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Phys. Rev. B **87**, 155123 — Published 11 April 2013

DOI: [10.1103/PhysRevB.87.155123](https://doi.org/10.1103/PhysRevB.87.155123)

Stability of Weyl metals under impurity scattering

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We investigate the effects of bulk impurities on the electronic spectrum of Weyl semimetals, a recently identified class of Dirac-type materials. Using a T -matrix approach, we study resonant scattering due to a localized impurity in tight binding versions of the continuum models recently discussed by Burkov, Hook, and Balents, describing perturbed four-component Dirac fermions in the vicinity of a critical point. The impurity potential is described by a strength g as well as a matrix structure Λ . Unlike the case in d -wave superconductors, where a zero energy resonance can always be induced by varying the impurity scalar and/or magnetic impurity strength, we find that for certain types of impurity (Λ), the Weyl node is protected, and that a scalar impurity will induce an intragap resonance over a wide range of scattering strength. A general framework is developed to address this question, as well as to determine the dependence of resonance energy on the impurity strength.

Pathbreaking discoveries in the areas of graphene and topological insulators have focused attention on a new class of materials, known as *Dirac materials*¹⁻⁴. The hallmark of these systems is the existence of one or more symmetry-protected Dirac nodes in the electronic band structure, where the density of states (DOS) becomes vanishingly small, and which have topological implications for the existence of gapless chiral edge states⁵. Such gapless bulk (three-dimensional) band structures have been considered in a number of recent investigations⁶⁻¹². A more general taxonomy was advanced by Burkov, Hook, and Balents (BHB)¹³, who described the effects of various homogeneous perturbations on a $3 + 1$ -dimensional system with a massive Dirac point described by the four-component Hamiltonian $H_0 = \sum_{a=1}^3 k_a \Gamma^a + m \Gamma^4$ written in terms of Dirac matrices. This provides a minimal model of a system with both time-reversal (\mathcal{T}) and inversion (\mathcal{I}) symmetries, and with a single tuning parameter m which distinguishes the massless Dirac point from the normal and topological insulating phases when $m \neq 0$. BHB found that for sufficiently strong \mathcal{T} or \mathcal{I} breaking perturbations, an intermediate *Weyl semimetal* phase generally arises, in which the electronic structure is gapless and characterized by point or line nodes.

In this paper we consider the effect of localized impurities on the electronic structure in the Weyl semimetal (WS) phase. In particular, we are interested in the occurrence of resonances in the vicinity of zero energy, where the density of states vanishes as ω^2 in the WS. We say that the energy node of a Dirac/Weyl material model $H^{(0)}$ is *stable* if it does not result in a low energy resonance in the presence of a local impurity potential $g\Lambda\delta(\mathbf{x})$ with arbitrary g , where g is coupling strength and Λ is a matrix describing the scattering potential. Such resonances give rise to sharp peaks in the density of states (DOS) which disrupt the pristine Dirac spectrum¹⁴. In addition to its characteristic low energy

electronic structure, the WS is also characterized by its topological properties, which interpolate between those of the non-topological insulator (NI), where the bulk and edge spectra are both gapped, and the topological insulator (TI) or - when \mathcal{T} is broken - the Chern insulator (CI), where the bulk is gapped but gapless edge states participate in quantized surface transport. Bulk transport consequences for scalar impurities were considered in refs.^{13,15}.

