Fast nuclear spin relaxation rates in tilted cone Weyl semimetals: Redshift factors from Korringa relation

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(Dated: March 24, 2022)

Spin lattice relaxation rate is investigated for 3D tilted cone Weyl semimetals (TCWSMs). The nuclear spin relaxation rate is presented as a function of temperature and tilt parameter. We find that the relaxation rate behaves as $(1 - \zeta^2)^{-\alpha}$ with $\alpha \approx 9$ where $0 \leq \zeta < 1$ is the tilt parameter. We demonstrate that such a strong enhancement for $\zeta \approx 1$ that gives rise to very fast relaxation rates, is contributed by the combined effect of a new hyperfine interactions arising from the tilt itself, and the anisotropy of the ellipsoidal Fermi surface. Extracting an effective density of states (DOS) $\tilde{\rho}$ from the Korringa relation, we show that it is related to the DOS $\rho$ of the tilted cone dispersion by the ”redshift factor” $\tilde{\rho} = \rho/\sqrt{1 - \zeta^2}$. We interpret this relation as NMR manifestation of an emergent underlying spacetime structure in TCWSMs.

I. INTRODUCTION

Weyl semimetals (WSMs) such as TaAs [1–3], NbAs [4, 5], TaP [6, 7], NbP [8–10] and YbMnBi$_2$ [11] are materials realizations of the Weyl fermions in condensed matter physics in the sense that their low energy excitations are Weyl fermions and identified by Weyl equation [12]. Whereas Weyl fermions have yet to be found as free particles in particle physics, condensed matter is the only platform where they exist. In condensed matter realization of Weyl fermions, the right-handed and left-handed fermions (corresponding to those with their momentum parallel or anti-parallel to their spins) are organized around two different points in the Brillouin zone, and as such their Lorentz symmetry is broken [13]. Indeed, Weyl semimetals are non-degenerate analogs of Dirac semimetals which can be emerged by breaking either time-reversal or inversion symmetry in Dirac semimetals [14, 15]. WSMs feature pairs of Dirac cone type electronic band structure in their bulk and Fermi arcs on the surface which lead to exotic phenomena including negative magnetoresistance [16], nonlocal transport [17], quantum anomalous Hall effect [18, 19], and unconventional superconductivity [20–22].

The Lorentz symmetry can be broken in more interesting ways in WSMs that can be interpreted as a new spacetime structure [23–30]. This deviation from Lorentz symmetry at the basic solid-state physics level, manifests as the deformation of cone shaped band structure resulting in tilted cone Weyl semimetals (TCWSMs) with point/hyperbolic Fermi surfaces (zero/nonzero density of states at the node) dubbed type-I and type-II WSMs respectively [31]. The tilt deformation of Weyl equation can be formalized by an additional term in the Weyl Hamiltonian via an dimensionless tilt parameter $\zeta = (\zeta_x, \zeta_y, \zeta_z)$ of magnitude $\zeta$ where $0 < \zeta < 1$ and $\zeta > 1$ correspond to type-I and type-II respectively [25, 28, 31]. The tilt term of the Hamiltonian being proportional to the unit matrix in k-space, reshapes spherical Fermi surface to ellipsoidal one which results in increasing of the DOS at energies away from the Weyl node. This is how the tilt deformation can alter the solid state properties of TCWSMs by modifying their energy levels.

The nuclear magnetic resonance (NMR) as a powerful bulk spectroscopy exploits the weak interaction between nuclear spins and surrounded electrons (Hyperfine interaction) to probe electronic properties of the materials [32]. Evidently, interaction between nuclear spins and spin angular momentum of quasiparticles have dominant contributions to the hyperfine interaction [33]. Nevertheless, recent theoretical and experimental studies find that in Dirac and Weyl semimetals hyperfine interaction is different from the case of parabolic band structure which arises from the coupling of the spin and orbital degrees of freedom in linear band structure of Weyl/Dirac materials. In these systems the interaction between nuclear spins and electron orbital angular momentum comes into play and overwhelms the spin hyperfine interaction which leads to anomalous temperature dependence of spin lattice relaxation rate [34–37]. Indeed, recent $^{13}$C NMR experiment on the quasi-two-dimensional organic conductor $\alpha - (BEDT - TTF)_2J_1$ has revealed that the local spin susceptibility and electron correlations are strongly angular dependent on the cone [38].

