Antiferromagnetism and spin density waves in Dirac metals

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In this paper we perform mean-field study of possible magnetic instabilities in Dirac metals. We find that Dirac electrons naturally host antiferromagnetic or SDW ground states, though their specific configurations may vary depending on specific model, as well as chemical potential and temperature. We also discuss paramagnetic susceptibility in Dirac metals. In certain cases, the magnetic properties may be \( \mu \) and \( T \) independent.

I. INTRODUCTION

Weyl and Dirac metals (see [1] for review) have attracted significant attention during the last years. Both of them are prominent for their band structure having effectively gapless excitations described by Weyl/Dirac equation. In the former case, their spectrum contains two non-degenerate bands, and in the latter case their two bands are doubly degenerate. Because of that, Weyl metals are realized, when either time-reversal or inversion symmetry is broken, whereas Dirac metals are realized in the presence of both of them.

It is known, that Weyl points in WMs [2–5] can be viewed as monopoles of Berry curvature, which makes them topologically stable. Weyl points cannot be gapped under any local perturbations. The only way to destroy them is via annihilation, which can happen after moving two WP of opposite charges together. In contrast, in Dirac metals, the Dirac points are not protected topologically. In type I Dirac metals [6–11] (two experimentally discovered examples are Na\(_3\)Bi and Cd\(_3\)As\(_2\)), there are two Dirac points located opposite to each other on the \( z \) axis, which are protected by crystal rotational symmetry relative to \( z \) axis. In type II Dirac metal ZrTe\(_5\) [12, 13] there is a single Dirac point at the center of the Brillouin zone, which is not protected at all: in fact the Dirac point is gapped, but the gap can be neglected because, accidentally, it is very small.

Dirac metals necessarily possess time-reveral and inversion symmetries, which ensure double degeneracy of their bands. By breaking one of these symmetries, the degeneracy can be lifted, and thus the Dirac point can be split into a pair of Weyl points. It can also lead to more complicated combinations of Weyl points and rings [3, 14]. The most natural way to achieve it, is to add intrinsic Zeeman field into the system. The behavior of Dirac metals under extrinsic magnetic fields applied in specific directions has been extensively studied, and for instance, it was found that, in the simplest model of ZrTe\(_5\), the Dirac point can split into two Weyl points, if the Zeeman field is applied in \( z \) direction, or into a nodal ring if the Zeeman field is applied in \( xy \) plane [15].

However, it is not yet fully understood whether magnetization in Dirac metals may happen spontaneously. Recently, magnetic properties of Dirac electrons interacting with magnetic impurities have been studied [16–19]. Magnetic impurities are known to obey RKKY interaction, which has complicated oscillating and anisotropic structure, and thus does not make it possible to find the resulting magnetic ground state. In the works [20, 21], magnetic susceptibility of Dirac metals at small external magnetic fields was studied, and a few remarkable properties were found. In particular, it was found that the susceptibility in Dirac metals is determined not only by the Fermi surface, but by the whole Brillouin zone, and it may be independent on the Fermi energy, but dependent on the boundary properties of the Brillouin zone.

Magnetic instabilities have also been studied in various systems, similar to Dirac metals, such as 3D fermi gas with Weyl-like spin orbit coupling [22] and Dirac electrons on a surface of topological insulator [23–25] and particularly Weyl metals [26–34]. It was found, that in these systems, various phases can emerge, including spin-density waves [22, 24, 29].

On the other hand, in the recent years a large number of antiferromagnetic Dirac metals has been discovered experimentally, which include CuMnAs [35–38], and also CaMnB\(_2\), SrMnB\(_2\) [39, 40], and NdSb [41–44]. These materials are currently widely explored in the context of possible spintronics applications [38, 45–47] (see [48] for review). However, their electronic structure is rather complicated and incudes both localized and conduction electrons. Their phase diagrams are also non-trivial.

Motivated by this knowledge, we study a simple problem of spontaneous magnetization in Dirac metals (which can arise either due to magnetic impurities or due to interactions) using mean field approximation [49, 50]. Similar approach was previously used to find preferred magnetic states in semiconductors with quadratic band touching [51, 52]. We find that Dirac metals may host antiferromagnetic or spin density wave ground states, depending on their Fermi level. We observe transitions between different magnetic ground states as functions of Fermi energy and temperature.

Specifically, we consider two most commonly used models of Dirac metals: a Hamiltonian describing type II Dirac metal ZrTe\(_5\) with one Dirac point at the BZ center, and a Hamiltonian describing type I Dirac metal Na\(_3\)Bi...
with two Dirac points separated in momentum space. We compute their effective actions up to quadratic order in external momentum, and thus demonstrate that the magnetic instabilities are spatially modulated. After it, we place these models on a lattice, and compute their susceptibilities numerically. In this way, we are able to see that at small chemical potentials, their magnetic ground states are antiferromagnetic, but as the chemical potential increases, the ground state becomes SDW. Also we compute the effective action at finite temperature and obtain that, typically, the paramagnetic susceptibility decreases \( \propto T^2 \). However, in certain cases, particularly when Dirac electrons do not have orbital momentum, the susceptibility may be \( \mu \) and \( T \)-independent. Finally, we compute the effective action numerically at finite temperatures and see that the wavevector of SDW changes as a function of temperature. This leads us to conclusion that there may exist transition between AFM and SDW ground states as a function of temperature.

