**Graphene Devices for Beyond-CMOS Heterogeneous Integration**

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Abstract

Semiconductor manufacturing is the workhorse for a wide range of industries. It lies at the heart of consumer electronics, telecommunication equipment and medical devices. Most semiconductor electronics are made from Silicon, and are fabricated using CMOS technology. The versatility of semiconductor electronics stems from the ever-reducing cost of integrating more computing and memory functions on chip. The small cost for adding extra functions has been maintained in the past 50 years through transistor scaling. Transistor scaling focuses on shrinking the size of transistors integrated on chip. This reduction in transistor size, while keeping the overall cost of the chip fixed allowed us to reduce the cost per function with scaling, and is what is celebrated as Moore’s law. Scaling has been working gracefully up to the last decade, where the exponential rise in manufacturing cost and diminishing gains of scaling on device performance reduce its economic benefit. To revive the cost reduction trend, different techniques were proposed such as augmenting CMOS manufacturing with new materials (Beyond CMOS), 3D integration, and integrating more non-transistor elements on-chip (More than Moore).

In this work, we focus on the efficient implementation of several circuit functions using an allotropy of carbon known as graphene. Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has unique electronic properties that has been taken the solid-state electronics community by a storm since its first experimental conception in 2004. Despite its promising electronic properties, namely the very high charge-carrier mobility and reduced scattering by impurities, graphene circuits has been held back by a plethora of nonidealities and technological roadblocks that hamper its use in traditional transistor-based circuits. In this work, we attempt to leverage the unique physical properties of graphene to implement non von-Neumann neuromorphic computing architectures, low-loss diodes and evaluate the behavior of diffusive-transport graphene couplers. We focus on the the design, fabrication and characterization of graphene devices in the presence of the current performance-limiting technological nonidealities in heterogeneous graphene-CMOS systems. We present the design, fabrication and characterization of all-graphene resistive data converters devices and diodes, discussing their performance and application as building elements of all-graphene brain-inspired computing architectures. We evaluate the performance of graphene couplers operating in the diffusive transport regime, which serve as a method to analyze the cross-coupling between adjacent graphene interconnects. We also discuss the current technological limitations hampering the performance of graphene devices, and the roles of different processing non-idealities on the characteristics of graphene devices.

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# Diffusive-Transport Graphene Couplers

The similarity between the dispersion relation of photons and charge carriers in graphene appeals to designing optics-inspired electronic devices. An interesting optics-inspired analog is the electronic directional coupler. Optics directional couplers allow coupling light between two branches, where the coupling coefficient varies periodically with the coupling distance[1]. The electronic wave modes in graphene ribbons and the resistive coupling between graphene ribbons in close proximity has been analyzed for ballistic transport [2]–[4]. The problem of analyzing resistive coupling in diffusive graphene ribbons is different from that in ballistic graphene ribbons. The successive scattering events randomize the wavefunction phase information [5]–[7] prohibiting the direct application of the coupled-mode theory. A direct consequence of this phase randomization is losing the spatial periodicity of the coupling coefficient predicted in ballistic devices.

Modeling of resistive coupling is also crucial for deeply scaled interconnects, in which transport will inadvertently be diffusive due to line-edge roughness[8]–[10]. Graphene interconnects in close proximity has been studied previously to evaluate their cross-talk performance[11]–[17]. Prior work focused on analyzing the delay and energy metrics of a single graphene interconnect, accounting only for the capacitive coupling among interconnects.

In this chapter, we study the coupling between graphene ribbons operating in the diffusive transport regime. We start by developing an analytical model for the coupling resistance between two graphene ribbons separated by a dielectric, highlighting the impact of different fabrication non-idealities on the coupling. We then evaluate the spatial dependence of such coupling coefficient, showing its monotonic saturating behavior, and assess the impact of such coupling on the performance of deeply scaled interconnects.

## Modeling Diffusive-Transport Current Coupling

An electronic current coupler consists of two graphene ribbons in close proximity as shown in Figure 1. The phase incoherence associated with diffusive transport devices prohibits the direct application of coupled mode theory to evaluate the coupling between two coupled graphene ribbons. A more direct approach would be to model the coupling using the tunneling resistance between the two branches of the coupler; this emphasizes the diffusive nature of the transport and the lack of phase coherency in the associated wave functions.