What else can we learn from NMR reveal when the tilt is introduced to WSMs to make them TCWSMs? The purpose of this work is to focus in the $k_BT \ll \mu$ limit of a TCWSm and to show that in the NMR spectroscopy of these materials, in addition to the effects arising from deformation of the spherical Fermi surface to ellipsoidal Fermi surface (with eccentricity $\zeta$), there is a unique term arising from the tilt of TCWSms that generates its own coupling to nuclear spin degrees of freedom. Such a term has no analogue in the rest of solid state systems. In this study we theoretically illustrate how tilt parameter along with orbital magnetism, significantly contributes to the spin lattice relaxation rate in TCWSMs and leads to a $(1 - \zeta^2)^{-\alpha}$ dependence on the tilt parameter $\zeta$ with $\alpha \approx 9$, which strongly diverges for $\zeta \gg 1$. This suggests that the tilt can be considered as an additional relaxation channel in the electronic degree of freedom, through which nuclear spins relax back to the equilibrium. Indeed the DOS, $\rho$ is enhanced

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by a factor of \((1 - \zeta^2)^{-2}\) whose square – having Korringa relation in mind – contributes an exponent 4 to the total \(\alpha \approx 9\). The tilt parameter further shows up explicitly in NMR via electron-spin hyperfine interaction. The orbital and tilt parts of the hyperfine interaction couple to the nuclear spins in a same way and the tilt term as well as orbital term jointly contribute to the NMR rate. As such, it is not possible to separate the individual contributions of electron spin, orbital and tilt degrees of freedom. We show that the resulting complicated matrix elements will contribute another exponent to the redshift factors appearing in NMR measurements. Another purpose of this paper is to show that this discrepancy come from? Another purpose of this paper is to show that this discrepancy contains the physics of gravitational redshift.

This paper is structured as follows: In section II we formulate the hyperfine interaction in TCWSMs and show how the presence of the tilt itself generates an additional terms in the hyperfine interaction giving rise to new relaxation mechanism. In section III we apply our formulation to a TCWSM and find that the tilt enhances the relaxation rate via both a density of states (DOS) and an additional effect arising from the hyperfine interaction. We end the paper by a discussion of the redshift factors appearing in NMR measurements.

II. TILTED WEYL FERMIONS IN THE LOCAL FIELD OF NUCLEAR SPIN

The isotropic low energy effective Hamiltonian for a tilted Weyl semimetal is described by three dimensional Weyl equation of e.g. +1 chirality \([39, 40]\).

\[
H(k) = \hbar v_F [\sigma \cdot (k + \zeta \cdot k) \sigma_0],
\]

where \(k\) is the momentum measured from the Weyl node, \(\sigma = (\sigma_1, \sigma_2, \sigma_3)\) are Pauli matrices which present physical spin of quasiparticles and \(\sigma_0\) denotes \(2 \times 2\) identity matrix. \(v_F\) and \(\zeta\) are Fermi velocity and tilt parameter respectively. The eigenvalues of Eq.(1) read

\[
\varepsilon_{\pm}(k) = \hbar v_F (\zeta \cdot k \pm |k|),
\]

where \(\pm\) denote the upper/lower bands touching at the Weyl nodes and correspond to the spinors eigenstates \(|k, \pm\rangle = (k_x \pm ik_y \pm k_z)\)\(^T\). The dimensionless tilt parameter \(|\zeta| < 1\) and \(|\zeta| > 1\) of magnitude \(\zeta\) represent type-I and type II Weyl materials respectively. The tilt transforms the spherical Fermi surface of WSMs into ellipsoidal surfaces with eccentricity \(\zeta\) and therefore changes the the density of states per unit volume (DOS). The DOS in tilted Weyl materials at energy \(\varepsilon\) above or below the Weyl node is given by \(\frac{\pi k_B^2 \varepsilon^2}{\hbar^2 (1 - \zeta^2)^2}\) which is trivially enhanced by a factor \((1 - \zeta^2)^{-2}\) compared to non-tilted ones.