We will focus on the stability of a 4-band tight binding model of Weyl materials under local impurity scattering. One might guess, based on the more familiar single-band problems, that an impurity resonance or bound state can be induced at arbitrary energy, *i.e.*, no energy is stable. This is not true for Weyl materials. Instead, we find that stability depends crucially on the type of impurity, which mathematically can be classified by its commutation relations with the Γ matrices appearing in the local Green's function. Typically an impurity is a foreign atom or local crystalline defect in an otherwise pristine material. Thus, the impurity potential should always involve a local scalar scattering component. We find that potential scattering (local chemical potential on-site change) will induce an intragap resonance and therefore will break stability at a single particle level. We will present a general framework to address the existence of impurity resonances and bound states, and the dependence of their energies on impurity strength. We will illustrate this first with a simpler case where both time reversal (\mathcal{T}) and inversion (\mathcal{I}) symmetries are conserved in the impurity-free system. There, the (fine-tuned) Dirac node is found to be unstable with \mathcal{I} -even impurities, but stable with \mathcal{I} -odd ones. The same approach can be used when \mathcal{T} and/or \mathcal{I} are broken by a homogeneous term $\eta\Gamma^{\mu\nu}$, and the Dirac node is replaced by a pair of Weyl nodes (or a line node) for sufficiently strong η . In these cases, stability depends not only on the impurity type, but also on η , the strength of the symmetry breaking term. Results will

be presented for the physically motivated Burkov-Balents model⁸ of alternating topological/normal insulator layers in an external magnetic field (η) along the stacking direction. The impurity classification can be found in Table I, and the stability phase diagram in Fig. 3. The critical field strength η_c is found to be related a form of band inversion.

Weyl material model – The models we study are lattice versions of the continuum models discussed by BHB¹³, and are defined by the following \mathbf{k} -space Hamiltonian in the Γ -matrix basis,

$$H^{(0)}(\mathbf{k}) = \xi(\mathbf{k}) \mathbb{I} + \sum_{i=1}^3 d_i(\mathbf{k}) \Gamma^i + m(\mathbf{k}) \Gamma^4 + \eta \Gamma^{\mu\nu} \quad (1)$$

where $\xi(\mathbf{k}) = -2t \sum_i \cos k_i - \varepsilon_0$, $d_i(\mathbf{k}) = -2t_1 \sin k_i$, $m(\mathbf{k}) = -4t' \sum_i (1 - \cos k_i) - \lambda$, and η is taken to be \mathbf{k} -independent for simplicity. We adopt the following Γ matrix convention: $\Gamma^i = \tau^x \otimes \sigma^i$ ($i = 1, 2, 3$), $\Gamma^4 = \tau^z \otimes \mathbb{I}$, $\Gamma^5 = -\tau^y \otimes \mathbb{I}$, and $\Gamma^{\mu\nu} = i[\Gamma^\mu, \Gamma^\nu]/2$. τ^i and σ^i are two sets of Pauli matrices acting on the orbital and spin degrees of freedom, respectively. In the model, t and t' are hoppings between same orbitals, and t_1 is the (spin-mixing) hopping between different orbitals. For $\lambda = \eta = 0$, there is a confluence of the four bands at the single Dirac node $\mathbf{k} = 0$ with energy $E = -6t - \varepsilon_0$. Such a Dirac node results from parameter fine-tuning, as nonzero λ will open up a gap. With $\eta = 0$, the model is both time-reversal and inversion symmetric. Time reversal is defined as $\mathcal{T} = \mathcal{K}\mathcal{R}$, where \mathcal{K} is complex conjugation and $\mathcal{R} = \mathbb{I} \otimes i\sigma^y$. Inversion is defined as $\mathcal{I} = \Gamma^4$ (the two “orbitals” being opposite inversion eigenstates). The model will exhibit a semimetal phase over a range of η values.

T-matrix and single impurity – The effect of localized impurities can be studied in the standard T -matrix formalism^{16,17}. We briefly recall the procedure here to establish notation. The Green’s function of the Hamiltonian $H = H^{(0)} + V$ is $G = G^{(0)} + G^{(0)}TG^{(0)}$ where $G^{(0)}(z) = (z - H^{(0)})^{-1}$ and $T = V(\mathbb{I} - G^{(0)}V)^{-1}$ is the T -matrix. Assume $H^{(0)}$ is translationally invariant, and the impurity potential is localized at the spatial point $r = 0$: $V_{\mathbf{r}\mathbf{r}'} = g\Lambda\delta_{\mathbf{r},0}\delta_{\mathbf{r}',0}$. Then the Green’s function connecting \mathbf{r} and \mathbf{r}' is $G_{\mathbf{r}\mathbf{r}'} = G_{\mathbf{r}\mathbf{r}'}^{(0)} + G_{\mathbf{r}0}^{(0)}T_0G_{0\mathbf{r}'}^{(0)}$, where $T_0(z) = (g^{-1}\Lambda^{-1} - G_{00}^{(0)}(z))^{-1}$ is the local T matrix, and $G_{00}^{(0)}(z) = \frac{1}{N} \sum_{\mathbf{k}} (z - H_{\mathbf{k}}^{(0)})^{-1}$ is the unperturbed local Green’s function. Here $H_{\mathbf{k}}^{(0)}$ is the Fourier transform of $H^{(0)}$ and N is the number of \mathbf{k} points.

