Phenomenology of a semi-Dirac semi-Weyl semi-metal

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(Dated: May 2, 2014)

We extend the study of fermionic particle-hole symmetric semi-Dirac (alternatively, semi-Weyl) dispersion of quasiparticles, \( \varepsilon_K = \pm \sqrt{(k_x^2/2m) + (vk_y)^2} = \pm \varepsilon_0 \sqrt{K_x^2 + K_y^2} \) in dimensionless units, discovered computationally in oxide heterostructures by Pardo and collaborators. This unique system a highly anisotropic sister phase of both (symmetric) graphene and what has become known as a Weyl semimetal, with \( v_y \gtrsim v \) independent of energy, and \( v_x \gtrsim m^{-1/2} \) being very strongly dependent on energy \( (\varepsilon) \) and depending only on the effective mass \( m \). Each of these systems is distinguished by bands touching (alternatively, crossing) at a point Fermi surface, with one consequence being that for this semi-Dirac system the ratio \( |\chi_{orb}/\chi_{sp}| \) of orbital to spin susceptibilities diverges at low doping. We extend the study of the low-energy behavior of the semi-Dirac system, finding the plasmon frequency to be highly anisotropic while the Hall coefficient scales with carrier density in the usual manner. The Faraday rotation behavior is also reported. For Klein tunneling for normal incidence on an arbitrarily oriented barrier, the kinetic energy mixes both linear (massless) and quadratic (massive) contributions depending on orientation. Analogous to graphene, perfect transmission occurs under resonant conditions, except for the specific orientation that eliminates massless dispersion. Comparisons of the semi-Dirac system are made throughout with both other types of point Fermi surface systems.

PACS numbers:

I. INTRODUCTION

The isolation of single layers of graphite (graphene) and its unique linear (massless Dirac, properly called Weyl) low energy band structure have far-reaching implications, have in the past in-cluded half metallic ferromagnets and compensated half metals (“half metallic antiferromagnets”), and more recently topological insulators. Each of these systems provide the promise of not only new physical phenomena but also new applications of their unconventional properties.

Another key feature of graphene is the point Fermi surface aspect. The touching (or crossing) of bands is accompanied by a gap throughout the rest of the Brillouin zone that pins the Fermi level \( (E_F) \) in the intrinsic material to lie precisely at the point of crossing – the point Fermi surface (two of them in graphene). This point Fermi surface aspect has been well studied in conventional zero gap semiconductors where a touching of the valence band maximum and conduction band minimum is symmetry determined and occurs at a high symmetry point. The dielectric susceptibility of such a system is anomalous – neither metallic nor semiconductor in character – and unusual consequences of the touching bands and residual Coulomb interaction promise unusual phases, such as excitonic condensates including excitonic superconductors and excitonic insulators.

The linear dispersion at the zone boundary in graphene has been known for many decades; it took the ability to prepare the delicate material and perform a variety of experiments to ignite interest. There are quasilinear (and potentially truly linear) band structure features in certain materials, viz. skutterudites that have been known for some time and with recent development may attract new attention. To actually discover a feature in a band structure that provides the quasiparticle dispersion of a new and unexpected type is rare, and the discovery of a semi-Dirac dispersion pinned to the Fermi energy is a very recent example.

Pardo and one of the authors reported such a finding in ultrathin (001) \( \text{VO}_2 \) layers embedded in \( \text{TiO}_2 \). This new point Fermi surface system, dubbed ‘semi-Dirac,’ is a hybrid of conventional and unconventional: dispersion is linear (‘massless’, Dirac-Weyl) in one of the directions of the two-dimensional (2D) layer, and is conventional quadratic (‘massive’) in the perpendicular direction. At directions between the axes the dispersion is intermediate and highly direction-dependent. Interest in this unique, maximally anisotropic, dispersion arises for several reasons. The (topologically determined pinning at the) point Fermi surface is itself of interest. The highly anisotropic dispersion (from massive to mass-
less depending on angle) is unique to this system. The fact that it arises in an oxide nanostructure of the general type that is grown and studied regularly these days also strengthens the promise of applications. Another layered superstructure, a double cell layer of Ti$_3$SiC$_2$ embedded in SiC, has displayed a point Fermi surface, but the dispersion is of the convention type. As alluded to above, an unusual point Fermi surface at zero momentum, with linear bands degenerate with quadratic bands, has been discovered in the skutterudite class of semimetals.

Such a spectrum had been noted earlier in different contexts. Volovik obtained such a spectrum at the point node in the A-phase of superfluid $^3$He and studied its topological robustness. More relevant to solids was the discovery by Montambaux’s group of this spectrum in a graphene-like model. The model has a broken symmetry such that hopping to two nearest neighbors is $t$ but to the third neighbor is $t’$. When $t’$ differs from $t$, the graphene “Dirac points” wander away from the $K$ and $K’$ points, and at $t’=2t$ they merge, resulting in the semi-Dirac spectrum. This group began a study of low energy properties of such a system which was continued by Banerjee et al. and will be extended in the present paper.

In this paper we first provide results for the Hall coefficient and plasma frequency versus doping level, finding some new behavior along with some somewhat conventional results. In the final section we provide selected results for Klein tunneling of semi-Dirac particles, a problem that acquires extra richness due to the variable angle of the barrier with respect to the anisotropic dispersion.

