Appendix A
2D–2D Tunneling in the Zero-Coherence-Length Limit

We briefly comment on one additional aspect of the tunneling formalism introduced in Chap. 7, namely, the use of the density-of-states formula of Eq. (7.1) for computing tunneling current [1]. This formula is commonly used in tunneling computations, although obtaining an absolute magnitude of the current is problematic with this approach since it is not obvious what the appropriate pre-factors in front of the integral should be. Of course, with the full theory of Eq. (7.2), we can obtain a current with well-defined magnitude. Also, in the limit of $L \to 0$ of that theory, it is easily shown that we recover Eq. (7.1). However, when we compute currents in that limit, i.e. for smaller and smaller $L$ values, then the currents that we obtain (actually they are current densities, since the computation is for a specific $L^2$ area) become unphysically small. The question we must address is, what is the fundamental source of this decrease in current density for $L \to 0$, and can we somehow produce a current density whose magnitude is physically meaningful even in this limit.

The origin of the unphysical $L \to 0$ limit of the full theory of Eq. (7.2), when evaluated together with Eq. (7.4) or (7.6) and Eq. (7.7) or (7.10), arises from our assumption of limiting the area over which the surface integral in Eq. (7.2) is performed. For very small $L$ values, we then encounter a situation in which the tunneling is restricted to a small area of one electrode over to the same small area of the opposite electrode. This restriction is invalid since we are ignoring the tunneling to neighboring areas in the opposing electrodes. That is, we must consider spreading (dispersion) of these states as they extend across the barrier. To properly deal with this situation, we construct states on each electrode that are restricted to an area $L$, hence with wavefunctions proportional to $[\Theta(x + L/2) - \Theta(x - L/2)][\Theta(y + L/2) - \Theta(y - L/2)]e^{ikr}$ where $\Theta(x)$ is a Heaviside step function. We Fourier transform these wavefunctions in order to deduce their dispersion in the barrier, with each Fourier component extending into the barrier with an exponential decay constant

$$\kappa' = \sqrt{\kappa^2 + \eta^2}, \quad (A.1)$$
(assuming effective masses in the lateral and perpendicular directions) where \( \eta \equiv |\eta| \) denotes the lateral wavevector variable in the Fourier transform. On each electrode the total wavefunction is written as a summation of such states, localized on adjoining areas. We then work through the Bardeen formalism.

For a given state restricted to an area \( A = L^2 \) of the left-hand electrode, we can evaluate contributions to the matrix element Eq. (7.3) from the overlap of that state with states from all areas of the right-hand electrode. To illustrate our result, we compare it to the surface integral in Eq. (7.7), for the case of zero misorientation and where we include a \( \kappa e^{-\kappa d} \) term in that integrand (i.e. from the prefactor of Eq. (7.4)). Whereas Eq. (7.8) was obtained by using an ad hoc restriction of this surface integral over the area \( A \), we now have a more rigorous treatment using our constructed wavefunctions. The term analogous to Eq. (7.7) then becomes

\[
\frac{1}{A} \int dS \kappa e^{-\kappa d} e^{i\Delta k \cdot r} \rightarrow \frac{A}{(2\pi)^2} \sum_{m,n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\eta_x d\eta_y \kappa' e^{-\kappa'd}
\]

\[
\times \text{sinc} \left( \frac{(\eta_x - k_{R,x})L}{2} \right) \text{sinc} \left( \frac{(\eta_y - k_{R,y})L}{2} \right)
\]

\[
\times \text{sinc} \left( \frac{(\eta_x - k_{L,x})L}{2} \right) \text{sinc} \left( \frac{(\eta_y - k_{L,y})L}{2} \right)
\]

\[
\times e^{i[(\eta_x - k_{R,x})mL(\eta_y - k_{R,y})nL]}
\]

(A.2)

where \( m \) and \( n \) label areas of the right-hand electrode, both extending over \( 0, \pm 1, \pm 2, \ldots \).