The impurity effect at energy ω can numerically be characterized by the matrix norm $\|T_{00}\| = \sqrt{\sum_a |\lambda_a|^2}$ where λ_a are eigenvalues of $T_{00}(\omega + i0^+)$. For instance, if $\|T_{00}(\omega + i0^+)\|$ is large, the local density of states (LDOS) $\rho(\omega) = \rho_{\mathbf{r}}(\omega) = -\text{Im} \text{Tr} G_{\mathbf{r}\mathbf{r}}(\omega + i0^+)/\pi$ will in general deviate significantly from the unperturbed one close to the impurity, yielding a sharp resonance peak. In Fig. 1, we plot $\log \|T_{00}\|$ for three impurity forms, showing two qualitatively different cases: in (a) the Dirac node is sta-

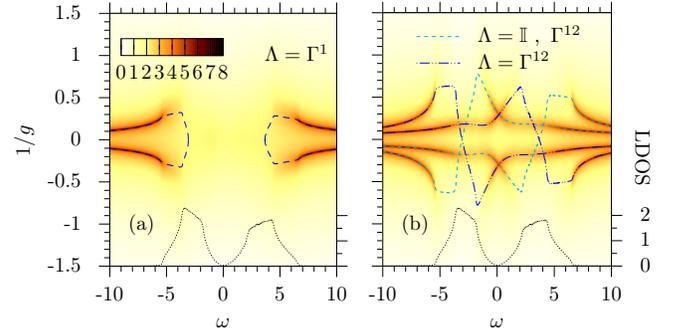


FIG. 1: (Color online) Background image: $\log \|T_{00}(\omega + i\epsilon)\|$ for \mathcal{T} and \mathcal{I} symmetric case ($\eta = 0$). Darker color corresponds to stronger impurity effect. Unperturbed DOS is shown at the bottom. Colored lines interpolating the dark curves are obtained by replacing $G_{00}^{(0)}$ with $\mathcal{G}_{00}^{(0)}$ (see text). For $\Lambda = \Gamma^1$ (a), the Dirac node is stable. Panel (b) shows results for $\Lambda = \Gamma^{12}$ (all curves) and for $\Lambda = \mathbb{I}$ (blue dashed curve only); the Dirac node is unstable. Parameters used are $t = 0.05$, $t_1 = -0.5$, $t' = -0.25$, $\lambda = 0$, $\varepsilon_0 = -0.3$, and lattice size $N_x = N_y = N_z = 50$. Spectral broadening ϵ is set to 0.05.

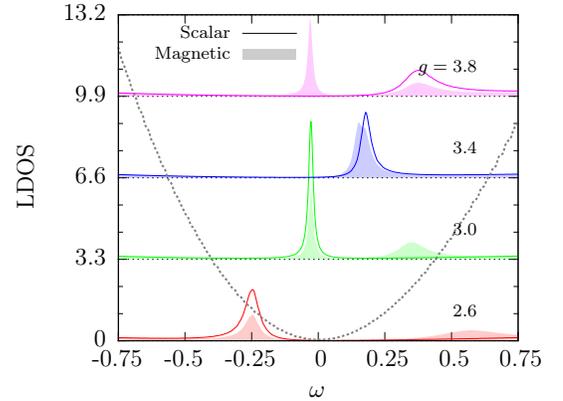


FIG. 2: (Color online) Resonance LDOS at nearest neighbor site $[x, y, z] = [0, 0, 1]$ by scalar and magnetic impurities. Solid curves: scalar impurity ($\Lambda = \mathbb{I}$). Shaded curves: magnetic scattering ($\Lambda = \Gamma^{12}$). LDOS with different g couplings are plotted on different base lines. Gray dotted curve: unperturbed LDOS rescaled. Same parameters as used in Fig. 1.