II. SEMI-DIRAC DISPERSION

SemiDirac dispersion is quadratic along one symmetry direction in the Brillouin zone and linear along the direction perpendicular to it: massless Dirac (i.e., Weyl). Choosing $k_x$ and $k_y$ to be the momentum variables and taking $h=1$ except occasionally for clarity, the semi-Dirac dispersion is given by:

$$\varepsilon_k = \pm \sqrt{\frac{k_x^2}{2m} + [vk_y]^2}$$

where the effective mass $m$ applies along $k_x$ and $v$ is the velocity along $k_y$ (the massless direction). For intermediate angles $\beta = \arctan(k_y/k_x)$, the dispersion is of an entirely new type. Two natural scales are introduced, one for the momentum and the other for the energy: $p = 2mv$ (momentum scale) and $\varepsilon_0 = \frac{p^2}{2m} = 2pv$. (Untidy factors of 2 appear because of the clash between the natural classical $\frac{p^2}{2m}$ and relativistic $pv$ units for energy.) One can then define the dimensionless momenta $K_x = \frac{hk_x}{p}$ and $K_y = \frac{hk_y}{p}$ in terms of which the semi-Dirac dispersion given by Eq. (1) becomes

$$\varepsilon_k = \pm \varepsilon_0 \sqrt{K_x^2 + K_y^2},$$

(2)

The corresponding velocity $\vec{v}_k = \nabla_k \varepsilon_k$ can be scaled to a dimensionless form $\vec{V}_K$ using

$$\vec{V}_K = \frac{\vec{v}_k}{v} = \nabla K \xi_k$$

(3)

Figure shows semi-Dirac Fermi surfaces as well as contour plots of $\vec{V}_K$.

We first compute $\langle v_x^2 \rangle$ and $\langle v_y^2 \rangle$, which are the averages of the Fermi surface velocity $v_F = \frac{(\langle v_x^2 \rangle + \langle v_y^2 \rangle)^{\frac{1}{2}}}{2}$ for the semi-Dirac dispersion in the non-relativistic and the relativistic directions respectively, which will prove to be useful later, and will also give the semiclassical conductivity tensor $\sigma_{\alpha\beta} = e^2 T D(\varepsilon) \langle v_{\alpha} v_{\beta} \rangle$. They are defined as follows

$$\langle v_{\alpha} v_{\beta}(\varepsilon) \rangle = \sum_k v_{\alpha} v_{\beta} \delta(\varepsilon_k - \varepsilon) / \sum_k \delta(\varepsilon_k - \varepsilon)$$

$$= \frac{1}{2\pi^2 D(\varepsilon)} \int dk |v_{\alpha} v_{\beta}|$$

where $D(\varepsilon)$ is the density of states. For semi-Dirac dispersion the density of states was obtained earlier as

$$D(\varepsilon) = I_1 \frac{\sqrt{2m\varepsilon}}{\pi^2 v} = I_1 \frac{2m}{\pi^2 v} \sqrt{\varepsilon - \varepsilon_0},$$

(5)

with proportionality coefficient $\sqrt{m/v^2}$. The integral $I_1$ is given by

$$I_1 = \int_0^1 ds (1 - s^4)^{-\frac{1}{2}} \approx 1.3110.$$

 Bácsy et al. have studied the quantum critical exponents of point Fermi surface semimetals with $D(\varepsilon) \propto |\varepsilon|^r$ for a continuous range of $r$ including this $r = 1/2$ case.

The squared Fermi velocities for semiDirac dispersion are obtained as

$$\langle v_x^2 \rangle = \frac{4I_1 \varepsilon}{I_1 m},$$

(7a)

$$\langle v_y^2 \rangle = \frac{I_1 \varepsilon_0}{I_1 m} \approx 1.3v^2,$$

(7b)
FIG. 1: Fig. a: Fermi-surfaces of semi-Dirac dispersion, along with arrows representing $\vec{v}_K$. The length of an arrow is proportional to the magnitude of $\vec{v}_K$. As can be seen from the figure, the arrow-length is constant along the $K_y$ axis indicating a constant velocity in the relativistic ($y$) direction. $\vec{v}_K$s are all normal to the constant Fermi energy contours, as they should be. Fig. b: The surface and contour plot of the magnitude of $\vec{v}_K$. The magnitude is constant in the $y$ direction as opposed to the monotonically changing values in the non-relativistic ($x$) direction, with rapid variation of other directions of propagation.

note that the former involves only $m$, the latter only $v$. The integrals $I_2$ and $I_3$ are given by

$$I_2 = \int_0^1 ds (1 - s^4)^{1/2} \approx 0.8740, \quad (8a)$$
$$I_3 = \int_0^1 ds \frac{s^6}{(1 - s^4)^{3/2}} \approx 0.3595, \quad (8b)$$

Thus the ratio of $\langle v_x^2 \rangle$ to $\langle v_y^2 \rangle$ scales as $\varepsilon/\varepsilon_0$, which reflects the extreme anisotropy at small doping. For the VO$_2$ system where semi-Dirac dispersion was discovered only very small doping levels will remain within the energy range represented by the semi-Dirac dispersion ($\epsilon/\varepsilon_0 \sim 10^{-4}$) but we consider more general cases.

