Impurities in three-dimensional quadratic band-touching Luttinger semimetals: Friedel and RKKY oscillations

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We investigate the response of three-dimensional Luttinger semimetals to localized charge and spin impurities as a function of doping. The strong spin-orbit coupling of these materials strongly influences the Friedel oscillations and RKKY interactions. This can be seen at short distances with an $1/r^4$ divergence of the responses and anisotropic behavior. Certain of the spin-orbital signatures are robust to temperature, even if the charge and spin oscillations are smeared out, and give an unusual diamagnetic Pauli susceptibility. We compare our results to the experimental literature on the bismuth-based half-Heuslers such as YPtBi and on the pyrochlore iridate $Pr_2Ir_2O_7$.

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I. INTRODUCTION

Luttinger semimetals [1] such as HgTe, α -Sn, YPtBi [2], and Pr₂Ir₂O₇ [3] play an important role in the field of threedimensional (3D) topological materials. Their conduction and valence bands meet quadratically at a time-reversal-invariant and inversion-symmetric point. This degeneracy can be lifted, for example, by applying strain, to obtain a Dirac semimetal [4,5] or a topological insulator [6]. In these materials, the nontrivial topology is responsible for unusual magnetic [7–9], surface [10–12], and transport [7,13,14] properties, which can also be met in Luttinger semimetals [15]. In particular, a way to probe the strong spin-orbit properties of these materials is through their response to charge and spin impurities, respectively, referred to as Friedel oscillations [16,17] and RKKY interactions [18–20].

The Friedel oscillations and RKKY interactions are a consequence of the sharp Fermi surface of the conduction electrons. In a 3D normal electron gas they typically scale as $\cos(2k_F r)/r^3$, where *r* is the distance from the impurity and k_F the Fermi wave vector [21]. But in general, this response depends on the dimension [17,22,23], band dispersion [24–30], and temperature [31,32]. For example, in Dirac and Weyl semimetals these responses decay more rapidly at large separations, r^{-5} [25–27], when the carrier density vanishes. The quadratic dispersion of Luttinger semimetals leads to a slower decay, which may prove useful to explore the consequences of the strong spin-orbit interaction. Also, on the contrary to a Luttinger metal with heavy and light carriers [33], the chemical potential can serve to explore the spin-orbit coupling of each band separately.

In this work we study the Friedel oscillations and RKKY coupling of 3D Luttinger semimetals at finite doping. This is

inspired by recent experimental results on the bismuth-based half-Heuslers [2] and the tentalizing phase diagram of the pyrochlore iridate $Pr_2Ir_2O_7$ [3,34,35]. We compute the charge and spin response analytically at zero temperature and numerically at finite temperature. Also, because it was recently shown that Luttinger semimetals have a paramagnetic Landau susceptibility [36], which is opposite to what is expected for a normal electron gas, we compute the Pauli susceptibility and find that it is diamagnetic.

This work is organized as follows. In Sec. II we introduce and discuss the underlying model of a Luttinger semimetal. Section III contains our main results, with the expression of the charge and of the spin response to a localized inhomogeneity. We discuss our results at zero temperature and as a function of the temperature and compute the spin susceptibility of a Luttinger semimetal. In Sec. IV, we compare our results to the existing litterature on Luttinger semimetals like bismuth-based half-Heuslers (YPtBi, LuPtBi, etc.) and the pyrochlore $Pr_2Ir_2O_7$. We compare our results with the known literature on Dirac semimetals.

II. MODEL

At a quadratic band touching, the behavior of noninteracting electrons can be described with the Luttinger Hamiltonian [1]

$$\hat{H}_0(\mathbf{k}) = \frac{\hbar^2}{2m} \left[-\frac{5}{4} \mathbf{k}^2 \,\hat{\mathbb{1}} + (\mathbf{k} \cdot \hat{\mathbf{J}})^2 \right] - E_F, \qquad (1)$$

where the band mass is *m* and $\hat{\mathbf{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$ are the j = 3/2 total angular momentum operators. This model has rotation, inversion, and time-reversal symmetries [1]. The four eigenstates of $\hat{H}_0(\mathbf{k})$ can be labeled with the eigenvalues $\lambda = \pm 1/2, \pm 3/2$ of the helicity operator $\hat{\lambda} = \mathbf{k} \cdot \hat{\mathbf{J}}/k$, and the corresponding spectrum $\xi_{\pm}(\mathbf{k}) = \pm \hbar^2 k^2/(2m) - E_F$ is drawn

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FIG. 1. Spectrum of a Luttinger semimetal for (a) m > 0 and (b) m < 0. The Fermi surface is in the lower band, and depending on the sign of the band mass m, it crosses different eigenstates, (a) $|\pm 1/2\rangle_{\mathbf{k}}$ and (b) $|\pm 3/2\rangle_{\mathbf{k}}$, of the helicity operator $\hat{\lambda} = \mathbf{k} \cdot \hat{\mathbf{J}}/k$. This influences the intraband and interband scattering in the presence of a magnetic impurity. We refer to the lower and upper bands as the conduction and valence bands, respectively, in the text, since we consider hole doping.

in Fig. 1. The precise expression of the corresponding eigenvector is cumbersome and in the following we use the thermal Green's function

$$\hat{G}(\mathbf{k}, i\omega_n) = -\frac{i\omega_n + \hat{H}_0(\mathbf{k})}{(\xi_+(\mathbf{k}) + i\omega_n)(\xi_-(\mathbf{k}) + i\omega_n)}, \qquad (2)$$

where $\hbar \omega_n = (2n+1)\pi k_B T$ is the Matsubara frequency at temperature *T*.

