

Floquet Topological Phase Transitions in Lieb Lattice with Intrinsic Spin-Orbit Coupling

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Abstract

We use Floquet theory to theoretically investigate the influence of the external circularly polarized light on the topological properties of the Lieb lattice with intrinsic spin-orbit coupling. Firstly, we use numerical calculation method to compute the spin Chern number to study the topological properties of the Lieb lattice. The variations of the spin Chern number with the amplitude of the circularly polarized light are obtained for different amplitudes of the next nearest-neighbor hopping of the model. Next, the effective Hamiltonian in the high-frequency limit is given, and the variations of the energy gaps at different high-symmetry points with the amplitude of the circularly polarized light are theoretically calculated. It is shown that the results from the theoretical calculating in the high-frequency limit are qualitatively consistent with those by numerical calculations. Finally, based on the computation of the Bott index, the influence of disorder on the topological properties of the Lieb lattice with the external circularly polarized light is investigated.

Keywords

Lieb Lattice, Intrinsic Spin-Orbit Coupling, Floquet Theory, Topological Phase Transition, Disorder

具有内禀自旋 - 轨道耦合的Lieb晶格中 Floquet拓扑相变

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摘要

我们基于Floquet理论研究了外加圆偏振光对具有内禀自旋-轨道耦合的Lieb晶格拓扑性质的影响。首先, 我们采用数值方法计算自旋陈数分析Lieb晶格的拓扑性质。给出了当模型中次近邻格点间跃迁强度取不同值时, 自旋陈数随着圆偏振光振幅变化关系。接着, 我们在高频极限下给出了体系有效哈密顿量, 理论计算了不同高对称点处能隙随者圆偏振光振幅变化的关系。计算结果表明, 在高频极限下的理论结果与直接数值计算结果定性一致。最后, 基于Bott指数的计算, 我们研究了无序对外加圆偏振光作用下的Lieb晶格拓扑性质的影响。

关键词

Lieb晶格, 内禀自旋-轨道耦合, Floquet理论, 拓扑相变, 无序

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1. 引言

Lieb晶格也被称为线心正方晶格, 其中每个元胞中包含了三个不等价格点[1]。这种特殊的几何结构导致了一种具有零能平带的特殊能带结构。由于它独特的能带结构和拓扑性质, 近年来Lieb晶格在理论和实验上都吸引了广泛的研究兴趣。Lieb晶格可以被看作是研究量子多体物理的理想平台。在铜基高温超导体中CuO₂平面内, 原子正是按照Lieb晶格排列[2][3]。最近, 文献报道在光晶格[4][5][6]和光子晶体中[7][8][9][10]可以实现Lieb晶格。令人感兴趣的是, Qiu等人理论上提出可以在热铜表面形成Lieb晶格[11][12], 随后该理论设计得到了实验证实[13][14], 这为人们基于电子型Lieb晶格研究新奇的物理特性提供了实际可行方案。自量子自旋霍尔效应(即二维拓扑绝缘体)在理论上被提出[15][16]及很快被实验所证实[17]后, 拓扑物态的研究目前已成为凝聚态物理研究领域中的一个热点方向[18][19]。有研究者提出在Lieb晶格中引入内禀自旋-轨道耦合效应将会出现量子自旋霍尔效应和量子反常霍尔效应[6][20]-[26]。最近, 在Lieb晶格中由不同参数变化驱动的拓扑相变吸引了人们研究兴趣[6][21][22][23][24]。例如, 研究发现Lieb晶格中次近邻跃迁强度的变化可以引起伴随着更高陈数变化的拓扑相变[21]。

在拓扑物态的理论与实验研究中, 人们非常关注外加含时周期场和无序对在拓扑性质的影响。通过周期驱动的外场, 如圆偏振光照射, 可以调控材料的电子能带结构, 甚至可以引起材料能带拓扑性质的改变[27][28][29][30]。理论上有人提出Floquet拓扑绝缘体的概念[31], 即在一个周期驱动外场的作用下, 可以使得一个静态的拓扑平庸材料变为一个拓扑绝缘体。人们在理论与实验上对Floquet拓扑相变也开展了广泛的研究[32]-[54]。最近, Du等人理论研究了在扩展的Kane-Mele模型中圆偏振光诱导的Floquet拓扑相变[54]。在低维电子体系中, 无序对电子输运性质有着重要的影响。一般情况下, 拓扑非平庸相对弱无序有着很强的抗干扰性; 而在强无序作用下, 体系出现了安德森局域化, 使得拓扑非平庸相转变为拓扑平庸相。在另一方面, Li等人研究发现无序也可以诱导拓扑平庸相转变为拓扑非平庸相, 提出体系

出现了拓扑安德森绝缘体相[55]。随后, 人们在不同体系中对拓扑安德森绝缘体开展了大量的理论研究[26] [56]-[65]。最近, 拓扑安德森绝缘体在无序的一维冷原子链和光学体系中被实验观察到[66] [67]。

本文将基于 Floquet 理论研究外加圆偏振光对具有内禀自旋 - 轨道耦合的 Lieb 晶格拓扑性质的影响。我们采用数值方法计算自旋陈数, 给出自旋陈数随着模型中次近邻格点间跃迁强度与圆偏振光振幅的变化关系。在高频极限下给出了体系有效哈密顿量, 理论计算不同高对称点处能隙随着圆偏振光振幅变化的关系。另外, 我们也研究了无序对外加圆偏振光作用下的 Lieb 晶格拓扑性质的影响。