This paper is organized as follows: in Sec. II, we compute analytically the effective action at zero temperature. In Sec. II A we focus on the case of Dirac metal with one Dirac point (i.e. type II) and in Sec. II B, we consider Dirac metal with two Dirac points (i.e. type I). In Sec. III we compute paramagnetic susceptibility at finite temperatures for both type II and I Dirac metals. We summarize our findings and their possible implications in Sec. IV. Finally we present our numerical results in Sec. A.

II. SPONTANEOUS MAGNETIZATION AT ZERO TEMPERATURE

In this section we study spontaneous magnetization in two simple models of type II and I Dirac metals. Specifically, we introduce the magnetization field, compute its effective action up to the second order over the field and its momentum, and use it to find possible magnetic instabilities. We start from the simplest model of type II Dirac metal containing a single Dirac point and use it to illustrate our method. After it, we repeat the calculations in the case of slightly more complicated model of type I Dirac metal, which contains a pair of Dirac points separated in momentum space.

A. Type II Dirac metal

Here we analyze the model of type II Dirac metal, which has a single Dirac point at the center of the Brillouin zone. We note that an experimental example of such Dirac metal is ZrTe\(_5\). Its band structure is invariant under time-reversal, inversion, and also under three mirror symmetries. The Hamiltonian [12] can be written as:

\[
H_0 = \sum_k d_i(k) \Gamma_i, \quad i = 1, 2, 3, 4, 5
\]

where \( \Gamma_i \) are five gamma-matrices defined as:

\[
\Gamma_1 = -\tau_z \sigma_z, \quad \Gamma_2 = \tau_y, \quad \Gamma_3 = \tau_z \sigma_x, \\
\Gamma_4 = -\tau_z \sigma_y, \quad \Gamma_5 = -\tau_x.
\]

The coefficients \( d_\mu \), have, in general, complicated form determined by the whole structure of the Brillouin zone, but near the Dirac point, they can be approximated as linear functions of momentum:

\[
d_1 = 0, \quad d_2 = v_z k_z, \quad d_3 = v_y k_y, \\
\quad d_4 = v_x k_x, \quad d_5 = m \approx 0. \quad (2)
\]

Here \( v_{x,y,z} \) are Fermi velocities in all possible directions, which, in general, may be different, since the crystal structure is anisotropic, and \( m \) is a gap in the Dirac point, which, strictly speaking exists, but can be neglected, because it is very small.

We are interested in computing mean-field effective action for the magnetization of Dirac electrons. Since, in the experimentally discovered example of type II Dirac metal ZrTe\(_5\), electrons have spin 1/2, we can define the magnetization simply as:

\[
M = \hat{b} \sigma.
\]

Furthermore, since the linear term \( \text{tr}(GM) \) is zero, the leading contribution to the effective action is written as:

\[
S = \frac{1}{\beta} \sum_{w, k, q} \text{tr} G(k)(-q) G(k + q) M(q).
\]

Here, \( k \) is an internal momentum, and \( q \) is the external momentum, corresponding to the spatial modulation of the magnetization. We note that, in this section, we are primarily interested in a possible spontaneous magnetization, but, strictly speaking, the same Eq. (3) describes momentum dependent spin susceptibility \( \chi_{ij}(q) = -\partial^2 S_{\sigma} / \partial w \partial q \).

After performing Matsubara summation, and taking the limit of zero external Matsubara frequency, the Eq. (3) evaluates as:

\[
S = \sum_k \left\{ \frac{\text{tr} M^2}{2(d_k^2 - d_p^2)} \left[ d_k n_F(d_k - \mu) - d_k n_F(-d_k - \mu) \right. \\
- d_p n_F(d_p - \mu) + d_p n_F(-d_p - \mu) \bigg] \\
+ \frac{\text{tr}(d_k \Gamma) M (d_p \Gamma) M}{2(d_k^2 - d_p^2)} \right\} \\
\left[ d_k \left\{ n_F(d_k - \mu) - n_F(-d_k - \mu) \right\} \\
- \frac{n_F(d_p - \mu)}{d_p} + n_F(-d_p - \mu) \frac{d_k}{d_p} \right], \quad (4)
\]

where for shortness we have introduced \( p = k + q \), and \( d_{k,p} = d(k,p) \). One can see, that in the limit of zero external momentum, i.e. at \( q \to 0 \), this expression contains two contributions: one from the bulk of the Brillouin zone, proportional to \( n_F(\pm d - \mu) \) (interband), and the
other from the Fermi surface, which is proportional to \( \frac{\partial n_{\mu}(\mathbf{q}, \mathbf{d} - \mu)}{\partial \mu} \) (intraband). We note that the fact, that magnetization contains the contribution from outside of the Fermi surface is a special property of Dirac metals. We explain this peculiarity by the fact that, in Dirac metal, different bands approach very closely each other near the Dirac points, which is in contrast to conventional metals, where a band containing the Fermi surface is assumed to be well-separated from the others.

