Universal Scaling and Signatures of Nodal Structures in Electron Tunneling from Two-Dimensional Semimetals

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We present the theory of out-of-plane electron thermal-field emission from 2D semimetals. We show that the current (J) - field (F) - temperature (T) characteristic is captured by a universal scaling law applicable for broad classes of 2D semimetals, including monolayer and few-layer graphene, nodal point semimetals, nodal line semimetals and Dirac semimetals at the verge of topological phase transition. The low-temperature scaling takes the universal form, \( \log(J/F^\gamma) \propto -1/F \) with \( \gamma = 1 \) for 2D semimetals, which is in stark contrast to the classic Fowler-Nordheim scaling of \( \gamma = 2 \) for 3D metals. Importantly, the Fermi level dependence of the tunneling currents depends sensitively on the nodal structure through the electronic density of states, thus serving as a probe for detecting the various possible nodal structures of 2D semimetals. Our findings provide a theoretical basis for the understanding of tunneling charge transport phenomena in solid/vacuum and solid/solid interfaces, critical for the development of 2D-material-based vacuum and solid-state electronic devices.

**Introduction.**— In two-dimensional (2D) materials, the confinement of electrons within atomic-scale thickness and the emergence of fermions with exotic dispersions lead to unusual transport properties unique to 2D \([1, 2]\) such as Klein tunneling \([3]\), unconventional quantum Hall \([4]\) and spin Hall effects \([5]\), valley contrasting transport \([6]\) and spontaneous berryogenesis \([7]\). Particularly in thermonic emission, where electrons are emitted from a surface via semiclassical thermal excitation, the universal current-temperature scaling law represents another fascinating transport manifestation of the reduced dimensionality of 2D materials \([8]\), challenging the century-old Richardson-Dushman thermionic emission theory \([9]\) in the 2D flatland.

Apart from thermonic emission, electron can undergo quantum mechanical field emission \([10]\) when an external applied field strongly enhances the electron tunneling from a solid surface by “narrowing” the interface potential barrier. Fowler-Nordheim (FN) theory \([11]\) has been the key theoretical foundation for electron field emission in bulk (3D) materials, and stood as a central pillar of vacuum device technology. Remarkably, field emission physics remains highly important to solid-state devices today due to its critical role in interfacial charge injection processes across the metal/insulator and metal/semiconductor interfaces \([12]\), which are omnipresent in modern electronic and optoelectronic devices. Due to its technological importance in both vacuum \([13]\) and solid-state device technology, FN theory has been continually refined over the past decades \([14–18]\).

In 2D materials, the validity of FN-type theories need to be scrutinized since their fundamental assumption of 3D parabolic dispersions are fundamentally incompatible with 2D materials \([19]\). Despite ongoing experimental \([20–30]\) and theoretical \([31–34]\) efforts in unearthing the physics of electron emission from graphene, a comprehensive understanding of electron emission from the broader family of 2D semimetals remains largely incomplete. The following questions remain open: (i) How does the field emission current relate to the applied electric field strength and emitter temperature? (ii) What are radical differences between the electron field emission in 2D and 3D materials? (iii) Is there a unifying scaling relation, counterpart to the universal current-temperature scaling law of semiclassical thermionic emission \([8]\), that encompasses field emission characteristics for generic 2D semimetals? (iv) Can emission characteristics reveal the nature of nodal structures of 2D semimetals?

In this work, we address the above questions by developing the theory of out-of-plane electron thermal-field emission from 2D semimetals. We present full numerical and approximate analytical expressions of the thermal-field emission current \([14]\) for various 2D semimetals, including monolayer and few-layer graphene \([1]\), nodal point semimetals \([35]\) of generalized pseudospin vorticity \([36]\), Dirac semimetals at the verge of topological phase transi-
plane direction, respectively; \( \varepsilon \) energy and the quantized wavevector along the out-of-plane direction, respectively, and \( c \) is a field-dependent parameter (defined below), and \( \varepsilon \equiv dF/k_BT \). In particular, Eq. (1) departs from the 3D material thermal-field emission scaling law \( \mathcal{J}_{3D}(F, T) \approx A (dF/F)^\varepsilon \sin \left( \pi \varepsilon \right) \exp \left( -B/F \right) \),

where \( A \) and \( B \) are material-dependent parameters, \( F \) is the electric field strength, \( T \) is the emitter temperature, \( dF \propto F \) is a field-dependent parameter (defined below), and \( c \equiv dF/k_BT \). In particular, Eq. (1) departs from the 3D material thermal-field emission scaling law \( \mathcal{J}_{3D} = A dF/F \sin (\pi/c) \exp (-B/F) \), which reveals the fundamental incompatibility of classic FN-type theories with 2D semimetals.