2. 模型与方法

本文我们研究二维 Lieb 晶格的拓扑性质。Lieb 晶格又被称为线心正方晶格, 其结构示意图由图 1 给出。图 1 中正方形虚线所围区域表示一个元胞, Lieb 晶格中的每个元胞包含三种不等价原子(分别记为 A、B 和 C)。在紧束缚近似下(取晶格常数 $a=1$), 我们研究的 Lieb 模型的哈密顿量写为[21]:

$$\hat{H} = \hat{H}_{NN} + \hat{H}_{NNN} + \hat{H}_{ISO}, \tag{1}$$

其中

$$\hat{H}_{NN} = -t \sum_{\langle i,j \rangle; \alpha} c_{i,\alpha}^\dagger c_{j,\alpha}, \tag{2}$$

$$\hat{H}_{NNN} = -t' \sum_{\langle\langle i,j \rangle\rangle; \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} c_{i,\alpha}^\dagger c_{j,\alpha}, \tag{3}$$

$$\hat{H}_{ISO} = i\lambda_{ISO} \sum_{\langle\langle i,j \rangle\rangle; \alpha\beta} c_{i,\alpha}^\dagger (\mathbf{e}_{ij} \cdot \boldsymbol{\sigma}_{\alpha\beta}) c_{j,\beta}. \tag{4}$$

这里, t 为最近邻格点间跃迁强度, t' 为次近邻格点间跃迁强度, λ_{ISO} 为内禀自旋 - 轨道耦合强度。 $\alpha(\beta) = \uparrow, \downarrow$ 为自旋指标, $c_{i,\alpha}^\dagger (c_{i,\alpha})$ 表示在格点 i 上具有自旋 α 的粒子的产生(湮灭)算符。 $\langle i, j \rangle$ 代表格点间最近邻求和, $\langle\langle i, j \rangle\rangle$ 代表格点次近邻求和。单位向量 $\mathbf{e}_{ij} = (\mathbf{d}_{ik} \times \mathbf{d}_{kj}) / |\mathbf{d}_{ik} \times \mathbf{d}_{kj}|$, \mathbf{d}_{ik} 为格点 i 指向格点 k 的矢量。 $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ 是泡利矩阵。

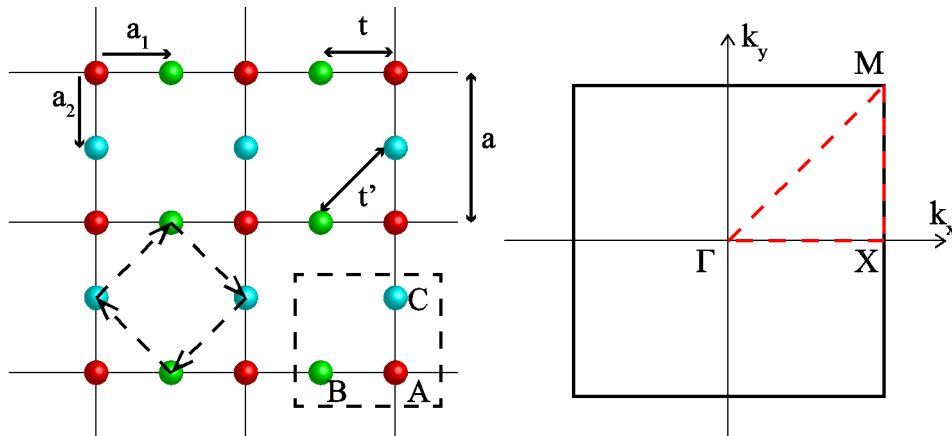


Figure 1. (a) The geometry structure of Lieb lattice. The dashed black arrow stands for spin-orbit coupling, and a square dashed line surrounds one unite cell; (b) First Brillouin Zone of the Lieb lattice

图 1. (a) Lieb 晶格几何结构。黑色虚线表示自旋 - 轨道耦合项, 正方形虚线所围的是一个元胞; (b) Lieb 晶格的第一布里渊区

通过傅里叶变换 $\hat{H} = \sum_k \psi_k^\dagger H_k \psi_k$, 其中 $\psi_k = (c_{kA\uparrow}, c_{kB\uparrow}, c_{kC\uparrow}, c_{kA\downarrow}, c_{kB\downarrow}, c_{kC\downarrow})$, 实空间的哈密顿量可以

转化成动量空间的形式。另一方面, 我们选取的体系满足时间反演对称性, 哈密顿量矩阵形式由自旋上和自旋下两个块对角项构成, 其中 $H_{k\downarrow} = H_{-k\uparrow}^*$,

$$H_{k\uparrow} = \begin{pmatrix} 0 & f_1(\mathbf{k}) & f_2(\mathbf{k}) \\ f_1^*(\mathbf{k}) & 0 & g(\mathbf{k}) \\ f_2^*(\mathbf{k}) & g^*(\mathbf{k}) & 0 \end{pmatrix}, \quad (5)$$

其中, $f_1(\mathbf{k}) = -2tc_x$, $f_2(\mathbf{k}) = -2tc_y$, $g(\mathbf{k}) = -4t'c_x c_y - 4i\lambda_{ISO}s_x s_y$, $c_u = \cos(k_u/2)$, $s_u = \sin(k_u/2)$ ($u = x, y$)。

当我们考虑一束圆偏振光垂直照射 Lieb 晶格时, 实空间含时的哈密顿量具体形式为:

$$\hat{H}(t) = -t \sum_{\langle i,j \rangle; \alpha} e^{-iA_{ij}(t)} c_{i,\alpha}^\dagger c_{j,\alpha} - t' \sum_{\langle\langle i,j \rangle\rangle; \alpha} e^{-iA_{ij}(t)} c_{i,\alpha}^\dagger c_{j,\alpha} + i\lambda_{ISO} \sum_{\langle\langle i,j \rangle\rangle; \alpha\beta} e^{-iA_{ij}(t)} c_{i,\alpha}^\dagger (\mathbf{e}_{ij} \cdot \boldsymbol{\sigma}_{\alpha\beta}) c_{j,\beta}, \quad (6)$$

其中, $A_{ij}(t) = \mathbf{A}(t) \cdot (\mathbf{R}_j - \mathbf{R}_i)$, $\mathbf{A}(t) = A_0 [\sin(\omega t), \cos(\omega t)]$ 是矢量, A_0 为圆偏振光的振幅, ω 为圆偏振光的频率, \mathbf{R}_i 是第 i 个格点的位置矢量。本文我们采用自然单位制, 设普朗克常数 $\hbar = 1$, 光速 $c = 1$, 电子电荷 $e = 1$, 以及使用标度势为零的库仑规范。光的效果相当于引入了含时的全空间均匀电场 $\mathbf{E}(t) = -\partial_t \mathbf{A}(t)$, 忽略圆偏振光的磁场的微弱效应[68]。单位能量设为最近邻跃迁的振幅 t , 取 $t = 1$ 。

