GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

Graphene online 2020 October 19-23

DILUTED RANDOM IMPURITIES DESTABILISE 3D SEMI-METALLIC PHASES

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INTRODUCTION

The recent discovery of Dirac and Weyl semimetals (DWSMs) has provided a rich arena for probing the exotic electrodynamic properties of 3D gapless electrons, including their unique topological features [1]. Several types of gapless systems featuring Dirac or Weyl points in the three-dimensional (3D) momentum space have been observed experimentally (e.g. see Ref. [2]). The simplest DWSMs are 3D analogues of graphene, exhibiting two- or four-fold degenerate linear-band touching at the Fermi level, with isotropic velocities, and a possible replication into disjoint momentum-space valleys. Their point-like Fermi surface is protected against band gap opening due to either topological constraints (for Weyl systems with broken time-reversal ($\mathcal{T}$) or inversion symmetries ($\mathcal{P}$)) or crystal symmetries (for $\mathcal{TP}$-symmetric Dirac systems). Different DWSMs' varieties are depicted in Figure 1.

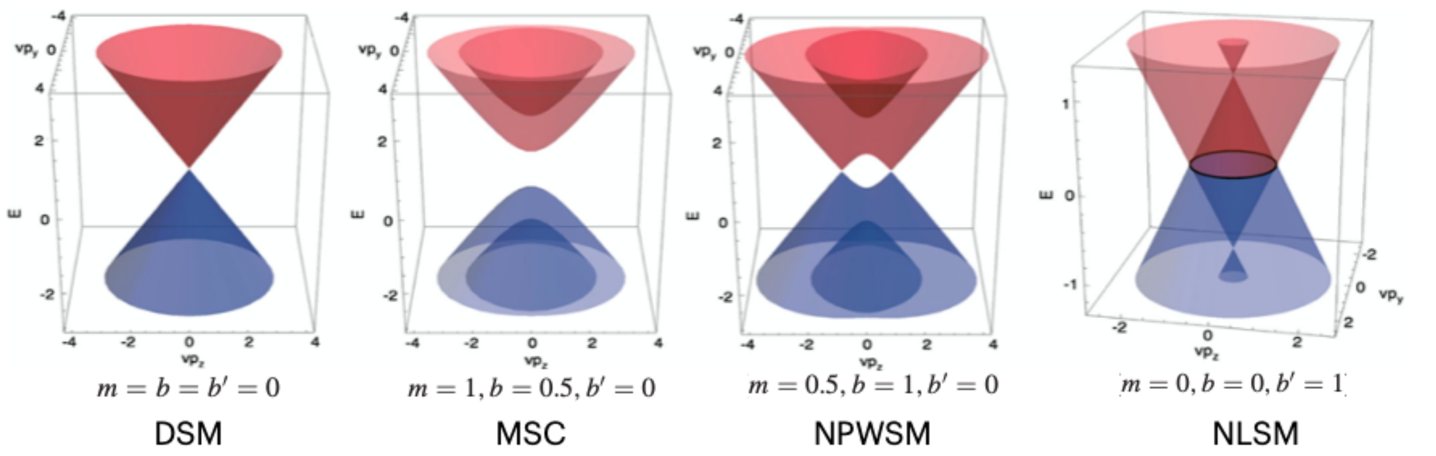

Figure 1: Depiction of the different types low-energy band structures which can happen in 3D four-band electronic systems. From left to right: Dirac Semimetal, Magnetic Semiconductor, Nodal-Point Weyl and Nodal-loop Weyl Semimetal. In M. Koshino and I. F. Hizbullah, *Phys. Rev. B* 93 045201 (2016).

DISORDERED DIRAC/WEYL SEMIMETALS

Similar to graphene, a clean DWSM is a semimetal with an electron density of states (DoS) vanishing as $\rho(E) \propto (E - E_F)^2$, near the node. This character crucially differentiates the dc-transport properties from those of an ordinary (diffusive) metal. An outstanding question is whether the semi-metallic phase survives the ubiquitous presence of disorder or impurities. Fradkin's early result [3] indicated weak random potentials as irrelevant perturbations in 3D nodal semimetals, which would suffer a non-Anderson semimetal-to-metal transition at finite disorder strength – this is the Quantum-Criticality (QC) picture, shown in the upper Figure 2.

The QC picture was more recently put into question by deeper analysis, which considered the effects of zero-energy bound-states which can appear at either fine-tuned impurities or rare-regions of a disordered landscape [4]. It was argued that these effects destabilise the semi-metal phase even for weak uncorrelated scalar disorder, provided the local potential's distribution is unbounded. This Avoided-Quantum-Criticality (AQC) picture is supported by numerical simulations [7,8] and depicted in the lower Figure 2.