To derive an expression for the relaxation rate in TCWSMs, we first investigate hyperfine interaction which has notable al-

\[
\frac{1}{T_1} = \frac{\pi k_B}{\hbar} \int \frac{dk'}{(2\pi)^3} \int \frac{dk}{(2\pi)^3} |\langle k', n' | H_{hf} | k, n \rangle|^2 \left[ -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right] \delta(\varepsilon - \varepsilon' + \hbar \omega_0),
\]

III. SPIN LATTICE RELAXATION RATE FOR TILTED WEYL SEMIMETALS

The nuclear spin lattice relaxation time \(T_1\) is determined by the part of the hyperfine interaction which nuclear spins flip to relax back to the equilibrium denoted by \(H_{hf}^\alpha\). The NMR rate is given by the following formula \([32]\),

\[
H(k) = v_F \hbar [\sigma \cdot (k + eA) + \zeta \cdot (k + eA)] + g\mu_B S \cdot B,
\]

where

\[
A = -i\mu_0 \frac{\mu_n \times q}{q^2},
\]

is the vector potential that leads to the local nucleus magnetic field \(B\), \(g\) is the electron g-factor, \(\mu_B\) is the Bohr magneton, and \(q = k' - k\). Hence, the hyperfine interaction consists in three terms given by

\[
H_{hf}^{\text{spin}} = \frac{g\hbar \mu_B \mu_0}{2} \mu_n \cdot \left( \frac{q \times q \times \sigma}{q^2} \right),
\]

\[
H_{hf}^{\text{orbital}} = -iev_F \mu_0 \mu_n \cdot \frac{q \times \sigma}{q^2},
\]

\[
H_{hf}^{\text{tilt}} = -iev_F \mu_0 \mu_n \cdot \frac{q \times \zeta}{q^2}.
\]

Although the Eq. (5) and Eq. (6), the interaction between nuclear spin, and spin and angular momentum of Weyl fermions, are well investigated in the NMR parameters of the Weyl and Dirac materials \([36, 37]\), but the \(H_{hf}^{\text{tilt}}\) is the new player in the nuclear relaxation rate of TCWSMs that is directly caused by the tilt parameter \(\zeta\). Since the tilt parameter in the Eq. (7) follows the same coupling pattern as orbital angular momentum in Eq. (6), \(H_{hf}^{\text{tilt}}\) is expected to have equally important contribution to the NMR rate. This is the essential conceptual point of this paper. Since we will be interested in highly doped TCWSMs where \(k_B T \ll \mu\), the vector \(q\) connecting two states on the Fermi surface will not be small, and therefore the \(H_{hf}^{\text{spin}}\) will have comparable contribution to the other two terms. So we keep all the terms. Furthermore, ellipsoidal Fermi surface of tilted Weyl fermions will modify the natural coordinate system describing the Fermi surface (see the appendix) whose Jacobian generates further implicit dependence on \(\zeta\) that affects the matrix elements of \(H_{hf}^{\text{spin}}\) and \(H_{hf}^{\text{orbital}}\) terms.
where $|k\rangle$s and $|n\rangle$s denote quantum states of the electrons and nuclear spin, $f(\varepsilon)$ is Fermi Dirac distribution function, and $\omega_0$ is Larmor frequency. For a TCWSM the scattering matrix elements obey the following expression

$$
\langle n'k'|H_{\text{hf}}|kn\rangle = \frac{\hbar e\mu_0\gamma_n F_N}{q^2} \left[ ivF\langle k'|q \times \sigma\rangle_{-}|k\rangle + ivF\langle k'|q \times \zeta\rangle_{-}|k\rangle - \frac{\hbar}{2m_e} \langle k'|q \times q\rangle_{-}|k\rangle \right],
$$

(9)

where $F_N = \langle n'|I^-|n\rangle$ is a constant coefficient for local isotropic interactions. In this paper, we consider the Fermi level in the upper branch of the Weyl node band far enough from Weyl node. For $\mu$ more than a fraction of an electron volt, even the room temperature satisfies $k_BT \ll \mu$ which allows for further simplifications of the Fermi-Dirac functions. Then only excitations in upper band are relevant. We further choose the momenta axis such that $\zeta = (0, 0, \zeta)$ and the unit which in $\hbar = v_F = k_B = 1$.