In the following we set $\hbar = k_B = 1$ and write energies in units of the Fermi energy, $|E_F|$, and wave vectors in units of the Fermi wave vector, k_F . We consider that the Fermi energy is in the lower band, $E_F = -k_F^2/(2|m|) < 0$, but we should keep in mind that, depending on the sign of *m*, the Fermi surface can cross eigenstates with either helicity $\pm 1/2$ if m > 0 or helicity $\pm 3/2$ if m < 0 (see Fig. 1). These two situations will alter the RKKY coupling.

III. RESPONSE TO CHARGE AND SPIN IMPURITIES

In the presence of a charge impurity with potential $V_0\delta^{(3)}(\mathbf{r})$ and a magnetic impurity with potential $V_1\mathbf{S}(\mathbf{r}) \cdot \hat{\mathbf{J}}\delta^{(3)}(\mathbf{r})$, a Luttinger semimetal is perturbed by the Hamiltonian [1]

$$\hat{H}_1(\mathbf{r}) = (V_0 \hat{\mathbb{1}} + V_1 \,\mathbf{S} \cdot \hat{\mathbf{J}})\delta^{(3)}(\mathbf{r}), \qquad (3)$$

where $\mathbf{S} = \{S_x, S_y, S_z\}$. We neglect the anisotropic contributions, such as $\mathbf{S} \cdot \hat{\mathbf{J}}^3$ [1], which is a reasonable approximation for most Luttinger semimetals with the exception of $\Pr_2 Ir_2 O_7$ [1,4,5].

In linear perturbation theory, the carrier density $J_0(\mathbf{r}) = \langle \hat{n}(\mathbf{r}) \rangle = \langle \hat{\psi}_{\mathbf{r}}^{\dagger} \hat{\psi}_{\mathbf{r}} \rangle$ and the j = 3/2 pseudospin operators $J_i(\mathbf{r}) = \langle \hat{J}_i(\mathbf{r}) \rangle = \langle \hat{\psi}_{\mathbf{r}}^{\dagger} \hat{J}_i \hat{\psi}_{\mathbf{r}} \rangle$ are

$$J_{\mu}(\mathbf{r}) = \sum_{\nu=0}^{3} \chi_{\mu\nu}(\mathbf{r}) S_{\nu}, \qquad (4)$$

where $\mu \in \{0, 1, 2, 3\}$ and $S_0 = 1$. The generalized susceptibility at a temperature *T* is a sum over Matsubara frequencies,

$$\chi_{\mu\nu}(\mathbf{r},T) = -T \sum_{\omega_n} \text{Tr}[\hat{G}(\mathbf{r},i\omega_n)\hat{J}_{\mu}\hat{G}(-\mathbf{r},i\omega_n)\hat{J}_{\nu}].$$
 (5)

Here, for the sake of clarity we introduce $\hat{J}_0 \equiv \hat{1}$. Note that in the present work we only consider the static regime, i.e., Eq. (5) does not depend on the frequency, which is appropriate in the study of impurities. The dynamic charge polarizability at T = 0 was derived in [37,38]. In a previous work [37] we also show that the Hamiltonian, (1), has no chargespin coupling, that is, $\chi_{i0} = \chi_{0i} = 0$ for $i \in \{1, 2, 3\}$. In Weyl semimetals, this coupling between charge and spin degrees of freedom allows for spin polarization of charge fluctuations [39]. The generalized susceptibility in the unperturbed, homogeneous gas depends only on $(\mathbf{r} - \mathbf{r}')$ and (t - t'). In Eq. (5) and what follows we express χ_{00} in units of $V_0 E_F N_0^2$ and χ_{ij} in units of $V_1 E_F N_0^2$, where $N_0 = 1/(4\pi^2)$ is the density of states per spin of an electron gas.

The real-space representation of the Green's function in Eq. (5) is derived in Appendix A. We use rotation symmetry to absorb the angular dependence in a unitary transformation $\hat{U}_{\theta\phi}$ on the spinor subspace, i.e., $\hat{G}(\mathbf{r}, i\omega_n) = \hat{U}_{\theta,\phi} \hat{G}(r\mathbf{e}_z, i\omega_n) \hat{U}_{\theta,\phi}^{\dagger}$ and

$$\hat{G}(r\mathbf{e}_{\mathbf{z}}, i\omega_n)/N_0 = \left[(i\omega_n - \operatorname{sgn}(m))I_0(r, i\omega_n) + \frac{5}{4} \left(\frac{2}{r} \partial_r I_0(r, i\omega_n) + \partial_r^2 I_0(r, i\omega_n) \right) \right] \hat{\mathbb{1}} \\ - \partial_r I_0(r, i\omega_n) \left(\hat{J}_x^2 + \hat{J}_y^2 \right) - \partial_r^2 I_0(r, i\omega_n) \hat{J}_z^2,$$
(6)

where the radial dependence of the Green's function is described by $I_0(r, i\omega_n) = -\frac{1}{r}(A_2(r, i\omega_n) + B_2(r, i\omega_n))$ and its derivatives.