The universal thermal-field emission scaling law identified here reveals an important feature of thermal-field emission in 2D: It is fundamentally determined by the density of states and dispersion profile of the 2D material, and hence exhibits strong Fermi level dependence. In particular, it is the topology of nodal structure, not band topology, that corresponds to markedly distinct transport regimes, as presented in Fig. 2. This contrasts with various other electronic, optical, electrical, mechanical and thermodynamical properties, where signatures of nontrivial band topology are also manifested in the density of states [39], transport [40, 41], optical response [42–44], quantum oscillations [46, 89], many-body behavior [48–50], and shear viscosity [36]. As electron field emission is a key charge transport mechanism in both solid/vacuum [51] and solid/solid interfaces [54, 55], the model developed here shall offer a pivotal theoretical foundation for both the fundamental understanding of nanoscale surface physics, and the design of novel vacuum [52] and solid-state devices based on 2D materials heterostructures [53].

2D electron emission theory.— In a 2D system, the confinement of electrons within the 2D plane lead to the formation of discrete subbands. The energy dispersion and the wavevector of the ith-subband are, \( \varepsilon_{i,\parallel} = \varepsilon_{i,\parallel}(k_{i,\parallel}) + \varepsilon_{i,\perp}(k_{i,\perp}) \) and \( k_{i,\parallel} = k_{i,\parallel} + k_{i,\perp}, \) respectively, where \( \varepsilon_{i,\perp} \) and \( k_{i,\perp} \) denote the discrete subband energy and the quantized wavevector along the out-of-plane direction; respectively; \( \varepsilon_{i,\parallel} \) and \( k_{i,\parallel} \) denote the continuously-dispersing in-plane energy dispersion and wavevector, respectively. The out-of-plane electron emission current density can be generally expressed as [36]:

\[
\mathcal{J}_{2D}(F, T) = \frac{g \varepsilon}{(2\pi)^3} \sum_{i} \tau_{i,\perp}^{-1} \int_{B.Z.} d^2k_{\parallel} D(k_{i}, F) f(k_{i}, k_{F}),
\]

where \( g \) is the degeneracy factor, \( k_{F} \) is the Fermi wavevector, \( D(k) \) is the out-of-plane tunneling probability, \( f(k_{i}) \) is the Fermi-Dirac distribution function, the \( k_{\parallel}-\)integral spans the whole Brillouin zone, \( \sum_{i} \) runs over all subbands, and \( \tau_{i,\perp}^{-1} \) is the vertical electron injection rate, which is affected by the intrinsic material properties and the device configuration, and can be experimentally extracted from the transport measurements [69–71]. The transmission probability, \( T(k_{i}, F) \), is a function of the total wavevector, \( k_{i} \), instead of only the out-of-plane component \( k_{i,\perp} \), due to the \( k_{i,\perp}\)-nonconserving scatterings [56–62], which can arise extrinsically from electron-electron [56], phonon [63], magnon [64], and defects [57, 65] scatterings. Such momentum nonconservation leads to the coupling of the \( k_{i,\perp} \) and \( k_{i,\parallel} \) during the out-of-plane tunneling process [8].

For thermal-field emission, the tunneling potential barrier is modeled, with inclusion of the image-charge effect across a dielectric interface, as \( U(z) = \Phi_{B0} - eFz - e^2
\beta/16\pi\varepsilon_{B}z \), where \( \Phi_{B0} \) is the intrinsic interface potential barrier height measured from zero-energy, \( \nu \equiv (\varepsilon_{s}-1)/(\varepsilon_{s}+1) \), and \( \varepsilon_{s} \) is the dielectric constant of the substrate material (see Fig. 1). The corresponding transmission probability can be accurately approximated as [14],

