Phase diagram of the Quantum Electrodynamics of 2D and 3D Dirac semimetals

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We study the Quantum Electrodynamics of 2D and 3D Dirac semimetals by means of a self-consistent resolution of the Schwinger-Dyson equations, aiming to obtain the respective phase diagrams in terms of the relative strength of the Coulomb interaction and the number $N$ of Dirac fermions. In this framework, 2D Dirac semimetals have just a strong-coupling instability characterized by exciton condensation (and dynamical generation of mass) that we find at a critical coupling well above previous theoretical estimates, thus explaining the absence of that instability in free-standing graphene samples. On the other hand, we show that 3D Dirac semimetals have a richer phase diagram, with a strong-coupling instability leading to dynamical mass generation up to $N = 4$ and a line of critical points for larger values of $N$ characterized by the vanishing of the electron quasiparticle weight in the low-energy limit. Such a marginal Fermi liquid boundary signals the transition to a strongly renormalized electron liquid having very unstable quasiparticles, with large decay rates implying an increasing departure at strong coupling from the Fermi liquid picture.

I. INTRODUCTION

The discovery of graphene has marked the beginning of a new chapter in condensed matter physics, with the appearance of new fundamental concepts and materials with unconventional properties. We have known about other genuine 2D materials like the transition metal dichalcogenides, and we have learned about the features hidden in the band structure of the topological insulators. Lately, we have also discovered the existence of 3D Dirac semimetals which are the higher-dimensional analogue of graphene, and we are in the search of Weyl semimetals with a built-in breakdown of parity and time-reversal invariance.

In the above instances, most part of the unconventional features of the materials come from the peculiar geometrical and topological properties of the band structure. Moreover, these are electron systems that are prone to be placed in the strong coupling regime, with a large relative strength of the Coulomb interaction. Graphene should be a clear example of electron system with strong interaction, given the large ratio between the square of the electron charge and the Fermi velocity in the 2D material. However, graphene is not a prototype of strongly correlated system, even in the case of the free-standing material in vacuum, as experimental observations have shown no sign of electronic instability at very low doping levels.

On the other hand, most part of theoretical studies have estimated that 2D Dirac semimetals should have an excitonic instability at a critical point below the maximum interaction strength attained in graphene suspended in vacuum. The absence of any signature of a gap in the electronic spectrum, even below the meV scale, is certainly a puzzling evidence regarding the behavior of the 2D material. Given that the theoretical analyses have been mainly based on a ladder approximation to the electron self-energy corrections, the discrepancy between theory and experiment calls into question the use of such approximate methods in electron systems that are placed in the strong-coupling regime.

In this paper, we apply a nonperturbative approach to the investigation of the effects of the Coulomb interaction in both 2D and 3D semimetals, with the aim of mapping more confidently the different phases that may appear in those electron systems. More precisely, we carry out the self-consistent resolution of the Schwinger-Dyson equations, aiming to obtain the respective phase diagram, with a strong-coupling instability leading to dynamical mass generation up to $N = 4$ and a line of critical points for larger values of $N$ characterized by the vanishing of the electron quasiparticle weight in the low-energy limit.

In this framework, we will see that 2D Dirac semimetals have just a strong-coupling instability characterized by exciton condensation (and dynamical generation of mass) that we find at a critical coupling well above the estimates based on a ladder approximation, thus explaining the absence of that instability in free-standing graphene samples. On the other hand, we will show that 3D Dirac semimetals have a richer phase diagram, with a strong-coupling instability leading to dynamical mass generation up to $N = 4$ and a line of critical points for larger values of $N$ characterized by the vanishing of the electron quasiparticle weight in the low-energy limit. We will see that such a marginal Fermi liquid boundary marks the transition to a strongly renormalized electron liquid having very unstable quasiparticles, with large decay rates implying an increasing departure at strong coupling from the Fermi liquid picture.
II. QUANTUM ELECTRODYNAMICS OF DIRAC SEMIMETALS