The modeling of the tunneling resistance between the two graphene ribbons must take into account the difference in energy dispersion relations across the tunneling barrier. The energy dispersion relation of charge carriers changes from a linear dispersion relation in graphene, to a parabolic dispersion relation with an energy gap in the oxide regions, as shown in Figure 2. The lack of states in the dielectric energy gap translates to decaying wavefunctions from the graphene ribbons on either side of the dielectric. In other words, despite the linear energy dispersion relation of graphene, the lack of states in energy gap region of the parabolic dielectric gives rise to a decaying wavefunction, reminiscent of tunneling in parabolic systems.

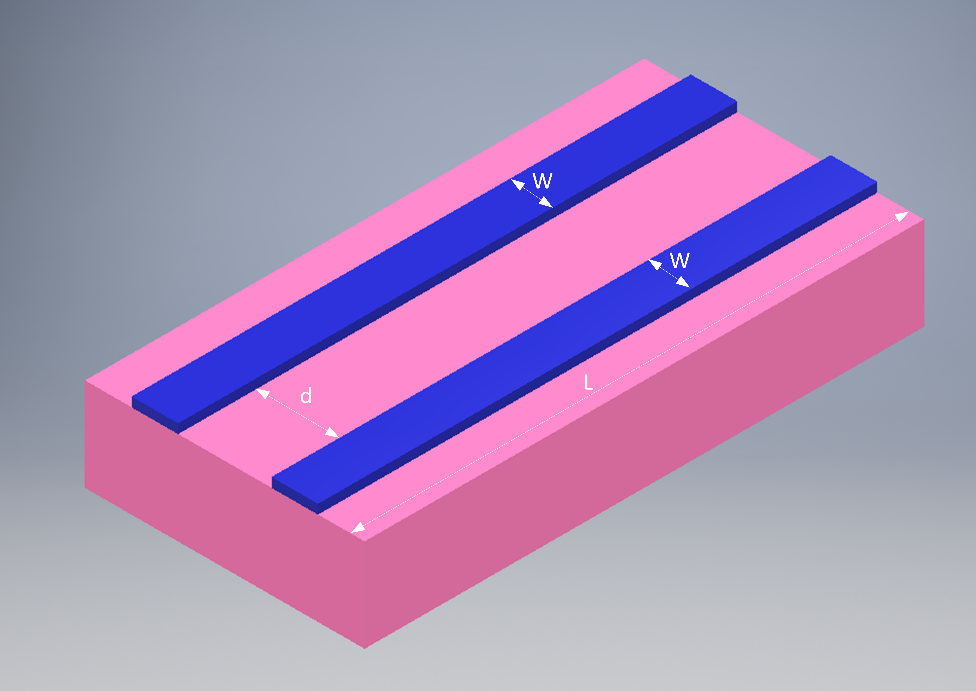


Figure . Schematic representation of an electronic graphene coupler. The ribbons are spaced by a distance d apart, over a length of L, while each ribbon has a width of W. The graphene is shown in blue while the surrounding oxide is shown in pink. The oxide is only shown below the graphene ribbon for clarity.

The calculation of the tunneling resistance is based on the analysis of Graphene-Insulator-Graphene (GIG) junctions[18], [19]. The major difference between the prior work on GIG junctions and the current problem is that in this device tunneling occurs between the edges of the graphene ribbons rather than normal to them. The edge tunneling nature modifies the results presented in [18], [19] slightly, but follows its essence otherwise. We defer the estimation of the tunneling resistance to Section ‎5.1.1, but stress on the fact that it is a tunneling resistance; its value is limited by how small the two ribbons can be spaced apart, and for all practical purposes, this tunneling resistance value is significantly larger than the resistance of the graphene ribbons. This observation will proof useful when analyzing the electrical model of the device.