ble because T_{00} has no poles near $\omega = 0$. For scalar or purely magnetic impurities (b), the stability of the Dirac node is disrupted by low energy resonances. Fig. 2 plots for case (b) the LDOS on the nearest neighbor site of the impurity. The positions of the resonance peaks agree with the large $\log \|T_{00}\|$ line in Fig. 1(b).

Bound states and resonances – Bound states appear as poles in $G(\omega)$, which is to say zeros of $T_{00}^{-1}(\omega) = g^{-1}\Lambda^{-1} - G_{00}^{(0)}(\omega)$. This may occur when ω lies outside the bulk bands. Resonances are solutions where ω is extended to have a finite imaginary part, which is inversely proportional to the resonance lifetime. In solving numerically for the resonances, it is convenient to de-

Λ	commutation with $\Gamma^4, \Gamma^{12}, \Gamma^4\Gamma^{12}$	g^{-1} yielding $\det(\Lambda/g - \mathcal{G}_{00}^{(0)}) = 0$	physical types
$\mathbb{I}, \Gamma^4, \Gamma^{12}, \Gamma^{35}$	(+, +, +)	$s_\Lambda/g = a + s_4b_1 + s_{12}b_2 + sb_3$	scalar, J_z and/or layer-swapping
$\Gamma^{13}, \Gamma^{15}, \Gamma^{23}, \Gamma^{25}$	(+, -, -)	$1/g^2 = (a + s_4b_1)^2 - (b_2 + s_4b_3)^2$	J_\parallel with or without layer-swapping
$\Gamma^3, \Gamma^5, \Gamma^{34}, \Gamma^{45}$	(-, +, -)	$1/g^2 = (a + s_{12}b_2)^2 - (b_1 + s_{12}b_3)^2$	layer-mixing with or without J_z
$\Gamma^1, \Gamma^2, \Gamma^{14}, \Gamma^{24}$	(-, -, +)	$1/g^2 = (a + sb_3)^2 - (b_1 + sb_2)^2$	J_\parallel with layer-mixing

TABLE I: Impurity classification for point-node Weyl semi-metal, with $\Gamma^{\mu\nu} = \Gamma^{12}$ in eqn. 1. In the second column, + denotes commute and - anticommute. a and b_i are defined after eqn. 3, principal values are implicitly taken. s_4, s_{12} and s_Λ are eigenvalues of Γ^4, Γ^{12} and Λ , respectively, and take the value ± 1 . $s \equiv s_4s_{12}$. In the last column, J_z refers to magnetic impurities in the z (stacking) direction, and J_\parallel those in the xy (layer) direction. See Fig. 3 for stability phase diagram of the last three classes.

fine $\mathcal{G}_{00}^{(0)}(\omega) = \frac{1}{2}(G_{00}^{(0)}(\omega + i\epsilon) + [G_{00}^{(0)}(\omega + i\epsilon)]^\dagger)$, where $\epsilon \rightarrow 0$ is always greater than the energy spacing between consecutive quantized levels. We then seek solutions to $u_a(\omega) = g^{-1}$, where $\{u_a(\omega)\}$ are the eigenvalues of $\mathcal{G}_{00}^{(0)}\Lambda$. This prescription works well when the bulk DOS is small, as we show in Fig. 1, and is exact when the DOS vanishes. Thus, if, for a given real value of ω , at least one of the eigenvalues $\{u_a(\omega)\}$ is real, and if the bulk DOS is small, then a bound state or resonance exists for coupling $g = 1/u_a(\omega)$. If all $u_a(\omega)$ have imaginary part, then ω is a stable energy. An immediate consequence is that an impurity with $[\Lambda, \mathcal{G}_{00}^{(0)}] = 0$ will for some g disrupt the stability at ω , because product of commuting Hermitian matrices has real eigenvalues. Single-band problems fall in this category as $\Lambda = \mathbb{I}$.