We focus on the QED of Dirac semimetals, for which the Fermi velocity $v_F$ is much smaller than the speed of light. The dynamics of these systems can be then described by the interaction of a number $N$ of four-component Dirac spinor fields $\psi_i(\mathbf{r})$ representing the electron quasiparticles and the scalar part $\phi(\mathbf{r})$ of the electromagnetic potential. The Hamiltonian can be written in general as

$$H = iv_F \int d^D r \bar{\psi}_i(r) \gamma \cdot \nabla \psi_i(r) + e \int d^D r \bar{\psi}_i(r) \gamma_0 \gamma_i(r) \phi(r)$$

(1)

where $\{\gamma_\alpha\}$ is a set of Dirac matrices satisfying $\{\gamma_\alpha, \gamma_\beta\} = 2\eta_{\alpha\beta}$ (with the Minkowski metric $\eta = \text{diag}(-1, 1, \ldots, 1)$) and $\bar{\psi}_i = \psi_i^\dagger \gamma_0$.

The expression (1) holds equally well for dimension $D = 2$ and 3, but the propagator of the $\phi$ field is very different in the two cases. The scalar field has to mediate the $e$-$e$ interaction with long-range Coulomb potential $V(\mathbf{r}) = 1/|\mathbf{r}|$, irrespective of the spatial dimension. At $D = 2$, this leads to a bare propagator $D_0(q, \omega)$ for the $\phi$ field

$$D_0(q)|_{D=2} = \frac{1}{2|q|}$$

(2)

while in 3D space the bare propagator is instead

$$D_0(q)|_{D=3} = \frac{1}{q^2}$$

(3)

The effects of the interaction can be characterized through the corrections undergone by the scalar and the Dirac field propagators. The full Dirac propagator $G(k, \omega_k)$ has in general a representation of the form

$$G(k, \omega_k)^{-1} = (\gamma_0 \omega_k - v_F \gamma \cdot k) - \Sigma(k, \omega_k)$$

(4)

in terms of a self-energy correction $\Sigma(k, \omega_k)$ that contributes to renormalize the bare quasiparticle parameters. This object is given in turn by the equation

$$i\Sigma(k, \omega_k) = -e^2 \int \frac{d^D p}{(2\pi)^D} \frac{d\omega_p}{2\pi} D(p, \omega_p) \gamma_0 G(k - p, \omega_k - \omega_p) \Gamma(p, \omega_p; k, \omega_k)$$

(5)

where $D(p, \omega_p)$ stands for the full propagator of the scalar potential and $\Gamma(q, \omega_q; k, \omega_k)$ represents the irreducible three-point vertex. More precisely, this function is defined by the expectation value

$$ie\Gamma(q, \omega_q; k, \omega_k) = \langle \phi(q, \omega_q) \psi_i(k - q, \omega_k - \omega_q) \bar{\psi}_i(k, \omega_k) \rangle_{1PI}$$

(6)

where 1PI means that we must take the irreducible part of the correlator.

Furthermore, $D(p, \omega_p)$ has also its own equation representing it in terms of the irreducible vertex and the full propagators. We can write

$$D(q, \omega_q)^{-1} = D_0(q)^{-1} - \Pi(q, \omega_q)$$

(7)

turning out that the polarization $\Pi(q, \omega_q)$ is given by

$$i\Pi(q, \omega_q) = -Ne^2 \int \frac{d^D p}{(2\pi)^D} \frac{d\omega_p}{2\pi} \text{Tr} [\gamma_0 G(q + p, \omega_q + \omega_p) \Gamma(q, \omega_q; p, \omega_p) G(p, \omega_p)]$$

(8)

On the other hand, the form of the irreducible vertex $\Gamma(q, \omega_q; k, \omega_k)$ is constrained by the Ward identity related to the reduced gauge invariance of the model, admitting also representations in terms of the full propagators.

