Valley-Controlled Anomalous Nernst Effect in an Optically Driven Biased Dice Lattice

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Abstract

We study the anomalous Nernst coefficient (ANC) in a biased dice lattice under the application of a circularly polarized off-resonant light within the Berry phase formalism. We employ the Floquet theory to study the effect of off-resonant light. The off-resonant light provides a Haldane-type mass term, which breaks the time reversal (TR) symmetry. The photoinduced mass term is valley dependent and can be tuned by changing the frequency of the off-resonant light. We find that the interplay between the bias term and the off-resonant light-induced mass term results in a tunable valley-dependent Berry curvature. The valley-controlled ANC is calculated as a function of the chemical potential for different values of the mass terms. We find that the total ANC, the sum of the contributions from the Dirac points K and K', no longer vanishes due to the breaking of TR symmetry. Our results demonstrate the control of the valley degree of freedom using the off-resonant light in a biased dice lattice, which can have a potential application in valley caloritronics.

Keywords: *Anomalous Nernst Effect, Berry Phase, Floquet Theory, Dirac Points.*

1. Introduction

Ever since the discovery of the Berry phase, a new paradigm in condensed matter physics has emerged [1]. The Berry phase has introduced a new approach to understand the behaviour of particles by taking into account the geometry of the wave function in the parameter space. The Berry phase describes a global phase acquired by a wave function when it undergoes adiabatic evolution in a parameter space. Based on the Berry phase effect numerous anomalous transport phenomena have been studied over the last decades. A non-zero Berry curvature of the energy bands has been considered a critical factor in explaining various transport phenomena like the anomalous Hall effect (AHE) and the anomalous Nernst effect (ANE) [2-9]. Here we are interested in ANE. In the conventional Nernst effect, a transverse voltage is generated when there is a longitudinal temperature gradient and an external magnetic field. However, the Nernst signal can be detected even without a magnetic field in the ANE. This is due to a nontrivial Berry curvature, which acts as an effective magnetic field in reciprocal space. As a result, charge carriers experience a transverse anomalous velocity, leading to the observation of the ANE. This connection between the Berry curvature and the anomalous Nernst effect emphasizes the intriguing interplay between topology and transport phenomena. The discovery of the substantial Nernst coefficient in a high-temperature cuprate superconductor [10] led to increased attention towards the Nernst effect. Since then, several studies [11-15] have been carried out to explore and understand the mechanism to produce a Nernst signal. Our system of interest is a biased dice lattice [16], where the bias term breaks the inversion symmetry and opens a gap in the energy spectrum. The breaking of inversion symmetry is essential to observe the valley contrasting physics. Since in the linear regime, the Berry phase-mediated ANE vanishes due to the presence of time-reversal symmetry [17]. Therefore, we consider our system driven by circularly polarized off-resonant light.

The effect of the off-resonant light is to provide a Haldane type mass term that breaks the TR symmetry. Similar to the two-dimensional crystals with hexagonal lattice structures like graphene [18], silicene [19], etc., the dice lattice also hosts a quasi-particle with a valley degree of freedom in addition to their charge and spin. The valley degree of freedom represents a spin-like quantity associated with two inequivalent Dirac points K and K', in the Brillouin zone. The lattice geometry of a dice lattice is shown in Fig. 1. It has a honeycomb lattice structure with an additional atom at the center of each hexagon. A dice lattice can be realized experimentally in a tri-layer structure of cubic lattices as well as optical lattices. [20,21]. Although the zero-field spectrum of dice and graphene lattices is the same, these two systems are fundamentally different as the former system hosts a zero-energy flat band. The low energy excitation of quasiparticles in dice lattice is described by the Dirac-Weyl Hamiltonian with pseudo-spin $\mathrm{S} = 1$, as compared to pseudo-spin S=1/2 in graphene. Additionally, a notable difference arises in the context of quasiparticle behaviour as they traverse a closed path around a high symmetry point in momentum space. In contrast to the Berry phase of π in graphene, quasiparticles in the dice lattice do not pick any nontrivial Berry phase. Therefore, it would be interesting to study the Berry phase mediated anomalous transport phenomena in a biased dice lattice.