The \( m = n = 0 \) term of the summation on the right-hand side of Eq. (A.2) dominates for large \( L \), and in that case the expression on the left-hand side of the equation (evaluated as in Eq. (7.8)) is recovered. The additional terms in that sum are negligible for \( L > 10 \text{ nm} \), but they make important contributions for smaller \( L \) values. Performing the complete summation for small \( L \) values becomes computationally demanding. However, we find for the parameters of our simulations described in Sect. 7.4 (1.34 nm-wide tunnel barrier with tunneling decay constant 6 nm\(^{-1}\)), the results of the full summation for \( L \to 0 \) match well to the result of including only the \( m = n = 0 \) term but with the fixed value of \( L = 1.4 \text{ nm} \). Therefore, to incorporate an absolute scale of current densities on computations employing Eq. (7.1), we can simply adjust the magnitude of the results so that they match that of a computation employing Eq. (7.4) together with Eq. (7.10) using \( L = 1.4 \text{ nm} \).

We note that the voltage-dependence of the computation using Eqs. (7.4) and (7.10) with \( L = 1.4 \text{ nm} \) is very close to that obtained with Eq. (7.1), so in principle we could simply use the former to report the results. Nevertheless it is desirable to use the latter for computations in which no trace of momentum conservation is evident in the experimental data, while at the same time including an estimate of the absolute magnitude for those current densities. We achieve that
goal by matching the magnitudes of the two computational results. Of course, this same procedure would be necessary (and would yield similar results) if employing the theory of Ref. [2], i.e. Eq. (7.6) together with Eq. (7.9) or (7.10), for very large $q_c$ values.

References


Appendix B
Details of Resonant Tunneling Model for Graphene and Its Bilayers

The following sections provide additional details regarding the analytic portion of the momentum-conserving 2D–2D tunneling calculation, including wavevector matching (for computing current) and densities-of-states (for solving electrostatics).

B.1 Monolayer Graphene

For comparison to the more complicated cases, I will reproduce the equations that govern resonant tunneling for the monolayer graphene case with elastic scattering. Using the Bardeen formalism, we have for the tunneling current

$$I_{\text{elas}} = g_{VGS} \frac{2\pi e}{\hbar} \sum_{\alpha\beta} |M_{\alpha\beta}|^2 \left[ f_L(E_{\alpha}) - f_R(E_{\beta}) \right] \delta(E_{\alpha} - E_{\beta}).$$  \hspace{1cm} (B.1)

which involves a sum over all states $\alpha, \beta$ in each graphene electrode. The matrix element $M_{\alpha\beta}$ is evaluated using graphene basis functions in Bloch form to obtain

$$M_{k_Rk_L} = \frac{\hbar^2}{2m} \frac{\kappa e^{-\kappa d}}{D} g_{\omega}(\theta_R, \theta_L) \frac{1}{A} \int dS e^{iQ \cdot r} e^{i(k_R - k_L) \cdot r},$$  \hspace{1cm} (B.2)

which allows us to write the current as a sum over wavevectors,

$$I_{\text{elas}} = g_{VGS} \frac{2\pi e}{\hbar} \left( \frac{\hbar^2}{2m} \right)^2 \sum_{k_Rk_L} \left( \frac{\kappa e^{-\kappa d}}{D} \right)^2 |\Lambda(\Delta k)|^2 \left[ f_L(E_L) - f_R(E_R) \right] \delta(E_L - E_R).$$  \hspace{1cm} (B.3)
with $\Lambda(\Delta k) = \frac{e\omega}{\mathcal{A}} \int dS \, e^{iQ \cdot r} e^{i\Delta k \cdot r}$ where $\Delta k = k_R - k_L$ and the surface integral is taken over an area defined by the phase coherence length, $L$. To evaluate the delta function which enforces energy conservation, we must convert the sums over all states to integrals, and rewrite $\delta(E_L - E_R)$ in terms of wavevectors. Using the linear approximation to the monolayer graphene dispersion $E(k) \approx \hbar v_F k$, we write the energy in each electrode as $E_i = E(k_i) + \phi_i$, where $\phi_i$ is the electrostatic potential at the Dirac point, and hence for the energy range above both Dirac points (REGION I),

$$E_L - E_R = E(k_L) - E(k_R) + \phi_L - \phi_R = \hbar v_F (k_L - k_R) + eV',$$  \hfill (B.4)

where $eV' = \phi_L - \phi_R$ is the electrostatic potential difference between the graphene electrodes. We replace the delta function of $E_L - E_R$ with a version in terms of $k$,

$$\delta(f(k_R, k_L)) \rightarrow \frac{\delta(k_R - k_0)}{|f'(k_0)|}, \hfill (B.5)$$