III. FARADAY ROTATION IN THE CONTEXT OF THE SEMI-DIRAC SYSTEM

A. The semiclassical equation of motion

The behavior of point Fermi surface semimetals in a magnetic field has stimulated lively interest due to unusual quantum Hall effect behavior, with the case of graphene having been reviewed recently by Goerbig.\textsuperscript{18} The semiclassical equation of motion of an electron in a magnetic field $\vec{B}$ is given by

$$\frac{d\vec{k}}{dt} = -\frac{e}{c} \vec{v}_K \times \vec{B}. \quad (9)$$

Using Eq. (3) for $\vec{v}_K$ in Eq. (9), one obtains the following expressions

$$\frac{dK_x}{dt} = -\omega_0 K_y, \quad (10a)$$
$$\frac{dK_y}{dt} = 2\omega_0 K_x^3, \quad (10b)$$

where $K_x$ and $K_y$ are the dimensionless variables associated with momentum introduced before, and $\omega_0$ is given by

$$\omega_0 = \frac{eBv_0^2}{c\varepsilon} = \frac{eB}{mc} \frac{\varepsilon_0}{\varepsilon}, \quad (11)$$

where $B$ is the magnetic field, and $\varepsilon$, the Fermi energy. The Fermi surface orbiting frequency diverges as the doping level decreases; the Fermi surface orbit length goes smoothly to zero whereas the mean velocity remains finite. Eliminating $K_y$ from Eqs. (10a) and (10b), the following differential equation is obtained

$$\frac{d^2K_x}{dt^2} = -2\omega_0^2 K_x^3, \quad (12)$$

In order to solve this second order differential equation, we multiply both sides of the equation by $K_x$ ($K_x$ denotes the time derivative of $K_x$). Both the right and the left sides of the equation can then be written as a total derivatives, which can be integrated to give

$$K_x^2 = -\omega_0^2 K_x^4 + C, \quad (13)$$
where the constant $C$ can be determined from the condition that $\dot{K}_x = 0$ when $K_x = K_{x,max}$. $K_{x,max} = (\varepsilon/\varepsilon_0)^{1/2}$ corresponds to $K_y = 0$, from the semi-Dirac dispersion given by Eq. 12, and the rest follows from Eq. 10a. Hence Eq. 13 becomes

$$\dot{K}_x = \pm \omega_0 \sqrt{K_{x,max}^2 - K_x^2}. \quad (14)$$

Integrating the above equation (numerically) one can get $K_x$ as a function of time. Once $K_x$ is known, $K_y$ can be obtained from Eq. 10b. The differential equation for the cyclotron orbit is obtained by dividing Eq. 10b by Eq. 10a. Solving for that, we obtain the semi-Dirac constant energy contour as an expression for the cyclotron orbit, which is expected, since the energy of an electron does not change when it moves under the influence of magnetic field.

B. The cyclotron frequency

Eq. 14 can be integrated using the limit $-K_{x,max}$ to $K_{x,max}$ for the variable $K_x$ to obtain the time period. The result for the time period $(T)$ thus obtained is

$$\omega_0 T = \frac{4I_1}{K_{x,max}} = 4I_1 \sqrt{\varepsilon/\varepsilon_0}, \quad (15)$$

where $I_1$ is given by Eq. 9. From Eq. 13, the fundamental semi-Dirac cyclotron frequency $\Omega_c \equiv \frac{\omega_0}{T}$ is obtained as

$$\Omega_c/\omega_0 = \frac{\pi}{2} I_1^{-1} \sqrt{\varepsilon_0 \varepsilon}. \quad (16)$$

The cyclotron frequencies for the parabolic and the linear dispersion cases are given by $(\mu_B B = \frac{2 e}{c \varepsilon_0})$ and $\frac{eBv^2}{c\varepsilon_0}$ respectively ($\mu_B$ is the Bohr magneton). Comparing with Eq. 10, we see that the cyclotron frequencies for all the three cases (the parabolic, linear, and semi-Dirac) depend linearly on the magnetic field. The cyclotron frequency is independent of the Fermi energy for parabolic dispersion, whereas it varies as $\varepsilon^{-\frac{1}{2}}$ for the semi-Dirac dispersion and as $\varepsilon^{-1}$ for the linear Dirac dispersion. One important aspect of the semi-Dirac dispersion is that the semi-Dirac dispersion being anisotropic in the momentum space can have harmonics of the fundamental cyclotron frequency given by Eq. 10. This feature is absent in the Dirac or the two dimensional parabolic dispersion where the energy momentum dispersion is isotropic giving rise to only one value for the cyclotron frequency.

C. Faraday Rotation

The Faraday rotation angle is given by the expression

$$\theta(\omega, B) = Z_0 f_s(\omega) \text{Re}[\sigma_{xy}(\omega, B)], \quad (17)$$

where $Z_0$ is the impedance of the vacuum, $f_s$ is the spectrally featureless function specific to the substrate, and $\sigma_{xy}$ is the dynamic Hall conductivity. According to the Drude formula the dynamic Hall conductivity is given by

$$\sigma_{xy} = \frac{-2D}{\pi} \frac{\omega_c}{\omega^2 - (\omega + \frac{1}{\tau})^2}, \quad (18)$$

where $D$ is the Drude weight, given by $D = \frac{\varepsilon_0}{\varepsilon} c^2 D(\varepsilon)(v_f^2)$. Taking the real part of Eq. 18 and using it in Eq. 17 we obtain

$$\theta(\omega, B) = \frac{-2Z_0 f_s(\omega) D \omega_c}{\pi} I(\omega), \quad (19)$$

where $I(\omega)$ is given by

$$I(\omega) = \frac{\omega^2 - \omega^2 + \frac{1}{\tau}}{(\omega_c^2 - \omega^2 + \frac{1}{\tau})^2 + \frac{4\omega^2}{\tau^2}} \quad (20)$$

Extremizing $I(\omega)$ and inserting the resulting expression for $I(\omega)$ in Eq. 19 we obtain the following expression for the maximum value of the Faraday rotation angle $\theta$

$$\theta(\omega, B) = \frac{-Z_0 f_s(\omega) D \omega_c \tau^2}{2\pi((\omega_c^2\tau^2 + 1)^{\frac{3}{2}} - 2)}. \quad (21)$$