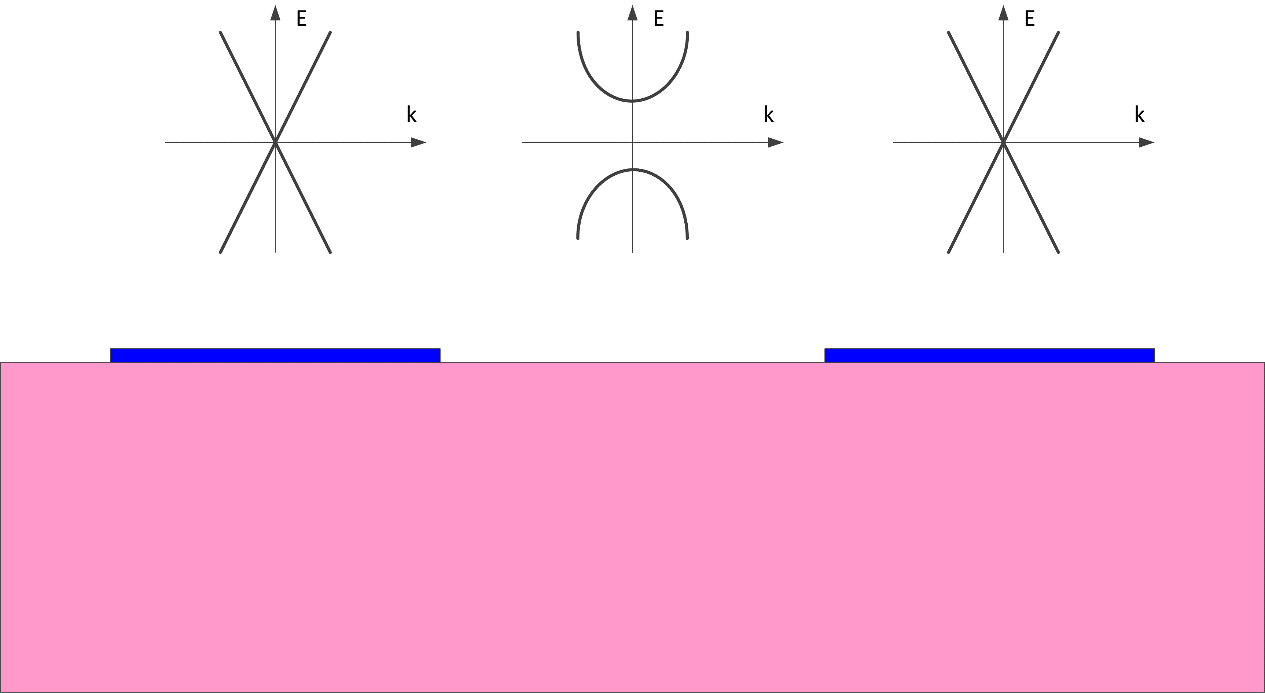


Figure . Cross Section of the graphene coupler with the bottom oxide only shown for clarity. The electronic energy dispersion relation for each region is shown above it; it is linear in each graphene region and parabolic with a band gap in the dielectric surrounding them. The energy gap in the parabolic region is significantly larger than the energy of charge carriers in each graphene ribbon.

The electrical model of the device is composed of three distributed resistors: a distributed resistor for each of the graphene ribbons with a distributed tunneling conductance connecting them together, as shown in Figure 3. We label one of the ribbons as the input ribbon, and the other as the output ribbon. For this analysis, we apply a current stimulus at the input ribbon and calculate the current at other end (output) of each ribbon.



Figure . Electrical model of graphene coupler. The graphene ribbons are modelled using two distributed resistors with a resistance per unit length of R1 and R2, and the tunneling resistance coupling them is modelled using a distributed conductance with conductance per unit length gc.

The coupling coefficient between the current in the two ribbons is defined as the ratio between the output ribbon and input ribbon branch currents as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

A detailed analysis of the electrical model and a derivation of the coupling coefficient is provided in ‎Appendix E. The current distribution and coupling are a strong function of the load at the output of each branch. This is expected due to the passive nature of the device that does not provide any buffering. Throughout this chapter, we assume that the ratio of the two loads matches the ratio of the ribbons’ resistance per unit length, that is . A more general analysis can be found in ‎Appendix E.

Under the matching load condition, we can approximate the current distribution in each branch of the coupler is:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Where .

## Dependence Current Coupling Coefficient on Coupling Distance

Under the condition of matching load ratios, , the current coupling coefficient is:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

In the limiting case when , Equation (‎5.3) reduces to:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Equations (‎5.2), (‎5.3) and (‎5.4) provides a very intuitive way of explaining the behavior of the diffusive-transport coupler: given enough length, the coupler will divide the current by the ratio of the resistances of the two branches, just as if they shorted only at the input end. Unlike the ballistic-transport coupler or the optical directional coupler, the coupling coefficient does not show any periodicity on the coupling coefficient. The lack of coupling coefficient periodicity is due to the loss of the phase information due to successive scattering associated with diffusive transport. The diffusive-transport coupler rather acts as a current divider that divides the current with according to the ratio of the two branch resistances. However, rather than being an ideal current divider, the current division takes places over a special distance dictated by the characteristic length, which is a function of the ratio between the coupling and branches conductance.