We proceed further by expanding the Eq. (4) in the powers of the external momentum \( q \), and integrating it over the internal momentum \( k \). In the zeroth order, i.e. at zero external momentum, we obtain, that the effective action acquires two contributions resulting from the bulk of the band and from the Fermi surface respectively:

\[
S^{(0)} = \frac{1}{2\pi^2 v_x v_y v_z} \int dk \left\{ \frac{2kb^2}{3} - \frac{4kb^2}{3} \right\} \theta(k - \mu),
\]

\[
+ \frac{1}{2\pi^2} \left\{ -\frac{4\mu^2 b^2}{3} - \frac{2\mu^2 b^2}{3} \right\}
\]

(5)

Interestingly, we find, that the 'bulk' contribution to the effective action is divergent at large \( k \). However, this divergence is resolved very easily: we were assuming that the dispersion is linear everywhere and unlimited, whereas in a real material, the range of momenta is limited by the size of the Brillouin zone, and furthermore, the dispersion becomes non-linear far away from the Dirac point. Thus, we can view the integral entering the Eq. (6) as large, but finite, and limited by nonlinearities in \( d \) and the size of the Brillouin zone. We can also track evolution of the effective action \( S^{(0)} \) with change of chemical potential \( \mu \). When the Fermi level is aligned with the Dirac points, i.e. at \( \mu = 0 \), the magnetic susceptibility is solely determined by the bulk of the Brillouin zone. In this special case, the \( z \) component of the magnetic field enters with the coefficient of larger magnitude, than \( b \), and thus we can infer that magnetic susceptibility in \( z \) direction is larger than in the perpendicular direction.

However, the contribution to \( S^{(0)} \) from the Fermi surface 'competes' against the contribution from the bulk. Indeed, the Fermi surface gives larger contribution to the perpendicular component of the susceptibility, than to its \( zz \) component. Thus, at sufficiently large Fermi energies, it is possible that the contribution from the Fermi surface is larger than from the bulk of the Brillouin zone, and as a result, the susceptibility in the perpendicular direction is larger than along \( z \) axis, oppositely to the case of small Fermi energy.

It is of interest to compute the change of effective action over the chemical potential explicitly. In the approximation of linear dispersion, it has the following expression:

\[
\Delta S^{(0)} = \frac{\mu^2 b^2}{2\pi^2 v_x v_y v_z}.
\]

This equation tells us, that the variation of the effective action due to finite chemical potential depends only on perpendicular component of the magnetic field. In other words, in the range of parameters, where the dispersion can be viewed as linear, the susceptibility in \( z \) direction does not depend on the chemical potential. We remark, that independence of observables on chemical potential is a common property of topological metals. The fact that susceptibility in Dirac metals does not depend on chemical potential, and even on the presence of superconductivity [53, 54].

In order to study possible spatial modulation of the magnetic ground state, we expand the effective action (4) up to quadratic order over external momentum. We obtain the following expression:

\[
S^{(2)} = \frac{1}{2\pi^2 v_x v_y v_z} \int \frac{dk}{k} \left\{ \frac{q_x b_x + q_y b_y}{6} + \frac{q_x b_y - q_y b_x}{6} \right\} \theta(k - \mu)
\]

\[
+ \frac{1}{2\pi^2 v_x v_y v_z} \left\{ \frac{q_x^2 b_x^2}{180} + \frac{43q_y^2 b_y^2}{180} - \frac{19q_z^2 b_z^2}{90} + \frac{q_z^2 b_z^2}{30}
\]

\[
- \frac{11(q_x b_x + q_y b_y)^2}{90} + \frac{11(q_x b_y - q_y b_x)^2}{90} \right\}.
\]

(6)

Similarly to the Eq. (5), this equation has two contributions from the bulk of the Brillouin zone, and from the Fermi surface respectively. They contain terms entering with the opposite signs, which implies that the bulk and the Fermi surface 'compete' against each other, and as a result, there exists possibility of crossovers between different phases at different Fermi energies. Specifically, at small Fermi energies, the 'bulk' contribution dominates, since the momentum integral in the Eq. (6) is determined by the UV cutoff of the Brillouin zone. However, this contribution decreases with increasing \( \mu \), whereas the Fermi surface contribution does not depend on the Fermi level \( \mu \), and thus, at sufficiently large \( \mu \), can become dominant.

