Simplified model for ballistic current–voltage characteristic in cylindrical nanowires

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A B S T R A C T
The ballistic regime gives the upper limit of an electron device performance. This paper proposes a fast and efficient model for calculating the current–voltage characteristic of a cylindrical nanowire within the framework of the non-equilibrium Green's function. Under certain assumptions, the calculation is simplified to a one-dimensional problem and the modes due to the radial confinement are given by an analytical equation. We further derive an analytical expression for the current–voltage characteristic at temperature approaching 0 K. The relationship between the radius of the nanowire and the electrical current is clearly shown in this expression. The effects of the radius on the current–voltage characteristic curve are also studied. Furthermore, we plot the trend of the saturation current as the radius is increased as predicted by both the numerical result and our analytical model. Our proposed model can be further used to include electron–photon interaction in the calculation of nanoscale optoelectronic devices.

1. Introduction

Semiconducting nanowires are among the most promising alternatives for future nano-electronics and optoelectronics [1,2]. The diameter of fabricated nanowires is controlled by the size of the catalyst, and the length is proportional to growth time. Moreover, specific dopants can be incorporated into nanowires to tune their electronic properties. Our capability to control these properties is essential for the development of electronic and optoelectronic nanodevices.

Nanowires have been fabricated with sizes within the nanometer range. For example, silicon nanowires with 1–2 nm diameters have been fabricated [3]. Moreover, the lengths of the nanowires are predicted to shrink as well [4]. At these length scales for the nanowires, ballistic calculations predict an upper limit to the device performance. The need for theoretical modeling and calculation then becomes essential. Theoretical calculations help us to design the properties of nanowires and to understand the physics behind the measurement results that are obtained.

In the calculation of nano-scale devices properties, the non-equilibrium Green's function (NEGF) framework has been widely used [5]. By using NEGF, the phase breaking phenomena such as electron scatterings due to phonon or photon can be included simply through its self-energy matrices. In this NEGF framework, the device region is discretized to form the Hamiltonian matrix. The size of the matrix can be extremely huge for two- or three-dimensional calculations. In order to increase the computational efficiency, a mode space approach has been proposed [6,7]. In this approach, the wavefunctions are expanded in the mode space. As a result, the transport calculation can often be simplified to a one-dimensional problem along the transport direction [8].

Even in this mode space approach, we still need to calculate the Schrödinger equation on every slice perpendicular to the transport direction. To simplify the calculation, Wang et al. proposed a fast uncoupled method where only one slice is computed [9]. Perturbation theory is used to obtain the potential at every grid along the transport direction.

In this work, we further simplify the non-equilibrium Green's function formulation for nanowires. We use an analytical solution to approximate the solution of the Schrödinger equation perpendicular to the transport direction. This increases the speed significantly since the numerical calculation is now only required along the transport direction. The benefit that we achieve from this simplification is faster calculation for predicting nanowire design. Our model is able to handle larger nanowire size which would take very long computational time when using the atomistic approach.

Another necessary step for nanowire design is knowing the effects of certain parameters on the transport properties. Such parameters include the diameter of the nanowires and their bandstructure. Yu et al. compared their ballistic model with experimental results for increasing values of nanowire diameter [4]. It was shown that the current increases as the radius increases. In this work we will provide...
a simple expression that relates the current and the nanowire diameter under certain assumptions.

It is important to note that the calculation in this paper is made for nanowires without gate electrode. We assume that the nanowire is isolated in vacuum and hydrogenated so that the wavefunction will diminish rapidly when going to vacuum. Applications of these kind of nanowires for optoelectronic comprise solar cells and photodetectors [10–12].

We will present the formulation of the non-equilibrium Green’s function calculation for the structure shown in Fig. 1. The source contact is connected to the left-hand side of the nanowire, and the drain is connected to the right-hand side. In this work, we assume that the contacts are ohmic, and no barriers are present. For simplicity, we study only the ballistic transport. As mentioned previously, ballistic calculations predict an upper limit to the device performance. Incorporating phase breaking phenomena into the calculation will be considered in future works.