The Drude weight $D \sim \varepsilon$ for Dirac dispersion (since $D(\varepsilon) \sim \varepsilon$, and $(v_f^2)$ is a constant). The Dirac cyclotron frequency $\omega_c \sim \varepsilon^{-1}$. Hence the product $D \omega_c$ that appears in the numerator of Eq. 21 is independent of the doping level for Dirac dispersion. For semi-Dirac dispersion, $D \sim \varepsilon^{\frac{1}{2}}$, which follows from the fact that the product $D(\varepsilon)(v_f^2) \sim D(\varepsilon)(v_f^2)$, where $v_f$ is the speed in the relativistic direction, and that $D(\varepsilon)(v_f^2) \sim \varepsilon^{\frac{3}{2}}$. The last step follows by combining Eq. 5 and Eq. 7b. For the same dispersion $\omega_c \sim \varepsilon^{-\frac{1}{2}}$ (From Eq. 16). Hence, like Dirac dispersion, $D \omega_c$ for the semi-Dirac dispersion is independent of the doping energy. For two dimensional parabolic dispersion, $\omega_c$ is independent of the doping energy, but $D \sim \varepsilon$. Hence $D \omega_c$ depends on the doping energy. This is a significant difference when
compared to the Dirac and the semi-Dirac dispersion.

For Dirac and semi-Dirac systems the dependence of the Faraday angle on the doping level arises from the term \( \omega_c \tau \) in the denominator of Eq. 21 whereas the numerator is independent of doping. For those dispersions one can fine tune the Fermi energy to obtain a large value of the Faraday angle by bringing the term \( \omega_c \tau \) close to three, so that the term \((\omega_c^2 \tau^2 + 1)^{1/2} - 2\) appearing in denominator goes to zero causing a significant value for the Faraday angle.

### IV. HALL COEFFICIENT

According to semiclassical Bloch-Boltzmann transport theory, the Hall coefficient of a two dimensional Fermi liquid (in the \( x - y \) plane) is

\[
R^H \equiv R^H_{xyz} = \frac{\Sigma_k v_y(k)[v(k) \times \nabla(k)]_z v_y(k)(\frac{\partial f}{\partial \varepsilon})}{[\Sigma_k v_x^2(k)(\frac{\partial f}{\partial \varepsilon})][\Sigma_k v_y^2(k)(\frac{\partial f}{\partial \varepsilon})]} \tag{22}
\]

Due to the algebraic complexity of the first and second derivatives of \( \xi_K \), this expression is formally unwieldy. We show however that general properties of this expression lead to a simple and familiar result for \( R^H \).

The numerator of Eq. 22 is the area \( A_x \) spanned by the velocity vector over the Fermi surface. In the zero temperature limit each term in the denominator reduces to a line integral along the Fermi-surface. The carrier density \( n \) is proportional to the area swept by the vector \( k \) over the Fermi surface, which is the area \( A_{FS} \) enclosed by the Fermi surface. Hence the quantity \( R^H n \) is given by:

\[
R^H n = \frac{A_x A_{FS}}{\int dk_l \frac{v_x^2}{v_k} \int dk_l \frac{v_y^2}{v_k}}. \tag{23}
\]

Using the fact that the gradient \( \nabla k \varepsilon \) is perpendicular to the vector line element \( dk_l \) along the Fermi surface, so that the dot product between them is zero, the denominator of Eq. 23 reduces to

\[
\int dk_l \frac{v_x^2}{v_k} \int dk_l \frac{v_y^2}{v_k} = \int dk_y v_x \int dk_x v_y. \tag{24}
\]

Using Eq. 24 in Eq. 23 we obtain

\[
R^H n = \frac{A_x A_{FS}}{\int dk_y v_x \int dk_x v_y}. \tag{25}
\]

\( R^H n \) as given by Eq. 25 is unity for the semi-Dirac dispersion. This result can be argued directly from equation Eq. 23 in the following way. The semi-Dirac dispersion is symmetric both in the \( x \) and the \( y \) directions. Hence we can restrict the limits of the integrals appearing in Eq. 23 to the first quadrant. For the first term in the denominator of Eq. 23, carrying out the integration by parts one obtains:

\[
- \int dk_y v_x = -k_y v_x |^f_i + \int dv_x k_y \tag{26}
\]

\( i \) and \( f \) correspond to the points on the Fermi surface with \( k_y = 0 \) and \( k_x = 0 \) respectively. The boundary terms in Eq. 26 at \( i \) and \( f \) are zero because \( k_y \) and the \( x \) component of the gradient at the semi-Dirac Fermi surface vanish at \( i \) and \( f \) respectively. Using the above reasoning the first term in the denominator of Eq. 23 is changed to \( \int dv_x k_y \). Making use of this along with the definition of area under a curve (for the terms in the numerator), Eq. 23 can be written as

\[
R^H n = -\int dk_x \int dv_x v_y. \tag{27}
\]

\( v_y \) for the semiDirac dispersion evaluated on the Fermi surface turns out to be proportional to \( k_y \) as can be seen from Eq. 2. Hence it is observed that in Eq. 27 the numerator and the denominator are equal except for a minus sign. That explains why we obtain \( R^H n = -1 \) for the semiDirac dispersion. Incidentally, \( v_y \) is proportional to \( k_x \) for the Dirac and the parabolic dispersion relations. Hence, \( R^H n \) is equal to \(-1\) for those dispersions too. So it can be said that the Hall coefficient times the carrier density is a topologically invariant quantity for a certain class of band structures, reminiscent of the geometrical representation of Ong.

