

Electron mobility in graphene without invoking the Dirac equation

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The Dirac point and linear band structure in graphene bestow it with remarkable electronic and optical properties, a subject of intense ongoing research. Explanations of high electronic mobility in graphene often invoke the masslessness of electrons based on the effective relativistic Dirac-equation behavior, which are inaccessible to most undergraduate students and are not intuitive for non-physics researchers unfamiliar with relativity. Here, we show how to use only basic concepts from semiconductor theory and the linear band structure of graphene to explain its unusual effective mass and mobility, and compare them with conventional metals and semiconductors. We discuss the more intuitive concept of transverse effective mass, which emerges naturally from these basic derivations, and which approaches zero in the limit of undoped graphene at low temperature and is responsible for its extremely high mobility. © 2019 American Association of Physics Teachers.

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I. INTRODUCTION

Graphene is often described in superlatives, with a multitude of extreme electronic, mechanical, and chemical properties of interest in disparate fields of research.^{1–3} This increasingly motivates exposure to graphene science at the undergraduate level,⁴ with excellent pedagogical resources introducing the calculation of its unique Dirac-point band structure,^{5,6} explaining novel transport phenomena such as Klein tunneling,⁷ and even outlining experimental demonstrations of the unique wave mechanics of honeycomb lattices in ripple tanks.⁸

Of graphene's extreme properties, its exceptional electrical conductivity and mobility, arising from the effective masslessness of electrons in the Dirac band structure are often discussed.⁹ Explaining the high mobility from a low effective mass is easily accessible at an undergraduate level with standard semiconductor physics derivations of Drude theory.¹⁰ However, explaining why the Dirac band structure corresponds to massless carriers is somewhat more challenging, and has not yet been discussed clearly in a pedagogical context. Specifically, the Dirac band structure contains a linear dispersion relation $E = v_F p$, corresponding to a constant electron speed $v = \partial E / \partial p = v_F$, independent of the momentum. Here, $v_F \approx 8.3 \times 10^5$ m/s is the Fermi velocity of graphene, the velocity of electrons at the Fermi energy up to which states are filled with electrons.¹¹ Naive application of the conventional semiconductor definition of effective mass, which corresponds to $(m^*)^{-1} = \partial v / \partial p = 0$ as we discuss below in further detail, leads to the opposite result of infinite mass! (See Fig. 1.)

Research papers invoke seminal work¹² that demonstrated that electron transport in graphene is essentially governed by the Dirac equation, with the charge carriers mimicking relativistic particles with zero rest mass. In the relativistic picture, linear dispersion corresponds to massless carriers by recognizing that $E^2 = (mc^2)^2 + (pc)^2$ for a particle of mass m reduces to $E = pc$ when $m = 0$. However, this is only an analogy⁶ and must be applied very carefully to graphene. For graphene, the electrons have a constant velocity $v_F \approx 8.3 \times 10^5$ m/s $\sim c/400$, as discussed above, instead of the speed of light c . Importantly, there is no Lorentz invariance for carriers in graphene: the frame in which the carbon nuclei are at rest is special! Therefore, explaining masslessness of graphene carriers using relativity, though valid when done

correctly, will likely lead to confusion especially at the introductory undergraduate level. Moreover, it is not an intuitive explanation for students from related fields in chemistry, materials science, or electrical engineering, who are all increasingly likely to encounter graphene in their careers.

Pedagogical descriptions that try to avoid the relativistic / Dirac explanation often rely on alternate definitions of the mass that work correctly for graphene, e.g., cyclotron effective mass,^{13,14} quaternion effective mass,¹⁵ etc. While these definitions work for a reason, as we will discuss below, they do not provide an intuitive picture of how electrons in graphene conduct remarkably well. Most importantly, some of these alternate approaches attempt to redefine the effective mass as the ratio of the *momentum to velocity*,¹³ $m^* = p/v$, rather than the ratio of *force to acceleration*, $m^* = F/a = \partial p / \partial v$. Such alternate definitions are correct only for a parabolic band structure, where the mass is independent of the momentum and the two expressions above become equivalent.