The expressions (5) and (8) correspond to the Schwinger-Dyson equations of the model. Together with a suitable representation of the irreducible vertex, they may lead to valuable information about the form of the full fermion and interaction propagators. In general, however, one has to resort to some kind of truncation to achieve a self-consistent resolution of the integral equations. In what follows, we will apply a common procedure, the so-called bare vertex approximation, by which we will set $\Gamma(q, \omega_q; k, \omega_k)$ equal to $\gamma_0$ in the resolution of (5) and (8). This will lead to a very convenient implementation of the self-consistent approach, allowing us to attain easily convergence in the recursive resolution of the equations.
Without the vertex corrections, (5) and (8) lead indeed to closed self-consistent equations, shown diagrammatically in Fig. 1. This representation allows to establish an easy comparison with other standard approaches used to deal with many-body corrections. In particular, it becomes clear that the contributions accounted for by the diagrams in Fig. 1 have a much more comprehensive content than other approaches dealing with the RPA sum of bubble diagrams for the polarization. This makes the present computational scheme much more reliable to describe the electron system away from the weak-coupling regime, incorporating effects like the renormalization of the Fermi velocity and the quasiparticle weight which are essential to capture the different critical points of the Dirac semimetals.

FIG. 1: Diagrammatic representation of the Schwinger-Dyson equations (in the bare vertex approximation). The thick (thin) straight line represents the dressed (free) Dirac fermion propagator and the thick (thin) wiggly line represents the dressed (undressed) interaction propagator.

### III. SELF-CONSISTENT RESOLUTION OF SCHWINGER-DYSON EQUATIONS

The integral equations represented in Fig. 1 can be solved numerically by applying a recursive procedure, after rotating first all the frequencies in the complex plane, \( \omega = -i\omega \), to make the passage to a Euclidean space in the variables \((\omega, k)\). In practice, the integrals can be done numerically by discretizing the frequency and momentum variables. By choosing a set of frequencies \( \omega = \pi(2n+1)T \) with \( n = 0, \pm 1, \pm 2, \ldots \), we can interpret such a discretization as the result of placing the theory at finite temperature \( T \). On the other hand, computing with a grid in momentum space is equivalent to describing a system with finite spatial size. In this case, we can check the finite-size scaling of the results in order to extrapolate the behavior in the long-distance limit.

For the self-consistent resolution, it becomes convenient to represent the fermion propagator in terms of renormalization factors \( z_\psi(k, i\omega) \) for the electron wave-function and \( z_v(k, i\omega) \) for the Fermi velocity, adding moreover another factor \( z_m(k, i\omega) \) to allow for the dynamical generation of a mass for the Dirac fermions. Thus we write the full Dirac propagator in the form

\[
G(k, i\omega) = (z_\psi(k, i\omega)i\gamma_0\omega - z_v(k, i\omega)v_F\gamma \cdot k - z_m(k, i\omega))^{-1}
\]

In this way, the resolution consists in finding the functions \( z_\psi(k, i\omega), z_v(k, i\omega) \) and \( z_m(k, i\omega) \) that attain the self-consistency in the Schwinger-Dyson equations.

One more important detail is that the polarization \( \Pi(q, \omega_q) \) may develop spurious divergences when computing the momentum integrals with a simple cutoff \( \Lambda_k \). In general, only a gauge-invariant regularization scheme can produce results without non-physical power-law dependences on the cutoff. These are anyhow additive contributions to the polarization, which makes possible to get rid of them by a suitable subtraction procedure. Thus, computing with the momentum cutoff, the polarization at \( D = 2 \) shows a contribution proportional to \( \Lambda_k^2 \), while the corresponding function at \( D = 3 \) has dependences growing as large as \( \Lambda_k^3 \). In our self-consistent resolution, we have dealt with expressions for \( \Pi(q, \omega_q) \) that are functionals of the renormalization factors, but with the unwanted cutoff dependences removed, displaying leading behaviors at small \( q \) proportional to \( |q| \) and \( q^2 \), respectively, for the polarization at \( D = 2 \) and \( D = 3 \).

