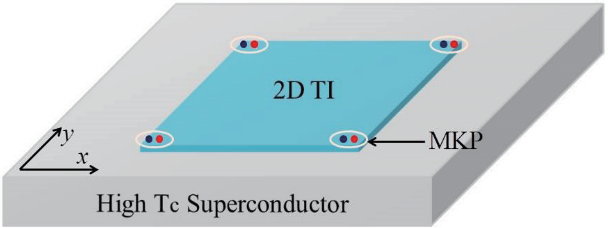

Figure: 示意图展示；一个 2D 拓扑绝缘体长在 d-波或者 $s_\pm$-波的高温超导体上，零能马约拉纳 Kramers 对 (MKP) 将会出现在 2D 拓扑绝缘体的角落。

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Edge Theory

首先将哈密顿量 (4) 在 $\Gamma = (0,0)$ 处做低能展开，并保留到二阶

$$H(\mathbf{k}) = (m + \frac{t_x}{2}k_x^2 + \frac{t_y}{2}k_y^2)\sigma_z\tau_z + \lambda_x k_x \sigma_x s_z + \lambda_y k_y \sigma_y \tau_z - \frac{1}{2}(\Delta_x k_x^2 + \Delta_y k_y^2) s_y \tau_y \tag{6}$$

取 x 方向在实空间 $k_x \to -i\partial_x$，将哈密顿量 (6) 分解成两部分 $H = H_0 + H_p$

$$\begin{aligned} H_0(-i\partial_x, k_y) &= (m - t_x\partial_x^2/2)\sigma_z\tau_z - i\lambda_x\sigma_x s_z\partial_x \\ H_p(-i\partial_x, k_y) &= \lambda_y k_y \sigma_y \tau_z + \frac{\Delta_y}{2} s_y \tau_y \partial_x^2 \end{aligned} \tag{7}$$

在边界条件 $\psi_\alpha(0) = \psi_\alpha(\infty)$ 下来求解 $H_0\psi_\alpha(x) = E_\alpha\psi_\alpha(x)$ 可以得到四个零能解，其形式为

$$\psi_\alpha(x) = \mathcal{N}_x \sin(\kappa_1 x) e^{-\kappa_2 x} e^{ik_y y} \xi_\alpha \tag{8}$$

归一化系数为 $|\mathcal{N}_x|^2 = 4|\kappa_2(\kappa_1^2+\kappa_2^2)/\kappa_1^2|$。(符号简记，$\kappa_1 = \sqrt{|(2m_x/t_x)| - (\lambda_x^2/t_x^2)}$，$\kappa_2 = (\lambda_x/t_x)$)。旋量部分 ξ_α 满足 $\sigma_y s_z \tau_z = -\xi_\alpha$，可以将旋量部分选取为

$$\begin{aligned} \xi_1 &= |\sigma_y = -1\rangle \otimes |\uparrow\rangle \otimes |\tau = +1\rangle \\ \xi_2 &= |\sigma_y = +1\rangle \otimes |\downarrow\rangle \otimes |\tau = +1\rangle \\ \xi_3 &= |\sigma_y = +1\rangle \otimes |\uparrow\rangle \otimes |\tau = -1\rangle \\ \xi_4 &= |\sigma_y = -1\rangle \otimes |\downarrow\rangle \otimes |\tau = -1\rangle \end{aligned} \tag{9}$$

在这个基矢的选取下，微扰部分 H_p 计算为

$$H_{I,\alpha\beta}(k_y) = \int_0^\infty dx \psi_\alpha^*(x) H_p(-i\partial_x, k_y)\psi_\beta(x); \tag{10}$$

最后得到有效哈密顿量为

$$H_I(k_y) = -A_y k_y s_z + M_I s_y \tau_y \tag{11}$$

$$M_I = \frac{\Delta_x}{2}\int_0^{\infty} dx \psi_\alpha^*(x)\partial_x^2\psi_\alpha(x) = \Delta_x \frac{m}{t_x} \tag{12}$$

其它三个边界上的有效哈密顿量也可以通过相似方式求解得到，结果为

$$\begin{aligned} H_I &= -A_y k_y s_z + M_I s_y \tau_y \\ H_{II} &= A_x k_x s_z + M_{II} s_y \tau_y \\ H_{III} &= A_y k_y s_z + M_{III} s_y \tau_y \\ H_{IV} &= -A_x k_x s_z + M_{IV} s_y \tau_y \end{aligned} \tag{13}$$

