第48回トポロジカル物質科学セミナー
Topological Materials Science Seminar (48)

Interference of the Bloch phase in stacked periodic structures

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Abstract:

The wave property of particles and interference of their wave functions represent the significant features of quantum mechanics. We address an interference effect for the electronic wave function in periodic systems [1]. Regardless of the crystal structure, the form of the eigenstate wave function must obey the Bloch theorem, which states that the wave function is written as a product of the plane wave (Bloch phase) and periodic function compatible with the crystal structure [exp(ikr)*u(r)]. Focusing on the Bloch-phase part, a general theorem is proved: In any multilayered systems with stacking shifts, the interlayer hopping is exactly canceled for some crystal wave numbers k, which is due to the interference of the Bloch phase. The correspondence between the positions of such k-points and stacking shift is thereby formulated. We demonstrate that this theorem governs the electronic properties of layered materials such as MoS_2 by first-principles electronic structure calculations and experiments [1, 2]. Some corollaries and implications derived from the theorem are also discussed.

References

[1] RA, Y. Iida, K. Yamamoto, and K. Yoshizawa, Phys. Rev. B **95**, 245401 (2017).

[2] RA, M. Ochi, S. Bordács, R. Suzuki, Y. Tokura, Y. Iwasa, and R. Arita, Phys. Rev. Applied **4**, 014002 (2015).

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