If we assume that the potentials in the radial direction do not vary significantly, the eigenstates are given by an analytical equation which can be readily obtained. We will then use this simplified model to compute the current–voltage characteristic curve of the nanowire. It turns out that this simplified model gives an excellent agreement with a previously published result.

To understand the effects of the diameter size of the nanowires on the ballistic current–voltage characteristic, we derived an analytical equation for an ideal case of the nanowire shown in Fig. 1 at low temperature. The equation can be expressed in terms of the electrochemical potential of the contacts and the radius of the nanowires. In this way, the relationship between the diameter size of the nanowire and its ballistic current is clearly shown.

We will also show the effects of the diameter size of the nanowire on the current–voltage characteristic curve of the ballistic cylindrical nanowire. It will be shown that the saturation current is linearly proportional to the saturation voltage. Moreover, our analytical model predicts pretty well the trend of the saturation current as the nanowire diameter increases.

2. Ballistic non-equilibrium Green’s function formulation

2.1. Hamiltonian in cylindrical coordinate

In this section, we present the formulation of the non-equilibrium Green’s function calculation for the cylindrical nanowire shown in Fig. 1. We start with the Hamiltonian

\[ H = -\frac{\hbar^2}{2m^*} \nabla^2 + V \]  

where \( m^* \) is the effective mass, and \( V \) is the potential. For simplicity in writing the equations, here we assume that the effective mass is uniform. The Laplacian in cylindrical coordinate is given by [13,14]

\[ \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2} \frac{\partial^2}{\partial z^2} \]  

Substituting (4), (5) and (2) into (1), it can be shown that

\[ -\frac{\hbar^2}{2m^*} \left\{ \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial \phi(r, z)}{\partial r} + \frac{\partial^2 \phi(r, z)}{\partial^2 \theta} - \frac{r^2}{r^2} \frac{\partial^2 \phi(r, z)}{\partial z^2} \right\} + V(r, z) \phi(r, z) \]

\[ = E \phi(r, z) \]

The wavefunction \( \phi \) can now be expanded in terms of the eigenfunctions of the Schrödinger equation in the transverse direction

\[ \phi(r, z) = \sum \phi_n(r) \xi_n(z) \]

where \( \xi_n(z) \) is the eigenstate solution of

\[ -\frac{\hbar^2}{2m^*} \left( \frac{d^2 \xi_n}{dz^2} + \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial \xi_n}{\partial r} \right) + V(z) \xi_n = E_n \xi_n \]

where \( m^*_n \) is the effective mass in the radial direction. The above equation is to be solved on the planes perpendicular to the transport direction. Solving this equation gives the eigenstates \( \xi_n(z) \) and the eigenenergies \( E_n(z) \). On this derivation we assume that the modes in different values of \( z \) are uncoupled.

We can substitute (7) into (6), and then multiply by \( \xi_m^* \) and integrate over \( r \) to give

\[ \int \sum \phi_m \xi_m^* \xi_m^* \phi_n \xi_n^* z^2 d\theta = \delta_{m,n} \]

so that the equation now becomes

\[ -\frac{\hbar^2}{2m^*_n} \frac{d^2 \phi_n}{dz^2} + E_n \phi_n = E \phi_n \]

It is important to note that the superscript \( n \) is just an integer index and is different from the effective mass along the transport direction \( m^*_n \). We can see that the resulting Hamiltonian becomes block diagonal, where for mode \( m \), the hamiltonian is given by

\[ h_{nm} = -\frac{\hbar^2}{2m^*_n} \frac{d^2}{dz^2} + E_n \]

Green’s function is simply calculated from the following relation:

\[ G = (ES - h_{nm} - \Sigma_1 - \Sigma_2)^{-1} \]

where \( S \) is the overlap matrix, and \( \Sigma_i \) is the self-energy matrix to take into account contact. In this calculation we assumed that the \( i=1 \) for the source contact, and \( i=2 \) for the drain contact.