对方程(6)进行傅里叶变换, 我们可以得到动量空间中含时的哈密顿量, 其中自旋向上部分写为:

$$H_{k\uparrow} = \begin{pmatrix} 0 & f_1(\mathbf{k}, t) & f_2(\mathbf{k}, t) \\ f_1^*(\mathbf{k}, t) & 0 & -i\lambda_{ISO}g_1(\mathbf{k}, t) + t'g_2(\mathbf{k}, t) \\ f_2^*(\mathbf{k}, t) & i\lambda_{ISO}g_1^*(\mathbf{k}, t) + t'g_2^*(\mathbf{k}, t) & 0 \end{pmatrix}, \quad (7)$$

其中

$$f_1(\mathbf{k}, t) = -te^{-ik \cdot a_1} e^{-iA(t) \cdot a_1} - te^{ik \cdot a_1} e^{iA(t) \cdot a_1}, \quad (8)$$

$$f_2(\mathbf{k}, t) = -te^{-ik \cdot a_2} e^{-iA(t) \cdot a_2} - te^{ik \cdot a_2} e^{iA(t) \cdot a_2}, \quad (9)$$

$$g_1(\mathbf{k}, t) = e^{-ik \cdot (a_1 - a_2)} e^{-iA(t) \cdot (a_1 - a_2)} + e^{-ik \cdot (a_2 - a_1)} e^{-iA(t) \cdot (a_2 - a_1)} - e^{ik \cdot (a_1 + a_2)} e^{iA(t) \cdot (a_1 + a_2)} - e^{-ik \cdot (a_1 + a_2)} e^{-iA(t) \cdot (a_1 + a_2)} \quad (10)$$

$$g_2(\mathbf{k}, t) = e^{-ik \cdot (a_1 - a_2)} e^{-iA(t) \cdot (a_1 - a_2)} + e^{-ik \cdot (a_2 - a_1)} e^{-iA(t) \cdot (a_2 - a_1)} + e^{ik \cdot (a_1 + a_2)} e^{iA(t) \cdot (a_1 + a_2)} + e^{-ik \cdot (a_1 + a_2)} e^{-iA(t) \cdot (a_1 + a_2)} \quad (11)$$

接下来, 我们将介绍本文所用到的几种方法。对一个含时系统, 我们可以运用 Floquet 理论[54] [68] 将含时体系转化为不含时体系。下面我们将简要介绍这一理论。含时的薛定谔方程写为

$$i \frac{d}{dt} |\psi_\alpha(t)\rangle = \hat{H}(t) |\psi_\alpha(t)\rangle. \quad (12)$$

含时哈密顿量 $\hat{H}(t)$ 满足 $\hat{H}(t+T) = \hat{H}(t)$, 其中 $T = \frac{2\pi}{\omega}$ 代表圆偏振光周期。其本征函数一般解的形式为

$$|\psi_\alpha(t)\rangle = e^{-i\varepsilon_\alpha t} |\phi_\alpha(t)\rangle, \quad (13)$$

其中 ε_α 是能带 α 对应的准能量, $|\phi_\alpha(t)\rangle = |\phi_\alpha(t+T)\rangle$ 为 Floquet 准模, 通过傅里叶级数展开可写为

$$|\phi_\alpha(t)\rangle = \sum_m e^{im\omega t} |\tilde{\phi}_\alpha^m\rangle. \quad (14)$$

将公式(13)和(14)代入公式(12), 可得

$$\sum_m (H_{nm} + m\omega \delta_{nm}) |\tilde{\phi}_\alpha^m\rangle = \varepsilon_\alpha |\tilde{\phi}_\alpha^m\rangle, \quad (15)$$

其中 Floquet 哈密顿量的矩阵元为

$$H_{nm} = \frac{1}{T} \int_0^T dt e^{-i(n-m)\omega t} \hat{H}(t). \quad (16)$$

这里, n 和 m 取值为从负无穷到正无穷的整数。本文的计算中 n, m 取值从-4 到+4, 计算表明这是一个很好的截断近似取值。

在接下里的章节中, 我们将采用数值方法计算自旋陈数[69]来讨论干净系统的拓扑性质。Lieb 格子由于几何结构具有三条能带, 我们将费米面放在下面两条能带的能隙中, 布里渊区划分为 $N \times N$ 个网格, $\Psi(k_x^i, k_y^j)$ 为网格点 (i, j) 对应波函数, 陈数表达式为[69]。

$$C = \frac{1}{2\pi} \sum_{i \in N, j \in N} \text{Im} \log \left[\left(\Psi(k_x^i, k_y^j) \Psi(k_x^{i+1}, k_y^j) \right) \left(\Psi(k_x^{i+1}, k_y^j) \Psi(k_x^{i+1}, k_y^{j+1}) \right) \right. \\ \left. \times \left(\Psi(k_x^{i+1}, k_y^{j+1}) \Psi(k_x^i, k_y^{j+1}) \right) \left(\Psi(k_x^i, k_y^{j+1}) \Psi(k_x^i, k_y^j) \right) \right] \quad (17)$$

当我们研究无序对 Lieb 晶格拓扑性质的影响时, 我们将采用 Bott 指数表征体系的拓扑性质。能隙以下电子占据态的投影算符定义为:

$$P = \sum_i^{N_{occ}} |\psi_i\rangle \langle \psi_i|, \quad (18)$$

其中 $|\psi_i\rangle$ 为第 i 个态的波函数, N_{occ} 为能隙以下电子占据态的总数。投影位置算符定义为

$$U = P e^{i2\pi X} P, \quad (19)$$

$$V = P e^{i2\pi Y} P, \quad (20)$$

其中 X, Y 分别是粒子横坐标和纵坐标所组成的坐标矩阵。由此 Bott 指数的表达式为[70] [71]

$$B = \frac{1}{2\pi} \text{Im} \left\{ \text{tr} \left[\log \left(V U V^\dagger U^\dagger \right) \right] \right\}. \quad (21)$$