where the zero of $f(k_R, k_L)$ is found using Eq. (B.4) to be

REGION I: \hspace{1cm} $k_0 = k_L + eV'/\hbar v_F = k_L + k'$, \hfill (B.6)

with $k' = eV'/\hbar v_F$. From this, it follows that $|f'(k_0)| = \hbar v_F$. This new delta function removes the integral over the magnitude of $k_R$, leaving two angular integrals and the integral over $k_L$. For the energy range below both Dirac points (REGION III), the energies are negative with respect to the charge neutrality point $E(k) \approx -\hbar v_F k$ and thus

$$E_L - E_R = -\hbar v_F (k_L - k_R) + eV',$$  \hfill (B.7)

which yields

REGION III: \hspace{1cm} $k_0 = k_L - k'$. \hfill (B.8)

Similarly, in the energy range between the two Dirac points (REGION II), one energy is positive while the other is negative, and generally

REGION II: \hspace{1cm} $k_0 = |k'| - k_L$. \hfill (B.9)

In order to properly determine the electrostatics, one must also compute the number of carriers in each electrode which requires the density of states. For a dispersion relation of $E(k) \approx \hbar v_F k$ in two dimensions with spin and valley degeneracy factors of 2, the occupation factor for each level is

$$n(k) = g_v g_s \frac{1}{(2\pi)^2} \pi k^2 = \frac{1}{\pi} \left( \frac{E}{\hbar v_F} \right)^2,$$  \hfill (B.10)
and thus the density of states is
\[ \rho(E) = \frac{dn}{dE} = \frac{2}{\pi} \frac{|E|}{(h \nu_F)^2}. \]  
(B.11)

From this, we calculate the electron and hole density in each electrode using
\[ n_i = \int_{\phi_i}^{\infty} dE \frac{\rho(E - \phi_i)}{e^{(E-\mu_i)/kT} + 1} = \frac{2}{\pi} \left( \frac{kT}{h \nu_F} \right)^2 \text{Li}_2 \left( -e^{(\mu_i-\phi_i)/kT} \right) \]  
(B.12a)
\[ p_i = \int_{-\infty}^{\phi_i} dE \frac{\rho(E - \phi_i)}{e^{(\mu_i-E)/kT} + 1} = \frac{2}{\pi} \left( \frac{kT}{h \nu_F} \right)^2 \text{Li}_2 \left( -e^{(\phi_i-\mu_i)/kT} \right), \]  
(B.12b)

with the second-order polylogarithm, Li\(_2\)(z). In the limit that T \(\to\) 0, the Fermi-Dirac function approaches a step-function, and the total number of carriers reduces to
\[ \lim_{T \to 0} n_i = \int_{\phi_i}^{\infty} dE \rho(E - \phi_i) \Theta(E - \mu_i) = \frac{1}{\pi} \left( \frac{\mu_i - \phi_i}{h \nu_F} \right)^2. \]  
(B.13)

**B.2 Bilayer Graphene: Parabolic Dispersion**

The simplest model for bilayer graphene assumes a parabolic dispersion \( E(k) \approx \alpha k^2 \), with the coefficient of proportionality \( \alpha = (h \nu_F)^2 / t_\perp \) (with interlayer hopping energy \( t_\perp \)) extracted from the tight-binding method. Borrowing Eq. (B.3) from the monolayer case, we proceed to evaluating the delta function \( \delta(E_L - E_R) \) for each of the relevant energy regions. In **REGION I**, above both Dirac points (conduction- to conduction-band tunneling) we have
\[ E_L - E_R = \alpha (k_L^2 - k_R^2) + eV', \]  
(B.14)
which tends to zero at
\[ \text{REGION I:} \quad k_0 = \sqrt{k_L^2 + eV' / \alpha} \]  
(B.15)
with the derivative \( |f'(k_0)| = 2\alpha k_0 \) evaluated at that point. In **REGION III** (valence- to valence-band tunneling) both energies are negative and therefore
\[ E_L - E_R = -\alpha (k_L^2 - k_R^2) + eV', \]  
(B.16)
which gives us \( f(k_0) = 0 \) for

\[
\text{REGION III: } \quad k_0 = \sqrt{k_L^2 - eV'/\alpha}. \tag{B.17}
\]