Here, we describe an alternate pedagogical approach to explain massless electrons in graphene, where we retain the standard definition of effective mass from semiconductor theory, albeit the full tensorial version. We demonstrate how to work through this definition to understand how graphene's effective mass and mobility vary with doping and temperature, and how it contrasts for conventional metals and semiconductors. We show how to arrive at the concept that the transverse effective mass, rather than the usual longitudinal one, dominates transport in graphene, and is the mass that approaches zero near the Dirac point in graphene. The approach presented here should be suitable for intuitively explaining the remarkable electronic properties of graphene—a topic of continuing research interest—at the senior undergraduate level.

II. DERIVATIONS

Electrons in materials with a band structure or dispersion relation $E(k)$ have group velocity $v = \partial E / \partial p$ and momentum $p = \hbar k$, using only basic principles in quantum mechanics. When an electric field is applied to the material, the electric force accelerates the electrons and generates a current. For the same force, lighter electrons will be accelerated more, and will result in higher mobility and conductivity. Consequently, the mass relevant for determining conduction

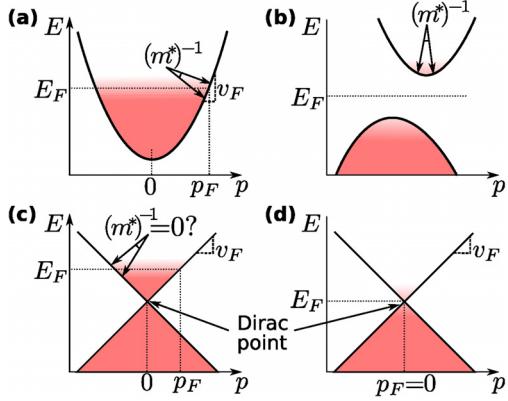


Fig. 1. Schematic band structure of (a) a free-electron metal, (b) a parabolic-band semiconductor, (c) doped graphene and (d) undoped graphene, with band velocity (E vs p slopes) and effective mass (inverse E vs p curvature) annotated. The shading denotes the Fermi occupation factors of electrons. Naively, the linear band structure yields zero curvature and an infinite effective mass in graphene, rather than zero or a low value.

by electrons is the ratio of force F to acceleration a (exactly as in Newton's second law). Now $F = dp/dt$ and $a = dv/dt$, which yield

$$\begin{aligned} (\bar{m}^*)^{-1} &\equiv \frac{dv/dt}{dp/dt} = \frac{\partial v}{\partial p} = \frac{\partial(\partial E/\partial p)}{\partial p} \\ &\equiv \frac{\partial^2 E}{\partial p^2} = \frac{\partial^2 E}{\hbar^2 \partial k^2}, \end{aligned} \quad (1)$$

the well-known expression in semiconductor theory that the effective mass is the inverse of the curvature of the band structure $E(k)$.^{10,11} The curvature and effective mass are both finite (non-zero and not infinite) for metals and semiconductors, as shown in Fig. 1. However, for graphene, the linear band structure has seemingly zero curvature corresponding to an infinite effective mass, in stark contrast to the massless carrier explanation for its high mobility.

The simplest correct explanation for massless electrons in graphene lies within the standard definition, but necessitates the full tensorial version,^{10,11}

$$(\bar{m}^*)^{-1} \equiv \frac{1}{\hbar^2} \nabla_{\vec{k}} \nabla_{\vec{k}} E(\vec{k}). \quad (2)$$

The mass tensor is just a matrix that connects how changes of momentum and velocity are related, $d\vec{p} = \bar{m}^* \cdot d\vec{v}$, or equivalently $d\vec{v} = (\bar{m}^*)^{-1} \cdot d\vec{p}$, which are not in the same direction for a general $E(\vec{k})$. For two-dimensional graphene near the Dirac point, the above definition reduces to

$$(\bar{m}^*)^{-1} = \frac{1}{\hbar^2} \begin{pmatrix} \partial_{k_x}^2 & \partial_{k_x} \partial_{k_y} \\ \partial_{k_x} \partial_{k_y} & \partial_{k_y}^2 \end{pmatrix} \hbar v_F \sqrt{k_x^2 + k_y^2}. \quad (3)$$