Now, let us discuss the form of possible magnetic configurations. First, we consider the magnetic instability in \( z \) direction. At small Fermi energies, the magnetic field component \( b_z \) enters the effective action with positive coefficient in front of the momentum, which implies that the magnetization in \( z \) direction is spatially independent. We note, however, that this is due to the fact that the bulk contribution does not have a term \( q_z b_z^2 \), which in turn happens due to linear dispersion. In principle, non-linear corrections to \( d(k) \) can lead to non-trivial 'bulk' term \( q_z b_z^2 \), which in turn may change the ground state into SDW modulated in \( z \) direction, as we will see in numerical calculations. In addition, at sufficiently large
Fermi energy, the term $q^3 b_z^2 \sigma$ may acquire negative coefficient, which means that magnetic field $b_z$ will be spatially modulated in the perpendicular direction.

In a similar way, if we look at the instability in perpendicular direction $b_{\perp}$, the Eq. (6) tells us that, at small Fermi energy, it will be spatially modulated in the transverse direction, since the effective action has negative momentum components in $z$ direction and in the $xy$ plane perpendicular to the magnetization. If the Fermi level is increased, its momentum may change: $q_z$ component may disappear, and, furthermore, it may change from transverse to longitudinal, i.e. the momentum vector may become aligned with the magnetization direction.

Thus, we have found that the magnetic state of the type II Dirac metal is spatially modulated, and its preferred configuration is determined by the competition between the 'bulk' (i.e. interband) and the Fermi surface (i.e. intraband) contributions to the effective action. As a result, the magnetic ground state may change as the Fermi level changes. Finding wavelength of the magnetic instabilities will require computing the effective action up to higher orders in the momentum $q$, but, in the case of strictly linear dispersion, we can guess its behavior from dimensional considerations. Indeed, we expect quartic over $q$ terms in the effective action to behave as $q^4 b_z^2 / \mu^2$, which in turn implies that the wavelength of the ground state scales inversely proportionally to $\mu$. In Sec. A we study possible magnetic ground states numerically and show, that Dirac metal can undergo phase transition between antiferromagnetic and SDW phases with increasing $\mu$.

B. Type I Dirac metal

Type I Dirac metal has two experimentally discovered examples: Na$_3$Bi and Cd$_3$As$_2$. It possesses a pair of Dirac points separated in momentum space in $z$ direction and protected by discrete rotational symmetry. We write the simplest Hamiltonian describing such a system as:

$$H_0 = d_i \Gamma_i,$$

and, to be consistent with the previous literature\cite{14}, we define the $\Gamma$-matrices as:

$$\Gamma_1 = \tau_z \sigma_x, \quad \Gamma_2 = \tau_z \sigma_y, \quad \Gamma_3 = \tau_z \sigma_z, \quad \Gamma_4 = \tau_x, \quad \Gamma_5 = \tau_y.$$ 

We take the simplest possible form of the coefficients $d_i$:

$$d_1 = v_F k_x, \quad d_2 = v_F k_y, \quad d_3 = m(k_z), \quad d_4 = d_5 = 0$$

Here $m(k)$ is chosen to capture the fact that it changes sign at two symmetric points separated in $z$ direction, which are indeed the Dirac points. We assume that $m$ is positive between the Dirac points (e.g. at $k = 0$) and negative away from them.

In type I Dirac metal, the Dirac points are protected by discrete rotational symmetry \cite{55} along the $z$ axis. Namely, states in the valence and conduction bands have different rotation eigenvalues, which makes it impossible to write a rotationally-invariant term, that would gap them out. This, in turn, results from the fact that, in type I Dirac metals, the valence and conduction band belong to different multiplets: the valence band is a singlet with total spin $J = 1/2$, whereas the conduction band is part of the triplet with total spin $J = 3/2$ (see e.g. \cite{7} \cite{14} for more details). The other bands from the triplet are separated by the energy gap, so we neglect them. Thus we write the magnetization operator as a sum:

$$M = M_s + M_p,$$

where $M_{s,p}$ are the singlet and triplet contributions, which have the following form:

$$M_s = \frac{g_s}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & b_z & b_z & 0 \\ 0 & b_z & b_z & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

and

$$M_p = \frac{3g_p}{2} \begin{pmatrix} b_z & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -b_z \end{pmatrix}.$$

We note that we include in the triplet contribution only $z$ component of the magnetic field. This is because interaction with $b_{x,y}$ can occur only through mixing of the different bands within the triplet, which are separated by an energy gap, but we are interested in scales smaller than the width of each band. We also note, that since, the conduction and valence band belong to different multiplets, they have, generally, different gyromagnetic factors, which we denote by $g_{s,p}$ respectively.