We introduce the functions $A_p(r, i\omega_n)$ and $B_p(r, i\omega_n)$, which are related to the contribution from the valence and from the conduction band for a given sign of *m* as shown schematically in Fig. 1:

$$A_p(r, i\omega_n) = \frac{\pi (-i \operatorname{sgn}(\omega_n))^p}{2(-\operatorname{sgn}(m) + i\omega_n)^{p/2}} e^{\operatorname{sgn}(\omega_n)ir\sqrt{-\operatorname{sgn}(m) + i\omega_n}},$$
(7)

$$B_p(r, i\omega_n) = \frac{\pi (-i \operatorname{sgn}(\omega_n))^p}{2(\operatorname{sgn}(m) - i\omega_n)^{p/2}} e^{-\operatorname{sgn}(\omega_n)ir\sqrt{\operatorname{sgn}(m) - i\omega_n}}.$$
 (8)

Thus, the generalized susceptibility, (5), is a sum over all excitations within or between the two bands, which are decomposed over the functions $AA_{k+p}(r, T) =$ $T \sum_{\omega_n>0} A_k A_p$, $BB_{k+p}(r, T) = T \sum_{\omega_n>0} B_k B_p$, and $AB_{k+p}(r, T) = i^k T \sum_{\omega_n>0} A_k B_p$: the expressions with the sum at negative frequencies are simply the complex conjugates of these. We numerically perform the summation on Matsubara's frequencies at $T \neq 0$. At T = 0 the sum becomes an integral and we compute these expressions explicitly in Appendix B. As expected we find that at zero temperature the intravalence band terms vanish, i.e., there are no contributions from intravalence band scattering since the band is empty. In what follows we separately discuss the charge response, related to the Friedel oscillations, and the magnetic response, related to the RKKY coupling. From the



FIG. 2. Friedel oscillations in response to an impurity that increases the potential at $\mathbf{r} = 0$ in a Luttinger semimetal with holelike doping at (a) T = 0 with both intraband and interband contributions and (b) $T \neq 0$, showing the damping as the temperature increases. The intraband contribution dominates at both short and long range and the interband coupling is only apparent at short range.

latter we compute the temperature dependence of the Pauli susceptibility.

In the following we express the susceptibilities in terms of the combinations $AA_p(r, T)$, $BB_p(r, T)$, and $AB_p(r, T)$ for a general value of the mass *m*. In Appendix B we explicitly compute the expression of these combinations at T = 0 in the case of a positive mass and deduce the corresponding expressions for a negative one.

A. Friedel oscillations

The charge response of a spin-degenerate normal electron gas at T = 0 in units of $V_0 E_F N_0^2$ is [21]

$$\chi_{00}^{3\text{DEG}}(r, T=0) = \frac{2\pi(\sin(2r) - 2r\cos(2r))}{r^4}.$$
 (9)

In a Luttinger semimetal, the generalized susceptibility also includes interband transitions due to the strong spin-orbit coupling. We compute the trace in Eq. (5) using the Green's function, (6), and we find

$$\chi_{00}(r,T) = -\frac{4}{r^6} (9(BB_4 + AA_4) + 18r(BB_3 - AA_3) + 15r^2(BB_2 + AA_2) + 6r^3(BB_1 - AA_1) + 2r^4(BB_0 + AA_0) - 18AB_4 - 18(1 - i)rAB_3 + 18r^2iAB_2 + 6r^3(1 + i)AB_1) + c.c., (10)$$

where the functions on the right-hand side are evaluated for (r, T) and c.c. stands for complex conjugate. We note here that the charge response is symmetric with respect to the sign of the mass.

At zero temperature T = 0, the charge susceptibility behaves as in Fig. 2(a). In this figure we decompose the charge susceptibility in terms of intraband contributions, given by AA_k or BB_k terms, and interband contributions, given by AB_k terms. The intraband contribution shows an oscillating behavior, which is expected from the sharpness of the Fermi surface, which forbids excitations with wave vector $q > 2k_F$, in the static regime. Oscillations in the interband contribution decay exponentially with distance since the only interband

contributions are virtual excitations in the static regime. At long range, $r \gg 1$, the response is dominated by the intraband contribution and is about half that in a normal electron gas given in Eq. (9). The consequences of spin-orbit coupling are more apparent at short range, $r \ll 1$, where the response is approximately

$$\chi_{00}(r \ll 1, T = 0) \approx -\frac{3\pi(\pi - 2)}{r^4}.$$
 (11)

This is in strong contrast with a normal electron gas where $\chi_{00}^{3\text{DEG}}(r \ll 1, T = 0,) \approx 16\pi/3r$. This is the result of a strong intraband coupling at short range, as we can see from the intraband and interband contributions of this asymptotic behavior. We find that the intraband contibution is $\chi_{00}^{(\text{intra})} \approx \frac{-3\pi^2}{r^4} + \frac{8\pi}{5r}$ and the interband one is $\chi_{00}^{(\text{inter})} \approx \frac{6\pi}{r^4} - \frac{8\pi}{5r}$ and we note that the intraband contribution dominates at small r. Also, the 1/r behavior associated with the 3DEG appears in both contributions, but they totally cancel each other. The power law in Eq. (11) can be related to the linear component of charge polarizability in momentum space [37]. This is of similar origin to the $1/r^5$ divergence observed in Dirac semimetals and the difference in power laws is a consequence of the difference in band dispersions.

At $T \neq 0$ we observe a change in the decaying behavior, from power-law to exponential decay, as shown in Fig. 2(b). There, we also observe the expected damping of Friedel oscillations with a change in their periodicity.