An example of the spatial variation of the current coupling coefficient and the voltage across the branches of a balanced coupler if shown in Figure ‎5.6 as obtained using SPICE simulations.

|  |  |
| --- | --- |
| (a) | (b) |

Figure . (a) Spatial variation of the current and (b) Spatial variation of the voltage across a balanced coupler. The simulations were performed using SPICE over a discretized model comprised of 1000 sections.

## Estimation of the tunneling resistance

The tunneling resistance can be estimated using the Bardeen Hamiltonian approach as in other Graphene-Insulator-Graphene junctions [18], [19]. The tunneling current evaluated using the Bardeen Transfer Hamiltonian [18], [19] is given as:

|  |  |  |
| --- | --- | --- |
|  |  | (‎5.3) |

Where is the valley degeneracy factor (2 in graphene), is the spin degeneracy factor (), is the tunneling matrix element, and are all the states in the electrodes in between which tunneling occurs, and is the Fermi Dirac distribution in the input and output electrodes respectively, and is the energy of the state. The matrix element is given as:

|  |  |  |
| --- | --- | --- |
|  |  | (‎5.4) |

Where is the reduced Planck constant, is the free-electron mass, is the wavefunction of state , is the direction of tunneling current flow and the integral is performed on a plane midway between the two tunneling electrodes. The matrix element in the case of graphene electrodes is given in [18], [19] as:

|  |  |  |
| --- | --- | --- |
|  |  | (‎5.5) |

Where is the wavevector of the decaying exponential function inside the parabolic region barrier (also known as the extinction coefficient), is the two tunneling electrodes separation, is the wavefunction normalization constant, is a scaling factor in the order of unity that accounts for the wave vector misalignment between the overlapping tunneling wavefunctions, is the misalignment vector with an angle similar to the in accounting for rotational misalignment between the tunneling bands, and and is the wavevector between the input and output electrodes. For low field transport in graphene, the wavevector of the charge carriers taking part in tunneling is quite close to the Dirac points ( and ).

The lateral tunneling and the use of lithography to form the junction requires some modifications to tunneling matrix element that significantly simplify its analysis:

1) Lithography creates rough edges. An example of the edge roughness of metal lines obtained when creating metal lines using PMMA photoresist is shown in Figure ‎5.4. The edge roughness standard deviation is 3 nm and there is no correlation between the edges. As such, the tunneling distance and corresponding tunneling resistance is a random variable, and the differential equations used to describe the transport in the electrical model should replace a constant with a random variable, converting Equation (‎E.1) into a set of coupled stochastic differential equation. This level of detail is only required when the edge roughness represents a considerable portion of the ribbon width or ribbon spacing, but should be kept into consideration when developing statistical models for the coupler. When the roughness of the edge is small relative to the ribbons separation or the width of each ribbon, using the average separation distance to derive a single constant value for tunneling conductance is enough.

|  |  |
| --- | --- |
| (a) | (b) |

Figure . SEM images of 25 nm metal lines created using PMMA photoresist. The images shows an edge roughness standard deviation of 3 nm and the lack of correlation between edges in close proximity; (a) single metal wire, and (b) two metal wires with a separation of 25 nm.

2) In this device, tunneling is from a 1D edge to the opposite 1D edge across a 2D barrier, not from a 2D surface of a graphene sheet to another across a 3D barrier. The tunneling probability across a 2D barrier falls exponentially away from the normal connecting the two closest points across the barrier. As such, a 1D model is suitable to describe the tunneling probability between the edges. In the 1D model the tunneling probability is:

|  |  |  |
| --- | --- | --- |
|  |  | (‎5.6) |

Where is a point midway the 2D barrier assumed to be in the x direction.

3) The two branches of the coupler are fabricated from a single CVD graphene sheet over SiO2 with a single common back gate. Since the devices are in close proximity, their Fermi level should be closely aligned. However, the surface roughness of the substrate will cause the formation of charge puddles, which causes random shifts in the Fermi level, and the barrier height, across the graphene ribbons. Our first order estimate will neglect these charge puddles and assumes Fermi level alignment, but a more elaborate analysis should account for charge puddles and roughness.