Dirac node – To illustrate the stability criteria, we consider first the case with $\eta = 0$, where both \mathcal{I} and \mathcal{T} symmetries are present. Inverting Eq. 1, one finds that the only Γ matrix appearing in $G_{00}^{(0)}$ is Γ^4 , which is also the inversion operator,

$$G_{00}^{(0)}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\omega - H^{(0)}(\mathbf{k})} = a(\omega)\mathbb{I} + b(\omega)\Gamma^4 \quad (2)$$

with $a = \frac{1}{N} \sum_{\mathbf{k}} [\omega - \xi(\mathbf{k})]/D(\mathbf{k})$, $b = \frac{1}{N} \sum_{\mathbf{k}} m(\mathbf{k})/D(\mathbf{k})$, and $D(\mathbf{k}) = [\omega - \xi(\mathbf{k})]^2 - \sum_i d_i^2(\mathbf{k}) - m^2(\mathbf{k})$. In the following, we will restrict to impurities where Λ is either the identity or a single Γ -matrix; linear combinations thereof can be analyzed in the same fashion. Λ belongs to one of two classes: Γ^C which commutes with Γ^4 , and Γ^A which anticommutes. Following our general criteria, we solve for real eigenvalues of $\mathcal{G}_{00}^{(0)}\Lambda$. The commuting case has already been discussed, thus inversion-even impurities may disrupt stability at any energy, including the Dirac node. As an example, the purely magnetic impurity $\Lambda = \Gamma^{12} = \mathbb{I} \otimes \sigma^z$ is shown in Fig. 1(b), where dashed lines are the eigenvalues u_a . The corresponding LDOS on the nearest neighbor site to the impurity is plotted in Fig. 2 for various g which induces resonance around the Dirac node. For inversion-odd impurities, we have $\mathcal{G}_{00}^{(0)}\Gamma^A = a\Gamma^A + b\Gamma^4\Gamma^A$, and $u(\omega) = \pm\sqrt{a(\omega)^2 - b(\omega)^2}$, where principal values of a and b are implicitly taken, as will be all such coefficients in the rest of the paper. Reality of $g^{-1} = u$ then requires $|a(\omega)| > |b(\omega)|$. A representative case with $\Lambda = \Gamma^1 = \tau^x \otimes \sigma^x$ is shown in

Fig. 1(b), where real u are the dashed blue lines.

The region between the two LDOS “towers” is stable in Fig. 1(b). This in fact is true for all inversion-odd impurities and is not accidental. This follows analytically from the *band center approximation* (BCA) in which the local Green’s function, $\mathcal{G}_{00}^{(0)}$, is replaced with the Green’s function of the local Hamiltonian, $\bar{G}(\omega) \equiv (\omega - H_{00}^{(0)})^{-1}$, where $H_{00}^{(0)} = \frac{1}{N} \sum_{\mathbf{k}} H^{(0)}(\mathbf{k})$. It is easy to verify that $H_{00}^{(0)}$ has eigenvalues $\Omega_{\pm} = -\epsilon_0 \pm \delta$, with $\delta = |12t' + \lambda|$, which are doubly degenerate due to inversion symmetry. We shall call Ω_{\pm} band centers as they represent in some sense the average position of the bands. The eigenvalues of $\bar{G}(\omega)$ are thus $1/(\omega - \Omega_{\pm})$. Comparing with eqn. 2, we find the BCA for a and b as $a^{BCA} = \frac{\omega + \epsilon}{(\omega + \epsilon)^2 - \delta^2}$ and $b^{BCA} = -\frac{\delta}{(\omega + \epsilon)^2 - \delta^2}$. Invoking our earlier results, $g = 1/u$ is imaginary for $\omega \in [\Omega_-, \Omega_+]$. Thus the Dirac node, being in between the band centers in general, is stable with \mathcal{I} -odd impurities.