B. RKKY coupling

In the absence of spin-orbit coupling, the magnetization profile of a normal electron gas in response to a magnetic impurity is isotropic (i.e., $\chi_{ij} = \chi_s^{3\text{DEG}} \delta_{ij}$) just like the charge response in Eq. (9) [21,40]. On the contrary, in a Luttinger semimetal, the spin response $\hat{\chi}_s$ is anisotropic. The angular dependence of $\hat{\chi}_s$ is absorbed in the rotation matrix $\hat{R}_{\theta\phi}$, where θ and ϕ are the angular coordinates of the separation



FIG. 3. Amplitude of the transverse, χ_T , and longitudinal, χ_L , RKKY coupling between two magnetic impurities for a single quadratic band ($\chi_L = \chi_T$, with m < 0) and a Luttinger semimetal (with holelike doping). (a, b) At T = 0, with m > 0 (a) and m < 0 (b). Insets: $10 \times$ zoom-ins. (c, d) At finite temperature with m > 0 (c) and m < 0 (d). Contrary to a normal electron gas, a Luttinger semimetal has opposite transverse and longitudinal couplings at short distances. This behavior is preserved at higher temperatures, where we also observe a change in the periodicity of the oscillations.

r to the impurity,

$$\hat{\chi}_{S}(\mathbf{r},T) = \hat{R}_{\theta,\phi} \begin{pmatrix} \chi_{T}(r,T) & 0 & 0\\ 0 & \chi_{T}(r,T) & 0\\ 0 & 0 & \chi_{L}(r,T) \end{pmatrix} \hat{R}_{\theta,\phi}^{T}.$$
(12)

The diagonal components $\chi_T(r, T)$ and $\chi_L(r, T)$ are, respectively, the transverse and longitudinal spin responses,

$$\chi_T(r, T) = \frac{1}{r^6} (9(BB_4 + AA_4) + 18r(BB_3 - AA_3)) + 3r^2(BB_2 + 9AA_2) - 6r^3(BB_1 + 3AA_1)) - 8r^4BB_0 - 18AB_4 - 18(1 - i)rAB_3 + 6(4 + 3i)r^2AB_2 + 6(3 - i)r^3AB_1 + 12r^4AB_0) + c.c.,$$
(13)

$$\chi_L(r, T) = -\frac{1}{r^6} (45(BB_4 + AA_4) + 90r(BB_3 - AA_3)) + r^2 (51BB_2 + 99AA_2) + 6r^3 (BB_1 - 9AA_1) + 2r^4 (BB_0 + 9AA_0) - 90AB_4 - 90(1 - i)rAB_3 + 6(8 + 15i)r^2 AB_2 + 6(9 + i)r^3 AB_1) + c.c.,$$
(14)

where the functions on the right-hand side are evaluated for (r, T) and c.c. stands for complex conjugate. The functions

 AA_p , BB_p , and AB_p are the same as the ones involved in computing the charge response in Eq. (10) and their expressions at T = 0 are reported in Appendix B.

We find that the spin response depends on the sign of the mass m in Eq. (1). We recall that this parameter does not affect the band dispersion but only the chirality of the states at the Fermi surface, which we illustrate in Figs. 1(a) and 1(b). We thus distinguish the situations where m is positive and negative with a superscript \pm on the spin response. In Figs. 3(a) and 3(b) we plot the transverse and longitudinal spin susceptibilities at zero temperature.

The intraband scattering dominates the long-range behavior, $r \gg 1$, and the spin response follows the same power law as in a normal electron gas. However, the spin response stays anisotropic even at long range with, for each sign of *m*,

$$\chi_T^+(r \gg 1, T = 0) \approx \chi_{00}^{3\text{DEG}}(r)/2,$$

 $\chi_L^+(r \gg 1, T = 0) \approx \chi_{00}^{3\text{DEG}}(r)/8;$ (15)

$$\chi_T^-(r \gg 1, T = 0) \approx -\frac{9\pi}{2r^4}\sin(2r),$$

 $\chi_L^-(r \gg 1, T = 0) \approx 9\chi_{00}^{3\text{DEG}}(r)/8.$ (16)

We note that in the long-range behavior, the longitudinal response has an amplitude $\lambda^2/2$, with λ the helicity crossing the Fermi surface (see Fig. 1), compared to the normal electron gas. This does not happen for the transverse response, where we even observe that χ_T^- decreases in $1/r^4$ instead of the $1/r^3$ for a normal electron gas.

Close to the magnetic impurity, the short-range spin-spin response is anisotropic, with opposite transverse and longitudinal contributions:

$$\chi_T^{\pm}(r \ll 1, T = 0) \approx \frac{3\pi(2+\pi)}{4r^4} \mp \frac{2\pi}{3r},$$

$$\chi_L^{\pm}(r \ll 1, T = 0) \approx -\frac{15\pi(\pi-2)}{4r^4} \pm \frac{4\pi}{3r}.$$
 (17)

This, again, is related to the strong spin-orbit coupling and provides the possibility of observing both ferromagnetic and antiferromagnetic coupling between magnetic impurities, from the RKKY coupling.

We observe that for a positive mass, m > 0, the contributions to the transverse spin response χ_T^+ from intraband and interband coupling are, respectively, $\frac{15\pi^2}{4r^4} - \frac{6\pi}{r^3} + \frac{8\pi}{5r}$ and $\frac{3\pi(1-2\pi)}{2r^4} + \frac{6\pi}{r^3} - \frac{34\pi}{15r}$, and the corresponding behaviors of the longitudinal component χ_L^+ are $-\frac{39\pi^2}{4r^4} + \frac{12\pi}{r^3} + \frac{2\pi}{r}$ and $\frac{3\pi(5+4\pi)}{2r^4} - \frac{12\pi}{r^3} - \frac{2\pi}{3r}$. The intraband contribution then always dominates close to the magnetic impurity. On the contrary, for a negative mass, m < 0, the intraband and interband contributions to χ_T^- are, respectively, $\frac{-9\pi^2}{4r^4} + \frac{6\pi}{r^3} + \frac{8\pi}{5r}$ and $\frac{3\pi(1+2\pi)}{2r^4} - \frac{6\pi}{15r}$ and for χ_L^- they are, respectively, $\frac{9\pi^2}{4r^4} - \frac{12\pi}{r^3} + \frac{2\pi}{r}$ and $\frac{3\pi(5-4\pi)}{2r^4} + \frac{12\pi}{r^3} - \frac{10\pi}{3r}$. Then, close to the impurity, the two spin responses are instead dominated by the interband contribution. This indicates that the magnetic coupling at small separation is dominated by excitations involving the bands with the lowest helicities, $\lambda = \pm 1/2$.