The spin lattice relaxation rate in terms of the new coordinates can be rewritten as

$$
\frac{1}{T_1T} = \frac{\mu_0^2 \gamma_n^2 v^2 F_N^2}{65 \pi^5} \int \frac{d\varepsilon d\Omega_k d\Omega_{k'}}{(1 + \zeta \cos \theta)^2(1 + \zeta \cos \theta')^2} h(\varepsilon, \Omega_k, \Omega_{k'}) \left[ \frac{d f(\varepsilon)}{d\varepsilon} \right].
$$

(10)

In $k_BT \ll \mu$ regime, the Sommerfeld expansion reduces the integral in Eq. (10) to integration over solid angles $\Omega_k$ and $\Omega_{k'}$. For $k_BT \ll \mu$ and $\zeta = 0$ (non-tilted case) NMR rate has a weak dependence on temperature indicated in Fig.1 which is the conventional behavior (black solid line). Indeed within the Korringa relation the $1/(T_1T)$ is independent of $T$. This corresponds to $T \to 0$ in Fig. 1. The additional parabolic dependence on $T$ comes from our Sommerfeld expansion upon this order. Upon introducing the tilt ($\zeta \neq 0$) spin lattice relaxation rate acquires notably sensitive to temperature. This sensitivity is further enhanced upon further increasing the tilt parameter. One might argue that the enhancement of the NMR relaxation rate in TCWSMs is a DOS effect. This seems feasible, because according to Korringa relation, the relaxation rate is proportional to the square of the density of states. To investigate this, in the inset of Fig.1 we have excluded the $\rho^2$ factor in order to separate the sole effect of the tilt parameter. As can be seen even after excluding the effect of DOS, while preserving the parabolic temperature dependence, still the relaxation rate shows enhancement caused by tilt parameter $\zeta$. Even the low-$T$ part of this figure that corresponds to Korringa limit, shows tilt induced enhancement.

To further investigate the role of the tilt parameter in relaxation time, we split it into two types of enhancements. First type is the enhancement of the DOS by the tilt parameter which as discussed below Eq. (2) is proportional to $(1 - \zeta^2)^{-2}$. Within a Korringa formula, this will give rise to a $\rho^2 \sim (1 - \zeta^2)^{-3}$ factor. There is still a significant dependence on $\zeta$ that comes through the matrix elements of the hyperfine interaction. Fig. 2 illustrates that $(T_1T)^{-1}$ depends on $\zeta$. The inset is the same, excluding a $\rho^2$ factor. As can be seen, even after excluding the $\rho^2$ factor, still a divergence at $\zeta \to 1$ persists. It appears that the tilt parameter is acting as a new relaxation channel that paves the way for nuclear spins to relax back. Fitting a $(1 - \zeta^2)^{-\alpha}$ behavior gives a value of $\alpha_0 = 8.927 \pm 0.024$ for $T = 0$ when the 90 data points in the range $0.9 \leq \zeta < 0.99$ are used for the fit. For $T = 300K$ the exponent $\alpha = 9.07$.

What is the source of such a strong divergence with $\alpha = 9$
in the limit \( \zeta \to 1 \). To investigate this, note that in Eq. (10), there are two Jacobians containing \((1 + \zeta \cos \theta)^3\) factors in the denominator, if one deliberately drops these factors from the integral, the remaining integral, instead of diverging with \( \alpha = 9 \), the result will diverge with \( \alpha_{hf} = 3.927 \pm 0.025 \approx 4 \) at zero temperature, where the subscript “hf” is used to emphasize the part of divergence arising from the hyperfine matrix elements without including the Jacobian. Therefore the product of two Jacobian contributes an exponent \( \alpha_J = 5 \) leaving an exponent of 2.5 for each Jacobian factors. Therefore a strong divergence with an exponent of \( \alpha = 9 \) is composed of Jacobian part \( \alpha_J = 5 \) as well as hyperfine contributions \( \alpha_{hf} = 4 \).

