Interacting Dirac liquid in three-dimensional semimetals

Johannes Hofmann, Edwin Barnes, and S. Das Sarma
Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, Maryland 20742-4111 USA
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We study theoretically the properties of the interacting Dirac liquid, a novel three-dimensional many-body system which was recently experimentally realized and in which the electrons have a chiral linear relativistic dispersion and a mutual Coulomb interaction. We find that the “intrinsic” Dirac liquid, where the Fermi energy lies exactly at the nodes of the band dispersion, displays unusual Fermi liquid properties, whereas the “extrinsic” system with finite detuning or doping behaves as a standard Landau Fermi liquid. We present analytical and numerical results for the self-energy and spectral function based on both Hartree-Fock and the random phase approximation (RPA) theories and compute the quasiparticle lifetime, residue, and renormalized Fermi velocity of the extrinsic Dirac liquid. A full numerical calculation of the extrinsic RPA spectral function indicates that the Fermi liquid description breaks down for large-energy excitations. Furthermore, we find an additional plasmaron quasiparticle sideband in the spectral function which is discontinuous around the Fermi energy. Our predictions should be observable in ARPES and STM measurements.

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The low-energy excitations of metals or semiconductors are usually well described by a set of parabolic particle and hole bands characterized by an energy offset and an effective mass. The resulting system — the electron liquid — is one of the cornerstones of solid state theory. An old question, dating back to the works of Herring and Abrikosov and Beneslavskii, is whether the band structure of a solid can support more exotic structures where the valence and conduction band touch only at certain points in the Brillouin zone at the Fermi level. The system then forms a semimetallic phase where particle and hole bands are not gapped but at the same time no extended Fermi surface is present. Near the band-touching point, the dispersion takes a chiral relativistic linear form \( \varepsilon(p) = \pm \varepsilon_F p \), where \( \varepsilon_F \) is the Fermi velocity. Indeed, it turns out that such Dirac semimetallic phases can exist generically (i.e., without an artificial fine-tuning, for example, of lattice hopping parameters or spin-orbit coupling strength) and are protected by the crystal symmetry. In addition, if time reversal or inversion symmetry is broken, the Dirac cones are nondegenerate and possess quantized anomalous transport properties and topologically protected Fermi arc surface states. Very recently, three-dimensional Dirac semimetals (where time-reversal invariance implies a double-degeneracy of each Weyl node) have been realized in Na\(_3\)Bi and Cd\(_3\)As\(_2\), and the linear dispersion was demonstrated by angle-resolved photoemission spectroscopy (ARPES) measurements of the Dirac cones. These experiments realize a novel fundamental interacting many-body system, which we shall refer to as the Dirac liquid, where the kinetic term has a linear relativistic structure and the electron-electron interaction is the usual 1/r nonrelativistic Coulomb interaction.

In this Letter, we characterize this Dirac liquid by calculating its quasiparticle properties and spectral function. We compute the quasiparticle lifetime, residue, and renormalized Fermi velocity analytically using Hartree-Fock and the RPA, revealing a standard Fermi liquid behavior at finite carrier density (i.e., doped) and a strange, marginal Fermi liquid phase at zero density (i.e., undoped). We calculate the spectral function numerically at finite density and find that the quasiparticle peak is accompanied by sidebands corresponding to plasmaron modes. Our results further indicate a breakdown of the quasiparticle picture away from the Fermi surface.

The effective noninteracting two-band Hamiltonian describing the low-energy excitations at one Weyl node is

\[
H_0 = v_F \mathbf{k} \cdot \mathbf{\sigma},
\]