每条边界上的质量项满足 $M_{II} = M_{IV} = \Delta_y m/t_y$，$M_I = M_{III} = \Delta_x m/t_x$。这里以逆时针方向为绕行正方向，可以将低能边界理论整理为

$$H_{\text{edge}} = -iA(l)s_z\partial_l + M(l)s_y\tau_y \tag{14}$$

Edge Theory

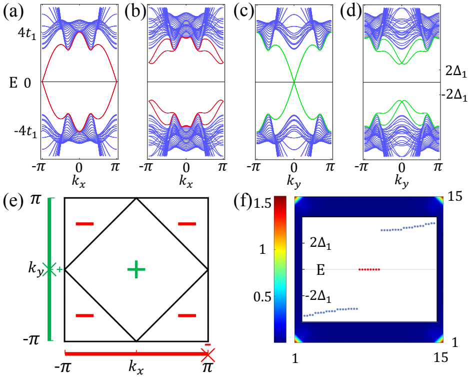
这里的动能系数 $A(l)$ 与 Dirac 质量项 $M(l)$ 都是阶跃函数：$A(l) = A_y, A_x, A_y, A_x$，$M(l) = \Delta_d m/t_x, -\Delta_d m/t_y, \Delta_d m/t_x, -\Delta_d m/t_y (l = \mathrm{I}, \mathrm{II}, \mathrm{III}, \mathrm{IV})$。
从这里可以看出，在系统的每个角落，系数 $A_{x,y}$ 并不会改变符号，但是 Dirac 质量项 $M_(l)$ 因为 d-波配对 $\Delta_x = -\Delta_y$ 的原因，在每个角落的位置都会反号，从而在每个角落处产生一个质量畴壁，形成类似于 Jackiw-Rebbi 零能模的束缚态。例如在边界 (I) 与 (II) 形成的角落中，零能束缚态波函数为

$$|\Psi^{\pm}_{\mathrm{MKP}}\rangle \sim e^{-\int^{l} dl' M(l')/A(l')} |s_x = \tau_y = 1\rangle \tag{15}$$

由于哈密顿量满足时间反演不变，它保证了这两个零能态之间不会相互耦合并产生能隙。

Method 2

$$
\begin{aligned}
H^{\mathrm{BdG}}(\mathbf{k}) &= (h^{\mathrm{TI}}(\mathbf{k}) - \mu)\tau_z + \Delta(\mathbf{k})\tau_x \\
h^{\mathrm{TI}}(\mathbf{k}) &= [2t(\cos k_x - \cos k_y) + 4t_1 \cos k_x \cos k_y]\,\sigma_z + 2\lambda(\sin k_x s_y - \sin k_y s_x)\sigma_x \qquad (16) \\
\Delta(\mathbf{k}) &= \Delta_0 + 2\Delta_1(\cos k_x + \cos k_y)
\end{aligned}
$$



Method 3

$$
\begin{aligned}
H(\mathbf{k}) &= 2\lambda_x \sin k_x \sigma_x s_z \tau_z + 2\lambda_y \sin k_y \sigma_y \tau_z + (\xi_k \sigma_z - \mu)\tau_z + \Delta_0 \tau_x + \mathbf{h}\cdot\mathbf{s} \\
\xi_k &= \epsilon_0 - 2t_x \cos k_x - 2t_y \cos k_y
\end{aligned} \tag{17}
$$