We can compute the trace of two Green functions in the same way, as in Sec. A, and obtain that, at zero external momentum $q$, the effective action can be also represented as a sum of contributions independent and proportional to the Fermi level respectively:

$$S^{(0)} = \left( \frac{3g_p}{2} \right) \frac{\mu^2}{8\pi^2 v_F v_z} \left\{ \left( 3g_p + g_s \right) b_z^2 + g_s^2 b_{\perp}^2 \right\}$$

We note, that we have obtained the last row of this equation in the limit of small Fermi level, i.e. when we can view dispersion within each Dirac cone as linear in all directions.

If we assume that the magnetic factors $g_{s,p}$ are close to each other: $g_s \approx g_p$, we can conclude that the coefficient
in front of $b_z^2$ has larger magnitude than the contribution to $b_z^2$, and thus magnetic susceptibility will be larger in the $z$ direction. Also, we can notice that, as the chemical potential increases, susceptibility always gets enhanced. This result is different from type II Dirac metal, whose susceptibility in one of directions does not depend on the magnetic Hamiltonian (7), which confirm our analytical results obtained from lattice regularization of the Brillouin zone and the Fermi surface, and therefore can change with Fermi level. In the Sec. A we consider the same problem numerically on a lattice and obtain that in most cases, the ground state is antiferromagnetic, though it can also undergo transitions to SDW.

III. MAGNETIC SUSCEPTIBILITY AT FINITE TEMPERATURES

In the previous section, we studied possible magnetic instabilities in Dirac metals at zero temperature and found that spontaneous magnetization occurs at finite wavevector, thus forming AFM or SDW phase. Now we would like to get an idea of its possible change, as the temperature becomes finite. Since the effective action cannot be computed analytically, when both temperature and wavevector are finite, we limit our analysis to the case of zero wavevector.

We start from the Eq. (1). Since we are only interested in the change of the effective action due to small temperature $T \ll \mu$, we leave only the terms, which contain $n_F(d - \mu)$ or its derivative. After taking the limit $q \to 0$, we obtain:

$$\Delta S^{(0)}_2 = \frac{\pi^2 q^2}{v_F^2 v_z} \left[ \frac{3g_y^2 b_z^2}{2} + \frac{g_z^2 b_z^2}{3} - \frac{59g_y g_z b_z^2}{10} \right] + \frac{\pi^2 q^2}{2v_F^2 v_z} \left[ (3g_y - g_z)^2 b_z^2 + g_z^2 b_z^2 \right].$$

We can see, that similarly to type II Dirac metal, $S^{(2)}$ contains momentum integral, which diverges in the limit of zero $\mu$, and thus becomes the dominant if $\mu$ is small. However, as $\mu$ grows, its contribution decreases. Thus, we can infer, that the $z$ component of the magnetic field is spatially modulated in both $z$ and perpendicular direction, but it can undergo crossovers, as $\mu$ is increased. Similarly, the perpendicular magnetization $b_\perp$, if present, is spatially modulated in $z$ direction, and again, with increasing $\mu$, it can undergo crossover. In the Sec. A we present numerical results obtained from lattice regularization of the Hamiltonian (7), which confirm our analytical calculation and also demonstrate that at small $\mu$ the spatially modulated magnetic state is antiferromagnetic, but as $\mu$ increases, it may undergo transition to a SDW state and even to ferromagnetic.

Overall, we have found that Dirac metals naturally host spatially modulated magnetic ground states, though their specific configuration may depend on details of the model. Furthermore, we have found that the ground state is determined by the competition between the bulk of the Brillouin zone and the Fermi surface, and therefore
metal in $z$ direction is temperature independent. This is the consequence of the fact that, in Dirac metal, bands are very close to each other, which makes intraband contribution to the susceptibility (Van-Fleck paramagnetism) comparable to the interband (Pauli paramagnetism). Moreover, we were assuming here that the dispersion is linear, which is just an approximation in real materials. However, since we obtained that the susceptibility is temperature-independent, it seems that by slight perturbing, it is possible to make it either decreasing or increasing with temperature.

In type I Dirac metal, the answer for the effective action has the form:

$$\Delta S_2^{(0)} = -\frac{1}{8\pi^2 v_x^2 v_z} \left\{ (3g_p + g_s) b_z^2 + g_s^2 b_\perp^2 \right\} \left( E_F^2 - \frac{\pi^2 T^2}{3} \right).$$

As we can see, the susceptibility is temperature dependent in all directions. However, we note that it becomes temperature independent in $z$ direction in the special case $g_s = -3g_p$, which could, in principle, happen if the band pseudospin were the same as physical spin.

To summarize our results, we have studied magnetic susceptibility of Dirac metals as a function of temperature and found that, in certain cases (namely, when pseudospin coincides with physical spin), it may be temperature independent. In this section, we did not study the behavior of the AFM or SDW instabilities at finite temperature, but we consider it numerically in Sec. A.2. We obtain that the ground state evolves, and, in principle, it may undergo a transition, e.g. from SDW to AFM phase.