Straightforward evaluation of the derivatives yields

$$(\bar{m}^*)^{-1} = \frac{v_F}{\hbar} \begin{pmatrix} \frac{k_y^2}{(k_x^2 + k_y^2)^{3/2}} & -\frac{k_x k_y}{(k_x^2 + k_y^2)^{3/2}} \\ -\frac{k_x k_y}{(k_x^2 + k_y^2)^{3/2}} & \frac{k_x^2}{(k_x^2 + k_y^2)^{3/2}} \end{pmatrix} \quad (4)$$

$$= \frac{v_F}{p^3} \begin{pmatrix} p_y^2 & -p_x p_y \\ -p_x p_y & p_x^2 \end{pmatrix}, \quad (5)$$

using $\vec{p} \equiv \hbar \vec{k}$. With the definition

$$\bar{M}(\phi) \equiv \begin{pmatrix} \sin^2 \phi & -\sin \phi \cos \phi \\ -\sin \phi \cos \phi & \cos^2 \phi \end{pmatrix}, \quad (6)$$

the inverse effective mass tensor can be written in polar coordinates as

$$(\bar{m}^*)^{-1} = \frac{v_F}{p} \bar{M}(\phi). \quad (7)$$

As with any symmetric tensor, the inverse mass tensor is best characterized in its principal axes or eigenvectors, so that it becomes diagonal. Solving the characteristic equation $\det[(\bar{m}^*)^{-1} - \lambda \mathbb{1}] = 0$ yields the two eigenvalues

$$\lambda = \left\{ 0, \frac{v_F}{p} \right\}, \quad (8)$$

and their corresponding eigenvectors can be derived to be

$$\vec{x} = \left\{ \frac{1}{p} \begin{pmatrix} p_x \\ p_y \end{pmatrix}, \frac{1}{p} \begin{pmatrix} p_y \\ -p_x \end{pmatrix} \right\}. \quad (9)$$

The first eigenvector is exactly \hat{p} , the unit vector along the momentum. This principal direction therefore corresponds to changes in momentum parallel to the momentum direction, which is a “longitudinal” change. The corresponding inverse mass eigenvalue is 0, therefore implying that the longitudinal mass $m_L \rightarrow \infty$, which is exactly the result we obtained in the non-tensorial analysis.

However, now we have the second eigenvector which is perpendicular to \hat{p} , corresponding to changes in momentum perpendicular to the momentum direction, which is a “transverse” change. The corresponding inverse mass eigenvalue is v_F/p , corresponding to a transverse mass $m_T = p/v_F$. As we approach the Dirac point $p \rightarrow 0$, the transverse mass $m_T \rightarrow 0$. Therefore, at the Dirac point, electrons in graphene have an infinite longitudinal mass, but are massless in the transverse direction.

This result can also be understood intuitively, directly from the linear dispersion relation, $E(\vec{p}) = v_F |\vec{p}|$. The corresponding velocity $\vec{v} \equiv \nabla_{\vec{p}} E(\vec{p}) = v_F \hat{p}$, is always parallel to the momentum \vec{p} , but has a constant magnitude v_F independent of p . As shown in Fig. 2(a), when the momentum is changed in the longitudinal direction, the momentum direction \hat{p} is unchanged, so the velocity direction and magnitude remain unchanged. No change in velocity with changing momentum yields zero inverse mass and an infinite longitudinal mass, $m_L \rightarrow \infty$. However, when momentum is changed in the transverse direction by $\delta \vec{p}_T$, the momentum and velocity directions both change by the angle $\delta\theta = \delta p_T/p$. Since the velocity magnitude is unchanged, the velocity vector changes by $\delta v = v_F \delta\theta = v_F \delta p_T/p$. Therefore, the ratio of velocity to momentum change is v_F/p which corresponds to the transverse mass, $m_T = p/v_F$. This can also be seen comparing radial (longitudinal) and transverse slices of the conical $E(\vec{k})$ near the Dirac point (Fig. 2(b)). The linear $E(k)$ along the longitudinal slice yields $m_L \rightarrow \infty$, while the parabolic $E(k)$ in the transverse slice yields finite m_T . The transverse curvature increases as the