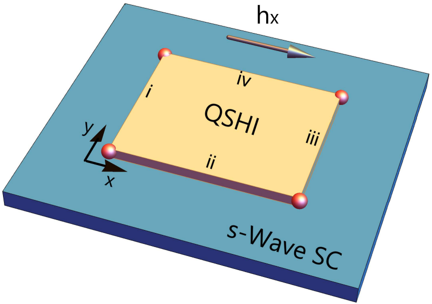


Figure: 量子自旋霍尔效应与 s-波超导构成异质结，并在面内存在一个各项异性的磁场，马约拉纳零能模出现在系统的四个拐角处。

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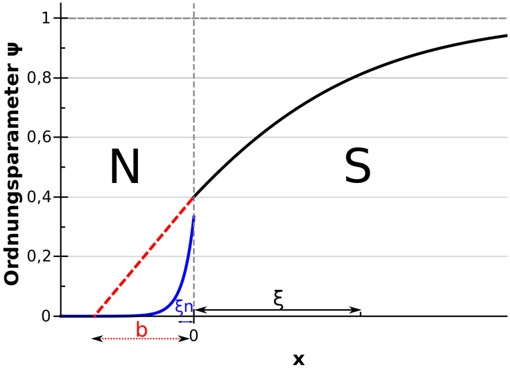
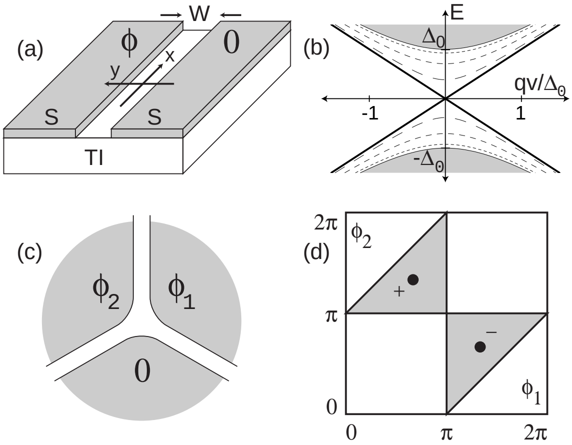
Proximity Effect





Proximity Effect

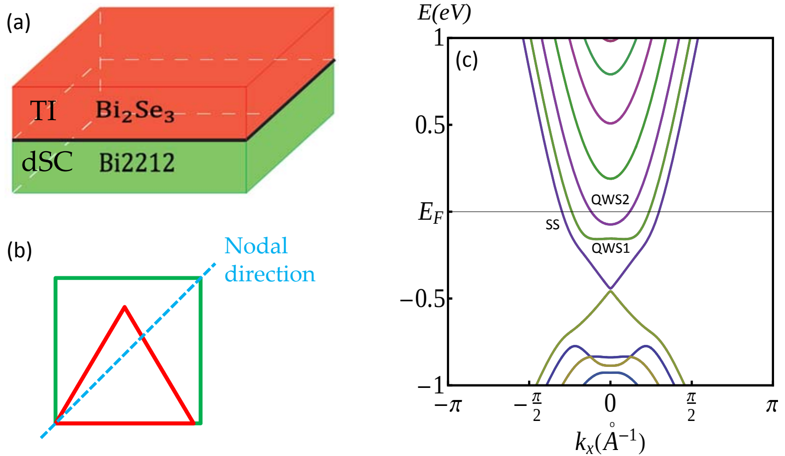


Figure: (a) 拓扑绝缘体/高温超导体异质结。(b)Bi_2Se_3 与 BSCCO 的相对晶格取向，沿着超导配对节线方向，体系波坏了 90° 旋转和反射对称。(c) 拓扑绝缘体 Bi_2Se_3 的能带结构

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Microscopic Model

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$$H = H_{\mathrm{TI}} + H_{\mathrm{SC}} + H_{\mathrm{I}} \tag{18}$$

$$H_{TI} = \sum_{\mathbf{k}} C_{\mathbf{k}}^{\dagger}(h_{\mathbf{k}}\sigma_3 s_0 + 2\lambda_0 \sin k_x \sigma_1 s_3 + 2\lambda_0 \sin k_y \sigma_2 s_0)C_{\mathbf{k}}, \tag{19}$$

$$H_{SC} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} d_{\mathbf{k}\sigma}^{\dagger} d_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}}(d_{\mathbf{k}\uparrow}^{\dagger} d_{-\mathbf{k}\downarrow}^{\dagger} + h.c.), \tag{20}$$

$$H_I = -t_{\perp} \sum_{\mathbf{k}\tau\sigma}(c_{\mathbf{k}\tau\sigma}^{\dagger} d_{\mathbf{k}\sigma} + h.c.). \tag{21}$$

这里 $h_{\mathbf{k}} = h_0 - 2t(\cos k_x + \cos k_y)$,$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$. 整个的哈密顿量可以被写成矩阵形式。在动量空间中它是一个 12×12 的矩阵 $\hat{M}$， $H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \hat{M} \Psi_{\mathbf{k}}$