IV. DISCUSSIONS AND SUMMARY

In this paper we studied the NMR relaxation rate for a tilted cone Weyl semimetal. We found that the contribution of tilt parameter is more than an additional coupling term in hyperfine interaction. Since in TCWSMs we have ellipsoidal Fermi surface whose eccentricity turns out to be given by the magnitude \( \zeta \) of the tilt parameter, the spin and orbital parts immediately imprint their \( \zeta \) dependence into the NMR relaxation rate as a very fast relaxation rate that diverges like \((1 - \zeta^2)^{-\alpha}\) with \( \alpha \approx 9 \) for \( \zeta \ll 1 \). The interpretation of the fast relaxation is that the tilt provides an additional relaxation channel for the nuclear spins via additional coupling of the spin and orbital hyperfine interaction on tilt parameter that accelerates the relaxation process.

In order to understand the exponent \( \alpha \approx 9 \) in the NMR relaxation rate, let us start by assuming that the tilt in the dispersion of TCWSMs that mixes energy-momentum is rooted in the metric \( ds^2 = -v_F^2 dt^2 + (dr - \zeta v_F dt)^2 \) [25, 28]. Let us further assume that in some part of this spacetime we have a given non-zero \( \zeta \) and in some other corner we have \( \zeta = 0 \). The time intervals in these two parts of the spacetime are \( dt \) and \( dt_0 \), respectively which are related by \( dt = dt_0/\sqrt{1 - \zeta^2} \) where \( \sqrt{1 - \zeta^2} \) is the "gravitational" redshift factor. Now let us turn our attention to the NMR rates in TCWSMs. The power 4 out of 9 was shown to arise from non-separable hyperfine matrix elements when they are all integrated together. Within the Korringa framework, insisting that the remaining power of 5 arises from a DOS squared, \( \rho^2 \), one concludes that \( \tilde{\rho} \sim (1 - \zeta^2)^{-2.5} \). But on the other hand, the DOS calculated from the tilted conic dispersion is \( \rho \sim (1 - \zeta^2)^{-2} \). We therefore find that \( \tilde{\rho} = \rho/\sqrt{1 - \zeta^2} \).

In the present NMR relaxation theory, the quantity \( 1/(T_1 T) \) contains the product of "time" and "energy" scales, and therefore one does not expect to directly observe the redshift factor in such quantity. However in one hand the density of states has the dimension of inverse energy (i.e. the dimension of "time" in units with \( \hbar = 1 \)) which makes it a suitable quantity to look for redshift factor in TCWSMs. On the other hand, the local nature of NMR experiments allows to compare the density \( \tilde{\rho} \) of states inferred from Korringa relation as a function of tilt parameter \( \zeta \) with the bare DOS \( \rho \) obtained from band structure at every point with a given \( \zeta \). Then these two "time scales" are related by "gravitational" redshift factor.

V. ACKNOWLEDGEMENTS

S.A.J. was supported by research deputy of Sharif University of Technology, grant no. G960214 and the Iran Science Elites Federation (ISEF). Z.F. was supported by ISEF post doctoral fellowship.

Appendix A

To obtain a proper coordinates for our system, we start with upper band dispersion for \( \zeta = \zeta \hat{z} \), that reads \( \epsilon = \zeta k_z + |\mathbf{k}| \), or alternatively, \( |\mathbf{k}| = \epsilon/(1 + \zeta \cos \theta) \) which gives the Cartesian components of the momentum as

\[
(k_x, k_y, k_z) = \frac{\epsilon (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)}{1 + \zeta \cos \theta} \tag{A.1}
\]

that provides a natural generalization of the spherical coordinate with \( \theta \) and \( \phi \) being polar and azimuthal angles. The Jacobian of the new coordinates transformation will be \( J(\epsilon, \theta, \phi) = \epsilon^2 \sin \theta/(1 + \zeta \cos \theta)^3 \). Integrating over the Fermi surface with a constant \( \epsilon = \epsilon_F \) gives rise to the density of states and the \((1 - \zeta^2)^{-2}\) enhancement. On the other hand by standard contour integration one can show that the strongest divergence in \( \zeta \to 1 \) that can be contributed by a factor like \((1 + \zeta \cos \theta)^{-\alpha}\) is given by \((1 - \zeta^2)^{0.5-\alpha}\).

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