Similarly to our observation for Friedel oscillations, this peculiar behavior in proximity to the magnetic impurity persists at higher temperatures as shown in Figs. 3(a) and 3(b). As the temperature increases, we observe a decrease in the periodicity of the RKKY oscillations and a decay in their amplitude. The long-range behavior of the spin oscillations shows an exponential decay at finite temperature. In order to complete this discussion, we now obtain the effective RKKY Hamiltonian between two impurities and also compute the Pauli susceptibility in a Luttinger semimetal.

C. Effective RKKY Hamiltonian

The interaction between two magnetic impurities S_1 and S_2 localized at, respectively, \mathbf{r}_1 and \mathbf{r}_2 , is described by the coupling Hamiltonian \hat{H}_{12} ,

$$\hat{H}_{12} = V_1 \mathbf{S}_1^T \hat{\chi}_S(\mathbf{r}, T) \mathbf{S}_2, \qquad (18)$$

where $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$, and $\hat{\chi}_S(\mathbf{r}, T)$ is given in Eq. (12). This can be rewritten in a more explicit way,

$$\hat{H}_{12}/V_1 = \chi_T \mathbf{S}_1 \cdot \mathbf{S}_2 + (\chi_L - \chi_T)(\mathbf{S}_1 \cdot \mathbf{e}_r)(\mathbf{S}_2 \cdot \mathbf{e}_r), \quad (19)$$

where \mathbf{e}_r is the unit vector that separates the two impurities and $\chi_{L,T}$ are evaluated for $r = |\mathbf{r}_2 - \mathbf{r}_1|$, the distance between the magnetic impurities. The first and second terms in Eq. (19) are, respectively, the Heisenberg and Ising contributions. There is no Dzyaloshinskii-Moriya interaction, which would be a consequence of asymmetric spin-orbit coupling [41,42] and which is absent in Eq. (1).

This effective spin-spin coupling Hamiltonian differs from that in a normal electron gas, where it is Heisenberg-like, i.e., only the first contribution in Eq. (19) is present. Here, in the



FIG. 4. Magnetic susceptibilities as a function of the temperature. The Pauli susceptibility of a normal electron gas (orange line) is paramagnetic, while it is diamagnetic in a Luttinger semimetal (solid blue line). Also shown is the Landau susceptibility in Luttinger semimetals [36], which we draw for a cutoff energy $E_0/E_F = 10$ (dashed line).

case of Luttinger semimetals, we obtain an additional coupling between the spin components parallel to their separation and in the next section we evaluate the amplitude of this term for various Luttinger semimetals. We also note that in Ref. [43], the coupling between the spin chiralities of a Luttinger semimetal is described by a Heisenberg Hamiltonian.

D. Spin susceptibility

In the presence of a uniform magnetic field, **B**, the Zeeman coupling will be [1]

$$\hat{H}_2 = -g\mu_B \hat{\mathbf{J}} \cdot \mathbf{B},\tag{20}$$

where we introduce the *g* factor and the Bohr magneton $\mu_B = e/(2m_ec)$. The spin magnetization $\mathbf{M} \equiv -\nabla_{\mathbf{B}} \langle \hat{H}_2 \rangle = g\mu_B \langle \hat{\mathbf{J}} \rangle = \hat{\chi}_P \mathbf{B}$ defines the Pauli susceptibility $\hat{\chi}_P$ [17],

$$\hat{\chi}_{P}(T) \equiv \lim_{k \to 0} \frac{\hat{\chi}_{S}(\mathbf{k}, T)}{4\pi^{2}} = \frac{1}{4\pi^{2}} \lim_{k \to 0} \int d^{3}\mathbf{r} \, \hat{\chi}_{S}(\mathbf{r}, T) e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{3\pi} \int_{0}^{\infty} dr \, r^{2} (2\chi_{T}(r, T) + \chi_{L}(r, T)) \hat{\mathbb{1}}, \qquad (21)$$

which we write in units of $(g\mu_B)^2 N_0$. Here, we perform the angular integral in position space and take the limit $k \to 0$.

We compute this integral numerically after subtracting the $1/r^4$ asymptotic contribution in Eq. (17) from χ_T and χ_L . These terms do not contribute to the Pauli susceptibility [44] and by substracting them we avoid numerical instabilities. We obtain the behavior reported in Fig. 4 and compare it to the Pauli susceptibility of a normal spin-degenerate electron gas. The response is diamagnetic instead of being paramagnetic, which is analogous to the unusual paramagnetic Landau susceptibility in Luttinger semimetals [36] that we reproduce in Fig. 4 for a cutoff energy $E_0/E_F = 10$. This diamagnetic Pauli susceptibility is a consequence of interband transitions and we find that the contribution of intraband and interband excitations to the susceptibility $\chi_P = \chi_P^{(intra)} + \chi_P^{(inter)}$ is, at T = 0, $\chi_P^{(intra)} = 5\chi_P^{3DEG}/4$ and $\chi_P^{(inter)} = -3\chi_P^{3DEG}/2$, where χ_P^{3DEG}

is the spin susceptibility of the normal electron gas. We also note that the Pauli susceptibility is independent of the sign of the mass. This behavior is also drastically different from that in Weyl semimetals, where the Pauli susceptibility cancels because a magnetic field only splits the cones in momentum space [45] and where the Landau susceptibility is diamagnetic [36,45].