3. 结果与讨论

3.1. 自旋陈数与 Floquet 能带结构

首先基于自旋陈数的数值计算, 我们讨论外加圆偏振光诱导的 Lieb 晶格中的拓扑相变。图 2 给出了在次近邻格点间跃迁强度取不同值时 ($t' = 0, 0.3, 0.6, 0.9$), 自旋陈数随着圆偏振光振幅变化的关系图, 其中, 最近邻格点间跃迁强度为 $t = 1$, 内禀自旋-轨道耦合强度为 $\lambda_{ISO} = 0.3$ 和圆偏振光频率 $\omega = 10$ 。

当不考虑次近邻格点间跃迁时, 由图 2(a) 可以发现, 没有外加圆偏振光时, 陈数为-1, 对应拓扑相; 随着圆偏振光振幅的增加, 陈数保持为-1, 直到圆偏振光振幅增加到 4.0, 陈数由-1 改变为 0, 表明发生拓扑相变, 由拓扑相转变为拓扑平庸相; 而圆偏振光振幅增加到 4.05, 陈数由 0 改变为+1, 拓扑平庸相转变为拓扑相; 圆偏振光振幅继续增加, 陈数为 1 的拓扑相继续保持; 同时, 发现在圆偏振光振幅为 4.9 附近时, 出现陈数为+3 的拓扑相。图 2(b) 给出了次近邻格点间跃迁强度为 0.3 时自旋陈数随着圆偏振光振幅变化情况。对比图 2(b) 与图 2(a), 发现陈数为 0 拓扑平庸相出现的范围略有扩大。仔细分析发现, 在次近邻格点间跃迁强度为 0.3 时, 陈数为 0 的拓扑平庸相对应的圆偏振光振幅为 4.0 到 4.17。

我们继续增大次近邻格点间跃迁强度时, 发现对于较大的次近邻格点间跃迁强度(如 0.6 和 0.9), 自旋陈数随着圆偏振光振幅变化的关系图有不同的性质(见图 2(c) 和图 2(d))。以次近邻格点间跃迁强度取 0.9 为例, 图 2(d) 给出没有外加圆偏振光时, 陈数为+1; 随着圆偏振光振幅的增加, 直到圆偏振光振幅增加到 2.5, 陈数由+1 改变为-1; 而圆偏振光振幅为 3.8 时, 陈数再次发生变化, 由-1 变为 0(对应拓扑平庸

相); 陈数为 0 的对应拓扑平庸相在圆偏振光振幅增至 4.25 时, 转变为陈数为+1 的拓扑相。同时, 发现在圆偏振光振幅继续增加时, 也会出现陈数为+3 的拓扑相。

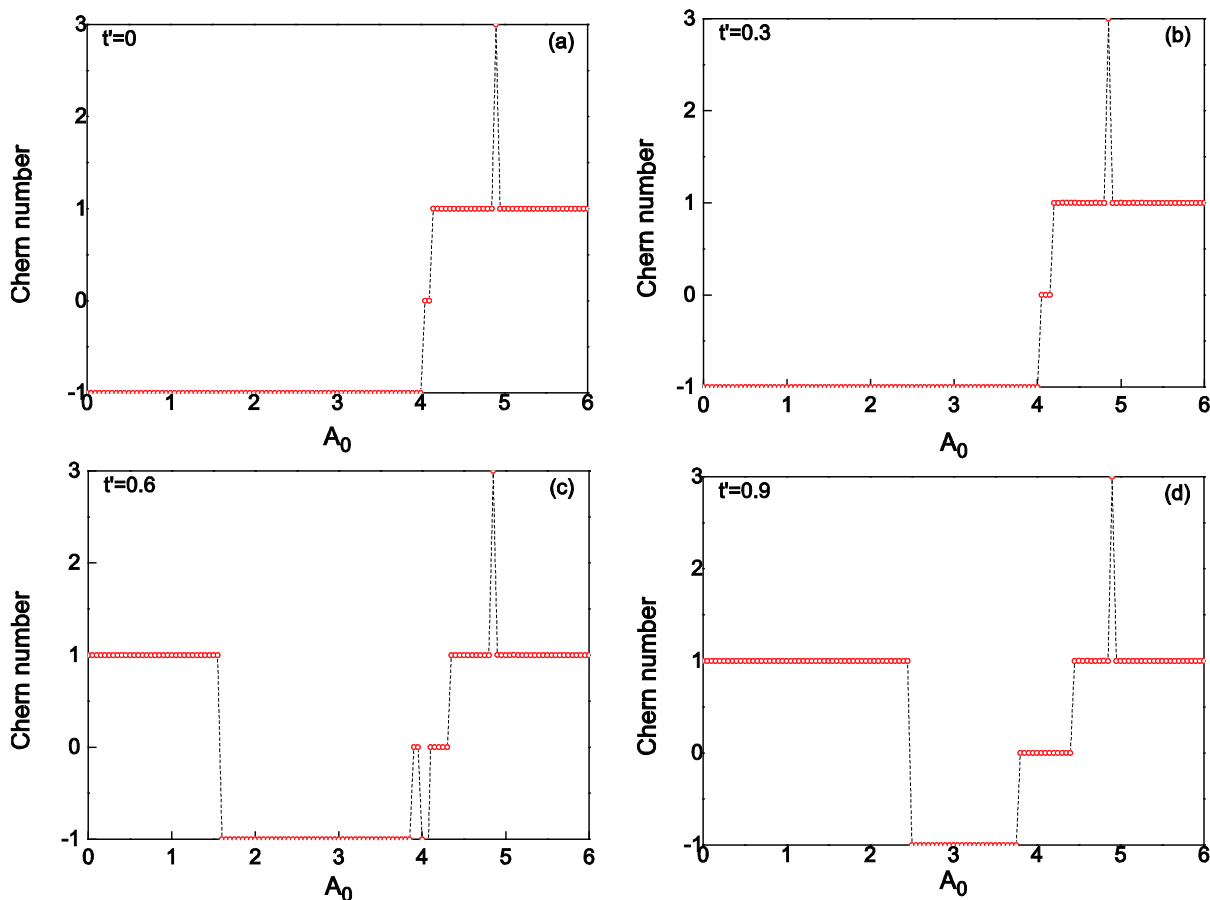


Figure 2. The spin Chern number as a function of the amplitude of the circularly polarized light. (a) $t' = 0$; (b) $t' = 0.3$; (c) $t' = 0.6$; (d) $t' = 0.9$. Here, the amplitude of the nearest-neighbor hopping, the spin-orbit coupling strength and the frequency of the circularly polarized light are taken as $t = 1$, $\lambda_{\text{ISO}} = 0.3$ and $\omega = 10$, respectively