### V. PLASMON FREQUENCY

The plasmon frequency for the semiDirac system can be computed by setting the random phase approximation expression for the dielectric constant

\[
\epsilon(q, \omega) = 1 - v(q) \chi_0(q, \omega) \tag{28}
\]

to zero. \( \chi_0(q, \omega) \) is the polarizability and \( v(q) \) is the Fourier transform of the Coulomb potential. \( \chi_0(q, \omega) \) is given by the Lindhard expression

\[
\chi_0(q, \omega) = \int \frac{d^2 k}{(2\pi)^2} \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\omega + \varepsilon_k - \varepsilon_{k+q}}. \tag{29}
\]

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Expanding $\varepsilon_{k+q}$ in Eq. (29) for small $q$ (we treat only this regime), the numerator in Eq. (29) takes the following form at low temperature

$$f(\varepsilon_k) - f(\varepsilon_{k+q}) = \tilde{v}_k \cdot \tilde{q} \delta(\varepsilon_k - \varepsilon).$$

Expanding the denominator as well, Eq. (29) becomes

$$\chi_0(q, \omega) = \int \frac{d^2k}{(2\pi)^2} \frac{\tilde{v}_k \cdot \tilde{q} (1 + \tilde{v}_k \cdot \frac{\tilde{q}}{\omega}) \delta(\varepsilon_k - \varepsilon). (31)}{\omega}.$$  

The Coulomb potential $v(q)$ in two dimensions is

$$v(q) = \frac{2\pi e^2}{\kappa q},$$

where $q = \sqrt{\tilde{q}_x^2 + \tilde{q}_y^2}$, and $\kappa$ is the background dielectric constant of the medium. Using Eq. (31) and Eq. (32) in Eq. (29), and setting $\epsilon(q, \omega) = 0$, the plasmon frequency is

$$\omega_p^2 = \frac{8I_3 e^2 q^3}{\pi \kappa} F(\theta),$$

where $F(\theta)$ is given by

$$F(\theta) = \xi^2 (\cos^2 \theta + \frac{1}{4} \varepsilon_{0}^{-1} I_2 I_3 \sin^2 \theta),$$

and $I_2, I_3$ are given by Eq. (33) and in Eq. (34) respectively. $\varepsilon_0$ is the energy scale defined earlier. $\theta$ denotes the angle that the plasmon wave-vector makes with the non-relativistic axis $k_x$ of the semi-Dirac dispersion. Recall that the Fermi energy variable is defined as $\xi = \frac{\varepsilon_0}{\omega_p}$, $\omega_p \propto \sqrt{\tilde{q}}$ is characteristic of a two-dimensional system.

The function $F(\theta)$ is plotted against $\theta$ in Fig. 2. Using Eq. (35) for the semi-Dirac density of states and Eq. (36) and Eq. (37) for the mean square Fermi velocities, Eq. (38) reduces to

$$\omega_p^2 = \frac{\pi^2 q \hbar D(\varepsilon)}{\kappa} ((v_x^2) \cos^2 \theta + (v_y^2) \sin^2 \theta).$$

The plasmon frequency is highly anisotropic and reaches its maximum along the relativistic direction, which could be a signature characteristic of a semi-Dirac system.

**VI. MAGNETIC SUSCEPTIBILITY**

In this section we consider the magnetic susceptibility for the semi-Dirac dispersion. The Pauli spin susceptibility is given by

$$\chi_{sp}/\mu_B^2 = D(\varepsilon),$$

where $D(\varepsilon)$ is the density of states. Using Eq. (3) for the semi-Dirac density of states Eq. (39) reduces to

$$\chi_{sp}/\mu_B^2 = \frac{2m}{\pi^2} \sqrt{\xi},$$

where $\xi$ is the same dimensionless variable related to the Fermi energy appearing in the previous section. For a non-interacting Fermi liquid the orbital susceptibility is given by

$$\chi_{orb}/\mu_B^2 = \frac{m^2}{12\pi^3} \int d^3k \frac{\partial^2 \varepsilon_k}{\partial k_x^2} \frac{\partial^2 \varepsilon_k}{\partial k_y^2} + 2(\frac{\partial^2 \varepsilon_k}{\partial k_x \partial k_y} \delta(\varepsilon - \varepsilon_k)),$$

Using Eq. (40) for $\varepsilon_k$ in Eq. (39) and doing the integral we obtain

$$\chi_{orb}/\mu_B^2 = \frac{2\sqrt{2}I_4 m^2 v}{3\pi^3} \frac{\varepsilon}{\varepsilon^2},$$

where the integral $I_4$ is given by

$$I_4 = \int_0^1 d\alpha - 33\alpha^{10} + 41\alpha^6 - 9\alpha^2 \frac{1}{(1 - \alpha^4)^{\frac{1}{2}}}. $$

Evaluating the numerical value for $I_4$ and using the dimensionless variable $\xi$, Eq. (41) reduces to

$$\chi_{orb}/\mu_B^2 = \frac{0.0798m}{\xi^2}.$$
We observe that the orbital susceptibility for the semi-Dirac system is always diamagnetic. The absolute value of the ratio of the spin to the orbital susceptibilities (the ratio of Eq. [57] to Eq. [11]) of the semi-Dirac dispersion is given by

$$\left| \frac{\chi_{\text{sp}}}{\chi_{\text{orb}}} \right| \sim 100\xi$$

(42)

Hence orbital magnetic susceptibility for the semi-Dirac dispersion dominates the spin susceptibility at low energy. This result is distinct qualitatively from both the Dirac and the parabolic dispersion cases. For the doped Dirac dispersion the orbital susceptibility vanishes identically. For conventional two dimensional parabolic dispersion the orbital susceptibility is calculated using Eq. 6 and turns out to be 6\(\pi\) times smaller than its paramagnetic susceptibility. Hence the unusually large orbital susceptibility can be considered a distinctive feature of the semi-Dirac dispersion.