**IV. DISCUSSION**

In this paper, we have explored the possibility of spontaneous magnetization in Dirac metals, and found that they naturally host antiferromagnetic or spin density wave ground state. We have also found that its specific structure may vary depending on a particular type of Dirac metal, as well as its Fermi energy, temperature, non-linear corrections to the Dirac spectrum. However, in a few special cases, magnetic properties of Dirac metals, including magnetic susceptibility, are Fermi energy and temperature independent.

The main reason, which makes Dirac metals different from other solids lies in the fact that, in contrast to conventional Fermi-liquid, magnetization in Dirac metal is created not only by electrons on the Fermi surface, but also by electrons from the whole Brillouin zone. In the limit of small chemical potential, i.e. when the Fermi level is close to the Dirac points, the Fermi surface gets reduced to a point(s), and thus the magnetization is created mainly by the bulk of the Brillouin zone. On the other hand, at finite Fermi level, the magnetization arises from competition between the 'bulk' and the Fermi surface contribution, which results in a possibility of phase transitions with varying Fermi energies.

We expect, that our findings may have a lot of implications. In fact, the problem of spatially inhomogeneous magnetization in Weyl/Dirac metals has also been extensively studied [57, 58], and it was found that it may lead to unusual properties. For example, in the presence of periodic magnetization, there appear novel electronic states, so-called pseudo-Landau levels, which have dispersion forming an 'open nodal line’. We suggest that such effects may arise due to spontaneous SDWs in Dirac metals, which we study in this work.

We note that type II Dirac cone has been experimentally observed in a material ZrTe$_2$ [13]. In fact, this material has been studied for a long period of time [59]. First, it was discovered as a material, which exhibits anomalous resistivity peak at $T = 150K$ [59], but soon after, it was claimed that such an anomaly is not attributed to SDW or CDW [60]. We suggest that such a conclusion may be reconsidered, for example, because in the work [62] it was implicitly assumed that SDW and CDW leads to suppression on carrier densities at Fermi level, but it may not be the case. As we mentioned, we expect that SDW will result in the formation of pseudolandau levels, which are gapless.

We mention that, in the recent years, antiferromagnetism was found to be common in Dirac and Weyl metals. A large number of materials, where antiferromagnetism coexists with Dirac electrons, was discovered. These materials include, for example antiferromagnetic NdSb [33, 34], where localized spins form ferromagnetic planes, which are antiferromagnetically aligned in one of the directions - similarly to the models considered in this paper. Weyl points were also theoretically predicted in antiferromagnets Mg$_3$Sn and Mg$_3$Ge. More interestingly, in Ref. [40] it was claimed that Dirac electrons enhance antiferromagnetic exchange interaction in the experimentally discovered Dirac metals CaMnBi$_2$ and SrMnBi$_2$. Another example of Weyl metal, which contains ferromagnetic planes aligned antiferromagnetically is BaMnSb$_2$ [61]. Perhaps, the most interesting material, where Dirac electrons coexist with antiferromagnetism is CuMnAs [35]. In this material, phase transition between commensurate and incommensurate antiferromagnetism has been observed as a function of temperature and chemical composition (i.e. chemical potential) [35]. Finally we mention the material Sr$_{1-x}$Mn$_{1-x}$Sb$_2$ [62]: this Dirac material exhibits canted antiferromagnetic order, when two spin components are antiferromagnetically ordered in such a way that the net magnetization is non-zero, but at higher temperatures it undergoes transition to a ferromagnetic phase. Interplay between antiferromagnetism and Dirac electrons is currently being actively studied, and it leads to novel effects, which have promising applications in spintronics [48].

In this paper, we have presented a simple mean-field picture, explaining why antiferromagnetism naturally appears in systems of Dirac electrons. We remark that our approach is not to be viewed as rigorous: mean-field is just a rough approximation, which does not al-
ways predict quantities (e.g. temperature dependencies) accurately. A significant contribution to the magnetization behavior may arise due to quantum corrections (e.g. magnons), the full electronic structure etc. Nevertheless, we have demonstrated that simple mean-field picture successfully explains the origin of antiferromagnetism in Dirac metals.

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Appendix A: Numerical calculation of possible magnetic ground states in Dirac metal

In this appendix, we consider lattice versions of the models of type II and I Dirac metals, introduced in the main text, and compute their effective actions (Eq. 3) numerically. In this way, we are able to find the momentum \( q \) of the magnetic ground state (determined by a minimum of the effective action \( S(q) \)) and its behavior at different \( \mu \) and \( T \), including the range, when non-linear corrections to the dispersion become important. We obtain that, typically, at small \( \mu \), the momentum \( q \) has one of the components equal to \( \pi \), which tells us that the ground state is antiferromagnetic, but at sufficiently large \( \mu \) (when non-linear corrections become important), \( q \) starts decreasing, thus forming a phase transition from AFM to SDW ground state. We note that, throughout our analysis, we do not consider the full 3D range of momenta, which would be computationally challenging, but instead we limit ourselves with just a few special directions of \( q \), which is sufficient for our illustrative purposes.