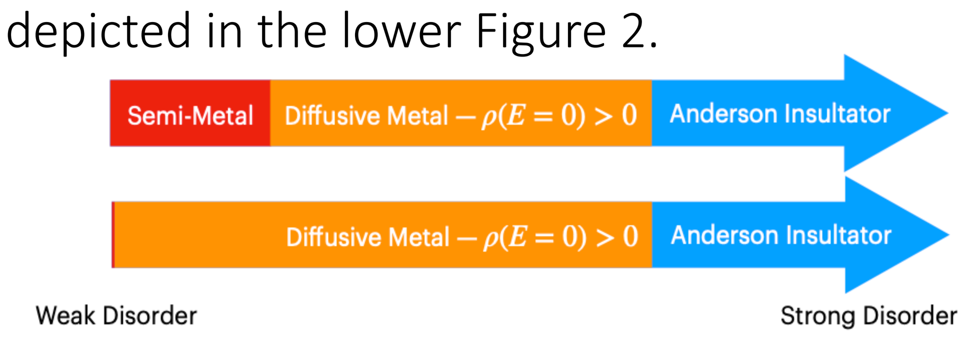

Figure 2: Depiction of the QC (upper arrow) and AQC (lower arrow) for the phase-diagram of a disordered DWSM.

STATISTICAL INSIGNIFICANCE OF RARE-REGIONS?

Granted their existence, the statistical significance of rare-region states for the bulk DoS of a DWSM have since been enquired by more sofisticated analytical means. These led to contradictory conclusions that either disprove [5] or support [6] the AQC paradigm. This state of affairs evidences the subtle issues that appear when the stability of DWSM phases is to be acessed.

In this work, we show that diluted random spherical impurities can lead to a finite zero-energy density of states (DoS) in a 3D Dirac system, destabilizing the semi-metallic node for arbitrary small impurity concentration [10].

SIMILAR VS DIVERSE IMPURITIES

Zero-energy bound states appear only for statistically insignificant fine-tuned scalar impurities - $J_j(b\lambda) = 0$ - where b/λ are the impurity radius/strength. It was argued [4] that, near these critical values ("*near-critical impurities*") the sharp low-energy resonances preceeding the bound states were enough to lift $\rho(0)$. However, this turns not to be the case [5,10] - individual resonances due to a dilute set of identical near-critical impurities always yield a zero DoS variation at $E = 0$.

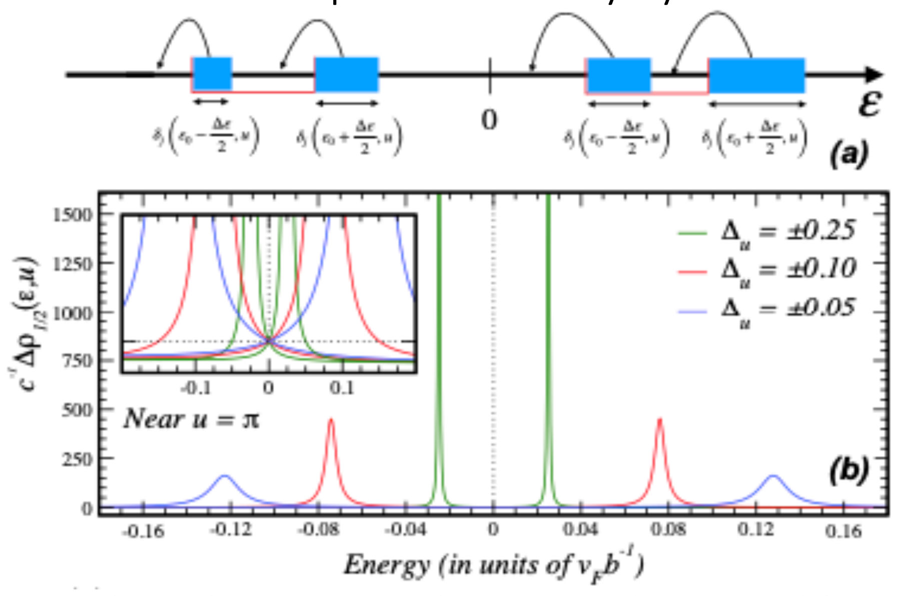

Figure 3: (a) Motion of energy levels triggered by a given central impurity, in terms of its scattering phase-shifts. (b) Plots of $\Delta\rho_{j=1/2}(E,u)$ obtained using FSR for selected deviations relative to the critical $u_c = \pi$. The inset shows the plots to have a zero pinned to the node.

The change in the DoS due to dilute impurities (for fixed impurity parameter u=λb) in Figure 3a was calculated using Friedel's Sum rule (FSR) — the change in the extensive DoS is given as a derivative of the scattering phase-shifts of a single impurity:

$$\Delta\nu(\varepsilon,u) = \frac{2}{\pi}\sum_{j=1/2}^{\infty}(2j+1)\frac{\partial\delta_j(\varepsilon,u)}{\partial\varepsilon}.$$

Our interest is not on identical impurities, but rather impurities of random strengths. In most instances, such case can be obtained simply by averaging the FSR over u (and include a concentration factor). However, if there is probability for impurity configurations around a critical u, this reasoning breaks down. Then the scattering phase-shifts become discontinuous at the node (Levinson's Theorem) and endow zero-energy modes with statistical significance. This way the semimetal phase is destabilized and gives way to a diffusive metallic phase.