\[
D(k_{i}, F) \approx D_F \exp \left\{ \left[ \varepsilon_{i}(k_{i,\parallel}) + \varepsilon_{i,\perp}(k_{i,\perp}) - \varepsilon_{F} \right]/\varepsilon_{F} \right\},
\]

where \( D_F \equiv \hbar eF/(8\pi m_{0})^{1/2} (\Phi_{B} - \varepsilon_{F})^{1/2} \), \( D_F \equiv \exp \left[-4(2m_{0})^{1/2} (\Phi_{B0} - \varepsilon_{F})^{3/2} \nu_{0}/3\hbar eF \right], \nu_{0} \) and \( t_{0} \) correction factors for the image charge effect, and \( m_{0} \) is the free electron mass (see [66] for detailed derivations). Considering the typical case where there is only one subband around the Fermi level \( \varepsilon_{F} \), Eq. (2) becomes

\[
\mathcal{J}_{2D}(F, T) = \frac{g e D_F}{4\pi^{2} \tau_{\perp}} \int_{B.Z.} d^2k_{\parallel} \frac{\exp \left( \varepsilon_{i,\parallel} - \varepsilon_{F} \right)}{\exp \left( \varepsilon_{i,\parallel} - \varepsilon_{F} \right) + 1},\]

where \( k_{\parallel} \) and \( \varepsilon_{\parallel} \) denote the in-plane wavevector and energy components of the subband undergoing emission.

We now express the emission current in Eq. (3) in terms of a 2D anisotropic density of states (DOS). The DOS is defined as \( \rho(\varepsilon_{\parallel}, \varepsilon_{\perp}) = \gamma / (2\pi m_{0}^2) \int_{0}^{2\pi} d\phi \rho_{\|}(\varepsilon_{\||}) \) where \( \varepsilon_{\||} \equiv |k_{\||}| \). Very generally, we can express the \( k_{\||}\)-differential as a two-variable polynomial, i.e. \( k_{\||} = \sum_{m=0}^{\infty} \beta_{ml} \varepsilon_{\||}^{m} \cos(l \phi) \varepsilon_{\||}^{m} \) where \( \beta_{ml} \) is an expansion coefficient of \( (m, l) \)-order in \( \varepsilon_{\parallel}, \cos \phi \), which yields

\[
\rho(\varepsilon_{\parallel}) = g \sum_{m=0}^{\infty} \beta_{m} \varepsilon_{\||}^{m},
\]

where \( m \in \mathbb{Z} \geq 0 \) and \( \beta_{m} \) is defined as [66],

\[
\beta_{m} = \frac{\beta_{ml}}{2\pi} \int_{0}^{2\pi} \cos(l \phi) d\phi = \frac{\beta_{ml}}{2\pi} \sum_{l \in \text{even},>0} \frac{\beta_{ml}}{2\pi} \sum_{k=1}^{l} \frac{2k-1}{2k}.
\]

Combining Eqs. (3) and (4), the universal thermal-field emission electrical current density from a 2D semimetal
becomes $J_{\text{uni}} = \sum_{m} J_{\text{uni}}^{(m)}$ where the $m$-component is,

$$J_{\text{uni}}^{(m)} = \frac{g_e D F}{\tau_{\perp}} \beta_m \int_{-\infty}^{\infty} d\varepsilon_{\parallel} \left|\varepsilon_{\parallel}\right|^{m} \exp \left(\frac{\varepsilon_{\parallel}-\varepsilon}{d F}\right) \frac{\exp \left(\frac{\varepsilon_{\parallel}-\varepsilon}{k_B T}\right)}{1 + 1},$$

(6)

which cannot be analytically solved except for the case of $m = 0$. An approximate analytical expression can be obtained by making the following ansatz. The term $\left|\varepsilon_{\parallel}\right|^{m}$ is replaced by $\xi_m \left|\varepsilon_{\parallel}\right|^{m}$ since field emission is dominantly contributed by electrons residing around $\varepsilon_{F}$. Here $\xi_m$ is a correction factor for the $m$-th order term which can be obtained by fitting the full numerical results with the analytical approximation derived below. By a substitution $u = \exp \left(\left|\varepsilon_{\parallel} - \varepsilon_{F}\right|/d F\right)$, Eq. (6) becomes [66]

$$J_{\text{uni}}^{(m)} \approx \xi_m \frac{g_e D F}{\tau_{\perp}} \beta_m \left|\varepsilon_{\parallel}\right|^{m} F \int_{0}^{\infty} \frac{du}{u^m + 1},$$