IV. DISCUSSION

The carrier density of Luttinger semimetals, such as YPtBi [46–49] and Pr₂Ir₂O₇ [50], is of the order of $n \approx (0.1-1) \times$ 10^{19} cm⁻³, that is, $k_F \approx 0.3-0.7$ nm⁻¹, which is comparable to the lattice constant, $a \approx 0.5-1$ nm [51]. Thus $ak_F \approx 0.1-1$, which is well within the region with unusual charge and spin responses due to spin-orbit coupling. With impurities separated by the lattice constant size, one can expect to see the stronger charge coupling near a charge impurity and opposite signs for the transverse and longitudinal spin-spin interactions. Note that YPtBi lacks a center of inversion and allows for additional asymmetric spin-orbit interactions in Eq. (1), which split the band structure. In the present discussion we neglect this effect, which is not always present [49] and leads to a Fermi surface splitting Δk of at most 8% of k_F in this material [46]. More specifically, in the case of $Pr_2Ir_2O_7$ the magnetic coupling occurs between the 4f orbitals of the Pr^{3+} ions described by J = 4 magnetic non-Kramers doublets with $J_z = \pm 4$ [52] and separated by a distance $ak_F \approx 1.7-2$ [3,50,53]. Then the ratio between the two contributions in the effective Hamiltonian, (19), given by $\frac{\chi_L - \chi_T}{\chi_T}$ is in the region [-2.5, -3] if one takes m < 0. In this interval of ak_F , one coupling is ferromagnetic while the other is antiferromagnetic, depending on the sign of V_1 as shown in Fig. 3(b).

However, this ratio fluctuates greatly and can reach large values if one takes m > 0 since χ_T is close to 0 according to our calculations [see Fig. 3(a). In this case χ_T can be positive or negative in this interval and $\chi_L - \chi_T > 0$. A similar analysis for the family of bismuth half-Heusler MXBi (M = Y, Lu; X = Pd, Pt), where the ions are separated by $ak_F \approx 0.1-0.5$ [51,54,55], gives ratios independent of the sign of the mass and of about -2, again with one coupling being ferromagnetic and the other antiferromagnetic. In a recent work we have pointed out the importance of these Friedel oscillations in the superconductivity from the Coulomb repulsion in Luttinger semimetals [56,57]. The anisotropic magnetic coupling may also be responsible for exotic magnetic phases [58,59]. However, these short-range effects may be strongly renormalized by interactions. Here, we neglect screening and vertex corrections, which are the strongest at short range and may push these effects to even shorter ranges, as in the normal electron gas [60].

The consequences of spin-orbit coupling for Friedel and RKKY oscillations in Luttinger semimetals have some similarities to those in isotropic Dirac semimetals. Dirac semimetals also have a strong spin-orbit coupling but with a linear band dispersion that leads to a $1/r^3$ decay of the oscillations [25–27,29]. These semimetals also show a spin-spin coupling with Heiseinberg and Ising contributions as in (19) and similar structures [22,23,33] and that can be made more anisotropic if the Weyl cones are split [25–27]. This

anisotropy also survives at long range, (16), and at higher temperatures [Figs. 3(c) and 3(d)]. The Weyl cones are characterized by a helicity operator, related to the cones' chirality, but the RKKY coupling is independent of this degree of freedom. This is in stark contrast to the behavior observed in our calculations for Luttinger semimetals, where the helicity at the Fermi surface matters for the profile of magnetic coupling.

It is also interesting to take the limit $\mu = 0$ at T = 0, in which case the carrier density vanishes and the model does not possess any energy scale. In Dirac and Weyl semimetals, this result in a nonoscillatory r^{-5} decaying RKKY behavior [25–27]. In the case of Luttinger semimetals, the Friedel and RKKY responses show a nonoscillatory r^{-4} decaying behavior, and we also note that the response is exactly the r^{-} terms from the expressions in Eq. (11) for Friedel oscillations and Eq. (17) for the RKKY responses. This difference in power law between Dirac and Luttinger semimetals could prove useful for experimentally probing the strong orbit coupling since the response is more long-ranged in Luttinger semimetals. In the previous subsection (Sec. III D) we also find a diamagnetic Pauli susceptibility, whereas in Weyl semimetals the Pauli susceptibility cancels [45]. Since the two band structures can be related by applying strain or a magnetic field [5,61-63], it is interesting to see that our results should still hold for energies higher than the energy scale of the Weyl cones. GdPtBi is an example of such a material, with an induced Weyl point from the rare-earth exchange field, but with a quadratic band dispersion far from the Fermi surface [64,65].

V. CONCLUSION

In this work we compute the response of a Luttinger semimetal to a charged and to a magnetic impurity. At large separations, the charge and magnetic oscillations are similar to those of a normal electron gas, up to an anisotropy for the magnetic response. The main difference between the two systems is at short distances, where spin-orbital effects are the most important and result in an r^{-4} divergence. In particular, we observe opposite transverse and longitudinal magnetic couplings, even if the model is isotropic. We obtain the RKKY interaction Hamiltonian between two impurities, compute the Pauli susceptibility, and find that it is diamagnetic instead of being paramagnetic, which is in line with previous calculations that find a paramagnetic orbital susceptibility in Luttinger semimetals [36].