To see this emergence of statistical weight, one cannot use FSR directly, but needs to go back to its derivation. For a DSM, one considers a single short-range impurity inside a finite spherical volume. The phase-shifts induced in the spherical scattering states by the impurity, translate into an E-dependent shift of the allowed energy levels. This motion of levels is related with the variation in the number of states inside a spectral window and, thus also the change in the DoS. A scheme of the argument is shown in Figure 3a and further details are found in [10].

CONFIRMATION BY LATTICE SIMULATIONS

In order to test our analytical theory, we performed ultra-high resolution simulations in lattices of up to 536 million orbitals, far beyond any previous work in 3D Dirac systems (only possible in the Kernel Polynomial Method, KPM, implementation of Quantum KITE [9]). For a direct comparison with the analytical theory, we implemented a 4-band simple cubic Dirac semimetal lattice model with 8 valleys. Spherical impurities of random strength were then scattered inside the simulated domain. Results are summed up in Figure 4 and caption (see also [10])

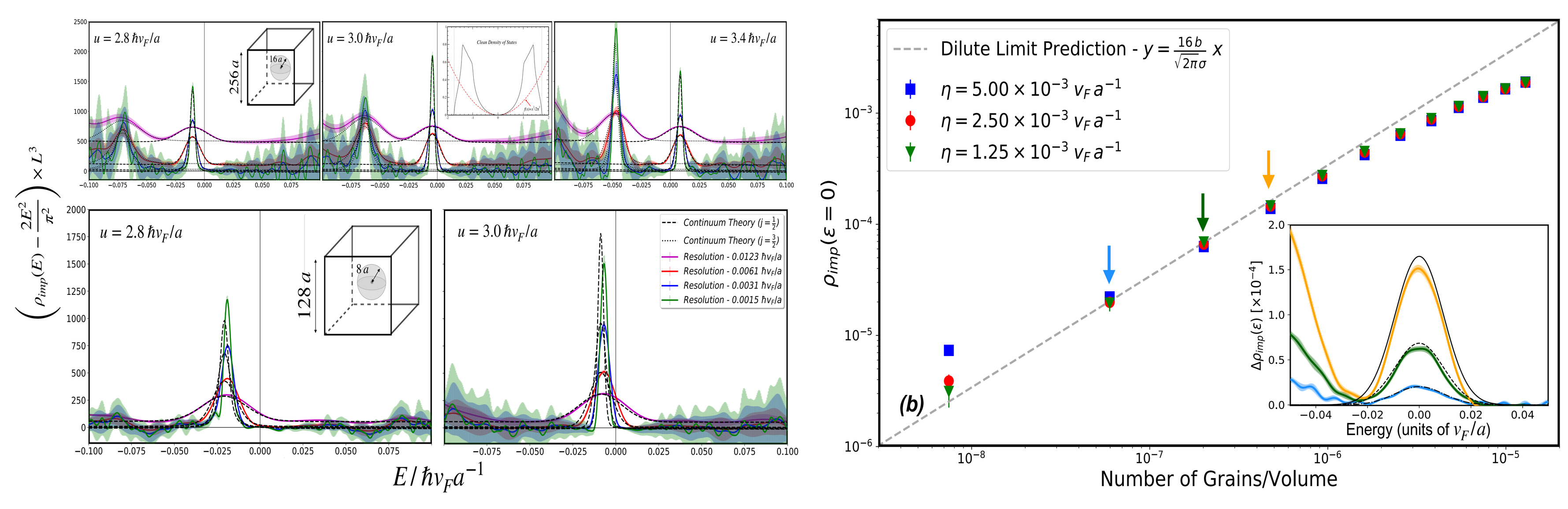

Figure 4: **Left Panel:** Change in the DoS with a single near-critical spherical impurity inside the simulated domain. Colored curves are simulated results (with error bars), while black curves are theory predictions corrected for the finite resolution (η) of the KPM simulations. For large enough spheres and simulation domains, the single-impurity results are fully repreoduced. **Right Panel:** Plot of $\langle\rho(E=0)\rangle$ with several impurities randomly placed inside the simulated supercell of 512^3 sites (without superpositions). The grey line is the theory prediction in the dilute regime - the first 4 points perfectly follow the diluted regime predictions, with deviations for larger concentrations due to multi-impurity interference effects. The inset shows the converged $\langle\rho(E)\rangle$ for 3 concentrations against the continuum theory's predictions (black lines).

J.P.S.P., B.A. and J.M.V.P.L. were supported by the Portuguese Foundation for Science and Technology (FCT) through funding **UIDB/04650/2020**, projects **POCI-01-0145-FEDER-028887** (J.P.S.P., J.M.V.P.L), **CEECIND/02936/2017** (B.A.) and grant Nr. **PD/BD/142774/2018** (J.P.S.P.). A.F. acknowledges financial support from the Royal Society through a Royal Society University Research Fellowship. The numerical calculations were performed on the Viking Cluster, which is a HPC facility provided by the University of York.

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Graphene online 2020

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