(7)

where $c \equiv d F/k_B T$. The above integral can be analytically evaluated for the thermal-field emission condition of $c > 1$ (i.e. $d F > k_B T$ which remains valid for $T \lesssim 550$ K at $F = 1 \text{ V/nm}$),

$$J_{\text{uni}} \approx \xi_m \frac{g_e D F}{\tau_{\perp}} \beta_m \left|\varepsilon_{\parallel}\right|^{m} \frac{\pi d F}{c \sin (\pi/c)} D F.$$  

(8)

We evaluate the full numerical solution [Eq. (6)] and the analytical approximation [Eq. (8)] for $m = 0, 1, 2, 3, 4$ (Fig. 2). The approximate solution agrees well with the full numerical results over the range of $F = 1 \text{ V/nm}$ to $F = 5 \text{ V/nm}$ with $\xi_m = (1, 1.22, 4, 24, 220)$ for $m = 0$ to $m = 4$. From Eq. (8), we obtain the following scaling law,

$$J \propto \frac{\pi d F}{c \sin (\pi/c)} D F.$$  

(9)

Equation (9) represents a universal current-field-temperature scaling law for 2D semimetals as long as the DOS near $\varepsilon_{F}$ can be captured by the anisotropic DOS model in Eq. (4). Equation (9) thus offer a simple unifying scaling law description of the thermal-field emission characteristics in 2D semimetals. Below, we derive the thermal-field emission characteristics for several representative 2D semimetals, including: (i) graphene and its few-layer; (ii) nodal point semimetal; (iii) Dirac semimetal near topological phase transition; and (iv) nodal line semimetal, and show that their current-field-temperature scaling relation universally converges to Eq. (9) (summarized in Fig. 2).

**Graphene.**—We first consider graphene, a 2D Dirac semimetal, which can be described by the effective Hamiltonian, $\hat{H}_{\text{Gr}}(k) = \hbar v_F (k_x \sigma_x + k_y \sigma_y)$ where $k \parallel = (k_x, k_y)$ is the in-plane wavevector, $\sigma_{x,y}$ are the Pauli matrices, and $v_F = 10^6 \text{ m/s}$. Using the procedure described above, the thermal-field emission current density can be solved as,

$$J_{\text{Gr}}/\psi \approx \frac{2e \Phi_B}{\tau_{\perp} \pi \hbar^2 v_F} \frac{\left|\varepsilon_{\parallel}\right|^{1+\eta}}{\Phi_B} \frac{\pi d F}{c \sin (\pi/c)} D F.$$  

(10)

where $\varepsilon_{F}$ (also implicit in $d F$, $c$ and $D F$) is a function of the applied electric field strength, i.e. $\varepsilon_{F} = \varepsilon_{F}(F)$, due to the field-effect tunable Fermi level in graphene [72]. Assuming a planar geometry and an undoped graphene with $\varepsilon_{F}(F = 0) = 0$, we obtain [66] $\varepsilon_{F}(F) = \sqrt{\pi^2 \hbar^2 v_F^2 / e}$ with $\eta = 0.176$ as fitted from the full numerical solution. Apart from exhibiting the universal scaling, $J_{\text{2D}}$ follows the $\varepsilon_{F}$-dependence, $J_{\text{Gr}}/\psi \propto \left|\varepsilon_{F}\right|^{1+\eta}$ where $\psi \equiv \pi d F D F/c \sin (\pi/c)$. As demonstrated below, the $J/\psi - \varepsilon_{F}$ scaling is sensitively influenced by the nodal structure, thus serving as a tool to probe different possible nodal structures of 2D semimetals (see Table I).