VII. HEAT CAPACITY

We show here how the heat capacity for the non-interacting two-dimensional semi-Dirac electron gas is similar to that of the three-dimensional non-interacting electron gas with the parabolic energy-momentum dispersion at both the low and the high temperature ends. The similarity becomes equality at high temperature. Relative to the natural energy scale \(\varepsilon_0\) introduced at the beginning, the low and the high temperatures can be considered. The low temperature heat capacity per particle for the semi-Dirac dispersion is:

$$c_v = \frac{2I_1}{3} \frac{mk_B^2 T}{\varepsilon_0} \sqrt{\varepsilon_0},$$

(43)

which is calculated using Sommerfeld expansion\(^{25}\) (\(I_1\) is given in Eq. [6]). It is observed that the heat capacity in Eq. [43] is proportional to \(D(\varepsilon) \propto \sqrt{\varepsilon}\), as it must be because \(c_v\) depends only on the spectrum of energy levels. A similar type of dependence with energy is observed for the three dimensional electron gas with the parabolic energy-momentum dispersion. The difference between them is in the prefactors. This difference disappears quite nicely in the high temperature end as is shown in the following. At high temperature, the heat capacity for the three dimensional electron gas is given by \(\frac{2}{3}k_B\). In order to emphasize a technique that will be used for the semi-Dirac problem, a derivation of the above result for the three-dimensional electron gas is first outlined in the following. The parabolic three dimensional Hamiltonian is given by

$$H_{\text{parabolic}} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2),$$

so it follows that

$$\frac{\partial H_{\text{parabolic}}}{\partial p_i} = \frac{p_i}{m} \quad [\text{where } i = x, y, z].$$

Hence

$$H_{\text{parabolic}} = \frac{1}{2}(p_x \frac{\partial H_{\text{parabolic}}}{\partial p_x} + p_y \frac{\partial H_{\text{parabolic}}}{\partial p_y} + p_z \frac{\partial H_{\text{parabolic}}}{\partial p_z}).$$

By the equipartition theorem, the ensemble average of each of \(p_x \frac{\partial H_{\text{parabolic}}}{\partial p_x}, p_y \frac{\partial H_{\text{parabolic}}}{\partial p_y}\), and \(p_z \frac{\partial H_{\text{parabolic}}}{\partial p_z}\) is \(k_BT\). Hence taking the ensemble average of the Hamiltonian in Eq. [44] one obtains

$$<H_{\text{parabolic}} = \frac{3}{2}k_BT.$$"
For example, a semi-Dirac nanostructure could be used as an efficient heat sink. More generally, a semi-Dirac system can function quite differently compared to other two dimensional systems for thermal management as well as for many other applications.

VIII. KLEIN PARADOX

The Klein paradox is the name given to the phenomenon of the complete transmission of a particle at selected energies or geometric configurations through a potential barrier even when the barrier is arbitrarily high. For the conventional tunneling problem, the probability of transmission decreases exponentially with the height and thickness of the barrier. In order for Klein tunneling to take place, there must be hole states having negative energies available to promote tunneling. The positive potential in the barrier region raises the hole states, making them available. For ‘relativistic’ Dirac-Weyl dispersion (as in graphene) Katsnelson and collaborators have shown that Klein tunneling can occur and that transmission is unusually robust at near-normal incidence. Klein tunneling is also possible in conventional (massive) zero-gap semiconductors including double-layer graphene, with an angular behavior that is distinct from that of graphene. Klein tunneling therefore is expected for particles with semiDirac dispersion, but there should be many distinctions. The low-energy Hamiltonian corresponding to the semiDirac dispersion can be taken as:

\[ H = v\hat{p}_y \tau_3 + \frac{\hat{p}_x^2}{2m} \tau_1, \] (49)

where the \( \tau \)'s are the Pauli matrices in orbital space and \( \hat{p}_{x(y)} \) are the momentum operators.

A. Rotation of the Frame

The semi-Dirac system is (highly) anisotropic. The potential barrier can be oriented at an arbitrary angle with respect to the \( \hat{x}, \hat{y} \) axes after which one might consider a particle impinging on the barrier from another arbitrary angle. This extension from the isotropic systems of graphene or zero-gap semiconductors leads to a rather complicated tunneling problem that could form the basis of a separate study. To keep the algebra and the physical picture as simple as possible, we consider only the special case of normal incidence of a semi-Dirac quasi-particle onto a potential barrier of width \( d \), which is inclined at an angle \( \frac{\pi}{2} + \alpha \) with respect to the \( x \) (nonrelativistic) axis as shown in Fig. 3. A set of orthogonal axes \( \xi \) and \( \eta \) with respect to the barrier are defined. \( \eta \) is the direction along which the potential is infinitely extended. An electron with energy \( E \) is incident normally on the potential, i.e., along the \( \xi \) direction.

FIG. 3: The top view of the potential barrier is shown. It extends infinitely in one direction (\( \eta \) direction), but limited to a spatial length \( d \) in the orthogonal direction (\( \xi \) direction), which makes an angle \( \alpha \) with the nonrelativistic direction. An electron with energy \( E \) is incident normally on the potential, i.e., along the \( \xi \) direction.
takes the following form:

\[ H = v \hat{p}_x \sin \alpha \tau_3 + \frac{\hat{p}_z^2}{2m} \cos^2 \alpha \tau_1 \]  

\[ = v_\alpha \hat{p}_x \tau_3 + \frac{\hat{p}_z^2}{2m_\alpha} \tau_1. \]  

This transformed kinetic “Hamiltonian” has both linear (massless) and quadratic (massive) contributions, governed an increased mass \( m_\alpha = m / \cos^2 \alpha \) and a decreased velocity \( v_\alpha = v \sin \alpha \). Thus the orientation of the barrier allows the tuning of the relative amounts of linear and quadratic dispersion.

