Role of electron correlations in some Weyl systems

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Abstract. We are discussing a model to understand previously obtained results on Weyl semimetals as realized in MoTe$_2$ using DFT and DFT+U calculations. The model is motivated from general principles and we use it to investigate the effects of Coulomb correlations originating from the localized nature of the Mo-$d$ orbitals. We find that such correlations can eliminate or create pairs of Weyl points as the strength of the Coulomb interaction is varied. The effect of the spin-orbit coupling (SOC) is to split each Weyl point, which is assumed present in the absence of SOC, into pairs of spin-chiral partners.

1. Introduction

Among several fascinating properties of transition metal dichalcogenides (TMDs) is that some are Weyl semimetals. In particular the band structure of MoTe$_2$ has been predicted by density functional theory calculations to contain pairs of Weyl points (WPs) not too far away from the Fermi level. While subsequent angular resolved photoemission spectroscopic (ARPES) studies seem to confirm that prediction, maps of the Fermi surface by detailed quantum oscillation experiments (QOE) seem to contradict such a scenario. Subsequent detailed calculations, within the GGA+U approximation, indicate that the effect of Coulomb electron corrections is significant in order to explain both the light-polarization dependence of ARPES and the angular dependence of the frequencies observed by the QOE. In addition, these calculations suggest that while the Weyl points nearest to the Fermi energy survive the inclusion of these correlations, interesting Lifshitz transitions occur which change the topology of the Fermi surface.

In the present paper, we present a rather simple analytical model based on the nature of the Weyl points in MoTe$_2$, to help understand the role of electron correlations in this material and the results obtained in Ref. [12].

First we begin by deriving the model based on the results of the GGA+U calculation presented in Fig. 1. The size of the dots in Fig. 1 gives the relative contribution of the $p$ and $d$ orbitals to the bands, while other orbitals have very small contribution. Notice that the two bands forming the Weyl-point far away from the Fermi-point are mostly of one of the two characters and near the Weyl-point there is hybridization. Therefore, it makes sense to construct a model containing just a pair of orbitals $A$ and $B$ representing the orbitals $d$ and $p$ respectively. The most general
Figure 1. Band structure of $\gamma$-MoTe$_2$ showing the projection onto (a) Mo-$d$ orbitals and (b) Te-$p$ orbitals. The size of the dots is proportional to the percentage of the corresponding orbitals.

The form of the tight-binding Hamiltonian in $k$-space is

$$\mathcal{H}(k) = \begin{bmatrix} \epsilon_A(k) & f_1(k) + i f_2(k) \\ f_1(k) - i f_2(k) & \epsilon_B(k) \end{bmatrix},$$

which can also be re-written as

$$\mathcal{H}(k) = \epsilon(k) \hat{I} + \vec{h}(k) \cdot \vec{\tau},$$
$$\epsilon(k) = (\epsilon_A(k) + \epsilon_B(k))/2,$$
$$\vec{h}(k) = (h_1(k), h_2(k), h_3(k)),$$
$$h_1(k) = (\epsilon_A(k) - \epsilon_B(k))/2, \quad h_2(k) = f_1(k), \quad h_3(k) = f_2(k),$$

where $\vec{\tau} = (\tau_x, \tau_y, \tau_z)$ and $\tau_{x,y,z}$ are the Pauli matrices. A Weyl point can exist when there is a $k_0$ which is the solution to the system of equations:

$$h_1(k_0) = 0, \quad h_2(k_0) = 0, \quad h_3(k_0) = 0.$$  

Each one of the equations above defines a “surface” in a $d$-dimensional $k$-space and, in principle, in $d \geq 3$ where there are $d$ unknowns, i.e., the $d$-components of $k_0$, there could be solutions independently of the nature of the symmetries of the Hamiltonian.

Let us ignore the SOC and add the on-site Coulomb Hubbard $U$ term on the $A$ orbital only:

$$\hat{H} = \sum_{\vec{k},\alpha,\beta,\sigma} \mathcal{H}_{\alpha\beta}(\vec{k}) C_{\beta\sigma}^\dagger(\vec{k}) C_{\alpha\sigma}(\vec{k}) + U \sum_{\vec{R}} n_{\downarrow}^{(A)}(\vec{R}) n_{\uparrow}^{(A)}(\vec{R})$$

where $n_{\sigma}^{(A)}(\vec{R}) = C_{A\sigma}^\dagger(\vec{R}) C_{A\sigma}(\vec{R})$. In mean field factorization, we write