**Nodal point semimetal.**—We next consider a general model of 2D nodal point semimetal with the effective Hamiltonian [36],

$$\hat{H}_{NP}(k) = \alpha_n \left(k_{x}^n \sigma_x + k_{y}^n \sigma_y \right),$$  

(11)

where $\alpha_n$ is a material-dependent parameter, and $n \in \mathbb{Z}^+$ denotes the pseudospin vorticity. Equation (11) also describes the low-energy quasiparticles in $n$-layer graphene of Bernal stacking configuration with $\alpha_n = (\hbar v_F)^n / t_{n-1}$ and $t_\perp = 0.39 \text{ eV}$ [1]. The thermal-field emission current density is,

$$J_{\text{NP}} \approx \xi_n \frac{g_e}{2\pi \tau_{\perp}} \frac{\left|\varepsilon_{\parallel}\right|^{2n-1}}{n \alpha_n^{2n}} \frac{\pi d F}{c \sin (\pi/c)} D F.$$  

(12)

Here the emission current density follows a particularly interesting $\varepsilon_{F}$-scaling of $J_{\text{NP}}/\psi \propto \left|\varepsilon_{F}\right|^{2n-1}$ which depends on the pseudospin vorticity, $n$.

**Dirac semimetal near criticality.**—We now consider a 2D Dirac semimetal near criticality, such as black phosphorus monolayer subjected to a strong vertical electric field [67]. Such system is captured by the effective semi-Dirac Hamiltonian,

$$\hat{H}_{SD}(k) = \hbar v_x k_x \sigma_x + (b k_y^2 + \Delta) \sigma_y,$$  

(13)

where $v_x$ and $b$ are band structure parameters. The system undergoes a critical phase transition when $\Delta$ is switched from $\Delta \leq 0$ to $\Delta > 0$, with two Dirac cones merging into one at $\Delta = 0$ and then gapping out. In the semimetallic phase ($\Delta \leq 0$), the thermal-field emission current density is

$$J_{\text{SD}} \approx \xi \frac{g_e}{(2\pi)^2 \tau_{\perp} b} \int_{\phi_{\text{cr}}} \frac{d \phi}{\pi} \left(\frac{\pi d F}{c \sin (\pi/c)} D F \right)$$  

(14)

where $\xi_0 \equiv \hbar^2 v_F^2 / b$ is a characteristic energy scale and $\phi = \tan^{-1}(k_y / k_x)$. The $\phi$-integral $\mathcal{I}_{\phi, \xi}(\mu) \equiv \int_{0}^{2\pi} d \phi \left[ \Lambda_{\phi, \mu} - 4 \sin^2 \phi \left( \mu^2 - \varepsilon_{F}^2 / \xi_0^2 \right) \right]^{1/2}$, where $\Lambda_{\phi, \mu} = \mu v_x k_x + (b k_y^2 + \Delta) \sin \phi$.
FIG. 2. Thermal-field electron emission from 2D semimetals, showing energy dispersion (column 1), density of states (column 2), numerical and approximate expressions of the thermal-field emission current density (column 3), and the normalized current (column 4) evaluated at $T = 300$ K, $\epsilon_s = 3.5$, and $\Phi_{B0} = 4.5$ eV. For nodal semimetal, Dirac semimetal near criticality and nodal line semimetal, $\varepsilon_F = 0.1$ eV is used. The full numerical and the analytical approximate solutions are denoted by circle and solid curves, respectively. The normalized currents are defined as $J_{NP} = c \varepsilon_F / n \tau_\perp \Delta \pi^2 \tau_\parallel b$, $J_{QCP} = \xi \varepsilon_F / \Delta \pi^2 \tau_\parallel b$, and $J_{unw} = \xi / \Delta \pi^2 \tau_\parallel b$. Here, $\xi = l_\parallel / l_\perp$, $\Phi_{B0} = d_F / \Phi_{B0}$, and $\Delta = \Delta_0 / \Delta_1$. The correction factors are $\eta = 0.176$ for graphene, and the $\xi$'s of other 2D semimetals are outlined in the Supplemental Material [66].
TABLE I. The current versus Fermi level scaling relation for various 2D semimetals.

| 2D System                          | $\varepsilon_F$ dependence of $J/\psi$ |
|-------------------------------------|----------------------------------------|
| Graphene                            | $|\varepsilon_F|^{1+\eta}$                 |
| Nodal point semimetal               | $|\varepsilon_F|^{2/n-1}$               |
| Dirac semimetal near criticality    | $|\varepsilon_F|=\varepsilon_F(\Delta/\varepsilon_0)$ |
| Nodal line semimetal                | constant in $\varepsilon_F$            |

$(\cos^2 \phi + 2\mu \sin^2 \phi)^2$, arises from the broken rotational symmetry of Eq. (13). In this case, $\mathcal{J}_{3D}/\psi \propto |\varepsilon_F|\mathcal{I}_0,\varepsilon_F(\Delta/\varepsilon_0)$.

