# Resistance calculation in metal-2D contacts: Accuracy of numerical integration

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## Introduction

Ab-initio modelling techniques provide ways to estimate the contact resistance of metal-2D contacts, and are important tools to understand and design these structures. However, due to the complicated nature of metal - 2D semiconductor contacts, the task of obtaining accurate, physically sound results that are consistent with experiment is daunting.

In this work, we investigate the validity of a widely used method for the calculation of contact resistance. Using our in-house quantum transport solver [1], [2], we compare the calculation of the transmission coefficient and contact resistance through a metal-2D contact using an analytical integration [2] and trapezoidal integration commonly used in ab-initio modelling approaches [3], [4]. It is necessary to carefully choose the integration method for the transmission coefficient [5].

## Calculation of contact resistance

Figure 1a shows the structure of the Au-$MoS_2$ contact we simulate, with the Au ($\phi_{\mathrm{Au}} = 5.2$ eV) in blue and the $MoS_2$ ($\chi_{\mathrm{MoS_2}} = 4.2$ eV) in red. Figures 1b and 1c show the Hartree potential and free charge density, respectively, obtained by self-consistently solving the Poisson and Schrödinger equations [1].

Figure 2 shows the band structures of the Au and $MoS_2$ at the left and right edges of the simulation domain, where semi-infinite leads provide electron baths from which electrons are injected in the simulated structure. We describe the materials using a continuum effective mass model. Therefore, the bandstructures are those of free electrons with an effective mass $m^*$ ($m^* = 1$ in this work).

We calculate the conductance from the transmission coefficient using

$$\sigma = \frac{2q^2}{h} \int_{-\infty}^{+\infty} dE \int_{-\infty}^{+\infty} dk_{\mathrm{y}} T(E, k_{\mathrm{y}}) \frac{\partial f_{\mathrm{FD}}(E)}{\partial E}. \tag{1}$$

Here, $\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}$ is the derivative of the Fermi-Dirac distribution, and $T(E, k_{\mathrm{y}})$ is the transmission coefficient in the transport ($x$) direction at a certain energy $E$ sampled at a value of $k_{\mathrm{y}}$ of the wave vector in the transverse direction.

Figure 3 shows the comparison between the analytical and trapezoidal integration methods for the calculation of $T(E) = \int dk_{\mathrm{y}} T(E, k_{\mathrm{y}})$. Using our effective mass model, we are able to perform a transformation where we obtain $T(E)$ analytically [2]. Crucially, Fig. 3 shows that a small $N_{k_{\mathrm{y}}}$ can result in over- as well as underestimation of the transmission coefficient.

## Conclusion

Figure 4 shows the convergence of the contact resistance w.r.t. the number of samples taken in the transverse ($k_{\mathrm{y}}$) direction. We see that the trapezoidal integration is able to capture the behavior of the contact well when $N_{k_{\mathrm{y}}}$ is well-chosen.

Figure 5 shows that the relative error in the calculated contact resistance is strongly dependent on the choice of $N_{k_{\mathrm{y}}}$. The choices for $N_{k_{\mathrm{y}}}$ that do not include the conduction band minimum are particularly erroneous at insufficiently large $N_{k_{\mathrm{y}}}$. We conclude that even in advanced models, e.g. DFT+NEGF, it is important to carefully choose $N_{k_{\mathrm{y}}}$.

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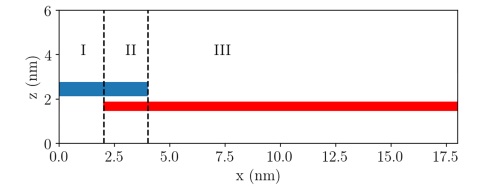
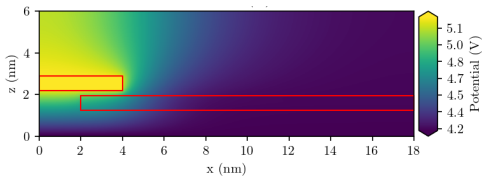



(a)

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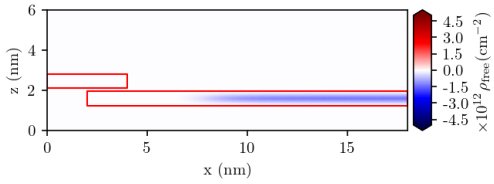


(c)

Fig. 1: (a) Schematic representation of our metal-2D semiconductor contact. Self-consistently calculated Hartree potential (b) and free charge density (c). The calculated Schottky barrier is 0.57 eV. We add a sheet doping of $\rho_{\text{sheet}} = 5 \times 10^{12}\ \text{cm}^{-2}$.

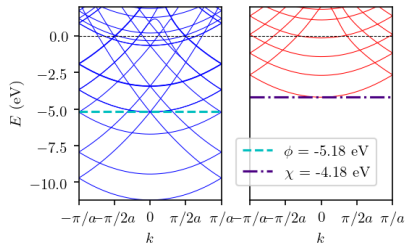


Fig. 2: Bandstructure of the materials at the left and right edges of the simulation domain and in the corresponding semi-infinite leads. The metal and semiconductor are at the left and right sides, respectively.

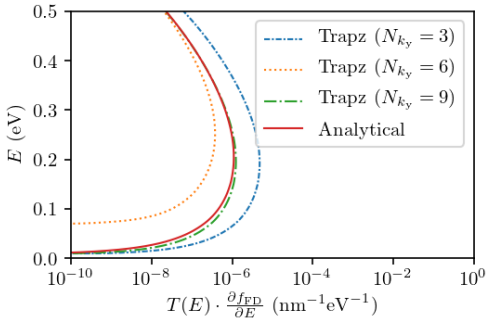


Fig. 3: The transmission coefficient, multiplied by the derivative of the Fermi-Dirac distribution, calculated using trapezoidal and analytical integration of $T(E) = \int dk_y T(E, k_y)$ for $N_{k_y} = 3$, $N_{k_y} = 6$ and $N_{k_y} = 9$.

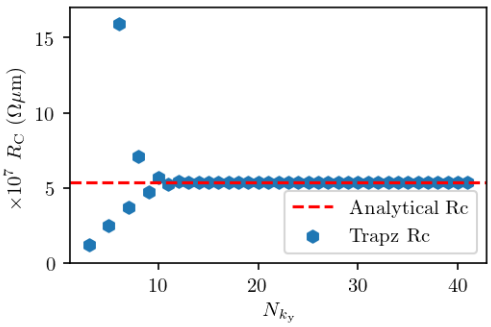


Fig. 4: Convergence of the contact resistance calculated using trapezoidal integration of the transmission coefficient, with varying number of samples in the transverse ($k_y$) direction. The analytically calculated value is shown as the dashed red line.

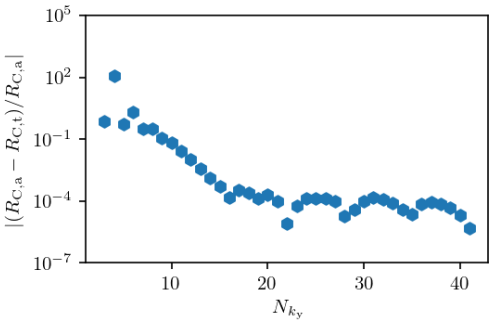


Fig. 5: Convergence of the relative error in the contact resistance between the trapezoidal and analytical integration methods for the transmission coefficient.