#### A. 2D Dirac semimetals

Solving the Schwinger-Dyson equations at \( D = 2 \), we find in general that the function \( z_\psi(k, i\omega) \) giving the quasiparticle weight remains bounded, while \( z_v(k, i\omega) \) diverges in the limit of small momentum \( k \to 0 \). As long as the effective
Fermi velocity depends on the energy scale, it is convenient to define the bare value \( v_B = z_v(\Lambda_k, 0)v_F \), which can be taken as a good measure of the Fermi velocity at the microscopic scale (it is always verified that \( z_v(\Lambda_k, 0) \approx 1 \)). We can then define the unrenormalized coupling giving the bare interaction strength as

\[
\alpha = \frac{e^2}{4\pi v_B}
\]

which can take different values depending on the particular Fermi velocities of the 2D Dirac semimetals.

As an illustration of the general behavior, Fig. 2 represents the results corresponding to \( z_v(0, i\omega) \) and \( z_v(k, \omega) \) for \( N = 2 \) and \( \alpha \approx 2.2 \), that is, for parameters that should correspond to the real instance of graphene samples suspended in vacuum. In this case, the self-consistency in the resolution of the equations is only attained when \( z_m(k, \omega) \) is set identically equal to zero. The behavior found for \( z_v(0, i\omega) \) and \( z_v(k, \omega) \) is in agreement with the general trend obtained from renormalization group methods at large \( N \), that found the divergence of the Fermi velocity in the low-energy limit as a most relevant feature\[24, 25\]. It can be observed anyhow that the plot in Fig. 2(b) follows the experimental results of Ref. 8 much more accurately than the scale dependence of the Fermi velocity obtained with that renormalization group approach in the large-\( N \) approximation.

![FIG. 2: Plot of the factors \( z_v(0, i\omega) \) and \( z_v(k, 0) \) for \( N = 2 \) and interaction strength \( \alpha = 2.2 \).](image)

![FIG. 3: Plot of the factors \( z_v(0, i\omega) \), \( z_v(k, 0) \) and \( z_m(k, 0) \) (measured in eV) for \( N = 2 \) and interaction strength \( \alpha = 3.37 \).](image)

With our nonperturbative approach, we can ask however whether the tendency towards a noninteracting Fermi liquid, implied by the growth of the Fermi velocity, can be arrested by some instability as the bare coupling \( \alpha \) is increased. The outcome of this search is that the other relevant feature of the 2D Dirac semimetals is the development of a nonvanishing mass \( z_m(k, \omega) \) at sufficiently large interaction strength, as illustrated in Fig. 3. This corresponds to the onset of a phase with chiral symmetry breaking and dynamical generation of a gap for the Dirac fermions, as predicted by several other methods\[9–20\]. The present approach has the virtue of allowing for an accurate determination of the critical coupling \( \alpha_c \) for the transition to the broken symmetry phase. We have represented in Fig. 4 the plot of the critical coupling as a function of \( N \), which can be taken as a map of the two different phases in the QED of the 2D Dirac semimetals. In agreement with earlier analyses, the critical coupling \( \alpha_c \) turns out to grow with \( N \), though in the present approach there seems to be no upper limit in the number of Dirac fermions for the development of the transition.
FIG. 4: Phase diagram of the QED of 2D Dirac semimetals showing the region with dynamically generated fermion mass \( m \neq 0 \).

Anyhow, the most relevant result regarding the phase diagram in Fig. 4 is that the point corresponding to real graphene samples suspended in vacuum falls in the region with no dynamical generation of mass. For the number \( N = 2 \) of Dirac fermions in graphene, the critical coupling obtained for chiral symmetry breaking turns out to be indeed well above most part of previous estimates relying on a restricted sum of many-body corrections. The present results explain therefore that no gap has been found in the electronic spectrum of graphene, even in experiments looking very close to the Dirac point [8]. The reason for the unexpectedly large values of the critical coupling can be traced back to the combination of the slight suppression of the quasiparticle weight and the large growth of the Fermi velocity at low energies. These two effects cooperate to reduce significantly the effective strength of the Coulomb interaction for the development of the gap, stressing the importance of a proper account of all the renormalization factors for the accurate determination of the transition to the broken symmetry phase.