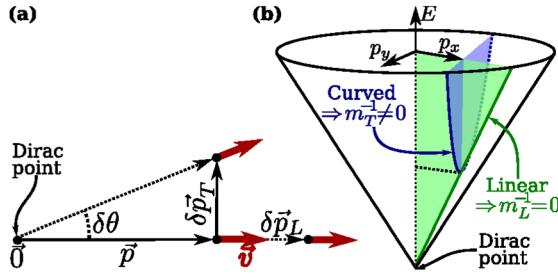


Fig. 2. (a) Velocity (thick red arrows) is always parallel to momentum (thin black arrows) with constant magnitude v_F . Therefore, velocity is unchanged for longitudinal changes in momentum $\delta \vec{p}_L$ yielding infinite longitudinal mass m_L . Velocity changes direction for transverse changes $\delta \vec{p}_T$, resulting in a small transverse mass m_T which $\rightarrow 0$ as $p \rightarrow 0$. (b) Linear $E(k)$ in the radial (longitudinal) slice of the conical $E(k)$ yields $m_L \rightarrow \infty$, while parabolic $E(k)$ in the transverse slice yields a small m_T that approaches zero as the slice gets closer to the Dirac point.

slice gets closer to the Dirac point, resulting in $m_T \rightarrow 0$ near the Dirac point.

The transverse mass is closely related to the cyclotron mass, which is the reason why the latter definition works for graphene.¹³ In a magnetic field, charged particles move in circles with centripetal force and acceleration perpendicular to the velocity. The cyclotron mass is the ratio of force to acceleration when they are both perpendicular to the momentum (velocity) direction, which is exactly the case for the transverse mass as discussed above.

When an electric field \vec{E} is applied to a material, this applies a force $-e\vec{E}$ on all the electrons, resulting in an acceleration $\vec{a} = -e(\bar{m}^*)^{-1} \cdot \vec{E}$. As the electrons move through the material, they scatter against defects and lattice vibrations (phonons), which cause the velocity to randomize due to collisions over the Drude relaxation time scale τ . With these two effects, the electrons pick up an average drift velocity $\vec{v}_d = \vec{a}\tau = -e\tau(\bar{m}^*)^{-1} \cdot \vec{E}$. The ratio of drift velocity to the applied electric field defines the mobility (excluding the sign due to negative charge)

$$\bar{\mu} = e\tau(\bar{m}^*)^{-1}. \quad (10)$$

The total current density in the electron is $\vec{j} = n(-e)\vec{v}_d = ne\bar{\mu} \cdot \vec{E}$, where n is the number density of electrons. The conductivity (tensor) is defined by $\vec{j} = \bar{\sigma} \cdot \vec{E}$, which implies $\bar{\sigma} = ne\bar{\mu}$, elucidating the mobility to be the conductivity per unit charge density.

In general, the effective mass m^* varies with \vec{k} (i.e., \vec{p}), and hence so does the mobility. The experimentally determined mobility is therefore an average over all charge carriers. First, consider the case of n-doped graphene, where a net excess of electrons over holes results in states being occupied up to an energy E_F above the Dirac point. (The discussion for excess holes with E_F below the Dirac point follows in exactly the same way, with exactly the same results, due to the electron \leftrightarrow hole symmetry in the band structure.) From the linear energy relation $E = v_F p$, we can see that this corresponds to a Fermi momentum $p_F = E_F/v_F$ and wave-vector $k_F = E_F/(\hbar v_F)$ (see Fig. 1(c)).