This response of Luttinger semimetals to impurities may lead to exotic phase transitions [66,67]. The Friedel oscillations contribute to the Kohn-Luttinger mechanism of superconductivity [68], which we have recently studied for Luttinger semimetals [56]. The peculiar RKKY coupling could be at the origin of exotic magnetic phases. In this work we focus on the bulk response of Luttinger semimetals, which may show a different behavior at their surface and is more relevant in scanning tunneling microscopy. Indeed, it was recently discussed that these materials may have surface states [69] with various band dispersions that could be responsible for a different surface response than described in the present paper.

While finishing the present work, we became aware of a similar one that has been published [70]. In that work the

authors explore the RKKY interaction in 2D Luttinger's systems with anisotropic electron-hole dispersion, in contrast to the present work, where we focus on 3D systems and where we observe anisotropy in the RKKY response even with electron-hole symmetry.

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APPENDIX A: FOURIER TRANSFORM OF THE THERMAL GREEN'S FUNCTION

In this Appendix, we compute the Fourier transform of the thermal Green's function, (2), for general m,

$$\hat{G}(\mathbf{r}, i\omega_n) \equiv \frac{N_0}{2\pi} \int d^3 \mathbf{k} \, \hat{G}(\mathbf{k}, i\omega_n) e^{i\mathbf{k}\cdot\mathbf{r}} = -\frac{N_0}{2\pi} \int d^3 \mathbf{k} \, \frac{\left(i\omega_n - \operatorname{sgn}(m) - \frac{5}{4}\mathbf{k}^2\right)\hat{\mathbb{1}} + (\mathbf{k}\cdot\hat{\mathbf{J}})^2}{(\xi_+(\mathbf{k}) + i\omega_n)(\xi_-(\mathbf{k}) + i\omega_n)} e^{i\mathbf{k}\cdot\mathbf{r}},\tag{A1}$$

with $\xi_{\pm}(\mathbf{k}) = \pm k^2 - \operatorname{sgn}(m)$. We write (A1) in terms of the auxiliary integral $I_0(r, i\omega_n)$ and its derivatives $I_{ij}(\mathbf{r}, i\omega_n) = \frac{\partial^2 I_0(r, i\omega_n)}{\partial r_i \partial r_j}$.

$$\hat{G}(\mathbf{r}, i\omega_n) = N_0 \bigg[\bigg((i\omega_n - \operatorname{sgn}(m))I_0(r, i\omega_n) - \frac{5}{4} \sum_{i=1}^3 I_{ii}(\mathbf{r}, i\omega_n) \bigg) \hat{\mathbb{1}} + \sum_{i,j=1}^3 I_{ij}(\mathbf{r}, i\omega_n) \hat{J}_i \hat{J}_j \bigg].$$
(A2)

The integral $I_0(r, i\omega_n)$ corresponds to the k-independent part of the numerator in (A1) and evaluates to

$$I_0(r, i\omega_n) = \int_0^\infty dk \, k^2 \int_{-1}^1 du \frac{e^{ikru}}{(k^2 - (\text{sgn}(m) - i\omega_n))(k^2 - (i\omega_n - \text{sgn}(m)))}$$
(A3)

$$= \frac{-i}{r} \int_{-\infty}^{\infty} dk \frac{k e^{ikr}}{(k^2 - (\operatorname{sgn}(m) - i\omega_n))(k^2 - (i\omega_n - \operatorname{sgn}(m)))}$$
(A4)

$$= \frac{\pi}{2r(-\operatorname{sgn}(m) + i\omega_n)} \left(e^{\operatorname{sgn}(\omega_n)i\sqrt{-\operatorname{sgn}(m) + i\omega_n}r} - e^{-\operatorname{sgn}(\omega_n)i\sqrt{\operatorname{sgn}(m) - i\omega_n}r} \right).$$
(A5)

The integration of the terms of the form $k_i k_j$ in the numerator of the Green's function can be written as the derivatives of this auxiliary integral:

$$I_{ij}(\mathbf{r}, i\omega_n) = -\frac{\partial^2 I_0(r, i\omega_n)}{\partial r_i \partial r_j} = \int_0^\infty dk \, k^2 \int_{-1}^1 du \frac{k_i k_j e^{ikru}}{(k^2 - (\text{sgn}(m) + i\omega_n))(k^2 + (\text{sgn}(m) + i\omega_n))}$$
(A6)

$$= -\frac{r_i r_j}{r^2} \left(\frac{\partial^2 I_0(r, i\omega_n)}{\partial r^2} - \frac{1}{r} \frac{\partial I_0(r, i\omega_n)}{\partial r} \right) - \frac{\delta_{ij}}{r} \frac{\partial I_0(r, i\omega_n)}{\partial r}.$$
 (A7)