Note that we have reduced the problem to a one-dimensional problem along the nanowire axis, i.e. \( z \). Moreover, the modes are...
decoupled, which can be seen clearly from the block diagonal structure of the Hamiltonian matrix. In the following section we will make some assumptions to obtain an expression for $E_{\text{sub}}$.

### 2.2. Solving the radial Schrödinger equation

Now, the next thing to do is to solve (8). This is where we will make some assumptions to simplify the calculations. For a cylindrical nanowire without a gate electrode, we assume that the potential does not vary significantly inside the nanowire along the radial direction. Moreover, it is assumed that the wavefunction terminates at the edge of the nanowire, i.e. at $r = R$. With this assumption, the potential profile along the radial direction can be simplified to a square infinite potential well. This assumption is reasonable since it was shown that the lattice is almost empty of charge for low gate biases [15], and the structure that is considered here does not have a gate bias at all. In this case the potential inside the well is not modified significantly from the square potential shape. We will further justify this by showing the results of calculating the energy subbands and the potential from a self-consistent Schrödinger–Poisson solver. With this assumption, we can write the potential profile as follows:

$$V(r) = \begin{cases} 0 & \text{for } r \leq R \\ \infty & \text{for } r > R \end{cases} \quad (14)$$

The solution of (8) for the given potential in (14) is given by the Bessel function of the first kind, $J_\nu$, where the quantum number $\nu$ is the order of the Bessel function and is the same as that found in (2) and (3) [16]. Now, to satisfy the condition that the wavefunction is zero at the edge of the nanowire, we must have $J_\nu(z_{nv}) = 0$ \quad (15)

where $z_{nv}$ is the $n$th root of the Bessel function of order $\nu$, and is related to the energy as

$$z_{nv} = k_m R = \frac{E_{\text{sub}} 2 m_r}{\hbar^2} R \quad (16)$$

In this equation, $k_m$ is the wave number and is related to the energy through a parabolic dispersion relation $E(k) = \hbar^2 k^2 / 2m_r$.

The benefit of making the assumption of an infinite potential well profile is that we obtain an analytical solution for the eigenenergies and the eigenstates. The eigenenergies that solve the radial Schrödinger equation are simply given by (16), or can be rewritten as

$$E_{\text{sub}} = \frac{k_m^2 \hbar^2}{2m_r} \quad (17)$$

It is significant to realize that the roots of the Bessel function are known once the two quantum numbers $n$ and $\nu$ are given. Table 1 gives the tabulated values of the roots of the Bessel function of the first kind for several values of $n$ and $\nu$.

The four lowest subband energies obtained from solving the radial Schrödinger equation are given by these quantum numbers $(n,\nu)$: $(1,0)$, $(1,1)$, $(1,2)$, and $(2,0)$. These correspond to the roots $z_{nv} = 2.4048, 3.8317, 5.1356$, and $5.5201$ (Table 1).

### Table 1

<table>
<thead>
<tr>
<th>$n = i$</th>
<th>$n = 2$</th>
<th>$n = 3$</th>
<th>$n = 4$</th>
<th>$n = 5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu = 0$</td>
<td>2.4048</td>
<td>5.5201</td>
<td>8.6537</td>
<td>11.7920</td>
</tr>
<tr>
<td>$\nu = 1$</td>
<td>3.8317</td>
<td>7.0156</td>
<td>10.1730</td>
<td>13.3240</td>
</tr>
<tr>
<td>$\nu = 2$</td>
<td>5.1356</td>
<td>8.4172</td>
<td>11.6200</td>
<td>14.7960</td>
</tr>
<tr>
<td>$\nu = 3$</td>
<td>6.3802</td>
<td>8.7610</td>
<td>13.0150</td>
<td>16.2230</td>
</tr>
<tr>
<td>$\nu = 4$</td>
<td>7.5883</td>
<td>11.0650</td>
<td>14.373</td>
<td>17.6160</td>
</tr>
</tbody>
</table>