Only electrons within a few $k_B T$ of the Fermi energy contribute to electronic conduction in materials. Intuitively, only these electrons have empty states available to “move” to, being close to the energy at which electronic states transition from filled to empty (Fig. 3(a)). In fact, a more detailed

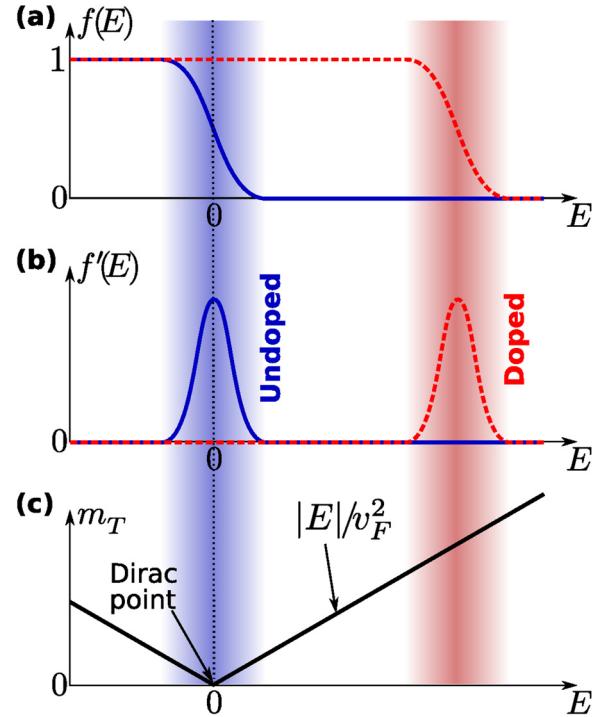


Fig. 3. (a) Fermi function and (b) its derivative for undoped and doped graphene. Shaded regions indicate the contribution to conduction, proportional to the Fermi function derivative. (c) Transverse effective mass in graphene as a function of electron energy, which is distributed around a non-zero value for doped graphene, but around zero for undoped graphene.

analysis based on the Boltzmann transport equation and the relaxation time approximation¹¹ shows that the contribution to conduction is proportional to the derivative of the Fermi function (Fig. 3(b)). If the number density of electrons due to doping is high enough that $E_F \gg k_B T$, then all the electrons that contribute to conduction have approximately the same magnitude of momentum, p_F . Correspondingly, they all have transverse mass $m_T \approx p_F/v_F = E_F/v_F^2$ (Fig. 3(c)), while the longitudinal mass remains ∞ (as shown above for all graphene electrons).

When the effective mass is anisotropic, the well-known simplified expression for mobility $\mu = e\tau/m^*$ remains valid provided an appropriate average of m^* in all directions is used. In particular, m^* should be the harmonic mean of all directions, i.e., if the contributions are m_1 , m_2 , and m_3 in three perpendicular directions (principal axes), the net effective mass should be $(m^*)^{-1} = (m_1^{-1} + m_2^{-1} + m_3^{-1})/3$. For example, in Silicon, $m_L = 0.89$ and there are two equal transverse values (in 3D) $m_{T1} = m_{T2} = 0.19$. The corresponding average value for mobility will then be $m^* = 0.26$. For graphene, we now have $m_L = \infty$ and $m_T = p_F/v_F$ (just one in 2D), which yields

$$m^* = \frac{2}{m_L^{-1} + m_T^{-1}} = \frac{2p_F}{v_F} = \frac{2E_F}{v_F^2}, \quad (11)$$

which is twice the transverse value. Correspondingly, we expect the mobility to be $e\tau/m^* = ev_F^2/(2E_F)$.