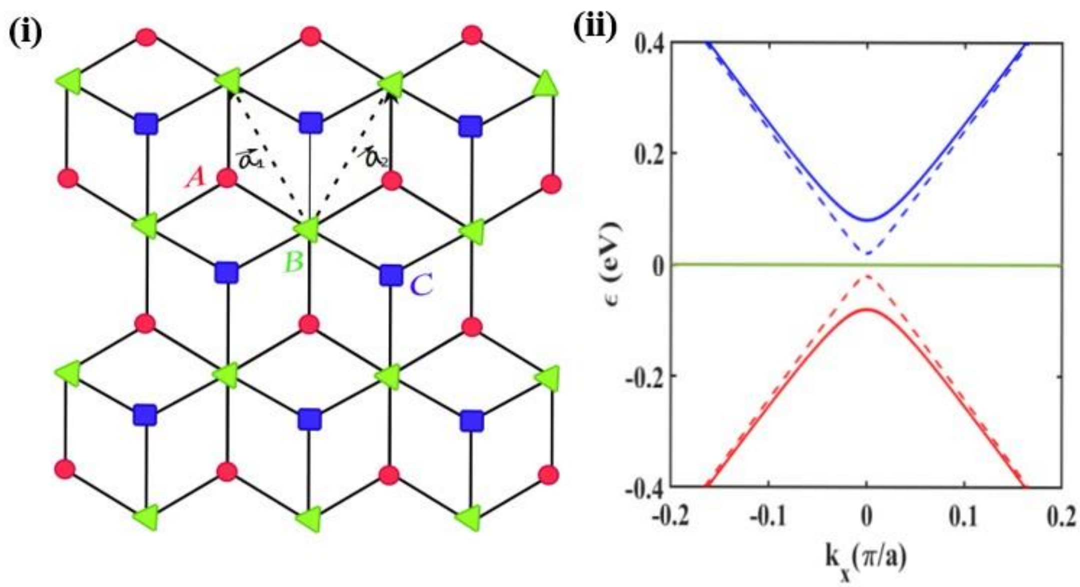

FIG 1. (i) The lattice geometry of Dice lattice, and (ii) Energy band structure of an optically driven biased Dice lattice at $\Delta = 50\ meV$ and $\Delta_\Omega = 30\ meV$. Blue, red, and green lines represent the conduction, valence and flat bands, respectively. Solid and dashed lines correspond to K and K'-valleys, respectively.

2. Results and Discussions:

The low-energy tight binding Hamiltonian of a symmetrically biased dice lattice can be written as [16]

$$H_0(\boldsymbol{k}) = \begin{pmatrix} \Delta & \frac{f_{\boldsymbol{k}}}{\sqrt{2}} & 0 \\ \frac{f_{\boldsymbol{k}}^*}{\sqrt{2}} & 0 & \frac{f_{\boldsymbol{k}}}{\sqrt{2}} \\ 0 & \frac{f_{\boldsymbol{k}}^*}{\sqrt{2}} & -\Delta \end{pmatrix}, \qquad (1)$$

where $f_k = \hbar v_F\,(\tau k_x - ik_y)$, $v_F = \frac{3a\gamma}{2\hbar}$ (γ is the hopping energy between the nearest neighbour lattice sites and a is the lattice constant) is the Fermi velocity, and $\tau = \pm 1$ is the valley index. The term Δ is the bias term that breaks the inversion symmetry and opens a gap in the energy spectrum. We consider the dice lattice irradiated with a normally incident circularly polarized off-resonant light. The vector potential of the off-resonant circularly polarized light can be written as $\boldsymbol{A}(t) = \frac{E_0}{\Omega}(\cos\Omega t\,, l\sin\Omega t)$, where E_0 is the amplitude of the electric field, Ω is the frequency of the radiation and $l = \pm 1$ represents the right (left) circularly polarized light. The effect of the off-resonant light can be introduced into the Hamiltonian (1) by Pierls substitution: $\boldsymbol{k} \to \boldsymbol{k} + \frac{e\boldsymbol{A}(t)}{\hbar}$. The free Hamiltonian (1) modifies to time-dependent Hamiltonian $H(\boldsymbol{k}, t)$, which is now time periodic with period $T = \frac{2\pi}{\Omega}$. The time periodicity of the Hamiltonian enables us to use the Floquet theory. Based on the Floquet theory, the effective time-independent Hamiltonian in the off-resonant regime ($\hbar\Omega \gg \gamma$) is given by [22]

$$H_{\text{eff}}(\mathbf{k}) = H_0(\boldsymbol{k}) + \frac{1}{\hbar\Omega}[H_{-1}(\boldsymbol{k}), H_{+1}(\boldsymbol{k})] + O\left(\frac{1}{\Omega^2}\right), \tag{2}$$

where $H_{\pm 1}(\boldsymbol{k}) = \frac{1}{T}\int_0^T e^{\mp i\Omega t} H(\boldsymbol{k}, t)dt$.