where \( v_F \) is the bare (i.e., single-electron) Fermi velocity, \( \mathbf{k} \) the momentum and \( \mathbf{\sigma} \) are Pauli matrices. \( H_0 \) is diagonalized with energy \( \varepsilon_s(k) = s v_F k \) by the chiral eigenstates \( |k_s\rangle = (\cos \vartheta_s/2, s e^{i \varphi} \sin \vartheta_s/2)^T \) (for \( k_z \neq 0 \)), where \( s = \pm 1 \) is the chirality. The angles \( \varphi = \arctan k_y/k_x \) and \( \cos \vartheta_s = k_z/|k| \) indicate the direction of the momentum in polar coordinates, and we define \( \vartheta_- = \pi - \vartheta_+ \). We allow for an arbitrary number \( g \) of Weyl nodes in our theory (for instance, lattice inversion symmetry implies that the Weyl nodes exist in pairs of opposite Chern number at opposite points of the Brillouin zone, implying twofold degeneracy). We distinguish between the undoped “intrinsic” case, where the chemical potential is exactly at the nodes of the Dirac dispersion, and the doped “extrinsic” case with finite chemical potential detuning. The extrinsic case is generic since the presence of impurities inevitably shifts the chemical potential away from half-filling. We note that the chemical potential can also be tuned experimentally by surface doping, as is, for example, done in recent experiments on Na\(_3\)Bi. Following these pioneering experiments, it is imperative to have a quantitatively predictive theoretical calculation of the spectral properties of Dirac liquids taking into account electron-electron interaction.
\[ \Sigma_s(\omega, k) = \sum_{s' \in \pm} \Sigma_s^{(\text{ex})}(\omega, k)|ks\rangle\langle ks| \]  

We compute the self-energy at zero temperature and decompose it into an exchange and correlation part:

\[ \Sigma_s(\omega, k) = \Sigma_s^{(\text{ex})}(\omega, k) + \Sigma_s^{(\text{corr})}(\omega, k). \]  

The exchange part (corresponding to the Hartree-Fock self-energy) contains the leading-order perturbative (i.e., the formal single-loop) interaction correction and is given by:

\[ \Sigma_s^{(\text{ex})}(k) = -\sum_{s'} \int\frac{d^3q}{(2\pi)^3} \Theta(-\xi_s'(q))V_{q-k} F_{ss'}(k, q). \]  

Here, the free dispersion is \( \xi_s(q) = v_F sl + \) with Fermi momentum \( k_F, V_k = 4\pi\epsilon^2/\kappa k^2 \) is the Coulomb matrix element, and \( F_{ss'}(k, q) = |\langle ks|qs'\rangle|^2 = \frac{1}{2}(1 + ss'\cos\theta) \) denotes the overlap of eigenstates of momentum \( q \) and \( k \) and chirality \( s \) and \( s' \). The exchange self-energy can be decomposed into an intrinsic part, which only contains the effects at zero chemical potential, and an extrinsic part, which corrects for the presence of a finite chemical potential:

\[ \Sigma_s^{(\text{ex})}(k) = \Sigma_s^{(\text{int})}(\omega, k) + \Sigma_s^{(\text{ext})}(\omega, k), \]

with

\[ \Sigma_s^{(\text{int})}(x) = -\frac{2\alpha v_F k_c}{\pi} \left[ f\left(\frac{k}{k_c}\right) - sh\left(\frac{k}{k_c}\right) \right] \]

\[ \Sigma_s^{(\text{ext})}(x) = -\frac{2\alpha v_F k_F}{\pi} \left[ f\left(\frac{k}{k_F}\right) + sh\left(\frac{k}{k_F}\right) \right]. \]

Here, \( k_c \) is the ultra-violet momentum scale beyond which we cut off the linear dispersion and

\[ f(x) = \frac{1}{4} + \frac{1 - x^2}{8x} \ln \frac{1 + x}{1 - x}, \]

\[ h(x) = -\frac{1}{12x} + \frac{x}{6} \ln \frac{1 - 1/x^2}{24x^2} \ln \frac{1 + x}{1 - x}. \]

We compute the correlation part in the RPA, or equivalently the \( G_0W \) approximation [13]:

\[ \Sigma_s^{(\text{corr})}(i\omega_n, k) = \frac{1}{\beta V} \sum_{\Omega_m, q} G_{ss'}(i\omega_n + i\Omega_m, q') \times V_q \left[ \frac{1}{\varepsilon(i\Omega_m, q)} - 1 \right] F_{ss'}(k, q'). \]