We can alternatively derive this result by averaging the mobility contributions due to all electrons contributing to conduction on this “Fermi circle” of radius p_F . This amounts to an average over ϕ

$$\bar{\mu} \equiv e\tau \frac{\int d\phi (\bar{m}^*)^{-1}(\vec{p}_F)}{\int d\phi} \quad (12)$$

$$= e\tau \frac{\int d\phi \frac{v_F}{p_F} \bar{M}(\phi)}{2\pi}$$

$$= \frac{e\tau v_F^2}{E_F} \cdot \frac{1}{2\pi} \int_0^{2\pi} d\phi \bar{M}(\phi) \quad (13)$$

$$= \frac{e\tau v_F^2}{2E_F} \frac{1}{2},$$

by substituting Eqs. (7) and (6), and noting that the angular integrals $\int_0^{2\pi} d\phi \cos^2 \phi = \int_0^{2\pi} d\phi \sin^2 \phi = \pi$ and $\int_0^{2\pi} d\phi \cos \phi \sin \phi = 0$. This also corresponds to an isotropic mobility $e\tau/m^*$, with the effective $m^* = 2p_F/v_F = 2E_F/v_F^2$ as argued above.

In pure (undoped) graphene, the electronic states switch from being occupied to unoccupied at the Dirac point (Figs. 1(d) and 3(a).) The contribution to conduction, proportional to the Fermi function derivative (Fig. 3(b)) as discussed above, is centered near $E=0$. Unlike the doped case, the corresponding effective mass is no longer of similar magnitude throughout the energy range with contributions to conduction, as shown in Fig. 3(c). In particular, the effective mass in the center of the distribution at the Dirac point is zero, while it is non-zero and linearly increasing away from the Dirac point. Therefore, we need to average over the carriers proportional to the Fermi function derivative to estimate the mobility for undoped graphene.

For undoped graphene with the Fermi energy at the Dirac point, $E_F=0$, the occupation of electrons is given by the Fermi function

$$f(E) = \frac{1}{1 + \exp \frac{E}{k_B T}}, \quad (14)$$

with derivative

$$f'(E) = \frac{\exp \frac{E}{k_B T}}{k_B T \left(1 + \exp \frac{E}{k_B T}\right)^2} = \frac{1}{4k_B T} \operatorname{sech}^2 \frac{E}{2k_B T}. \quad (15)$$

We can therefore determine the average mobility of undoped graphene as

$$\bar{\mu} \equiv e\tau \frac{\int dp_x dp_y f'(v_F p) (\bar{m}^*)^{-1}(\vec{p})}{\int dp_x dp_y f'(v_F p)} \quad (16)$$

$$= e\tau \frac{\int_0^\infty p dp \int_0^{2\pi} d\phi \operatorname{sech}^2 \left(\frac{v_F p}{2k_B T}\right) \frac{v_F}{p} \bar{M}(\phi)}{\int_0^\infty p dp \int_0^{2\pi} d\phi \operatorname{sech}^2 \left(\frac{v_F p}{2k_B T}\right)}$$

$$= \frac{e\tau v_F^2}{2k_B T} \cdot \frac{\int_0^\infty dx \operatorname{sech}^2 x}{\int_0^\infty dx x \operatorname{sech}^2 x} \cdot \frac{\int_0^{2\pi} d\phi \bar{M}(\phi)}{2\pi},$$

where we switched the integrals over momenta to polar coordinates and substituted $x = v_F p / (2k_B T)$ to simplify the integral over p . The integrals over x are standard definite integrals that evaluate to the constants 1 and $\ln 2$ in the numerator and denominator, respectively, while the final term is exactly what we evaluated above to be $1/2$. Putting that all together yields

$$\bar{\mu} = \frac{e\tau v_F^2}{2k_B T} \cdot \frac{1}{\ln 2} \cdot \frac{1}{2} = \frac{e\tau v_F^2}{(4 \ln 2) k_B T} \frac{1}{2}. \quad (17)$$

Note that the average mobility is isotropic (scalar) as expected and corresponds to an averaged effective mass

$$\bar{m}^* = \frac{(4 \ln 2) k_B T}{v_F^2}, \quad (18)$$

which is directly proportional to temperature. This is because the transverse mass $m_T \propto p$, and the average magnitude of momentum for electrons in graphene at finite temperature $\propto T$. This is in sharp contrast to conventional metals and semiconductors, and even doped graphene with $E_F \gg k_B T$ as considered above, where the effective mass depends only weakly on temperature.