We have compared the results of obtaining the subband energies using the Bessel function approach with that from a self-consistent Schrödinger–Poisson solver of ATLAS, a device simulator from SILVACO [17]. In our ATLAS simulation an oxide barrier was added at the outer layer of the nanowire to simulate a finite barrier. The ATLAS simulation gave us the value of 1.11 eV for the first subband while our Bessel function approach gave the value of 1.15 eV. These values are obtained by using the default bulk effective mass in ATLAS. The material used in the simulation was silicon. The small difference indicates that our assumption of infinite potential well is justified for undoped nanowires in calculating the subband energies. Fig. 2 also shows that the potential inside the nanowire can be approximated to zero as shown in Eq. (14).

We can summarize the calculations as follows. We first determine how many modes or subband energies are to be used in the calculation. The energies are then obtained from (17) and (16) as well as Table 1. Once the subband energies are known, the Hamiltonian matrix can be constructed from (12), and the Green’s function is calculated using (13). With the Green’s function obtained, the other parameters such as the current, transmission curve, electron density, etc., can be computed.

### 3. Current–voltage characteristic

We work out the calculation using silicon material parameters. The literature provides quite a number of non-equilibrium Green’s function simulation for nanowires, but most of them are for field effect transistors with gate electrodes. But, the case we are studying is for a single nanowire suspended in vacuum which is commonly used for optoelectronic devices. Current–voltage characteristic for this kind of silicon nanowires has been previously calculated using atomistic simulation by one of the authors [18]. In this paper, we will obtain the current–voltage characteristic using the simplified model. In order to obtain the nanowire current–voltage characteristic, the device shown in Fig. 1 is biased from 0 up to 1 V. The source contact is kept at ground potential, while the drain contact on the right is lowered by the bias. It is assumed that the potential falls linearly near the contacts and constants along the nanowire. This non-self-consistent calculation follows that in [19]. Fig. 3 shows the potential applied along the nanowire axis.
The current is then calculated from
\[
I = \frac{2q}{h} \int_{-\infty}^{\infty} T(E) [f_i(E) - f_j(E)] dE
\]  
(18)
where \( h = 2\pi \hbar \), \( T(E) \) is the transmission coefficient, \( f_i(E) \) is the Fermi function at the contact \( i \), where \( i = 1 \) is for the source contact, and \( i = 2 \) is for the drain contact. The transmission coefficient is calculated from the Green’s function of Eq. (13) as follows:
\[
T(E) = \text{Trace} \left[ \Gamma_{1} G(E) \Gamma_{2} C^{*} \right]
\]  
(19)
where
\[
\Gamma_i = j[\Sigma_i - \Sigma_i^{*}]
\]  
(20)
and we use the superscript * to indicate the conjugate transpose of a matrix.

The diameter of the nanowire was set to 3 nm while the length was set to 100 nm. It has been shown that effective mass approximation is valid for calculating nanowires with diameter down to about 3 nm [20,21]. Following the procedure in [22], we adjusted the Fermi level in the contacts so that the saturation current was about 6 µA. This method gave us a Fermi level value of around 0.39 eV. The result is shown in Fig. 4. Our simplified model has the same profile trend as the results plotted in Fig. 5(a) of [22].

Two effective mass values should be used for anisotropy bandstructure material such as silicon. One is for the radial direction and the other one is for the transport direction. In silicon, the radial effective mass can be approximated from the transverse and longitudinal effective masses following the approach used in ATLAS, SILVACO. For spherically symmetric bandstructure such as GaAs only one effective mass value is needed.

For this calculation, therefore, we set \( m_{t}^{*} = m_{r}^{*} \), which is the transverse effective mass in silicon and is about \( m_{t}^{*} = 0.19m_{0} \). The radial effective mass, on the other hand, was set as \( m_{r} = 2m_{t}m_{l} / (m_{t} + m_{l}) \). The longitudinal effective mass of silicon is \( m_{l} = 0.916m_{0} \). The approximation for the radial effective mass has been used in the literature [17,13,14].