In \textit{REGION II} (unlike-band tunneling), we must examine separate cases for each sign of \( eV' \). Doing this, we obtain one equation which holds for both zeros (here \( k^2 = |eV'|/\alpha \)),

\[
\text{REGION II: } \quad k_0 = \sqrt{|eV'|/\alpha - k_L^2} = \sqrt{k^2 - k_L^2}. \tag{B.18}
\]

For the electrostatics calculation, we can simply replace the \( k^2 \) in Eq. (B.10) with the rearranged dispersion relation \( k^2 = |E|/\alpha \) to obtain

\[
n(k) = g_V g_S \frac{1}{(2\pi)^2} \pi k^2 = \frac{|E|}{\pi \alpha}. \tag{B.19}
\]

Taking the derivative with respect to energy, we calculate the density of states

\[
\rho(E) = \frac{dn}{dE} = \frac{1}{\pi \alpha}, \tag{B.20}
\]

which is constant (a well-known result for parabolic dispersion in two dimensions). The charge densities for each graphene sheet are then easily obtained for finite temperature,

\[
n_i = \frac{1}{\pi \alpha} \int_{\phi_i}^{\infty} dE \frac{1}{e^{(E-\mu_i)/kT} + 1} = \frac{kT}{\pi \alpha} \ln(1 + e^{(\mu_i-\phi_i)/kT}) \tag{B.21a}
\]

\[
p_i = \frac{1}{\pi \alpha} \int_{-\infty}^{\phi_i} dE \frac{1}{e^{(\mu_i-E)/kT} + 1} = \frac{kT}{\pi \alpha} \ln(1 + e^{(\phi_i-\mu_i)/kT}), \tag{B.21b}
\]

as well as in the low-temperature limit,

\[
\lim_{T \to 0} n_i = \frac{1}{\pi \alpha} \int_{\phi_i}^{\infty} dE \Theta(E-\mu_i) = \frac{|\mu_i - \phi_i|}{\pi \alpha}. \tag{B.22}
\]

Curiously, when we calculate the net charge using the temperature-dependent forms shown in Eqs. (B.21a) and (B.21b), we find that the result is independent of temperature and equal to Eq. (B.22),

\[
n_i - p_i = \frac{kT}{\pi \alpha} \left[ \ln(1 + e^{(\mu_i-\phi_i)/kT}) - \ln(1 + e^{(\phi_i-\mu_i)/kT}) \right] = \frac{|\mu_i - \phi_i|}{\pi \alpha}. \tag{B.23}
\]
B.3 Bilayer Graphene: Hyperbolic Dispersion

Although the parabolic approximation to the bilayer graphene dispersion is appropriate for very small energies, the true bilayer dispersion quickly becomes non-parabolic as one extends out to energies that are relevant for off-resonance currents (high-voltage behavior). These effects can be captured by writing the dispersion in a hyperbolic form which is parabolic for $v_F k_F / t \ll 1$ and linear in the opposite limit $v_F k_F / t \gg 1$,

$$ E \approx \frac{t_\perp}{2} \left[ \sqrt{1 + \left( k / k_c \right)^2} \pm 1 \right], \quad (B.24) $$

with the transitional value $k_c = t_\perp / 2 h v_F$ between the two regimes, and where the upper (lower) sign corresponds to the higher (lower) energy sub-band. For convenience, we define $h(k) \equiv \sqrt{1 + (k / k_c)^2}$. Considering only the lower conduction bands of both electrodes, we write the argument of the delta function in Eq. (B.3) as

$$ E_L - E_R = \frac{t_\perp}{2} \left[ h(k_L) - h(k_R) \right] + eV', \quad (B.25) $$

and we find that the zero occurs when

**REGION I:** \quad $k_0 = k_c \sqrt{\left[ h(k_L) + 2 eV' / t_\perp \right]^2 - 1}$. \quad (B.26)

The derivative of Eq. (B.25) gives us $|f'(k_0)| = 2 \alpha k_0 / h(k_0)$. In **REGION III** (considering only the upper valence bands), we have negative energies and

$$ E_L - E_R = -\frac{t_\perp}{2} \left[ h(k_L) - h(k_R) \right] + eV'. \quad (B.27) $$

The zero of this equation is

**REGION III:** \quad $k_0 = k_c \sqrt{\left[ h(k_L) - 2 eV' / t_\perp \right]^2 - 1}$. \quad (B.28)

In the unlike-band tunneling region, we evaluate the two cases of positive and negative $eV'$ to obtain