In the limits \( \alpha = 0 \) and \( \pi / 2 \), the problem reverts to the problem for zero-gap semiconductors and for graphene, respectively.

For a value of \( \alpha \) between these limits the forward propagating wave, which is of the form \( e^{i k \xi} \) times a spinor, is still an admissible eigenstate of the Hamiltonian. Operating on the plane wave with the Hamiltonian in Eq. (51) gives an expression that can be written as

\[ H_k = v k \sin \alpha [\tau_3 + \tau_1 \tan \theta], \]  

where

\[ \tan \theta = \frac{\cos^2 \alpha}{\sin \alpha} \frac{k}{2m v_\alpha} = \frac{k}{2m_\alpha v_\alpha} = \frac{k}{p_\alpha}. \]  

Thus \( \tan \theta \) reflects the magnitude of the particle momentum relative to the scaled semi-Dirac momentum \( p_\alpha = 2m_\alpha v_\alpha \). When \( k \) goes to \( -k \) as is the case when one considers the backward propagating wave \( e^{-i k \xi} \), aside from the positive multiplicative factor \( v k \) which changes sign, the Hamiltonian in Eq. (51) changes from \( \tau_3 + \tau_1 \tan \theta \) to \( -[\tau_3 - \tau_1 \tan \theta] \). The corresponding eigensystems are given for quick reference in the Appendix.

**B. Derivation of the Resonance Condition**

The time independent Schrödinger equation in a given potential can be written as

\[ \hbar \psi = (E - V) \psi, \]  

where \( \hbar \) is the part of the Hamiltonian without the potential \( V \). In regions I and III \( (E - V) \) is positive, and the positive eigenvalue form of the solution as given by Eq. A2a in the Appendix for the forward propagating wave and by Eq. A4a for the backward propagating wave need to be considered in those regions. In region II, \( V \) being much larger than \( E \) results in \( (E - V) \) being negative. Hence the negative eigenvalue solutions as given by Eq. A2b and Eq. A4b appearing in the appendix are of importance in that region. Momenta in regions I and III are equal, denoted by \( k_1 \), and denoted by \( k_2 \) in region II. \( k_1 \) and \( k_2 \) are given by

\[ v k_1 \sin \alpha (\cos \theta_1)^{-1} = E, \]  

\[ v k_2 \sin \alpha (\cos \theta_2)^{-1} = V - E, \]  

where \( \theta_1 \) and \( \theta_2 \) are given by

\[ \tan \theta_{1(2)} = \frac{\cos^2 \alpha k_{1(2)}}{2m v_\alpha} = \frac{k_{1(2)}}{p_\alpha}. \]  

Finally, the wave functions in the three regions are

\[ \Psi_I = e^{i k_1 \xi} \left( \begin{array}{c} \cos(\theta_1/2) \\ \sin(\theta_1/2) \end{array} \right), \]  

\[ + r e^{-i k_1 \xi} \left( \begin{array}{c} \sin(\theta_1/2) \\ \cos(\theta_1/2) \end{array} \right), -\infty < x < 0, \]  

\[ \Psi_{II} = t_1 e^{i k_2 \xi} \left( \begin{array}{c} \sin(\theta_2/2) \\ -\cos(\theta_2/2) \end{array} \right) \]  

\[ + r_1 e^{-i k_2 \xi} \left( \begin{array}{c} \cos(\theta_2/2) \\ -\sin(\theta_2/2) \end{array} \right), 0 < x < d, \]  

\[ \Psi_{III} = t_2 e^{i k_1 \xi} \left( \begin{array}{c} \cos(\theta_1/2) \\ \sin(\theta_1/2) \end{array} \right), d < x < \infty, \]  

where \( r, t_1, r_1 \) and \( t_2 \) are constants determined by matching. The absolute square of \( t_2 \) gives the transmission coefficient. Matching the wave functions at the boundaries \( y = 0 \) and \( y = d \), one obtains for the transmission

\[ |t_2|^2 = \frac{(\sin \theta_2 \cos \theta_2 \cos \theta_1)^2}{A^2 + B^2 - 2AB \cos k_2 d}, \]

where \( A \) and \( B \) are given by:

\[ A = [\sin((\theta_2 - \theta_1)/2) \cos \theta_2 + \sin(\theta_2 + \theta_1)/2] \cos((\theta_2 - \theta_1)/2) \]  

\[ B = \sin \theta_2 \sin^2((\theta_2 + \theta_1)/2) \]

It can be shown that when

\[ \cos k_2 d = 1 \]  

the denominator in Eq. (58) becomes equal to the numerator. The resonance condition as given by Eq. (60) implies

\[ k_2 d = 2n\pi, n = npd \]  

(61)
where \( n \) is an integer and the characteristic momentum scale \( p_d = 2\pi/d \) has been introduced. From Eq. 50b and Eq. 61 we obtain the following condition for complete transmission of an incident wave:

\[
|n^2 \sin^2 \alpha + n^4 \cos^4 \alpha (\frac{\pi}{m\alpha d})^2|^{\frac{1}{2}} = \frac{(V - E)d}{2\pi v^\alpha} \quad (62)
\]
or equivalently in terms of “renormalized” constants

\[
n[1 + n^2 (\frac{p_d}{p_\alpha})^2]^{\frac{1}{2}} = \frac{(V - E)}{p_d v_\alpha}, \quad (63)
\]

Eq. 63 gives the resonance condition, either for resonant energies \( E_n(\alpha, d, V) \) or for orientations \( \alpha_n(d, V - E) \), for full transmission.