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Spectral Function

$$G_{ij}(E)=\sum_n \frac{u_{in}u_{jn}^*}{E-E_n+i\Gamma}. \tag{22}$$

这里 u_{in} 和 E_n 分别代表着矩阵的本征矢量和本征值。
在动量空间中，2D 拓扑绝缘体层的谱函数可以通过格林函数计算

$$A(\mathbf{k},E)=-\frac{1}{\pi}\sum_{p=1}^{4}\mathrm{Im}G_{pp}(\mathbf{k},E). \tag{23}$$

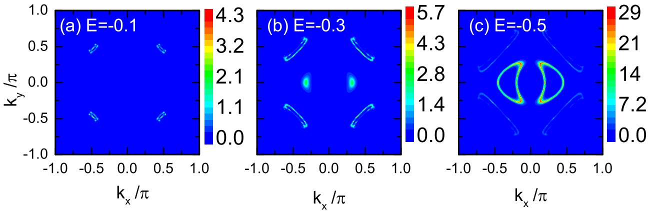

Figure: 2D 拓扑绝缘体层谱函数强度分布。(a)$E=-0.1$,(b)$E=-0.3$,(c)$E=-0.5$

$$C^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{r}\cdot\mathbf{k}} C^\dagger_{\mathbf{r}} \qquad C^\dagger_{\mathbf{r}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{r}\cdot\mathbf{k}} C^\dagger_{\mathbf{r}} \tag{24}$$

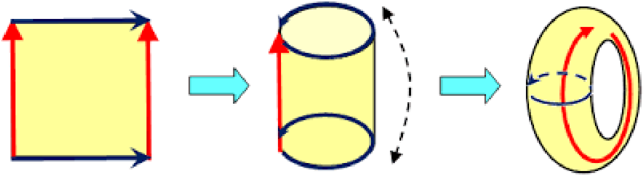

Figure: 圆柱形结构示意图

Edge state

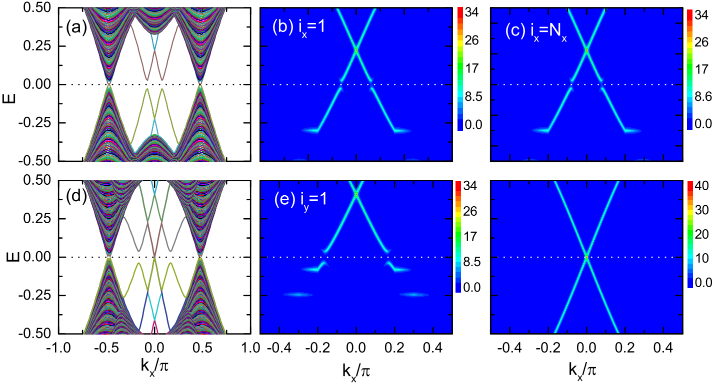

Figure: 考虑圆柱形结构的数值计算结果。(a) 沿 x 方向开边界时哈密顿量本征值,(b)$i_x = 1$ 边界处的谱函数,(c)$i_x = N_x$ 边界处的谱函数,(d) 沿 y 方向开边界时哈密顿量本征值,(b)$i_y = 1$ 边界处的谱函数,(c)$i_y = N_y$ 边界处的谱函数

$$\rho_i(E) = -\frac{1}{\pi}\sum_{p=1}^{4} \mathrm{Im}G_{m+p,m+p}(E). \tag{25}$$

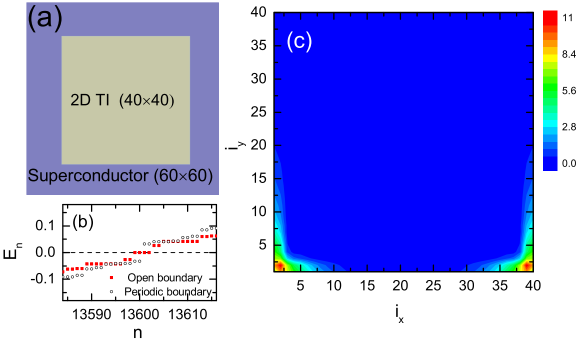

Figure: (a)2D 拓扑绝缘体生长在 d-波高温超导体上，(b) 实空间哈密顿量本征值 (c)2D 拓扑绝缘体实空间中零能态电子局域态密度

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$$\Delta_\tau(\mathbf{k}) = \langle c^\dagger_{\mathbf{k}\tau\uparrow} c^\dagger_{-\mathbf{k}\tau\downarrow} \rangle = \sum_n u^*_{\tau,n}(\mathbf{k}) u_{\tau+6,n}(\mathbf{k}) f(E_n), \tag{26}$$

$$\Delta_s(\mathbf{k}) = \frac{1}{2}\left[\Delta_1(\mathbf{k}) + \Delta_1(-\mathbf{k})\right] \qquad \Delta_t(\mathbf{k}) = \frac{1}{2}\left[\Delta_1(\mathbf{k}) - \Delta_1(-\mathbf{k})\right] \tag{27}$$