**REGION II:** \quad $k_0 = k_c \sqrt{\left[ h(k_L) - 2 |eV'| / t_\perp - 2 \right]^2 - 1}$. \quad (B.29)

Before we begin calculating the carrier densities required for electrostatics, we must first invert the dispersion shown in Eq. (B.24) (for the lower sign),

$$ k^2 = \left( \frac{2k_0}{t_\perp} \right)^2 |E| \left( |E| + t_\perp \right) = \frac{|E|}{(h v_F)^2} \left( |E| + t_\perp \right). \quad (B.30) $$
We use this equation to determine the occupation factor for each $k$,

$$n(k) = g_v g_s \frac{1}{(2\pi)^2} \pi k^2 = \frac{|E|}{\pi (h v_F)^2} (|E| + t_\perp),$$

(B.31)

and take the derivative to get the density of states

$$\rho(E) = \frac{d n}{dE} = \frac{2|E| + t_\perp}{\pi (h v_F)^2} = \frac{1}{\pi \alpha} + \frac{2}{\pi} \frac{|E|}{(h v_F)^2},$$

(B.32)

which is in fact a sum of the monolayer and parabolic densities of states. As such, the carrier densities will be sums of the monolayer and parabolic cases as well;

$$n_i = \frac{kT}{\pi \alpha} \ln(1 + e^{(\mu_i - \phi_i)/kT}) - \frac{2}{\pi} \left( \frac{kT}{h v_F} \right)^2 \text{Li}_2 \left( -e^{(\mu_i - \phi_i)/kT} \right),$$

(B.33a)

$$p_i = \frac{kT}{\pi \alpha} \ln(1 + e^{(\phi_i - \mu_i)/kT}) - \frac{2}{\pi} \left( \frac{kT}{h v_F} \right)^2 \text{Li}_2 \left( -e^{(\phi_i - \mu_i)/kT} \right),$$

(B.33b)

and in the low-temperature limit,

$$\lim_{T \to 0} n_i = \frac{1}{\pi \alpha} + \frac{1}{\pi} \left( \frac{\mu_i - \phi_i}{h v_F} \right)^2.$$

(B.34)
Appendix C
Resonant Tunneling Between Transition Metal Dichalcogenides

The following sections extend the band model for graphene–graphene interlayer tunneling to enable calculation of tunneling current between semiconducting transition metal dichalcogenides. The described model uses an approximate form for the semiconducting bands around the $K$ and $K'$ points of the Brillouin zone, and neglects the details of the TMD wavefunctions, which in general will be more complicated than those of graphene.

C.1 Tight-Binding Model and Dispersion

Following the discussion of a simple tight-binding model for monolayers of transition metal dichalcogenides (TMDs) by Liu et al. [1], we approximate the low-energy behavior of electrons by expanding the tight-binding Hamiltonian around the $K$-point. Keeping only the lowest order term, we write the reduced $\mathbf{k} \cdot \mathbf{p}$ two-band Hamiltonian as

$$H_0(k) \approx \begin{pmatrix} \Delta/2 & \hbar v(\tau k_x - ik_y) \\ \hbar v(\tau k_x + ik_y) & -\Delta/2 \end{pmatrix} = \begin{pmatrix} \Delta/2 & \tau \hbar v k e^{-i\phi} \\ \tau \hbar v k e^{i\phi} & -\Delta/2 \end{pmatrix},$$

(C.1)

where $k = |k|$, $\phi = \arctan(k_x/k_y)$, $\tau = \pm 1$ is a valley-index, $\Delta$ is the band gap of the TMD, and $\hbar v = at$ in the notation of Liu et al. The eigenvalues for this simple model are hyperbolic,

$$E(k) = \pm \frac{1}{2} \sqrt{(2\hbar v k)^2 + \Delta^2}.$$

(C.2)

It is possible at this stage to make a simple, parabolic “effective mass” approximation using this result by expanding to lowest order in $k$,
\[ E(k) = \pm \frac{1}{2} \left[ \Delta + \frac{(2\hbar v k)^2}{2\Delta} + \mathcal{O}(k^4) \right] \approx \pm \frac{\Delta}{2} + \frac{\hbar^2 k^2}{2m^*}. \]  

\[ \text{with } m^* = \frac{\Delta}{2v^2}, \text{ but the hyperbolic form is at least as compact and a bit more accurate.} \]