This section is organized as follows. In the Sec. A1 we describe our methods of finding the magnetic ground state at zero temperature by considering the model of type II Dirac metal, and then repeating the calculations for the case of type I Dirac metal. After it, in Sec. A2 we consider the effective action at finite temperatures. We start from describing our method, and after it we describe our results for type II and type I Dirac metals.

1. Magnetic ground states

Let us describe our approach of finding the magnetic ground states by using the example of type II Dirac metal. We replace the coefficients \( d_i \) from the Eq. 2 with their lattice counterparts, which, in type II case, have the form:

\[
\begin{align*}
    d_2 &= v_z \sin k_z, \\
    d_3 &= v_y \sin k_y, \\
    d_4 &= v_x \sin k_x.
\end{align*}
\] (A1)

We use these expressions to compute numerically the effective action (see Eq. 4) by using tetrahedral method (this method helps to resolve issues, which may happen due to divergences in the numerator and denominator of the Eq. 1). We present our findings on the Fig. 1. One can see that for some directions of the momentum \( q_i \), the effective action has minimum at zero \( q_i \), as was predicted by the Eq. 6, whereas for others, the minimum is reached at finite values of \( q_i \). For example, in the case of \( b \parallel x \), the effective action increases with \( q_x \), and the curvature decreases with increasing \( \mu \) consistently with the Eq. 6. Similarly, the effective action as a function of \( q_z \) has minimum away from zero.

One can see that magnetization \( b_z \) is spatially modulated in \( z \) direction (as we will see, this is due to non-linear corrections to the energy spectrum). Similarly \( b_x \) component of the magnetization is spatially modulated both in \( y \) and \( z \) directions. At small values of the chemical potential \( \mu \), both effective potentials have minima at the boundary of the Brillouin zone, which implies that the ground state is antiferromagnetic. However, at larger values of \( \mu \), spatial modulation of the ground state decreases, so that it starts forming SDW. Eventually, spatial modulation in the \( z \) direction disappears, but, on the other hand, it appears in \( x \) direction. Thus, as \( \mu \) increases, there appears a phase transition between two SDWs modulated in different directions.

We note that our numerical results have minor deviations from the analytical, but the difference is explained by the non-linearity of dispersion. For example, from the Eq. 6 we expect, that in the case of strictly linear dispersion, the term \( q_x^2 b_z^2 \) should have zero 'bulk' contribution and small positive contribution from the Fermi surface. However, since on a lattice, the dispersion is non-linear, it has indeed a large negative 'bulk' contribution responsible for the shape of the curves on the Fig. 1. Similarly, the wavelength of SDWs is not proportional to \( \mu \), but instead it is determined by scales of the band. In realistic metals, we expect non-linear corrections to play weaker role than in our simulations, since their scale is much larger than the chemical potential, but our main conclusion is that non-linear corrections to the band structure may change magnetic ground states in numerous ways, even though they are still expected to be spatially modulated.

Now, let us repeat the calculations in the case of type I Dirac metal. In a similar way, we compute the effective action 4 for the model placed on a lattice. We consider the Hamiltonian (Eq. 7), and choose the functions \( d \) as:

\[
\begin{align*}
    d_1 &= \sin k_x, \\
    d_2 &= \sin k_y, \\
    d_3 &= m_0 - m_1(1 - \cos k_z).
\end{align*}
\] (A2)
FIG. 1: Numerically computed $\text{tr}G(k)M(k + q)M$ for the model (A1) in the case of: (1a) $\vec{b} = (0, 0, 0.5)$ as functions of $\vec{q}$ in the form $\vec{q} = (0, q_x, 0)$ and $\vec{q} = (q_x, 0, 0)$; (1b) $\vec{b} = (0.5, 0, 0)$ as functions of $\vec{q}$ in the form $\vec{q} = (0, q_y, 0)$, $\vec{q} = (q_x, 0, 0)$; (1c) $\vec{b} = (0.5, 0, 0)$ as functions of $q = q_y = q_z$ and $\vec{q} = (0, 0, q_z)$. The plots are aligned vertically, so that one can see that, in the ground state, (1a) $b_z$ is modulated in $z$ direction, whereas (1b) $b_x$ is modulated in $y$ direction. Also, in the fig. (1a) one can see a special case of $\mu = 1.001$, when $b_z$ is modulated in $x$ direction. Thus, we conclude that as $\mu$ reaches band energy at the point $(\pi, 0, 0)$, phase transition occurs.