In the current calculation we used two subbands, though effectively only one subband was needed. The lowest calculated subband energies are around 0.31, 0.79, and 1.42 eV. Since the Fermi level is about 0.39 eV, only one subband is occupied.

Fig. 5 shows the transmission curve at two biases. Note that the transmission curve does not change when the drain contact is biased. The reason for this is explained in [8]. The transport for a ballistic device is mainly determined by the transport at the top of the barrier [23–26]. Since there is no barrier present along the nanowire, the top of the barrier for our device is simply the potential at the source. When the drain contact is biased, the potential at the drain is lowered by the bias voltage. However, the potential at the source remains the same. Hence, the transmission curve does not change at all. The only change is that the Fermi level. The transmission curve has a step-like shape. The jumps in the curve occur at the subband energies. Note that the transmission curve does not change significantly under bias.

With this understanding, we can further explain the shape of the \( I-V \) curve in Fig. 4. To help in the elaboration, we refer to (18). It appears that the ballistic current is simply the area under a curve. The curve is obtained by multiplying the transmission coefficient by the difference of the two Fermi functions. Fig. 6 shows the current calculation visually.

Note that the only curve that changes is the Fermi function at the drain contact. This is because the source is kept at the ground potential, and the transmission curve does not change under bias for this ballistic nanowire (Fig. 5). So now, the calculation of the current becomes simple and straightforward. In the next section, we will derive a simple analytical equation that relates the radius of the nanowire to the electrical current under certain assumptions.

### 4. Analytical equation

In this section we derive an analytical equation for the electrical current which relates the current to the radius of the nanowire. It is assumed that the temperature is 0 K. The reason for this assumption is to simplify the expression since the Fermi function at this temperature can be expressed by a step function as shown in Fig. 6. In addition, we will only consider one subband...
in the derivation. The extension to more subband will be elaborated at the end.

The analytical equation is derived by considering different regions and cases in Fig. 6. Let us start with the case when the lowest energy subband $E_1$ is higher than the electrochemical potential at the source, i.e. $E_1 > \mu_1$. In this case, there is no overlap region between the two Fermi functions and the transmission curve. In other words, there is no shaded area in Fig. 6d, and therefore, the current is zero for all bias.

Now consider the case when $E_1 < \mu_2$, which means that the lowest subband is lower than the electrochemical potential at the drain. For this case, the shaded area is fixed and is given by the difference between the two Fermi functions. Since the magnitude of the Fermi function is unity for energies lower than the Fermi level, the shaded area is simply given by the width of the area shown in Fig. 6b. This width is simply the bias voltage $V_D$. Hence for this region, we can write the current as

$$I = \frac{2q}{\hbar} V_D$$  \hspace{1cm} (21)

The equation above gives us the linear portion in Fig. 4, which happens when the drain is biased at a very low voltage. In a latter part, we will give the expression for the voltage where the current starts to saturate.

The last case is when the lowest energy subband is between the electrochemical potential at the source and the drain, i.e. $\mu_2 < E_1 < \mu_1$, as is shown in Fig. 6d. Note that as the drain is biased, the shaded area does not change. This is because the transmission curve and the source Fermi function do not change under bias. Hence, the current for this region is a constant and is given by the width of the shaded area in Fig. 6d. The width is given by the difference between the electrochemical potential at the source and the first lowest subband energy

$$I = \frac{2q}{\hbar} (\mu_1 - E_1)$$  \hspace{1cm} (22)

From (16), (17), and Table 1, we can write the first subband energy as

$$E_1 = \frac{2.4048^2 \hbar^2}{2m^*_1 R^2}$$  \hspace{1cm} (23)

Hence, the current in (22) can be expressed in terms of the electrochemical potential and the radius of the nanowire.