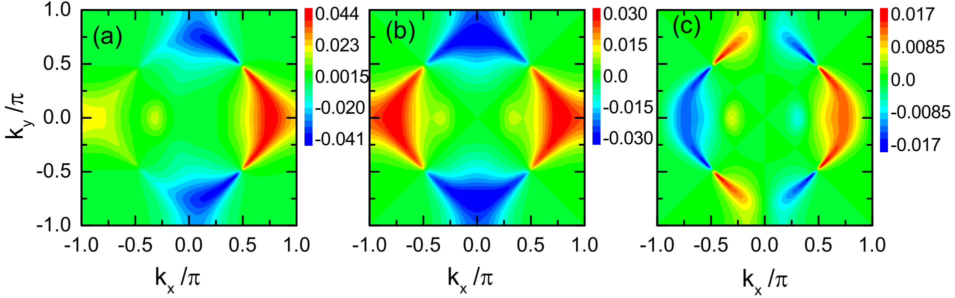

Figure: (a) 轨道 1 的超导序参量 (b) 轨道 1 单重态通道的序参量 (c) 轨道 1 三重态通道的序参量

Real Space Order Parameter

$$\Delta_{ij}^{\tau} = \sum_{n} u_{h(i),n}^{*} u_{h(j)+6,n} f(E_n), \tag{28}$$

$$\Delta_{i}^{\tau} = \mid \Delta_{i,i+\hat{x}}^{\tau} + \Delta_{i,i-\hat{x}}^{\tau} - \Delta_{i,i+\hat{y}}^{\tau} - \Delta_{i,i-\hat{y}}^{\tau} \mid . \tag{29}$$

在系统的边界上，Δ_i^{τ} 表示为

$$\Delta_{i}^{\tau} = \mid 2(\Delta_{i,i+\hat{\alpha}}^{\tau} + \Delta_{i,i-\hat{\alpha}}^{\tau}) \mid \qquad (\alpha = x, y). \tag{30}$$

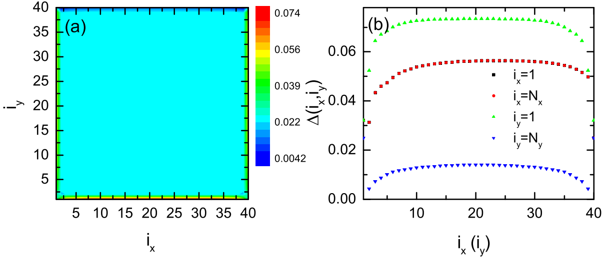

Figure: (a)2D 拓扑绝缘体轨道 1 实空间中的 d-波序参量 (b) 实空间四条边界上的 d-波序参量分布

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Anomalous Green's Function

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对于 2D 拓扑绝缘体，其轨道 τ 的有效配对可以由反常格林函数 $F_\tau(\mathbf{k},\omega)=\langle\langle c^\dagger_{\mathbf{k}\tau\uparrow}|c^\dagger_{-\mathbf{k}\tau\downarrow}\rangle\rangle$

$$F_\tau(\mathbf{k},\omega)=\sum_n\frac{u^*_{\tau,n}(\mathbf{k})u_{\tau+6,n}(\mathbf{k})}{\omega-E_n+i\Gamma} \tag{31}$$