III. RESULTS AND DISCUSSION

Table I compares the typical effective masses m^* , momentum relaxation time τ , and mobility μ of electrons in a prototypical metal (silver), semiconductor (silicon), and both doped and undoped graphene. The values for silver and silicon are based on experimental measurements, while that for graphene is based on the above derivation along with a first-principles calculated value¹⁶ of $\tau \approx 2$ ps for ideal undoped graphene and $\tau \approx 700$ fs for graphene (ideally) doped to a Fermi energy of 0.1 eV (limited only by electron-phonon scattering).

Metals have a short relaxation time because they have a large number of states at the Fermi level, which enhances electron-phonon scattering. Semiconductors and graphene have much smaller density of states at the energies of electrons that carry current, resulting in an increased relaxation time by one and two orders of magnitude relative to the metal. The typical effective mass is somewhat smaller in semiconductors than metals, but it is two orders of magnitude smaller at room temperature in graphene because the transverse mass approaches zero near the Dirac point. Consequently, the mobility $\propto \tau/m^*$ is smallest for metals. Semiconductor mobilities are one-to-two orders larger due both to larger τ and somewhat smaller m^* . However, in graphene both factors contribute two orders making the mobility at room temperature four orders larger!

Table I. Comparison of typical relaxation time, effective mass, and electron mobility for metals, semiconductors, doped graphene and (undoped) graphene at room temperature.

Material	τ (fs)	m^*/m_e	μ (cm ² /V · s)
Silver	30	1.0	50
Silicon	200	0.26	1400
Graphene with $E_F = 0.1$ eV	700	0.063	2×10^4
Undoped graphene	2000	0.018	2×10^5

Note that despite the much higher mobilities in semiconductors and graphene, the number density n of electrons in metals is sufficiently larger that the conductivity $\sigma = ne\mu$ is still much larger in metals. Specifically, in graphene, the mobility is higher for undoped graphene due to the lower effective mass (and additionally because of a lowered electron-phonon scattering rate¹⁶) than the doped case. However, mobility is effectively the conductivity per carrier available for conduction, and the number of carriers is much smaller for undoped graphene. Consequently, undoped graphene has a low conductivity despite the highest mobility, and graphene actually achieves a higher conductivity at an optimal doping level where the increasing effective mass and scattering rate are compensated by an increased carrier density.^{1,2}

As temperature changes, the scattering time τ is roughly inversely proportional to temperature near room temperature for pure materials, because the amplitude of lattice vibrations increases with temperature. The effective mass is mostly temperature dependent in metals and semiconductors, so that the temperature dependence of mobility follows the scattering time. However for undoped graphene, the effective mass is also temperature dependent causing an additional decrease of mobility with increasing temperature and resulting in an overall T^{-2} dependence near room temperature. The temperature dependence for doped graphene will be similar to conventional metals and semiconductors because the average momentum and hence the average transverse mass is set by the doping level and not by temperature, as derived above.

IV. CONCLUSIONS

We have presented a simplified approach to explain the remarkable mobility of electrons in graphene that relies only on the standard semiconductor theory definition, completely avoiding the conventionally invoked parallel to the Dirac equation and corresponding relativistic explanation. We discussed the calculation of the tensorial effective mass, the emergence of a zero transverse mass (but infinite longitudinal mass) upon approaching the Dirac point and the corresponding temperature-dependent mobilities. The full derivations require only basic concepts from calculus, thermodynamics and semiconductor theory, accessible to undergraduate students in physics, chemistry, materials science and electrical engineering. In addition, we pictorially discussed the concept of transverse effective mass and contrast it with the more intuitively familiar longitudinal mass, which

is critical for understanding the unusual electron transport in graphene.

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