We use rotation symmetry to simplify (A1) and introduce the unitary transformation $\hat{U}_{\theta\phi}$ generated by the pseudospin j = 3/2 operator $\hat{\mathbf{J}}$ to write $\hat{G}(\mathbf{r}, i\omega_n) = \hat{U}_{\theta\phi}\hat{G}(r\mathbf{e}_z, i\omega_n)\hat{U}^{\dagger}_{\theta\phi}$. The Green's function $\hat{G}(r\mathbf{e}_z, i\omega_n)$ can then be similarly decomposed into

$$\hat{G}(r\mathbf{e}_{z},i\omega_{n}) = N_{0} \bigg[\bigg((i\omega_{n} - \operatorname{sgn}(m))I_{0}(r,i\omega_{n}) - \frac{5}{4} \sum_{i=1}^{3} I_{ii}(r\mathbf{e}_{z},i\omega_{n}) \bigg) \hat{\mathbb{1}} + \sum_{i,j=1}^{3} I_{ij}(r\mathbf{e}_{z},i\omega_{n}) \hat{J}_{i} \hat{J}_{j} \bigg],$$
(A8)

where we write $I_{ii}(r\mathbf{e}_z, i\omega_n)$ in a matrix form,

$$I_{ij}(r\mathbf{e}_{z}, i\omega_{n}) = \begin{pmatrix} -\frac{1}{r} \frac{\partial I_{0}(r, i\omega_{n})}{\partial r} & 0 & 0\\ 0 & -\frac{1}{r} \frac{\partial I_{0}(r, i\omega_{n})}{\partial r} & 0\\ 0 & 0 & -\frac{\partial^{2} I_{0}(r, i\omega_{n})}{\partial r^{2}} \end{pmatrix}.$$
 (A9)

We substitute these expressions in (A8) and obtain the real-space Green's function reported in Eq. (6) in the text.

APPENDIX B: EXPLICIT CONTRIBUTIONS TO SUSCEPTIBILITIES AT T = 0, m > 0

The generalized susceptibility, (5), depends on multiple contributions from intra- and interband scattering. In this section we explicitly denote the combinations of the m > 0 case with a plus superscript, and in the following subsection we obtain the relationship between these expressions and those corresponding to the case m < 0, denoted by a minus superscript. In the limit $T \rightarrow 0$, with m > 0, the intra-valence-band contributions $AA_p^+(r, T = 0)$ in Eqs. (10), (13), and (14) vanish $\forall p$ and the

Matsubara sums

$$BB^{+}_{k+p}(r,T) = T \sum_{\omega_n > 0} B^{+}_k(r, i\omega_n) B^{+}_p(r, i\omega_n),$$

$$AB^{+}_{k+p}(r,T) = i^k T \sum_{\omega_n > 0} A^{+}_k(r, i\omega_n) B^{+}_p(r, i\omega_n)$$
(B1)

can be evaluated analytically with the Euler-MacLaurin summation formula $T \sum_{\omega_n} \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega$. These expressions are

$$BB_0^+(r, T=0) = \frac{1}{2\pi} \frac{\pi^2}{4} \int_0^\infty d\omega \ e^{-2ir\sqrt{1-i\omega}} = \frac{\pi(-i+2r)}{16r^2} e^{-2ir},$$
(B2)

$$BB_{1}^{+}(r, T = 0) = \frac{1}{2\pi} \frac{\pi^{2}}{4} \int_{0}^{\infty} d\omega \, \frac{e^{-2ir\sqrt{1-i\omega}}}{i\sqrt{1-i\omega}} = -\frac{i\pi \, e^{-2ir}}{8r},\tag{B3}$$

$$BB_{2}^{+}(r, T=0) = -\frac{1}{2\pi} \frac{\pi^{2}}{4} \int_{0}^{\infty} d\omega \, \frac{e^{-2ir\sqrt{1-i\omega}}}{1-i\omega} = \frac{\pi(-\pi+i\operatorname{Ei}(-2ir))}{4}, \tag{B4}$$

$$BB_{3}^{+}(r,T=0) = \frac{1}{2\pi} \frac{\pi^{2}}{4} \int_{0}^{\infty} d\omega \, \frac{ie^{-2ir\sqrt{1-i\omega}}}{(1-i\omega)^{3/2}} = -\frac{\pi(e^{-2ir} - 2\pi r + 2ir\operatorname{Ei}(-2ir))}{4},\tag{B5}$$

$$BB_4^+(r, T=0) = \frac{1}{2\pi} \frac{\pi^2}{4} \int_0^\infty d\omega \, \frac{e^{-2ir\sqrt{1-i\omega}}}{(1-i\omega)^2} = \frac{\pi (e^{-2ir}(i+2r) - 4r^2(\pi - i\operatorname{Ei}(-2ir)))}{8},\tag{B6}$$

where Ei(r) is the exponential integral, and using that

$$AB_{p}^{+}(r,T) = T \sum_{\omega_{n}>0} \frac{\pi^{2}}{4} \frac{(-i)^{p}}{(1-i\omega_{n})^{p/2}} e^{-2i\sqrt{1-i\omega_{n}}[(1-i)r/2]} = BB_{p}^{+}((1-i)r/2,T),$$
(B7)

one can deduce from (B2)–(B6) the corresponding expressions of $AB_p^+(r, T = 0)$.

Relationships to $m < 0, \forall T$

One can obtain the following relationships between the expressions corresponding to a positive mass and those or a negative mass,

$$AA_{p}^{-}(r,T) = (-1)^{p} (BB_{p}^{+}(r,T))^{*},$$
(B8)

$$BB_{p}^{-}(r,T) = (-1)^{p} (AA_{p}^{+}(r,T))^{*},$$
(B9)

$$AB_{n}^{-}(r,T) = (-i)^{p} (AB_{n}^{+}(r,T))^{*},$$
(B10)

where the minus and plus superscripts refer to the cases m < 0 and m > 0, respectively, and the asterisk denotes the complex conjugate. Then, for m < 0, the intra-valence-band contributions are associated with BB_p^- and do not contribute to Eqs. (10), (13), and (14) at T = 0 since it is empty.

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