We can summarize the ideal current equation as follows:

$$I = \begin{cases} 0, & E_1 \geq \mu_1 \\ \frac{2q}{\hbar} V_D, & E_1 \leq \mu_2 \\ \frac{2q}{\hbar} (\mu_1 - E_1), & \mu_2 < E_1 < \mu_1 \end{cases}$$  \hspace{1cm} (24)

where $E_1$ is given by (23).

What happens if there are more than one subband involved in the transport? We must compute the currents due to each subband using (24) and sum them up. For example, when a second subband is involved, (24) is used to calculate $I_i$ by replacing $E_1$ with $E_i$. The constant in (23) is also replaced with 3.8317 according to Table 1. Then the total current is simply given by

$$I_{\text{total}} = \sum_{i=1}^{M} I_i$$  \hspace{1cm} (25)

where $M$ is the last subband with energy lower than $\mu_1$, and the current for each contribution is given by replacing $E_1$ with $E_i$ in (22)

$$I_i = \frac{2q}{\hbar} (\mu_1 - E_i)$$  \hspace{1cm} (26)

and $E_i$ is the $i$th subband energy.

Fig. 7 shows the current–voltage characteristic calculated using the analytical model (24) with the same parameters as those used in the previous section. The agreement between the analytical model and the numerical calculation is not surprising. The analytical equation is able to model the current–voltage characteristic accurately in the linear and in the saturation regions. The only region where the analytical model differs from the numerical calculation occurs where the current starts to saturate.

The reason for this discrepancy seems to be caused by the assumption of 0 K temperature in the analytical model. When the temperature is finite, the Fermi function is no longer a step function. This causes the numerical results to have a lower value of current as the drain Fermi function passes through the lowest subband energy $E_1$.

The point where the current starts to saturate can be obtained by equating (21) and (22)

$$I = \frac{2q}{\hbar} V_S = \frac{2q}{\hbar} (\mu_1 - E_1)$$  \hspace{1cm} (27)

where $V_S$ is the drain voltage at which the current starts to saturate. Solving the above equation gives

$$V_S = \mu_1 - E_1$$  \hspace{1cm} (28)

Fig. 7. Current–voltage characteristic calculated using the analytical model in comparison with the result obtained numerically. We use the same parameters for both calculation. Note that the analytical model can be used to model the ballistic nanowire. The inset shows the region where the current starts to saturate. The difference could be caused by the finite temperature assumed in the analytical model.
Hence, $V_S$ depends on the electrochemical potential as well as on the lowest subband energy. The lowest subband energy, in turn, depends on the radius of the nanowire. Recall from (23) that the energy subband is proportional to the inverse square of the nanowire radius. This means that for the same electrochemical potential level at the source, $V_S$ decreases as the radius of the nanowire decreases.

We can also write the saturation current in terms of this voltage $V_S$. From (27),

$$I_S = \frac{2q}{\hbar} V_S$$

(29)

This means that the saturation current is proportional to the voltage $V_S$. Hence, as the radius of the nanowire is decreased, $V_S$ and $I_S$ will decrease.

Note that the analytical equations presented here are similar to those in Ref. [27] for low-temperature limits. The derivation of our expression, however, shows how the radius of the nanowire affects the current.

5. Electrical current dependencies on nanowire radius

In the previous section, we have derived an analytical equation for the ballistic current in cylindrical nanowires. Eqs. (24) and (23) show that for a given Fermi level in the contact, the current depends on the radius of the nanowire as well as on the effective mass. In this section, results for varying the radius of nanowires are presented.

Eq. (23) shows that the subband energy depends on the radius of the nanowires. More exactly, the subband energy is inversely proportional to the square of the radius of nanowires. This means that as the radius decreases, the subband energy increases. An increasing subband energy results in smaller $V_S$ and $I_S$ values as shown in (28) and (29).

Fig. 8(a) shows the current–voltage characteristic when the diameter of the nanowire is varied. It appears that the current decreases as the diameter of the nanowire decreases. This is consistent with our previous discussion. It is interesting to note that the slope in the linear region remains the same for various values of diameter. From (21), the slope is obviously given by

$$\frac{I}{V_D} = \frac{2q}{\hbar} = G_0$$

(30)

where $G_0$ is the quantum conductance.