We can go a bit further by including spin-orbit coupling (which is relevant in many 2D TMDs) according to the prescription by Liu et al.,

\[ H_{\text{SO}} \approx H_0(k) + \begin{pmatrix} 0 & 0 \\ 0 & \tau s \lambda \end{pmatrix}, \]  

for spin-orbit perturbation parameter \( \lambda \) (see Table IV of Ref. [1]) and spin-index \( s = \pm 1 \). The eigenvalues including spin-orbit coupling now take the form,

\[ E_{s,\tau}(k) = \frac{1}{2} \left[ \tau s \lambda \pm \sqrt{(2\hbar v k)^2 + (\Delta - \tau s \lambda)^2} \right]. \]

The valley-index \( \tau \) appears explicitly in the dispersion, indicating that the valley degeneracy has been lifted by spin-orbit splitting. However, we cannot distinguish between the spin-states in our device (or rather, between the states involved in spin-orbit splitting), so we can ignore the valley-index and retain a valley degeneracy factor of \( g_v = 2 \),

\[ E_s(k) = \frac{1}{2} \left[ s \lambda \pm \sqrt{(2\hbar v k)^2 + (\Delta - s \lambda)^2} \right]. \]

This dispersion relation is compact enough for direct use in our tunneling calculation, while also properly capturing the non-parabolicity of the bands at low energies as well as the primary effect of spin-orbit coupling, which is asymmetric for electrons versus holes (Fig. C.1). This model will likely be sufficient for computation for both like-band and unlike-band tunneling modes. In particular, the band-splitting from spin-orbit coupling will properly capture the effect on the density of states near the band edge, which governs the turn-on characteristic of a device based on unlike-band tunneling, a tunneling field-effect transistor (TFET).

### C.2 Energy-Conservation Between Tunneling States in Transition Metal Dichalcogenides

The modification in the energy-conservation term between monolayer graphene devices and TMD devices is straightforward. The delta function \( \delta(E_L - E_R) \) must be rewritten in terms of the wavevector in each electrode and summed over the available bands,

\[ \delta(E_L - E_R) \rightarrow \sum_i \frac{\delta(k - k_i)}{|F'(k_i)|}. \]
Fig. C.1 Energy versus wavevector $E_s(k)$ around the $K$-point using a first-order two-band effective Hamiltonian with spin-orbit coupling (solid, blue), and a parabolic effective mass approximation (dashed, red). Energy axis in units of eV and $k$-axis in nm$^{-1}$.

where the sum index $i$ runs over $s = \pm 1$ for both the conduction and valence bands (four terms in total). Here, $f$ refers to the original argument of the delta function and $k_i$ are the zeros of that function,

$$f \equiv E_L - E_R = E_s^\pm (k_L) - E_s^\pm (k_R) + \phi_L - \phi_R. \quad (C.8)$$

Solving this expression for zero will require the inversion of Eq. (C.6),

$$k_s(E) = \frac{1}{2\hbar v} \sqrt{(2E - s\lambda)^2 - (\Delta - s\lambda)^2}, \quad E \geq \frac{\Delta}{2} \text{ or } E \leq -\frac{\Delta}{2} + s\lambda. \quad (C.9)$$

Using Eq. (C.9) to evaluate the solution of $f = 0$ yields

$$k_i = k_s^\pm \left[E_s^\pm (k_R) - eV'\right], \quad (C.10)$$

with $eV' = \phi_L - \phi_R$ and where the band gaps $\Delta_L$, $\Delta_R$ and spin-orbit parameters $\lambda_L$, $\lambda_R$ are defined separately for each material. The zeros $k_i$ define the relationship between the magnitude of wavevectors imposed by energy conservation, and will differ for each of the three energy regions in the tunneling calculation. The limits of each region in TMDs will extend from the band edges instead of from the Dirac point, as in monolayer graphene. This is similar to the case of bilayer graphene, where the band gap creates bands of energy in which no tunneling can occur.