Figure 1 shows the RPA in a Feynman diagram representation. The RPA sums an infinite number of repeated polarization bubble diagrams, leading to a dynamically screened Coulomb interaction with a momentum and frequency-dependent dielectric function \( \varepsilon(i\Omega_m, q) \) given by the geometric series

\[ \varepsilon(i\Omega_m, q) = 1 + V_q \Pi(i\Omega_m, q), \]

with the polarizability of the noninteracting Dirac liquid:

\[ \Pi(i\omega_n, q) = \frac{g}{V} \sum_{kss'} \frac{n_F(\xi_s(k)) - n_F(\xi_{s'}(k'))}{i\omega_n + \xi_s(k) - \xi_{s'}(k')} F_{ss'}(k, k'), \]

where \( n_F \) is the Fermi-Dirac distribution. The infinite RPA summation removes an infrared divergence stemming from the low-momentum behavior of the polarizability [13]. Formally, the RPA, which is the leading-order expansion in the dynamically screened Coulomb interaction, is the leading-order term in a systematic large-\( g \) expansion, with higher-order corrections suppressed by powers of \( 1/g \). We note that for many Weyl semimetals, the degeneracy of Weyl nodes is exceptionally large.
\( g = 24 \) for pyrochlore iridates [9], implying that our calculation is essentially exact. In addition, in a previous work [16], we have explicitly computed the next-to-leading order contribution to the RPA in graphene (where \( \alpha \leq 2.2 \) and \( g = 4 \), which is a two-dimensional Dirac liquid, finding only a very slight correction to the leading-order results for any interaction strength. Therefore, we expect that the RPA provides an excellent description of many-body interaction effects in Dirac liquids.

Intrinsic Dirac liquid: To leading order in \( \alpha \), the Fermi velocity acquires a logarithmic renormalization which can be extracted from the asymptotic form of the exchange self-energy [5] after subtracting an irrelevant linear divergence:

\[
v_F^* = v_F \left[ 1 + \frac{2\alpha}{3\pi} \ln \frac{k_c}{k_F} \right],
\]

which agrees with previous results [17, 18]. To leading order in the RPA, the polarizability is given by [5]

\[
\Pi^-(\omega, k) = \frac{k^2}{12k_F^2} \ln \left| \frac{k_F^2 - \omega^2}{v_F^2 k^2 - \omega^2} \right| + i \frac{k^2}{12k_F^2} \Theta(\omega - v_F k),
\]

where \( \Pi = \Pi/D_0 \) with \( D_0 = g k_F^2/2\pi^2 v_F \) being the non-interacting density of states. Crucially, the logarithmic dependence of the dielectric function on the cutoff \( k_c \) induces a renormalization of the electron charge; the bare and renormalized charge are related via

\[
\frac{1}{e^2} = \frac{1}{e_0^2} + \frac{g}{3\pi \varepsilon v_F} \ln \frac{k_c}{\mu},
\]

where \( \mu \) is a renormalization scale. The charge renormalization here is similar to the renormalization of the electron charge in quantum electrodynamics [18]. Substituting this into Eq. [14] reveals a new pole at energy \( \omega = \sqrt{v_F^2 k^2 - \Lambda_L^2} \), where we define the Landau scale \( \Lambda_L = \mu e^3/\gamma \alpha \). This is a manifestation of the famous Landau pole in quantum electrodynamics [19]. However, this pole is unphysical, as can be seen for example by computing the residue at \( \Lambda_L \), which diverges as \( 1/\sqrt{v_F^2 k^2 - \Lambda_L^2} \). It is also in direct violation of the \( f \)-sum rule. Hence, the Landau pole does not indicate new physics but reflects a breakdown of the RPA expansion at momentum scales \( k \sim \Lambda_L \). This ambiguity can be resolved by choosing a cutoff \( k_c < \Lambda_L \).

In order to characterize the quasiparticle nature of the intrinsic Dirac liquid, we compute the lifetime at small momentum, which is given by the imaginary part of the self-energy. In the on-shell approximation \( \omega = v_F q \), the imaginary part of the intrinsic RPA self-energy vanishes because of phase-space restrictions [20]. At zero momentum, however, the self-energy is linear in frequency and given by

\[
\text{Im}\Sigma(\omega, 0) = -\frac{\pi \omega^2 q}{48} \frac{1}{1 + (\pi \gamma \alpha/12)^2}, \tag{16}
\]

as is characteristic for a marginal Fermi liquid. In what follows we show that this strange Fermi liquid behavior breaks down in the generic case of a finite chemical potential, i.e., the marginal Fermi liquid fixed point is unstable to infinitesimal finite doping.