B. 3D Dirac semimetals

Contrary to the case of the 2D Dirac semimetals, their higher-dimensional analogues have a natural tendency to develop an attenuation of the quasiparticle weight at low energies, with just a soft renormalization of the Fermi velocity [26]. This behavior has been already found in an analytical study of the 3D electron systems in the large-\( N \) limit, where it has been possible to establish rigorously the existence of a critical coupling at which the quasiparticle weight vanishes in the low-energy limit [22]. In Fig. 5 we can see the effect of the critical behavior in the functions \( z_\psi(k, i\omega) \) and \( z_v(k, i\omega) \), computed in the present approach for \( N = 6 \) close to the critical point. For smaller values of \( N \), there is however an interplay between that quasiparticle attenuation and the tendency to chiral symmetry breaking. For \( N \geq 2 \), this latter effect becomes actually dominant, leading to a phase with dynamical generation of mass that is the analogue of the broken symmetry phase found in the 2D Dirac semimetals [27].

FIG. 5: Plot of the factors \( z_\psi(0, i\omega) \) and \( z_v(k, 0) \) for \( N = 6 \) and \( g = 36.5 \).

From the self-consistent resolution of the Schwinger-Dyson equations, we have determined for each value of \( N \) the critical coupling at which the electron system becomes first unstable, either from the vanishing of the quasiparticle weight or from the dynamical generation of a gap. In the case of the 3D Dirac semimetals, one has to take special care to refer the parameters to a given scale, since quantities like the electron charge and the Fermi velocity are
renormalized at low energies. In this respect, we have chosen to define the bare electron charge $e_B$ at the highest value of the momentum cutoff, according to the relation $e_B^2 = \Lambda^2 D(\Lambda, 0)$, where $D(\Lambda, 0)$ is a function of the momentum cutoff $\Lambda$. Then, we can take for the microscopic parameter $e_B$ the standard value of the electron charge. As in the case of the 2D Dirac semimetals, we have also defined the bare Fermi velocity by $v_B = z_v(\Lambda, 0)v_F$. Thus, we have computed all the critical couplings referred to the relative interaction strength at the microscopic scale, given by

$$g = Ne_B^2/4\pi v_B$$

FIG. 6: Phase diagram of the QED of 3D Dirac semimetals, showing the region with dynamical generation of mass ($m \neq 0$) and the region corresponding to the strongly renormalized electron liquid (with $\text{Im}[z_\psi(k, i\omega)] \neq 0$).

The results we have obtained are condensed in the phase diagram shown in Fig. 6. We observe that there is always a phase connected to weak-coupling for all values of $N$, characterized by a gapless spectrum of quasiparticles whose parameters remain regular at low energies. This phase terminates for $N \leq 2$ with the dynamical generation of a fermion mass at sufficiently strong coupling, which in our approach is reflected in the onset of a nonvanishing $z_\psi(k, i\omega)$. This is shown in Fig. 7 where we have represented the different renormalization factors for $N = 2$ at a coupling above the critical point. For this value of $N$, we observe that the renormalization of the quasiparticle weight is a moderate effect as the gap opens up in the electronic spectrum.

FIG. 7: Plot of the factors $z_\psi(0, i\omega)$, $z_v(k, 0)/z_\psi(k, 0)$ and $z_m(k, 0)/z_\psi(k, 0)$ (measured in eV) for $N = 2$ and $g = 15.0$.

The case of $N = 4$ is however more interesting, since there is then an interplay between the dynamical generation of mass and the strong attenuation of the quasiparticle weight. This can be observed in Fig. 8 where we have plotted $z_\psi(k, i\omega)$, $z_v(k, i\omega)$ and $z_m(k, i\omega)$ for different couplings below and above the point where the mass develops. We see that, while the breakdown of chiral symmetry takes place before the system is completely destabilized by the large growth of $z_\psi(k, i\omega)$, this latter effect may still have a large impact in the observation of the quasiparticles in the electron system.