The increase in electrical current can also be explained in this way. As the subband energy is lowered by increasing the nanowire radius, the transmission curve shifts to the left, and the shaded area in Fig. 6(d) increases. This, in turns, causes the increase in the current. Since the first subband energy is the lowest energy where electron can flow, it acts like a barrier for the electron coming from the source that has energy lower than this first subband. When the electron barrier decreases, the current starts to flow. A closer look at Fig. 8(a) suggests that the current–voltage characteristic resembles that of a transistor. Indeed, a transistor current is controlled by a gate voltage which controls the barrier at the channel [28,23].

Fig. 8(b) shows the trend of the saturation current values with respect to the nanowire diameter. We also plot the values predicted by the analytical model. It can be seen that the analytical model predicts pretty well the saturation current computed numerically. It is to be noted that the analytical model was derived by assuming 0 K temperature. On the other hand, the non-equilibrium Green’s function simulation use a room temperature value. The good prediction of the analytical model is not surprising though. The reason is that the Fermi function is symmetric about the Fermi energy. Hence, even for non-zero temperature, the integration area for the saturation current calculation remains the same. This is shown in Fig. 9 where the two shaded areas are equal.

In this calculation, we use up to eight subband energies in both the numerical and the analytical calculation. This is sufficient for the diameter sizes considered in Fig. 8(b). As the diameter size increases, the subband energies decrease and more subbands...
contribute to electrical current. Using (17), we compute that the highest subband energy that is still below the source electrochemical potential is the eight subband, which is about 0.34 eV (recall that the $\mu_s = 0.39$ eV). Fig. 8, hence, shows the validity of the analytical solution amidst its simple expression.

6. Conclusion

In this work we have derived a formulation for calculating the ballistic transport in cylindrical nanowires using a simplified model. The result of this simplification is that the eigenstates due to the confinement along the radial direction are given by an analytical equation. The three-dimensional problem of a cylindrical nanowire is reduced to a one-dimensional problem along the transport direction.

To understand further the ballistic transport in cylindrical nanowires, we also derived an analytical equation for the current–voltage characteristic by assuming 0 K temperature. The current is expressed in terms of known parameters such as the electrochemical potential of the contacts and the radius of the nanowires. In this expression the relationship between the current and the radius of the nanowires is clearly shown. The current work then discusses the effect of the radius on the nano-scale optoelectronic cylindrical nanowires.

Interested readers can obtain the software for the calculation of nano-scale optoelectronic cylindrical nanowires. In a normal modern PC, the code computes the non-equilibrium Green’s function in a few minutes for 31 bias points, and the analytical equations in just a few seconds. The result of this simplification is that the eigenstates due to the confinement along the radial direction are given by an analytical equation. The three-dimensional problem of a cylindrical nanowire is reduced to a one-dimensional problem along the transport direction.

To understand further the ballistic transport in cylindrical nanowires, we also derived an analytical equation for the current–voltage characteristic by assuming 0 K temperature. The current is expressed in terms of known parameters such as the electrochemical potential of the contacts and the radius of the nanowires. In this expression the relationship between the current and the radius of the nanowires is clearly shown. The current work then discusses the effect of the radius on the nano-scale optoelectronic cylindrical nanowires.

Interested readers can obtain the software for the calculation from the author. In a normal modern PC, the code computes the non-equilibrium Green’s function in a few minutes for 31 bias points, and the analytical equations in just a few seconds. The work presented in this paper yields a fast and efficient model for designing nanowires, and is useful before a more elaborate and accurate simulation is performed. The source code used in this paper can be obtained for free from the author.

We intend to include the interaction between electron and photon into the calculation. When phase-breaking phenomena are introduced, the non-equilibrium Green’s function calculation generally takes a huge amount of time. Our proposed model, then, is able to reduce the computational burden of simulating nano-scale optoelectronic cylindrical nanowires.

References