Extrinsic Dirac liquid: We consider first the quasiparticle lifetime in the presence of an extended Fermi surface using the on-shell approximation for the quasiparticle dispersion \( \omega = v_F (k - k_F) \). We write the correlation self-energy as the sum of a line and a residue term:

\[
\Sigma_s(\omega, k) = \Sigma_s^{\text{line}}(\omega, k) + \Sigma_s^{\text{res}}(\omega, k)
\]

\[
\Sigma_s^{\text{line}}(\omega, k) = -\frac{1}{V} \sum_{q' s'} \int \frac{d\Omega}{2\pi} G_{s'}(\omega + i\Omega, q') \times \left[ \frac{V_{q}^{s}}{|\varepsilon(\Omega, q') - 1|} F_{s'}(k, q') \right] \tag{17}
\]

\[
\Sigma_s^{\text{res}}(\omega, k) = \frac{1}{V} \sum_{q'^{s'}} \left[ \Theta(\omega - \xi_{s'}(q')) - \Theta(-\xi_{s'}(q')) \right] \times \left[ \frac{V_{q}^{s}}{|\varepsilon(\xi_{s'}(q') - \omega, q) - 1|} F_{s'}(k, q') \right] \tag{18}
\]

where the line contribution is the self-energy [10] with the imaginary frequency replaced by its analytic continuation. The residue term modifies this expression so that is gives the correct analytic continuation of the retarded self-energy. Only the residue term contributes to the imaginary part and thus the quasiparticle lifetime is given by:

\[
\frac{1}{\tau(k)} = -2\text{Im}\Sigma_+(\xi_+(k), k) = -\frac{1}{(2\pi)^d} \int_{k_F}^{k} dq q^2 \times \int d\Omega (1 + \cos \theta) \text{Im} \left[ \frac{V_{q-k}^{s}}{|\varepsilon(v_F (q-k), q-k)|} \right]. \tag{20}
\]

Since we consider low-energy excitations above the Fermi surface, the dielectric function [21] can be expanded in powers of \( (k - q)/k_F \), i.e., small frequency density excitations determine the lifetime of the quasiparticle. Furthermore, the Coulomb matrix element implies that the integrand is strongly peaked for forward-scattering processes with \( k \approx q \). In this limit, we can expand \( \varepsilon^{-1}(\omega, q) = \pi q \omega / 2 g v_F k_F^2 \). This yields a standard Fermi liquid expression for the quasiparticle lifetime

\[
\frac{1}{\tau(k)} = \frac{\pi \xi_k^2}{3g \varepsilon_F}, \tag{21}
\]

which is quadratic in the excitation energy \( \xi_k = v_F (k - k_F) \). Hence, the system behaves as a Fermi liquid with a discontinuity in the occupation number at the Fermi surface.

The quasiparticle residue \( Z \) is related to the derivative of the self-energy as \( Z^{-1} = 1 - A \), where \( A = \lim_{\omega \to 0} \lim_{k \to k_F} \frac{d}{d\omega} \text{Re} \Sigma(\omega, k) \). We compute the self-energy derivative using the line and residue decomposition [17].
When integrating the line part by parts in \( \Omega \), it turns out that the integral boundary term cancels with the residue contribution. It remains to compute

\[
A = - \lim_{k \to k_F} \text{Im} \sum_{s'} \int_0^\infty dq q^{d-1} \int d\Omega d \int_0^\infty \frac{d\Omega}{\pi} \\
\times G_{s'}(i\Omega, q') F_{s'}(k, q') \frac{V_q}{\varepsilon^2(i\Omega, q')} \frac{\partial \varepsilon(i\Omega, q')}{\partial \Omega}, \tag{22}
\]

In the weak interaction small-\( \alpha \) limit, the integrand is concentrated in the region of small \( k \) and only the intraband excitations with \( s' = 1 \) contribute to the residue. This yields the result

\[
A = \frac{\alpha}{\pi^2} \int_0^{\varepsilon/2} dz \ln(1 - z \cot z) = -1.067 \frac{\alpha}{\pi}. \tag{23}
\]