For $N > 4$, the destabilization of the electron quasiparticles due to the divergence of $z_\psi(0, i\omega)$ takes place before the dynamical generation of mass, as already illustrated in Fig. 5. The present approach allows us moreover to investigate the phase of the electron system above the critical point. The self-consistent resolution of the Schwinger-Dyson equations gives rise in that case to renormalization factors that get in general large imaginary parts, as shown in Fig. 9. This has to be interpreted as the signature of dealing with very unstable quasiparticles whose decay rate, given by the imaginary part of the electron self-energy, does not vanish in the low-energy limit.
FIG. 8: Plot of the factors $z_\psi(0, i\omega)$, $z_\psi(k, 0)/z_\psi(0, i\omega)$ and $z_m(k, 0)/z_\psi(0, i\omega)$ (in eV) for $N = 4$ and $g = 30.6, 29.0$ and 26.0.

FIG. 9: Plot of the real and imaginary parts of the factors $z_\psi(0, i\omega)$ and $z_v(k, 0)$ for $N = 6$ and $g = 37.2, 37.4$ and 37.6.

Finally, we mention that the present approach can be also extended to study the phases of the QED of Weyl semimetals. These can be thought as a particular class of semimetals in which the Dirac points host fermions with a given chirality. In these conditions, a gap cannot open up at the Dirac cones, since the dynamical generation of mass requires mixing the two different chiralities of a Dirac fermion. The phase diagram for the Weyl semimetals can be obtained therefore by a simple modification of the previous analysis of the 3D Dirac semimetals, discarding the phase corresponding to chiral symmetry breaking. This implies that the electron systems with $N \leq 4$ can only have now a critical point at strong coupling characterized by the vanishing of the quasiparticle weight in the low-energy limit. The phase diagram obtained then from the self-consistent resolution of the Schwinger-Dyson equations is represented in Fig. 10. The phase boundary marking the destabilization of the Fermi liquid corresponds essentially to the extension of the line of critical points already present for $N \geq 4$ in Fig. 6 after taking into account the absence of the phase with chiral symmetry breaking.

FIG. 10: Phase diagram of the QED of Weyl semimetals (where $N$ corresponds to one-half the number of Weyl fermions).
IV. CONCLUSION

We have seen that the behavior of 2D and 3D Dirac semimetals is driven by quite different features in the two cases. In the 2D systems, there is in general a tendency of the Fermi velocity of quasiparticles to grow large in the low-energy limit, as already shown in renormalization group analyses carried out in the large-$N$ approximation. In the case of the 3D Dirac semimetals, we observe instead that the electron system is prone to develop an attenuation of the quasiparticle weight, with a less significant renormalization of the Fermi velocity. This tendency has been also identified in the large-$N$ limit of the 3D Dirac semimetals, which shows the existence of a critical coupling characterized by the divergence of the electron scaling dimension.

In the 2D Dirac semimetals, the divergence of the Fermi velocity in the low-energy limit is the dominant feature that explains for instance the absence of significant correlation effects in the graphene layer. Our nonperturbative solution of the Schwinger-Dyson equations has found indeed that the interaction strength has to be set to relatively large values, above those attained in the suspended graphene samples, in order to open up a phase with exciton condensation and dynamical generation of a gap in the electronic spectrum.

This picture is changed to a richer phase diagram for the 3D Dirac semimetals, as a consequence of the interplay between the tendency to exciton condensation, which is dominant at small $N$, and the attenuation of the electron quasiparticles that prevails at large $N$. Both effects seem to coexist at the interface found for a number of Dirac fermions $N = 4$. Most interestingly, our self-consistent resolution has also revealed the phase of the system above the large-$N$ critical point, allowing to characterize the properties of a strongly renormalized electron liquid and providing a paradigm for other instances of materials showing non-Fermi liquid behavior.

Finally, we have also obtained the phase diagram of the QED of Weyl semimetals as an extension of the analysis carried out for the 3D Dirac semimetals. In that case, the phase with exciton condensation is ruled out from the impossibility to combine the two different chiralities needed to build up a mass term for the electron quasiparticles. We remain then with a single strong-coupling phase corresponding to the mentioned strongly renormalized electron liquid, which should be susceptible of being experimentally observed in Weyl semimetals with suitably small Fermi velocity in their electronic dispersion.

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