In our case, the effective time-independent Hamiltonian becomes

$$H_{\text{eff}}(\mathbf{k}) = \begin{pmatrix} \delta_\tau & \frac{f_{\boldsymbol{k}}}{\sqrt{2}} & 0 \\ \frac{f_{\boldsymbol{k}}^*}{\sqrt{2}} & 0 & \frac{f_{\boldsymbol{k}}}{\sqrt{2}} \\ 0 & \frac{f_{\boldsymbol{k}}^*}{\sqrt{2}} & -\delta_\tau \end{pmatrix}, \tag{3}$$

where $\delta_\tau = (\Delta + \frac{\Delta_\Omega}{2})$ with $\Delta_\Omega = \frac{l\tau e^2 E_0^2 v_F^2}{\hbar\Omega^3}$ is the mass term induced by the off-resonant light. It breaks the time-reversal symmetry and has opposite signs in the two valleys. The eigenvalues of the effective Hamiltonian (3) can be obtained as:

$$\varepsilon_0^\tau(k) = 0 \text{ and } \varepsilon_{\pm 1}^\tau(k) = \pm\sqrt{E_k^2 + {\delta_\tau}^2} \tag{4}$$

where $E_k = \hbar v_F\, k$ and $k = \sqrt{k_x^2 + k_y^2}$ is the absolute value of the wave vector.

The eigenvalues $\varepsilon_0(k)$ and $\varepsilon_{\pm 1}(k)$ represent the off-resonant quasienergies corresponding to flat, conduction, and valence bands, respectively. The energy spectrum of the biased dice lattice for K and K' valley is shown in figure 1(ii). Due to the valley dependent mass term Δ_Ω induced by the off-resonant light, the band gaps between the conduction and valence bands in the two valleys are different.

The corresponding eigenfunctions are calculated as

$$\psi_0(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} -\frac{f_{\boldsymbol{k}} C_0}{\Delta_\tau} \\ \sqrt{2}C_0 \\ \frac{f_{\boldsymbol{k}}^*\, C_0}{\Delta_\tau} \end{pmatrix}, \psi_{\pm 1}(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} \frac{f_{\boldsymbol{k}}\, C_{\pm 1}}{\varepsilon_{\pm 1} - \Delta_\tau} \\ \sqrt{2}C_{\pm 1} \\ \frac{f_{\boldsymbol{k}}^*\, C_{\pm 1}}{\varepsilon_{\pm 1} + \Delta_\tau} \end{pmatrix}, \tag{5}$$

where $C_0 = \frac{\delta_\tau}{\sqrt{E_k^2 + {\delta_\tau}^2}}$ and $C_{\pm 1} = \frac{E_k}{\sqrt{2}\varepsilon_{\pm 1}}$ are the normalization constants.

The Berry curvature can be determined by $\Omega_n(\boldsymbol{k}) = i\,\langle\nabla_{\boldsymbol{k}}\psi_n(\boldsymbol{k})| \times |\nabla_{\boldsymbol{k}}\psi_n(\boldsymbol{k})\rangle$, for 2D materials, where $\nabla_{\boldsymbol{k}}$ is the directional derivatives with respect to the momentum $\boldsymbol{k}$, and $\psi_n(\boldsymbol{k})$ is the periodic part of the Bloch function. Berry curvature can be viewed as a magnetic field in reciprocal space and turns the motion of an electron by providing an anomalous velocity in the presence of an in-plane electric field. Under space inversion (IS) and time reversal (TR) symmetry operations, the Berry curvature transforms as $IS\ \Omega_n(\boldsymbol{k})$

$=\Omega_n(-\boldsymbol{k})$ and $TR\,\Omega_n(\boldsymbol{k}) = -\Omega_n(-\boldsymbol{k})$. Therefore, for a non-zero Berry curvature, either one of the symmetries must be broken. In our system, both the symmetries are broken.