$$n_{\downarrow}^{(A)}(\vec{R}) n_{\uparrow}^{(A)}(\vec{R}) \rightarrow \langle n_{\downarrow}^{(A)}(\vec{R}) \rangle \langle n_{\uparrow}^{(A)}(\vec{R}) \rangle + \langle n_{\downarrow}^{(A)}(\vec{R}) \rangle \langle n_{\downarrow}^{(A)}(\vec{R}) \rangle - \langle n_{\downarrow}^{(A)}(\vec{R}) \rangle \langle n_{\uparrow}^{(A)}(\vec{R}) \rangle \langle n_{\downarrow}^{(A)}(\vec{R}) \rangle$$

and if the system is not magnetically ordered we take $\langle \hat{n}^{(A)}_\uparrow (\vec{R}) \rangle = \langle \hat{n}^{(A)}_\downarrow (\vec{R}) \rangle = n_A$. In this case the Hamiltonian simply becomes

$$\hat{H} = \sum_{k,\alpha\beta\sigma} \mathcal{H}'_{\alpha\beta}(\vec{k}) C^\dagger_{\beta\sigma}(\vec{k}) C_{\alpha\sigma}(\vec{k}) + E_0$$

(6)

where $E_0$ is a constant and

$$\mathcal{H}'(\vec{k}) = \begin{bmatrix} e_A(k) + n_A U & f_1(k) + if_2(k) \\ f_1(k) - if_2(k) & e_B(k) \end{bmatrix}$$

(7)

for both up and down spins. However, Eqn. 7 is similar to Eq. 3 with the only difference is that $h_1(k)$ is replaced by:

$$h_1(k) = \frac{e_A(k) + n_A U - e_B(k)}{2}.$$  

(8)

Let us discuss the role of $U$, assuming that there were WP solutions before the introduction of the Hubbard term. Since, we have assumed that there is a WP solution before we introduce an non-zero $U$, it implies that the two surfaces in $k$-space defined by the equations $h_2(k) = 0$ and $h_3(k) = 0$ remain the same as in the case where $U=0$. Therefore, these two equations should define an intersection, which is a line $l$, which is unaffected by the addition of the Hubbard term, within mean-field treatment. For a small value of $U$ the modified equation $h_1(k) = 0$ defines a somewhat different surface which for a sufficiently small value of $U$ should continue to intersect the line $l$ at least in two points, the WPs. To highlight this point, that the WPs continue to exist for small value of $U$, although they change their relative positions, we illustrate the positions of the source and of the sink of the WPs for zero and non-zero $U$ value in Fig. 2.

Figure 2. Vector plot of the Berry curvature on $k_z = 0$ plane showing the source and sink of the WPs for $U = 0$ and $U = 0.75$ eV respectively as obtained from DFT calculations. The relative size of the length of the vector is proportional to the magnitude of the Berry curvature. Notice the shift of the WPs in (b) as compared to (a).

We can linearize the equations $h_1(k) = 0$, $h_2(k) = 0$, and $h_3(k) = 0$, around each of the band touching points $k_0$ where all three components of $\mathbf{h}(k_0)$ vanish as mentioned in Eqn. 3. A Taylor expansion around $k = k_0$ gives:

$$h_i(k) = h_i(k_0) + \sum_j v_{ij}(k_0)(k - k_0)_j + O((k - k_0)^2)$$

(9)
where, $v_{ij} = \frac{\partial h_i}{\partial k_j}$ is the Fermi velocity tensor. Hence, the Hamiltonian near the band touching point takes the form of:

$$H(k) = \begin{bmatrix} \tilde{h}_3(k) & \tilde{h}_1(k) + i\tilde{h}_2(k) \\ \tilde{h}_1(k) - i\tilde{h}_2(k) & \tilde{h}_3(k) \end{bmatrix}$$

(10)

where, $\tilde{h}_i(k) = v_{ix}k_x + v_{iy}k_y + v_{iz}k_z$ and $k_i = (k - k_0)_i$. Equivalently, Eqn. [10] can be written as:

$$H(k) = \sum_{ij} \tau_i v_{ij} k_j.$$  

(11)

A unitary transformation that diagonalizes the velocity tensor $v$ transforms Eqn. [10] into the familiar Weyl equation of the form $\vec{\tau}. \vec{k}$.

Therefore, we have shown that the most general form of the $2 \times 2$ Hamiltonian reduces to the Weyl Hamiltonian in the vicinity of the band touching point, even with the addition of the Hubbard term $U$ for some range of $U$.

The role of spin-orbit coupling was studied in Ref. [12] and it was found that it doubles the number of Weyl pairs and from a single pseudo-spin chiral pair it produces two real spin-chiral pairs of Weyl points.

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