The renormalized Fermi velocity is computed in a similar way. It is defined as \( v_F^{\ast}/v_F = (1+B)/(1-A) \), where \( A \) is given in Eq. (22) and \( B \) denotes the derivative of \( \text{Re}\Sigma \) with respect to momentum evaluated at zero energy at the Fermi momentum: \( B = \frac{\partial}{\partial q} \text{Re}\Sigma_s(\omega, q) \big|_{\omega=0,q=k_F} \). The calculation proceeds in the same way as for the quasiparticle residue and gives the result for small \( \alpha \)

\[
v_F^{\ast}/v_F = 1 - \frac{\alpha}{2\pi} \left[ \ln \frac{q\alpha}{2\pi} + 2 \right] + \frac{2\alpha}{3\pi} \ln \frac{k_F}{k_F}. \tag{24}
\]

The divergent part agrees with the exchange part [13]. We see that in addition to the cutoff-dependent term due to the renormalization, there is an additional finite contribution due to intraband interactions.

**Spectral function:** Having analytically calculated the quasiparticle properties, we proceed to present numerical results for the full spectral function. The full spectral function is given by \( A(\omega, q) = \sum_{s=\pm} A_s(\omega, q) \), where

\[
A_s(\omega, k) = \frac{1}{\pi} (\omega - \xi_s(k) - \text{Re}\Sigma_s(\omega, k))^2 + (\text{Im}\Sigma_s(\omega, k))^2. \tag{25}
\]

Figure 2(a) shows the spectral function as computed numerically from Eqs. (18) and (19) at an interaction strength \( \alpha = 0.15 \) and with a cutoff \( k_c/k_F = 100 \). As is standard for the \( G_0W \) approximation, we compute the real part of the self-energy relative to the chemical potential at the Fermi surface. As a consistency check of our calculation, we verify the normalization of the spectral function to within less than one percent. Beside the quasiparticle branch discussed in the previous sections, the coupling of electrons to the plasmon density modes induces an additional quasiparticle excitation, the plasmon [22], which forms sidebands to the quasiparticle dispersion. These plasmon satellite peaks are clearly visible in Fig. 2(b) which shows the spectral function as a function of frequency at fixed momentum \( k/k_F = 0.75, 1, \) and 1.25. For a momentum smaller than \( k_F \), the plasmon band is below the quasiparticle branch, whereas above \( k_F \), it lies above it. Right at the Fermi momentum, the quasiparticle peak has infinite lifetime and zero
width as indicated by the arrow. Since the plasmon mode is gapped in three dimensions with a dispersion of \( \omega_p(q) = \omega_0 + O(q^2) \), where \( \omega_0 > 0 \), low-energy excitations around zero frequency do not couple to the plasmon modes and, hence, there is a discontinuous jump in the plasmaron branch across the Fermi surface. The Fermi liquid nature of the system is also apparent in the occupation number shown in Fig. 2(c), which clearly displays the discontinuity of size \( Z \) at the Fermi momentum. We note that for excitations at small momentum or negative chirality, the quasiparticle description breaks down. In addition, we observe strong interaction effects on the density of states [Fig. 2(d)], the minimum of which is shifted with respect to the minimum of the noninteracting DOS which is located at \( \omega = -\varepsilon_F \). At high frequency, the DOS retains its noninteracting quadratic shape with a renormalized slope \( \sim v_F/v_F^* \).

In summary, we provide a comprehensive theory for the quasiparticle properties of the Dirac liquid in the random phase approximation. While we found that the intrinsic Dirac liquid displays marginal Fermi liquid behavior with an imaginary part that is linear in frequency, the experimentally relevant extrinsic Dirac liquid behaves as a Fermi liquid. We have computed the Fermi liquid properties – lifetime, residue, and renormalized Fermi velocity – both analytically in the on-shell approximation as well as numerically in a full calculation of the spectral function. The numerical calculation reveals the limit of the Fermi liquid description away from the Fermi surface and indicates the existence of an additional quasiparticle excitation, the plasmaron, which arises from a coupling to the plasmon density modes. Our predictions can be directly tested in spectroscopic measurements such as ARPES and STM.

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\* hofmann@umd.edu

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