Using Eq. (5), we obtained the Berry curvature as

$$\Omega_{\pm}^{\tau}(\boldsymbol{k}) = \mp\tau \frac{\hbar^2 v_F^2\, \delta_\tau}{\left(E_k^2+{\delta_\tau}^2\right)^{3/2}} \text{ and } \Omega_0^{\tau}(\boldsymbol{k}) = 0. \quad (6)$$

Although the Berry curvature of conduction and valence bands are non-zero and valley dependent, the Berry curvature of the flat band vanishes. Due to the dependency of the Berry curvature on Δ_Ω, it is possible to tune the Berry curvature by changing the frequency and polarisation of circularly polarized off-resonant light. Figures 2(i) and 2(ii) depict the valley dependency of Berry curvatures.

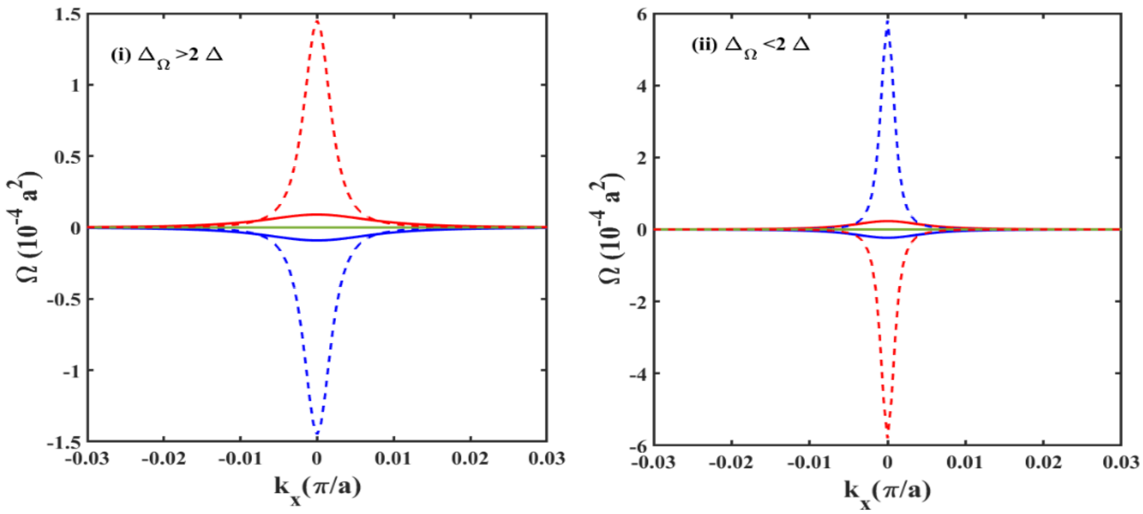

FIG 2. The distribution of Berry curvature around K and K′ valleys for (i) $\Delta_\Omega > 2\Delta$ and (ii) $\Delta_\Omega < 2\Delta$. Blue, red, and green lines represent the Berry curvatures of conduction, valence and flat bands, respectively. Solid and dashed lines correspond to K and K′ valleys. Here, we consider $\Delta = 30$ meV.

The distribution of Berry curvatures around both valleys is mainly centered around $\boldsymbol{k} = 0$. For $\Delta_\Omega > 2\Delta$, Berry curvature of the conduction band (valence band) is negative (positive) for both K and K′ valleys. However, as we tune Δ_Ω such that $\Delta_\Omega < 2\Delta$, the sign of the Berry curvature for the K valley becomes opposite to that of K′ valley.

The anomalous Nernst coefficient for a particular valley (τ) can be written as [13]

$$\alpha_{xy}^{\tau} = -\frac{k_B e}{h}\int \frac{d^2k}{(2\pi)} \sum_n \Omega_{\,n}^{\tau}(\boldsymbol{k})\, S_n^{\tau}(\boldsymbol{k}), \quad (7)$$

where n represents the band index, $S_n^{\tau}(\boldsymbol{k}) = [-f_n(\boldsymbol{k})\ln f_n(\boldsymbol{k}) - (1 - f_n(\boldsymbol{k}))\ln(1 - f_n(\boldsymbol{k}))]$ is the entropy density, and $f_n(\boldsymbol{k})$ is the Fermi-Dirac distribution function. Therefore, both Berry curvature and entropy generation around the Fermi surface can control the behaviour of α_{xy}^{τ}. The total ANC can be calculated by summing the contribution of both valleys.