**Nodal line semimetal.** In a 2D nodal line semimetal, the band touching of two bands extends from a discrete nodal point into a continuous one-dimensional open nodal line or closed nodal ring in phase space. We consider a representative 2D semimetal that hosts an isotropic iso-energy nodal loop, such as carbon nitride monolayer [68], as described by,

$$\mathcal{H}_{NL}(k_x) = \left( b k_x^2 - \Delta \right) \sigma_x \tag{15}$$

where $\Delta$ is a band inversion parameter. Solving Eq. (3) yields the approximate solution,

$$\mathcal{J}_{NL} \approx \xi \frac{g^e}{4\pi b r_\perp} \frac{\pi d_F}{c \sin (\pi/c) D_F}, \tag{16}$$

where $\mathcal{J}_{NL}/\psi$ is constant in $\varepsilon_F$.

Before closing this work, we make four remarks. Firstly, in the ‘cold’ field emission regime ($T \to 0$), Eq. (9) becomes $\mathcal{J}_{2D}(F,T \to 0) \propto d_F D_F$, which is in stark contrast to the FN law for bulk materials, $\mathcal{J}_{3D}(F,T \to 0) \propto d_F^2 D_F$. Ignoring the image-charge effect, the FN plot [73] widely used in characterizing electron field emission and solid-state tunneling charge injection can thus be generalized as,

$$\log \left( \frac{\mathcal{J}}{F^\gamma} \right) \propto -\frac{1}{F}, \tag{17}$$

where $\gamma = 1$ and 2, respectively, for 2D and 3D materials. Secondly, the scaling law is universal except in the case of a non-dispersing 2D flat bands in 2D systems such as Kagome [74], Lieb [75], $\alpha$-T$^3$ [76], Weierstrass-function-inspired [77] and Archimedian [78] lattices. For a flat band situated at $\varepsilon_\parallel = \varepsilon_{FB}$, the thermal-field emission current density is

$$\mathcal{J}_{FB} \propto D_F \exp \left( \frac{\varepsilon_{FB} - \varepsilon_F}{d_F} \right) \left[ 1 + \exp \left( \frac{\varepsilon_{FB} - \varepsilon_F}{k_B T} \right) \right]^{1/m}, \tag{18}$$

which clearly deviates from Eq. (9). Such deviation also explains the reduced accuracy of Eq. 8 in approximating $\mathcal{J}^{(m,l)}$ using Eq. 6 at large $m$ since each $|\varepsilon|^m$ term in Eq. (4) corresponds to $\varepsilon_\parallel \propto k_B^{2/(m+1)}$ and thus a larger $m$ corresponds to a ‘flatter’ dispersion. Thirdly, the thermal-field emission model developed here can be directly mapped onto the case of charge tunneling injection in the solid-state interfaces of metal/insulator and semiconductor/metal interfaces. Finally, we emphasize that although the $\mathcal{J}^{-}\mathcal{T}$ scaling does not offer distinctive signature of nontrivial band topology, the $\mathcal{J}^{-}\varepsilon_F$ scaling does contain rich scaling signatures for different nodal structures (see Table 1), which can represent cross sections of sophisticated topological structures classified by knot theory and singularity theory [79–83].

In conclusion, we developed the theory of out-of-plane thermal-field electron emission from 2D semimetals. We demonstrated the existence of a universal current-field scaling law broadly applicable for a large variety of 2D semimetals with different nodal structures. As thermal-field emission represents one of the key charge transport process across solid/vacuum and solid/solid interfaces, the universal scaling law developed here shall be a ubiquitous tool for the study and the design of vacuum electronics, nanoelectronics, optoelectronics and the emerging fields of spintronic [84], valleytronic [85] and neuromorphic [86] devices using 2D materials, and shall offer a theoretical basis for the understanding of complex electron emission phenomena, such as ultrashort-pulsed laser-induced internal photoemission [87] and photo-assisted hot carrier field emission [88, 89] in the 2D Flatland.

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