图 2. 自旋陈数随着圆偏振光振幅变化的关系图。(a) $t' = 0$; (b) $t' = 0.3$; (c) $t' = 0.6$; (d) $t' = 0.9$ 。这里, 最近邻格点间跃迁强度、自旋 - 轨道耦合强度和圆偏振光频率分别取为 $t = 1$, $\lambda_{\text{ISO}} = 0.3$ 和 $\omega = 10$

图 2 表明外加圆偏振光引起 Lieb 晶格能带自旋陈数较为复杂的变化, 其对应拓扑相的变化, 而这种变化可以通过分析 Floquet 能带结构来理解。实际上, 拓扑相的变化对应能隙的打开和闭合, 即在陈数发生突变时, 相应的能隙发生闭合。我们将以次近邻格点间跃迁强度等于 0.3 为例, 图 3 给出了与图 2(b)对应的 Floquet 能带结构。在图 3(a)~(c)中, 圆偏振光振幅分别为 0、2.0 和 3.0, 可以发现, 下面两个能带之间有明显的能隙, 对应图 2(b)中给出的陈数为-1, 即体系为拓扑绝缘体; 而且高对称点 M 处的能隙随着圆偏振光振幅增加而减小; 注意到图 3(d)给出了圆偏振光振幅为 4.0 的情况, 我们发现这时下面两个能带在高对称点 M 处的能隙闭合, 对应在图 2(b)中陈数由-1 变为 0; 圆偏振光振幅继续增大, 能隙重新打开, 如图 3(d)给出的圆偏振光振幅为 4.05 的情况(这时, 高对称点 M 处的能隙再次出现, 而这个能隙为拓扑平庸的能隙, 即体系为普通绝缘体); 圆偏振光振幅为 4.17 时(见图 3(f)), 高对称点 M 处的能隙再次闭合, 对应在图 2(b)中陈数由 0 变为+1; 在图 3(g)~(i)中, 圆偏振光振幅分别为 4.8、4.9 和 5.0。令人感兴趣的是, 我们发现, 圆偏振光振幅为 4.9 时, 下面两个能带的能隙闭合

点由之前的高对称点 M 处转变为在高对称点 X 处, 对应图 2(b)中陈数由+1 变为+3。

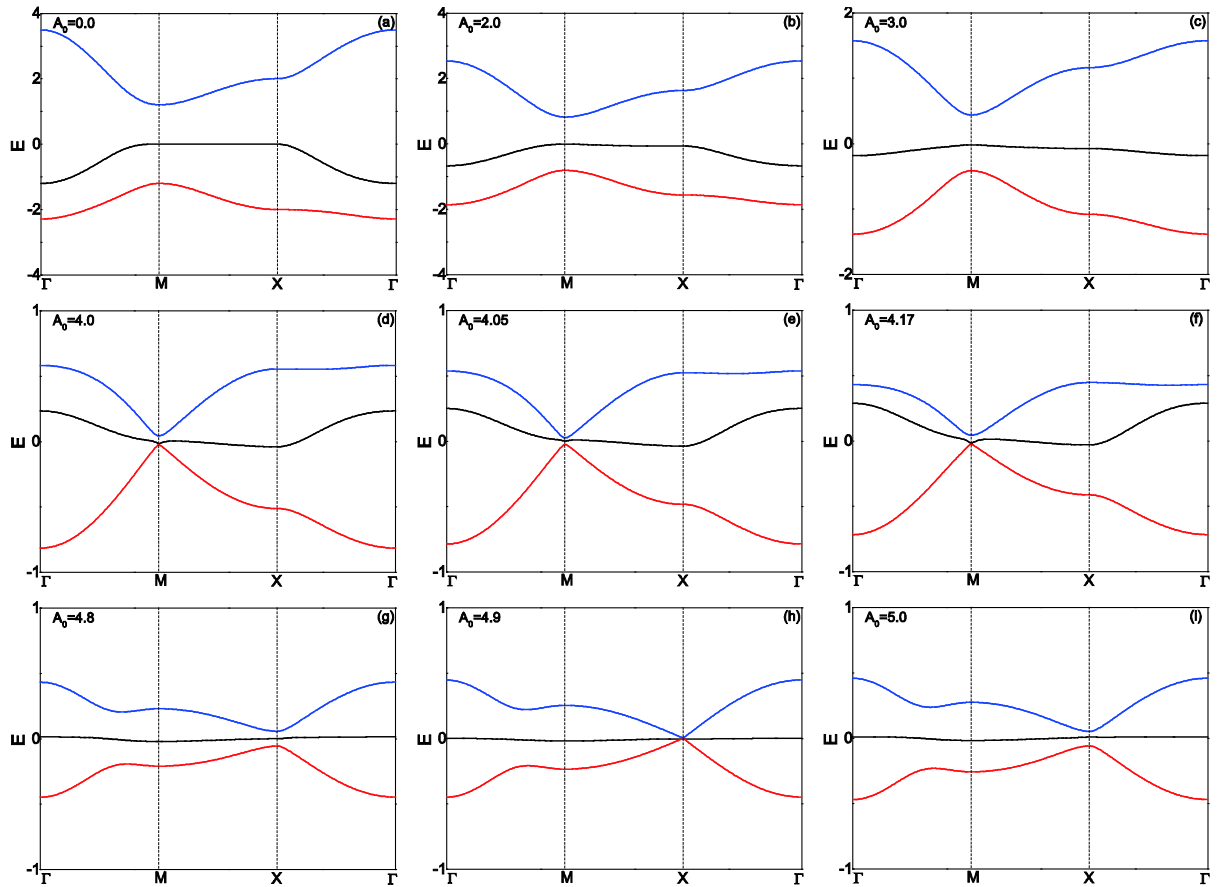


Figure 3. The Floquet-Bloch band structure of Lieb lattice model with parameters $t = 1$, $t' = 0.3$, $\lambda_{ISO} = 0.3$, and $\omega = 10$. (a) $A_0 = 0.0$; (b) $A_0 = 2.0$; (c) $A_0 = 3.0$; (d) $A_0 = 4.0$; (e) $A_0 = 4.05$; (f) $A_0 = 4.17$; (g) $A_0 = 4.8$; (h) $A_0 = 4.9$; (i) $A_0 = 5.0$