C.3 Density of States and Occupation of Levels

There are several ways to write the density of states; here, I will use

$$\rho_s = \frac{g_v}{2\pi} k_i \left| \frac{dk_s}{dE} \right|, \quad (C.11)$$
summing over spin states and the conduction and valence bands to get the total density of states. Using Eq. (C.9) we write

\[ \frac{dk_s}{dE} = \frac{2E - s\lambda}{\hbar \sqrt{(2E - s\lambda)^2 - (\Delta - s\lambda)^2}}. \]  

which gives

\[ k_s \left| \frac{dk_s}{dE} \right| = \frac{|2E - s\lambda|}{2\pi (\hbar v)^2}. \]  

In the conduction band, \( E > 0 \) (also \( E > \Delta / 2 \gg \lambda \)) and the density of electron states (summing over spin) takes the form

\[ \rho_e(E) = \frac{2}{\pi} \frac{E}{(\hbar v)^2} \Theta(E - \Delta / 2). \]  

Due to the splitting of hole bands, there are two terms for the hole density of states,

\[ \rho_h(E) = \frac{1}{2\pi (\hbar v)^2} \left\{ |2E - \lambda| \Theta(-\Delta / 2 + \lambda - E) + |2E + \lambda| \Theta(-\Delta / 2 - \lambda - E) \right\}. \]  

The total density of states is the sum of the electron and hole parts \( \rho = \rho_e + \rho_h \). There is a notable step in the hole density of states due to spin-orbit splitting. In Fig. C.2, we see that this effect is quite distinct from the equivalent density of states one gets in the effective mass approximation, as shown by the red, dashed line which exhibits a simple step-function behavior. This feature may be important for the TFET device since such operation always involves tunneling from one conduction band to the valence band in the other layer.
**Fig. C.3** Total carrier density (black, dashed line) $n + p$ (nm$^{-2}$) as a function of Fermi level (eV). Separate electron (red, solid) and hole (blue, solid) densities are shown as well.

For the electrostatics of TMD devices we will need carrier densities for each TMD layer. The electron density is obtained by integrating Eq. (C.14) with the Fermi occupation function,

$$n = \frac{2}{\pi (\hbar v)^2} \int_{\Delta/2}^{\infty} dE \frac{E}{1 + e^{(E-\mu)/kT}}$$

$$= \frac{\Delta}{\pi (\hbar v)^2} kT \ln(1 + e^{(\mu-\Delta/2)/kT}) - \frac{2}{\pi} \left( \frac{kT}{\hbar v} \right)^2 \text{Li}_2\left(-e^{(\mu-\Delta/2)/kT}\right). \quad (C.16)$$

The hole density is obtained similarly, albeit with a few more terms,

$$p = \frac{1}{2\pi (\hbar v)^2} \left\{ \int_{-\infty}^{-\Delta/2+\lambda} dE \frac{|2E - \lambda|}{1 + e^{(\mu-E)/kT}} + \int_{-\infty}^{-\Delta/2-\lambda} dE \frac{|2E + \lambda|}{1 + e^{(\mu-E)/kT}} \right\}$$

$$= \frac{(\Delta - \lambda)}{2\pi (\hbar v)^2} kT \ln(1 + e^{-(\Delta/2+\lambda-\mu)/kT}) - \frac{1}{\pi} \left( \frac{kT}{\hbar v} \right)^2 \text{Li}_2\left(-e^{-(\Delta/2+\lambda-\mu)/kT}\right)$$

$$+ \frac{(\Delta + \lambda)}{2\pi (\hbar v)^2} kT \ln(1 + e^{-(\Delta/2+\lambda+\mu)/kT}) - \frac{1}{\pi} \left( \frac{kT}{\hbar v} \right)^2 \text{Li}_2\left(-e^{-(\Delta/2+\lambda+\mu)/kT}\right). \quad (C.17)$$

The total carrier density $n + p$ is shown as a function of Fermi level in Fig. C.3, with a kink caused by the jumps in hole density for negative Fermi energies. Total charge is defined as $q = -en + ep$.

**Reference**

Vita

Sergio C. de la Barrera graduated from the University of Tennessee, Knoxville in May 2008 with a Bachelor of Science in Nuclear Engineering. He continued at Argonne National Laboratory as a Nuclear Engineering Associate from 2008 to 2011, developing novel methods of directional gamma ray radiation detection. In August 2011, he joined the Carnegie Mellon University Department of Physics to study two-dimensional tunneling physics and materials characterization as a Ph.D. student with Prof. Randall Feenstra. He defended this work in July 2016 and began working with Prof. Benjamin Hunt as a Postdoctoral Researcher in August 2016, investigating superconductivity and magnetism in two dimensions.