同样的，他可以解析的通过下面的运动方程来求解

$$\omega\langle\langle A|B\rangle\rangle=\langle[A,B]_+\rangle+\langle\langle[A,H]\,|B\rangle\rangle \tag{32}$$

$$H=H_{\mathrm{TI}}+H_{\mathrm{SC}}+H_{\mathrm{I}} \tag{33}$$

先做一些简化的记号 $x_1=\langle\langle c^\dagger_{\mathbf{k}1\uparrow}|c^\dagger_{-\mathbf{k}1\downarrow}\rangle\rangle_\omega$，$x_2=\langle\langle c^\dagger_{\mathbf{k}2\uparrow}|c^\dagger_{-\mathbf{k}1\downarrow}\rangle\rangle_\omega$，$x_3=\langle\langle d^\dagger_{\mathbf{k}\uparrow}|c^\dagger_{-\mathbf{k}1\downarrow}\rangle\rangle_\omega$，
$x_4=\langle\langle d_{-\mathbf{k}\downarrow}|c^\dagger_{-\mathbf{k}1\downarrow}\rangle\rangle_\omega$，$x_5=\langle\langle c_{-\mathbf{k}1\downarrow}|c^\dagger_{-\mathbf{k}1\downarrow}\rangle\rangle_\omega$，$x_6=\langle\langle c_{-\mathbf{k}2\downarrow}|c^\dagger_{-\mathbf{k}1\downarrow}\rangle\rangle_\omega$

Anomalous Green's Function

$$
\begin{aligned}
ax_1 &= fx_2 + t_\perp x_3 && \text{(34a)}\\
bx_2 &= ex_1 + t_\perp x_3 && \text{(34b)}\\
cx_3 &= gx_4 + t_\perp (x_1 + x_2) && \text{(34c)}\\
dx_4 &= gx_3 - t_\perp (x_5 + x_6) && \text{(34d)}\\
bx_5 &= 1 - fx_6 - t_\perp x_4 && \text{(34e)}\\
ax_6 &= -ex_5 - t_\perp x_4, && \text{(34f)}
\end{aligned}
$$

这里 $a = \omega - h_{\mathbf{k}}$, $b = \omega + h_{\mathbf{k}}$, $c = \omega - \varepsilon_{\mathbf{k}}$, $d = \omega + \varepsilon_{\mathbf{k}}$, $e = 2\lambda_0 \sin(k_x) - 2i\lambda_0 \sin(k_y)$, $f = 2\lambda_0 \sin(k_x) + 2i\lambda_0 \sin(k_y)$, 并且令 $g = \Delta_{\mathbf{k}}$.

$$
\langle\langle c^\dagger_{\mathbf{k}1\uparrow} | c^\dagger_{-\mathbf{k}1\downarrow} \rangle\rangle = \frac{\Delta_{\mathbf{k}} t_\perp^2 (a - e)(b + f)}{\Omega} = \frac{\Delta_{\mathbf{k}} t_\perp^2 (C_{even} + C_{odd})}{\Omega}, \tag{35}
$$

$C_{even} = \omega^2 - h_{\mathbf{k}}^2 - 4\lambda_0[\sin^2(k_x) + \sin^2(k_y)]$, $C_{odd} = 4\omega\lambda i \sin(k_y) - 4h_{\mathbf{k}}\lambda_0 \sin(k_x)$

Anomalous Green's Function

$$F_\tau(\mathbf{k}) = -\int_{-\infty}^{0} \mathrm{Im}F_\tau(\mathbf{k},\omega)d\omega. \tag{36}$$

$$\begin{aligned} F_s(\mathbf{k}) &= 1/2[F_1(\mathbf{k}) + F_1(-\mathbf{k})] \\ F_t(\mathbf{k}) &= 1/2[F_1(\mathbf{k}) - F_1(-\mathbf{k})] \end{aligned} \tag{37}$$

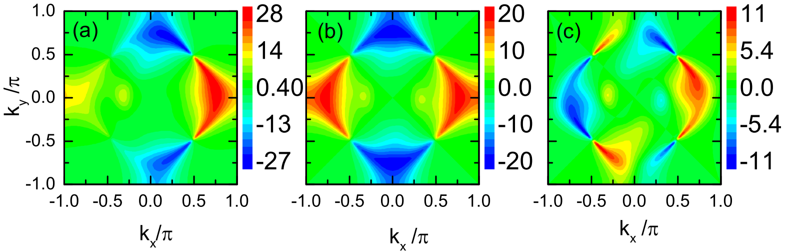

Figure: (a) 反常格林函数计算轨道 1 的超导序参量 (b) 轨道 1 单重态通道的序参量 (c) 轨道 1 三重态通道的序参量

Thank you for your attention!

Questions?