图 3. Lieb 晶格模型的 Floquet-Bloch 能带结构。模型参数分别为 $t = 1$, $t' = 0.3$, $\lambda_{ISO} = 0.3$, and $\omega = 10$ 。(a) $A_0 = 0.0$; (b) $A_0 = 2.0$; (c) $A_0 = 3.0$; (d) $A_0 = 4.0$; (e) $A_0 = 4.05$; (f) $A_0 = 4.17$; (g) $A_0 = 4.8$; (h) $A_0 = 4.9$; (i) $A_0 = 5.0$

3.2. 高频极限下的有效哈密顿量

由高频区的 Magnus 展开式出发, 有效哈密顿量可以写为[35] [39] [54]

$$H_{eff} = H_0 + \sum_n \frac{1}{n\omega} [H_n, H_{-n}] + O\left(\frac{1}{\omega^2}\right), \quad (22)$$

其中当频率趋于无穷大时, $H_{eff} = H_0$ 。在高对称点 $M \{\pi, \pi\}$ 处, 有效哈密顿量形式可以写为

$$H_{eff} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -4i\lambda_{ISO}J_0\left(-\sqrt{2}A_0/2\right) \\ 0 & 4i\lambda_{ISO}J_0\left(-\sqrt{2}A_0/2\right) & 0 \end{pmatrix}. \quad (23)$$

能量本征值为

$$E_{\pm} = \pm 4\lambda_{ISO}J_0\left(\sqrt{2}A_0/2\right), \quad (24)$$

$$E_0 = 0. \quad (25)$$

这里本征值仅取决于内禀自旋-轨道耦合强度 λ_{ISO} , 以及贝塞尔函数 $J_0(\sqrt{2}A_0/2)$ 。
在高对称点 $X\{\pi, 0\}$, 有效哈密顿量写

$$H_{eff} = \begin{pmatrix} 0 & 0 & -2J_0(A_0/2)t \\ 0 & 0 & 0 \\ -2J_0(-A_0/2)t & 0 & 0 \end{pmatrix}. \quad (26)$$

能量本征值为

$$E_{\pm} = \pm 2tJ_0(A_0/2), \quad (27)$$

$$E_0 = 0. \quad (28)$$

这里本征值仅与最近邻跃迁系数 t , 以及贝塞尔函数 $J_0(A_0/2)$ 有关。

在中心对称点 $\Gamma\{0, 0\}$, 有效哈密顿量为

$$H_{eff} = \begin{pmatrix} 0 & -2J_0(A_0/2)t & -2J_0(A_0/2)t \\ -2J_0(-A_0/2)t & 0 & -4J_0(\sqrt{2}A_0/2)t' \\ -2J_0(-A_0/2)t & -4J_0(-\sqrt{2}A_0/2)t' & 0 \end{pmatrix}. \quad (29)$$

能量本征值为

$$E_{\pm} = -2t'J_0(\sqrt{2}A_0/2) \pm 2\sqrt{2t^2J_0(A_0/2)^2 + t'^2J_0(\sqrt{2}A_0/2)^2}, \quad (30)$$

$$E_0 = 4J_0(\sqrt{2}A_0/2)t'. \quad (31)$$

可以看出在中心对称点 Γ 次近邻项对本征值有很大影响。为了与上一节的数值结果相比较, 我们讨论下面两个能带之间的能隙。图 4 给出了在不同高对称点的能隙随着圆偏振光振幅变化的关系图, 其中实线对应数值计算的结果, 虚线表示在高频极限下由有效哈密顿量计算的结果。

图 4 给出了不同高对称点(Γ 点, M 点和 X 点)处能隙随着圆偏振光振幅变化的关系图。图 4 中的虚线和实线分别是在高频极限下的理论计算和直接数值计算得到的能隙。从图 4 中可以看出, 在高频极限下的理论结果与直接数值计算结果定性一致。特别是, Γ 点和 X 点处能隙随着圆偏振光振幅变化的关系用上述两种方法得到的结果吻合得较好; 而 M 点处在高频极限下的理论计算得到的能隙与直接数值计算得到的能隙有些偏差, 说明对于高对称点 M 处而言, 有效哈密顿量的高阶修正需要进一步考虑。

3.3. 无序对拓扑性质的影响

为研究无序对 Lieb 晶格拓扑性质的影响, 我们在体系紧束缚模型哈密顿量中引入在位能无序项如下:

$$H_{dis} = \sum_i U_{dis}^i c_i^\dagger c_i, \quad (32)$$

其中 U_{dis}^i 随机分布在 $[-U_{dis}/2, U_{dis}/2]$ 范围内, U_{dis} 表示无序强度。我们数值计算无序体系的 Bott 指数, Bott 指数为 1 时对应拓扑非平庸相, 而 Bott 指数为 0 则对应拓扑平庸相。图 5 给出了次近邻格点间跃迁强度和圆偏振光振幅分别取不同值时, Bott 指数随无序强度变化的关系图。在我们的数值计算中, 样品