The limiting cases are \( \alpha \to 0 \) and \( \alpha \to \pi/2 \). The latter limit corresponds to normal incidence of a particle with ‘relativistic’ Dirac-Weyl dispersion which is treated in Ref. 27, where it was shown that there is complete transmission even if the potential barrier is large. The resonance condition for this limiting case can be obtained setting \( \alpha = \pi/2 \) in Eq. 63. The \( \alpha = 0 \) limit becomes the case of conventional massive particle tunneling, which must be treated separately (see the following subsection). The semi-Dirac system provides for, and interpolates between smoothly, the two very different limits. Figure 4 provides a schematic illustration where there is a single resonant orientation of the barrier.

C. Limiting case \( \alpha = 0 \)

This case corresponds to the potential being perpendicular to \( x \) (the non-relativistic direction), so \( k_y = 0 \). The Hamiltonian admits evanescent as well as propagating wave solutions only in this case; in a sense the relativistic character dominates the behavior except at \( \alpha = 0 \). It is instructive to follow the mixing of the positive and negative energy components. Operating on propagating waves \( e^{\pm ik_xx} \) the Hamiltonian in Eq. 19 takes the following form in the \( k \) space:

\[
H = \frac{k^2}{2m} r_x, \quad (64)
\]

with the conventional massive eigenvalues \( \pm \frac{k^2}{2m} \). For evanescent waves the eigenvalues are interchanged, resulting in a mixing of positive and negative energy functions in a way that does not occur with non-zero \( k_y \).

The energy of the incident particle for both the propagating and the evanescent cases are the same: \( E = \frac{k^2}{2m} \). The momenta in regions \( \{I, III\} \) and \( II \) are denoted by \( k_1^2 = \sqrt{2mE} \) and \( k_2^2 = \sqrt{2m|V - E|} \) respectively. The form of the wave function in the three regions are

\[
\Psi_I = e^{ik_1^a x} \frac{1}{1} + r'' e^{-ik_1^a x} \frac{1}{1} \quad (65)
\]

\[
\Psi_{II} = t''_1 e^{ik_1^a x} \frac{1}{1} + r''_1 e^{-ik_1^a x} \frac{1}{1},
\]

\[
\Psi_{III} = t''_2 e^{ik_1^a x} \frac{1}{1} + r''_2 e^{-ik_1^a x} \frac{1}{1},
\]

where \( r'', t''_1, t''_2, r''_1, r''_2 \) are constants. In Eq. 60 for regions \( I \) and \( III \) the evanescent waves are constructed in such a way that they don’t diverge when \( |x| \) becomes large. There is no backward traveling wave in region \( III \). \( |t''_2|^2 \) is the transmission coefficient.

Equating the wave function and its derivative at the boundaries \( x = 0 \) and \( x = d \), for the transmission coefficient we obtain

\[
|t''_2|^2 = \frac{4ik''_1 k''_2 e^{-ik_2^a d}}{e^{-k_2^a d}(k_2^2 + ik''_2)^2 - e^{k_2^a d}(k_2^2 - ik''_2)^2} \quad (66)
\]

Eq. 66 is the same as that given by Katsnelson et al. 27 in the context of the tunneling probability for the bilayer graphene dispersion. \( k_2^a \) gets large as the potential \( V \) gets large. Because of the presence of the exponential factor \( e^{k_2^a d} \) in the denominator, the transmission coefficient given by Eq. 66 goes to zero as the potential goes to infinity. Thus there is no perfect transmission when the potential is in the non relativistic direction and the particle is incident normally, as mentioned above.

IX. SUMMARY

In this paper several low energy properties of the semi-Dirac, semi-Weyl degenerate semimetal have been studied. Whereas some of the properties are intermediate between the conventional parabolic and the linear “Dirac” dispersion, as is the case for the
FIG. 4: Complete transmission for various orientations of the potential

cyclotron frequency, some other properties can be distinct and rather unusual. The results for the Klein scattering for the semi-Dirac dispersion have been obtained for normal incidence on an arbitrarily oriented barrier in the 2D plane, revealing that an electron can tunnel through the barrier with probability one, subject to a resonance condition being met, except for the direction where linear dispersion does not enter the problem. The extreme anisotropy of the plasmon frequency is a distinctive feature of a semi-Dirac system. Intriguing behavior for the Faraday rotation, Hall coefficient and heat capacity have been provided. Finally, we note that the behavior of the orbital susceptibility is distinct from both quadratic and linear systems, being strongly dependent on doping level.

X. ACKNOWLEDGMENTS

This project was supported by DOE grant DE-FG02-04ER46111 and was facilitated by interactions within the Predictive Capability for Strongly Correlated Systems team of the Computational Materials Science Network.

Appendix A: $2 \times 2$ eigensystems

I. The eigenvalues $\lambda_{\pm}$ and eigenstates $\Lambda_{\pm}$ of the 2 by 2 real matrix

$$\tau_z + \tan \theta \tau_x$$

are given by:

$$\lambda_+ = (\cos \theta)^{-1}; \quad \Lambda_+ = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}$$

$$\lambda_- = -(\cos \theta)^{-1}; \quad \Lambda_- = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix}$$

II. For the matrix

$$- [\tau_z - \tan \theta \tau_x],$$

the eigensystems are

$$\lambda_+ = (\cos \theta)^{-1}; \quad \Lambda_+ = \begin{pmatrix} \sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}$$

$$\lambda_- = -(\cos \theta)^{-1}; \quad \Lambda_- = \begin{pmatrix} \cos(\theta/2) \\ -\sin(\theta/2) \end{pmatrix}$$

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