4) The region between the two branches of the coupler is typically composed of an oxide. The effective mass of the oxide should be taken into account when calculating the tunneling matrix element, not the free-electron mass.

5) The tunneling resistance is a function of the Fermi level separation between the two ribbons, which is a function of the potential different between them. The voltage drop between the two ribbons is small, thus the variation of tunneling resistance due to the spatial variation of the Fermi level difference can be neglected. This is further justified by the fact that we are interested in the low-field transport phenomena occurring across lithographically defined barriers (roughly nm apart), a condition under which electrode charging occurs.

Taking the above points into consideration we can rewrite the tunneling current in the low-field transport regime at T=0 K as:

|  |  |  |
| --- | --- | --- |
|  |  | (‎5.7) |

Where is a constant in the order of unity that captures the effects of misalignment and normalization constants (it has the units of m-1), and V is the applied voltage. Equation (‎5.7) yields the tunneling current per unit length of the ribbons in the low field transport regime. The conductance per unit length of the ribbon is thus given as:

|  |  |  |
| --- | --- | --- |
|  |  | (‎5.8) |

Evaluating Equation (‎5.8) without the constant to estimate the order of and the extinction factor , we find it is a strong function of the separation distance and weak function of the ribbon’s Fermi level as shown in Figure ‎5.5.

|  |  |
| --- | --- |
| (a) | (b) |

Figure . (a) Logarithm of tunneling coupling conductance (), and (b) Extinction coefficient () while varying the Fermi level from 0 to 0.3 eV and the separation distance from 1 to 25 nm.

The numbers obtained show that the coupling is extremely weak. This is due to the use of a non-resonant tunneling device [18], [19]. In addition, with the separation distances achievable in the order of 10 nm, the extinction of the coupling wave function is very weak to yield appreciable coupling ( nS/m). This translates to a very large, impractical, coupling characteristic length, which means that the device operates essentially as two independent ribbons.

## Impact of Current Coupling on Deeply Scaled Interconnects

Resistive coupling between neighboring interconnects is a hazard to signal integrity. Deeply scaled graphene interconnects will not suffer because of current coupling before the spacing between them falls well below 5 nm laterally. However, care should be taken when discussing the limits on stacking graphene interconnects [11], [13]–[17], [20], [21]. Resonant-tunneling [18], [19], can play a significant role in the engineering of graphene interconnects.

Resonant tunneling between neighboring interconnects would increase the coupling conductance and cause resistive leakage of current among neighboring interconnects. and should be prevented if the interconnects do not belong to the same route.

Similarly, resonant tunneling can be used to reduce the overall interconnect resistance. It can be used to reduce the overall resistance of a stacked, multi-layer graphene interconnect, where the layers belong to the same route and carry the same signal. The large coupling distributed conductance will help shunt the resistance of each layer and reduce the overall resistance.

Proper design of stacked graphene interconnects, or different graphene-metallization layers in multi-layer graphene chips should take into account the resonant stacking constraints. If two ribbons are routed normal to each other on successive graphene-metallization layer (Manhattan Routing), the spacing between the layers should be carefully chosen to prevent resonant tunneling as long as they carry independent signals.

## Conclusion

A graphene-insulator-graphene electronic coupler operating in the diffusive-transport regime does not show a spatially periodic dependence on the coupler length. Diffusive-transport coupler show an asymptotic, monotonic dependence of the coupling coefficient on the coupling length due to the loss of wavefunction phase information by successive scattering events.

Diffusive-transport graphene couplers are not practically viable without creating a resonant tunneling structure. Otherwise, the tunneling-based coupling conductance between the graphene ribbons will be too small to yield any practically significant effect.

The analysis of the graphene coupler shows that graphene interconnects are highly scalable laterally, where resistive coupling will not be effective even when the inter-ribbon spacing falls below 5 nm. However, care should be taken when stacking graphene interconnects to prevent resonant tunneling between independent routes when using multi-layer graphene interconnects. Similarly, resonant tunneling can be used in multi-layer graphene interconnects to reduce the overall interconnect resistance..

# Current Technological Limitations on Graphene Devices and Circuits

## Contact Engineering

### Electrical Resistance

### Thermal Interface Conductance

## Interface Roughness

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## Impact of Metal-Ion Containing Developers on the Performance of Graphene FETs

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## Mixing 2D Materials for Optimized Contacts

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# Measurement Setup for Dual-Gated Graphene FETs

# Measurement Setup for Graphene Diodes

# Derivation of the Current Coupling Coefficient in a Diffusive-Transport Graphene Coupler



Figure . Electrical model of graphene coupler. The graphene ribbons are modelled using two distributed resistors with a resistance per unit length of R1 and R2, and the tunneling resistance coupling them is modelled using a distributed conductance with conductance per unit length gc.