取为 20×20 , 无序构型取 500 次平均。

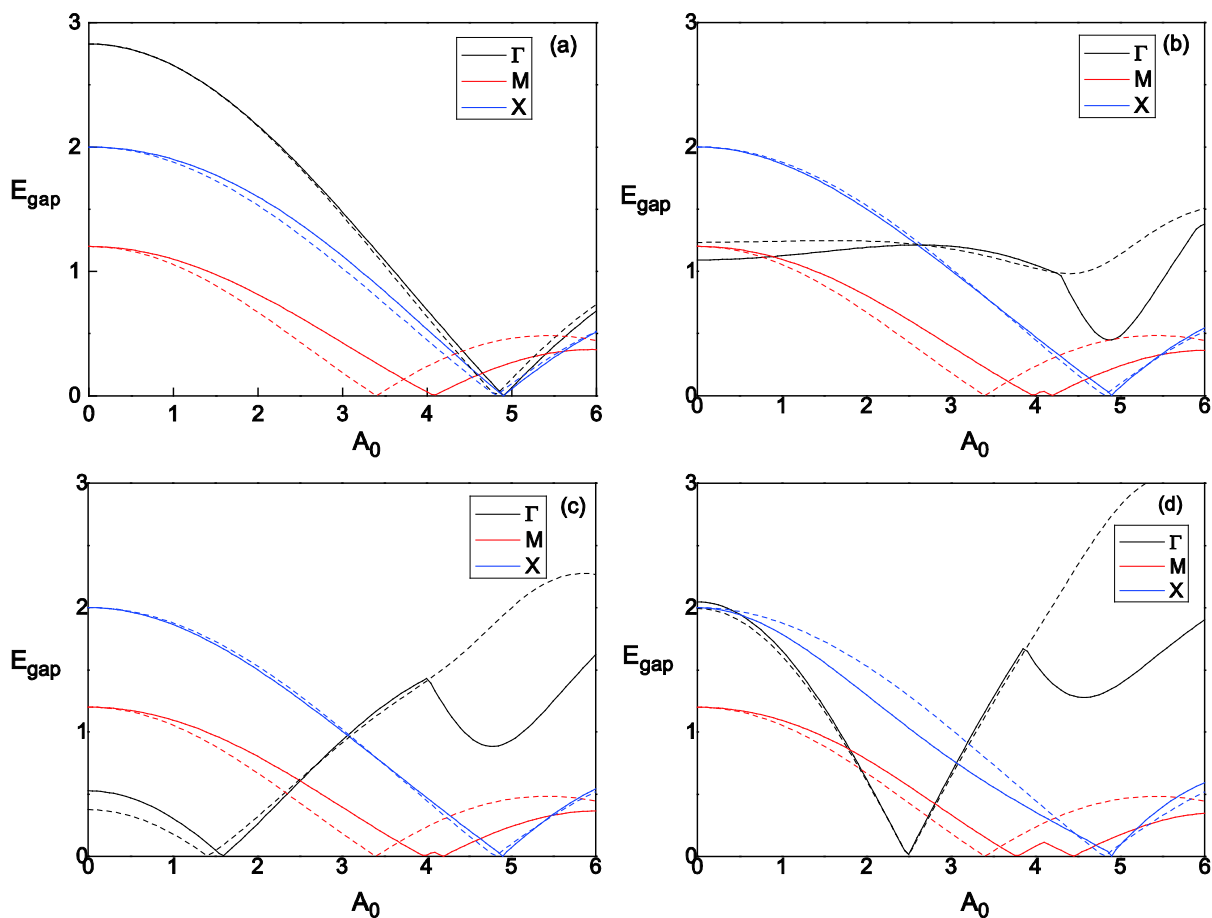


Figure 4. The energy gaps at the different high symmetry points as a function of the amplitude of the circularly polarized light. (a) $t' = 0$; (b) $t' = 0.3$; (c) $t' = 0.6$; (d) $t' = 0.9$. Here, the amplitude of the nearest-neighbor hopping, the spin-orbit coupling strength and the frequency of the circularly polarized light are taken as $t = 1$, $\lambda_{iso} = 0.3$ and $\omega = 10$, respectively. The dashed line indicates the energy gap in the theoretical infinite-frequency limits, and the solid line denotes the gap obtained by numerical calculation

图 4. 不同高对称点处能隙随着圆偏振光振幅变化的关系图。(a) $t' = 0$; (b) $t' = 0.3$; (c) $t' = 0.6$; (d) $t' = 0.9$ 。这里, 最近邻格点间跃迁强度、自旋 - 轨道耦合强度和圆偏振光频率分别取为 $t = 1$, $\lambda_{iso} = 0.3$ 和 $\omega = 10$ 。虚线表示在高频极限下的理论计算得到能隙, 而实线是数值计算给出的能隙

由图 5 可以看到, 选取适当的模型参数, 弱无序并不会改变在外加圆偏振光作用下的拓扑非平庸相, 即证实了拓扑非平庸相在弱无序条件下的稳定性。同时也发现, 随着无序强度的增加, 在强无序条件下, 出现安德森局域化, 体系变为拓扑平庸的绝缘体。我们首先具体分析圆偏振光振幅变化带来的影响。我们观察到, 在一定范围内圆偏振光振幅的增强降低了拓扑非平庸相的稳定性。以图 5(a)为例, 这里不考虑次近邻格点间跃迁(即 $t' = 0$), 当圆偏振光振幅 A_0 分别为 0.5、1.0、1.5 和 2.0 时, 体系由拓扑非平庸相转变为拓扑平庸安德森局绝缘体相对应的无序强度 U_{dis} 分别为: 6.4、5.8、4.6 和 2.6。

接下来我们考虑次近邻格点间跃迁的影响。从图 5 中我们发现, 次近邻格点间跃迁强度的增加有利于拓扑非平庸相的稳定性。我们以圆偏振光振幅 $A_0 = 2.0$ 为例, 当次近邻格点间跃迁强度分别为 0、0.3、0.6 和 0.9 时, 体系由拓扑非平庸相转变为拓扑平庸安德森局绝缘体相对应的无序强度 U_{dis} 分别为: 2.6、3.4、4.0 和 4.8。