Weyl semimetal phase – BHB¹³ found a WS phase intervenes when \mathcal{T} or \mathcal{I} is broken sufficiently strongly. Depending on $\Gamma^{\mu\nu}$ in Eq. 1, degeneracy of the two central bands may occur either at discrete points or along a line in the Brillouin zone. We now consider the effect of local impurity on the WS phase induced by the \mathcal{T} -breaking term $\Gamma^{\mu\nu} = \Gamma^{12} = \mathbb{I} \otimes \sigma^z$. A complete classification will be presented elsewhere¹⁸. The Hamiltonian Eq. 1 can be used to model an alternating stack of topological insulator and normal insulator layers immersed in a magnetic field along the stacking direction (the Γ^{12} term), as proposed in Ref. 8. The local Green’s function is

$$G_{00}^{(0)}(\omega) = a(\omega)\mathbb{I} + b_1(\omega)\Gamma^4 + b_2(\omega)\Gamma^{12} + b_3(\omega)\Gamma^4\Gamma^{12} \quad (3)$$

where all coefficients can be obtained analytically¹⁸. Note that all four terms in Eq. 3 mutually commute.

Following the general stability criteria, we find that impurities fall into four classes, based on the commutation relations of Λ with the three Γ matrices in eqn. 3. The results are summarized in Table I. The fully commuting class (+, +, +) always yields a real g solution for any ω and η . For the other three classes, there are stable zones in the ω - η plane where g is imaginary. A phase diagram

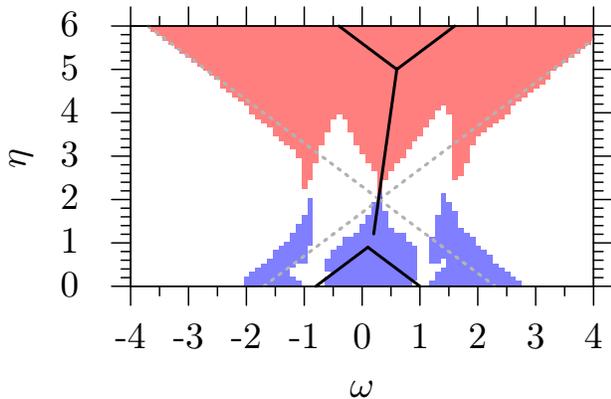


FIG. 3: (Color online) Stability of \mathcal{T} -breaking Weyl semimetal. The vertical axis η is the strength of the \mathcal{T} -breaking term. Red: stable zone for impurity classes $(+, -, -)$ and $(-, -, +)$. Blue: stable zone for impurity classes $(-, +, -)$ and $(-, -, +)$. See Table I for impurity classification. Solid black lines mark the two band edges bounding the central gap. They touch from around $\eta = 1$ to 5, corresponding to the Weyl semimetal phase. The black lines are broken around $\eta = 1$ due to the closing of the indirect gap. Dotted gray lines are the stable zone boundaries given by the band center approximation. Parameters used are $t = 0.05, t_1 = -0.5, t' = -0.25, \lambda = 1, \varepsilon_0 = -0.3$, on a lattice of $N_x = N_y = N_z = 50$.

is shown in Fig. 3, where red is the stable zone of the class $(+, -, -)$, blue of $(-, +, -)$, and $(-, -, +)$ is stable in both red and blue zones. The general shape of the zone boundary can be understood by invoking the band center approximation again, *viz.* $\mathcal{G}_{00}^{(0)}(\omega) \simeq (\omega - H_{00}^{(0)})^{-1}$. This yields the two dotted lines in Fig. 3 given by

$$\omega = \Omega_{\pm} = -\varepsilon_0 \mp (|\delta| - |\eta|), \quad (4)$$

which are nothing but the central two of the band centers (eigenvalues of $H_{00}^{(0)}$). A band center inversion occurs when $\eta_c = \pm\delta$, at which point $\Omega_+ = \Omega_-$. It may be viewed as a stability critical point (critical external magnetic field) in the sense that the stable zones of the classes $(+, -, -)$ and $(-, +, -)$ are each restricted to only one side of η_c . One may think of impurity levels as forming an energy band parameterized by the strength g , then stable zones in the phase diagram are gaps of the “impurity band”, and η_c marks a transition between gapless and gapped phases. This is reminiscent of the Bloch band inversion associated with the topological phase transition in Chern insulators.