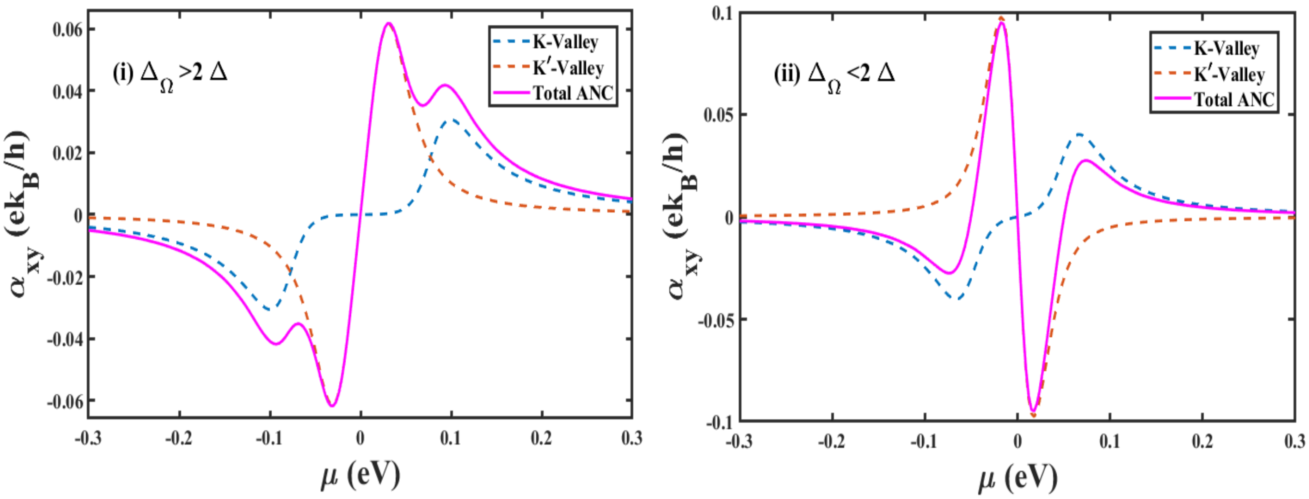

FIG 3. The Anomalous Nernst coefficient as a function of chemical potential (μ) for (i) $\Delta_\Omega > 2\Delta$ and (ii) $\Delta_\Omega < 2\Delta$. Dashed lines represent the ANC around K and K′ valleys, and the solid line corresponds to the total ANC, which is the sum of the contributions from both valleys. Here, we consider $\mathrm{T} = 100\mathrm{K}$, and $\Delta = 30$ meV.

The ANC is evaluated numerically using Eq. (7), and its variation with the chemical potential (μ) at $\mathrm{T} = 100$ K around each valley is shown in Fig. 3 (i) and (ii). Due to the breaking of TR symmetry, the total ANC is non-zero. As μ scans the energy bands, the ANC exhibits peaks/dips features. The occurrence of the peaks/dips features in the ANC can be attributed to both Berry curvature and entropy density. The Berry curvature is mainly centered in the band gap region around $\boldsymbol{k} = 0$ and decreases rapidly on either side. However, the entropy density sharply peaks at the Fermi surface and vanishes for completely filled and completely emptied bands. Therefore, the combined distribution of the Berry curvature and the entropy density in the momentum space leads to the peaks/dips features in the Nernst coefficient. It is worth noting that altering the values of Δ_Ω has a considerable impact on the ANC. Interestingly, as we change Δ_Ω from $\Delta_\Omega > 2\Delta$ to $\Delta_\Omega < 2\Delta$, the ANC for K′ valley changes its sign.

3. Conclusions:

In this work we have studied the Anomalous Nernst effect in an optically driven biased dice lattice. Tunability of the band gap is achieved by means of circularly polarised off-resonant light. We find that the interplay between the mass term induced by the off-resonant light and the bias term led to a tunable valley-dependent Berry curvature. The ANC is calculated for each valley and its behaviour is analysed by considering different positions of the chemical potential. The ANC is found to be strongly dependent on the value of Δ_Ω. It is observed that the ANC for K′ valley changes its sign for a particular value of Δ_Ω. Our findings demonstrate the optical manipulation of the valley degree of freedom in a biased dice lattice, which can have potential applications in valley caloritronics.

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