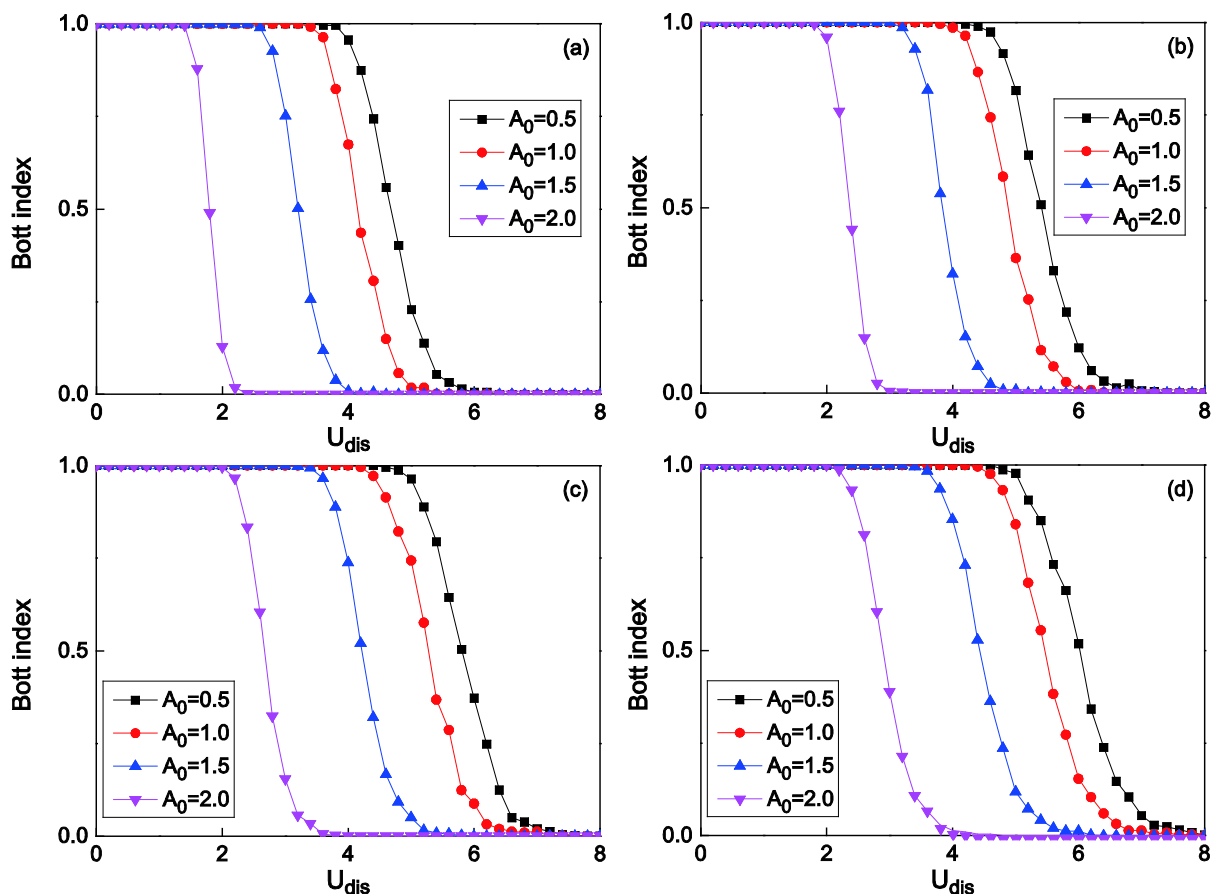


Figure 5. The Bott index as a function of the disorder strength. (a) $t' = 0$; (b) $t' = 0.3$; (c) $t' = 0.6$; (d) $t' = 0.9$. Here, the amplitude of the nearest-neighbor hopping, the spin-orbit coupling strength and the frequency of the circularly polarized light are taken as $t = 1$, $\lambda_{iso} = 0.3$ and $\omega = 10$, respectively

图 5. Bott 指数随着无序强度变化的关系图。(a) $t' = 0$; (b) $t' = 0.3$; (c) $t' = 0.6$; (d) $t' = 0.9$ 。这里, 最近邻格点间跃迁强度、自旋 - 轨道耦合强度和圆偏振光频率分别取为 $t = 1$, $\lambda_{iso} = 0.3$ 和 $\omega = 10$

4. 总结

在 Lieb 晶格中引入内禀自旋 - 轨道耦合, 将使体系能带结构出现拓扑非平庸的能隙, 从而出现量子自旋霍尔效应, 即 Lieb 晶格成为二维拓扑绝缘体。本文中, 我们基于 Floquet 理论研究了外加圆偏振光对具有内禀自旋 - 轨道耦合的 Lieb 晶格拓扑性质的影响。首先, 我们采用数值方法计算自旋陈数, 分析 Lieb 晶格能带结构中下面两条能带的能隙的拓扑性质。给出了当模型中次近邻格点间跃迁强度取不同值时, 自旋陈数随着圆偏振光振幅变化关系。研究发现次近邻格点间跃迁强度和圆偏振光振幅的变化对 Lieb 晶格的拓扑性质有着明显的调制作用。外加圆偏振光引起 Lieb 晶格能带自旋陈数较为复杂的变化, 其对应拓扑相的变化, 拓扑相的变化对应能隙的打开和闭合, 而这种变化通过具体计算 Floquet 能带结构得到证实。接着, 我们在高频极限下给出了体系有效哈密顿量, 理论计算了不同高对称点处能隙随着圆偏振光振幅变化的关系。计算结果表明, 在高频极限下的理论结果与直接数值计算结果定性一致。最后, 我们基于 Bott 指数的计算, 研究了无序对外加圆偏振光作用下的 Lieb 晶格拓扑性质的影响。计算表明, 选取适当的模型参数, 弱无序并不会改变在外加圆偏振光作用下的拓扑非平庸相, 而在强无序条件下, 体系出现安德森局域化, 由拓扑绝缘体转变为拓扑平庸的普通绝缘体。在一定参数范围内, 圆偏振光振幅的增强会降低拓扑非平庸相的稳定性, 而次近邻格点间跃迁强度的增加有利于拓扑非平庸相的稳定性。

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