FIG. 2: Numerically computed $\text{tr}G(k)M(k + q)M$ for the model (A2) as functions of $q_z$, $q_x$. The parameters of the model are: $m_0 = 1.0$, $m_1 = 1.0$, $g_s = g_p = 1.0$. The magnetic field is: (2a) $\vec{b} = (0, 0, 0.5)$, and (2b) $\vec{b} = (0.5, 0, 0)$. One can see, that $b_z$ has minima at either $p_x = \pi$ or $p_z = \pi$, which suggests that the magnetic ground state is spatially modulated. Also, one can see (2a) that at large $\mu$, the local minimum gets displaced away from the boundary of the BZ. Similarly, one can see that $b_x$ forms an antiferromagnetic configuration modulated in $x$ direction, but with increasing $\mu$, it changes into SDW.

We present our findings on the Fig. 2b. One can see that in the case of magnetization in $z$ direction, the effective action has local minima either at $X$, or at $Z$ point of the BZ (i.e. at $q = (\pi, 0, 0)$ or $q = (0, 0, \pi)$ ), which suggest that $b_z$ can be spatially modulated either in $x$ or in $z$ direction. On the other hand, $b_x$ is modulated in $z$ direction: at small $\mu$, it forms an antiferromagnet, but as $\mu$ increases, a transition to SDW phase occurs. Eventually, at large $\mu$, a phase transition occurs: spatial modulation in $z$ direction disappears, and the system becomes spatially modulated in the $x$ direction.

2. Magnetic ground states at finite temperatures

Once we found the magnetic ground states at zero temperature, we can try to study their evolution, when tem-
perature becomes finite. Specifically, we would like to compute numerically the effective action (Eq. 4) at finite temperatures. Since \( n_F \) and its derivative significantly deviate from constant only in a narrow range of parameters, straightforward tetrahedral integration is challenging. For this reason, to obtain the effective action at finite temperature, we first compute it for various chemical potentials at zero temperature, and then obtain the answer at finite temperatures by applying the following relation [64]:

\[
S(T, \mu) = - \int d\xi \frac{\partial n_F(\xi - \mu)}{\partial \xi} S(0, \xi). \tag{A3}
\]

In addition, we have to account explicitly for the change of chemical potential with temperature, and we do it in the following way. First, we numerically compute particle number at zero temperature as a function of chemical potential \( N = \int \frac{d^3 k}{(2\pi)^3} \theta(\mu - k) \). Then, by using the Eq. (A3), we obtain particle number \( N(\mu, T) \) at finite temperatures and various chemical potentials and use it to find the dependency \( \mu(T) \). Namely, for a given chemical potential at zero temperature \( E_F \), we take number of particles \( N(E_F, T = 0) \), then, for given nonzero \( T \), find two closest values of \( N(T) \) and their corresponding \( \mu \) and finally obtain the answer for \( \mu(T) \) through their linear interpolation. In total, we find \( \mu(T) \) for given \( E_F \) and then use it to compute the effective action through the Eq. (A3).

In the case of type II Dirac metal, we present our findings on the Fig. 3. At \( q = 0 \) we expect that the effective action will be temperature-independent for \( b \parallel z \), but will increase e.g. for \( b \parallel x \). Our numerical plots are consistent with these predictions at small \( T \), but as \( T \) increases, the numerical plots start behaving differently because of nonlinearities in the dispersion. More interestingly, our numerical findings confirm that wavevector of the magnetization changes with temperature, and even more, as temperature grows, the system may undergo a phase transition from SDW to AFM phase.

The results for type I Dirac metal are qualitatively similar to type II case and are shown on the Fig. 4. As expected, the magnitude of the effective action decreases with temperature, and its shape evolves. Specifically, its minimum may shift, so that the system undergoes a transition from SDW to AFM phase.

Thus, we have demonstrated that Dirac electrons may have a large variety of possible magnetic phases. Most commonly, these phases are antiferromagnetic or SDW, and there are possible transitions between them, as chemical potential or temperature varies.

![FIG. 3: Numerically computed effective action for the model (A1) at various temperatures. The magnetic field and momentum have are directed: (left) \( b = (b_x, 0, 0) \), \( q = (0, q, q) \); (right) \( b = (0, 0, b_z) \), \( q = (0, 0, q_z) \). We choose \( \mu = 0.7 \) and the other parameters are the same as on the Fig. 1 One can see that, at zero \( T \), the effective action has minimum away from the boundary of the Brillouin zone, but as \( T \) increases, the minimum shifts towards it. Thus the system undergoes a phase transition from AFM to SDW phase.](image)

![FIG. 4: Numerically computed effective action for the model (A2) at various temperatures. We choose: (left) \( b = (b_x, 0, 0) \), \( q = (0, 0, q_z) \); and (right) \( b = (0, 0, b_z) \), \( q = (0, 0, q_z) \). Here \( \mu = 0.7 \) and the other parameters are the same as on the Fig. 2.](image)

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