The electrical model of the device is composed of three distributed resistors: a distributed resistor for each of the graphene ribbons with a distributed tunneling conductance connecting them together, as shown in Figure 3. We label one of the ribbons as the input ribbon, and the other as the output ribbon. For this analysis, we apply a current stimulus at the input ribbon and calculate the current at other end (output) of each ribbon.

We start by solving the voltage differential equation for the distributed system then relating it to the current.

Applying KCL at any node the node (i), we get:

This can be rewritten as:

Taking the limit as , we get:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Substituting from the two equations together to decouple the equations we get:

Accordingly, the differential equation for each branch after substitution:

The resulting decoupled equations are:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

The two differential equations are the same. The general solution is written as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

The above equation can be rewritten by setting to be:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Current conservation dictates the boundary conditions on the current as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Ohm’s law relates the current and voltage at any given position as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

In addition, Ohm’s law as relates the voltage and current at the output end of each ribbon:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

The coupling coefficient between the current in the two ribbons is defined as the ratio between the output ribbon and input ribbon branch currents as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Equations (‎E.1) and (‎E.4) can be solved for the relation between the constant to give:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Before proceeding to solve the equation, we note that the voltage and current equation present a system of two coupled second order linear equations, reducible to two fourth order decoupled ordinary differential equations. Ohm’s law relates the voltage gradient to the current and hence, the current continuity equation poses a condition on the first derivative of the voltage, while Equation (‎E.8) serves as a Robin boundary condition relative the voltage to its derivative at the boundary. Accordingly, the current system cannot be completely solved analytically; we will not be able to obtain the values of the four constants needed to fully determine a unique solution, but it can be solved numerically. In this discussion, we provide an incomplete solution that does not determine all the unknown constants, but reveals the functional form of the solution.

By letting , we can write the current in each branch using the left side of Equation (‎E.7) as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

From the current conservation equation (‎E.6) we obtain the requirement on the constant , allowing us to rewrite Equation (‎E.11) as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

The voltage across each ribbon is this given as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Although it is quite tempting to null the increasing exponential constant , its presence is important in maintaining the consistency of the equations. This is can be seen through applying the boundary condition given by Equation (‎E.8):

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

If the constant, is set to zero the while , Equation (‎E.14) reduces to:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Equation (‎E.15) can only be satisfied if D is also nulled. This result is erroneous as it means that the current will not change regardless of the values of if the output of the device is shorted. In line with Equation (‎E.14), we can extract the value of as:

|  |  |
| --- | --- |
|  | (.) |

Equation (‎E.16) shows that the coefficient of the exponential increasing term decays exponentially with the length of the device and will not cause an unphysical increase in the voltage or current across the device length.

To sum up, we can write the functional form of the voltage and current across the coupler as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

The solution reveals the functional form of the current to distribute between the two lines in an asymptotic fashion. The current asymptote is roughly given by the current division ratio had the two branches been connected only at the input end. The asymptotic behavior roughly follows an exponentially decaying function with a characteristic length.

To demonstrate the functional behavior, we study the case when the coupler branches have matched impedance with their loads, i.e. when. In such a case, Equation (‎E.16) reduces to:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

For all practical purposes, the value of and thus the contribution of the exponentially increasing term in Equation (‎E.17) and Equation (‎E.18) can be neglected to give:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

A useful approximation that simplifies the analysis considerably is to assume . This assumption is valid especially when. This assumption is especially valid in our analysis, as is a tunneling conductance that is considerably small relative to the conductance of the either branches of the coupler. Under this assumption, and thus we can rewrite Equation (‎E.21) as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

Equation (‎E.22) demonstrates the behavior of the coupler under the matching approximation, while neglecting . The current in each branch asymptotically approaches its value had the two ribbons been connected only at the input side, with an asymptotic behavior following an exponential function with a characteristic length of . In this case the current coupling coefficient is given as:

|  |  |  |
| --- | --- | --- |
|  |  | (.) |

In the limit when , the current coupling coefficient at the output end of the coupler is given as :

|  |  |  |
| --- | --- | --- |
|  |  | (.) |