Average T-matrix approximation (ATA) – The resonance/bound states as discussed before will broaden into a “band” when multiple impurities are present. Here we consider an ensemble of local impurities of the same ma-

trix form, with a homogeneous spatial concentration c and a distribution of strength $f(g)$. We find that average DOS is enhanced at resonance energy $\omega_{\text{res}}(g)$ obtained from a single impurity when $f(g)$ is relatively

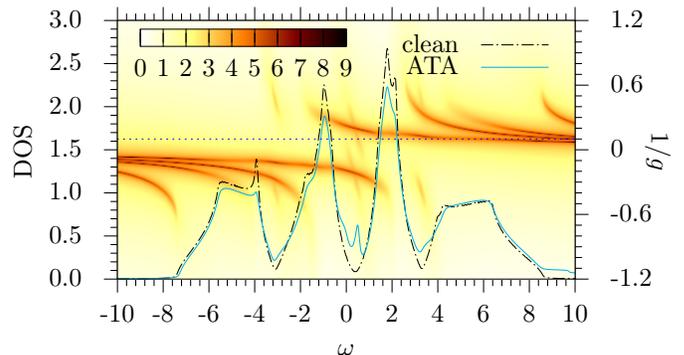


FIG. 4: (Color online) Average DOS using ATA for $\Gamma^{\mu\nu} = \Gamma^{12}$ (external magnetic field along \hat{z}) and scalar impurity $\Lambda = \mathbb{I}$. Impurity concentration is $c = 10\%$ and impurity strengths are uniformly distributed in $g \in (0, 10]$. Solid blue line: ATA result. Dash-dot black line: DOS of clean system. Background color image: $\log ||T_{00}||$ of single impurity as a function of ω and g^{-1} , similar to Fig. 1. Dotted horizontal line marks maximum g used in ATA ($g^{-1} = 0.1$), the ATA DOS is significantly enhanced in the range of ω in which the high $\log ||T_{00}||$ lines exist above $g^{-1} = 0.1$. η is set to 3, putting the clean system in the WS phase (Fig. 3). Other parameters used are the same as in Fig. 3.

high. In the ATA formalism^{16,17}, translational invariance is restored after statistical averaging, and the effect of the impurity ensemble is captured by the local self energy $\Sigma_{\text{loc}} = c \langle T_{00} \rangle [1 + c G_{00}^{(0)} \langle T_{00} \rangle]^{-1}$, where $\langle \dots \rangle$ denotes averaging over $f(g)$. The local Green’s function is $G_{\text{loc}}(z) = \frac{1}{N} \sum_k 1/(z - H^{(0)}(k) - \Sigma_{\text{loc}})$ and the average DOS is $\rho(\omega) = -\text{Im Tr } G_{\text{loc}}(\omega + i0^+)/\pi$. In Fig. 4, we show the average DOS of a sample immersed in an external magnetic field ($\Gamma^{\mu\nu} = \Gamma^{12}$) with magnetic impurities breaking local inversion symmetry ($\Lambda = \Gamma^3$). The impurity strengths are uniformly distributed in $g \in (0, 10]$. The difference in DOS with the clean system agrees with the single impurity $||T_{00}||$ (shown as colored background).

a. Acknowledgement We are grateful to A. Vishwanath, R. Biswas, and A. Black-Shaffer for useful discussions. This work was supported in part by the NSF through grant DMR-1007028. Work at LANL was supported by US DoE Basic Energy Sciences and in part by the Center for Integrated Nanotechnologies, operated by LANS, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. Work at Nordita was supported by ERC and VR.

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