# Analytic solution of Ando's surface roughness model with finite domain distribution functions

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In this abstract we present two variants of a new approach to simulate surface roughness (SR) scattering with Ando's model and the multi-subband Boltzmann transport equation (BTE) [1]. An crucial step to obtain the SR matrix element is the integration of the product of wave functions (of the initial and final state) over the length of the SR deviation in the direction normal to the boundary surface. Typically one expands this integral up to first order of the SR deviation, usually even taking the limit of an infinite barrier height, known as the Prange-Nee (PN) approximation [2]. The validity of these approximations can be seriously doubted when applied in metal nanowires, as small diameters lead to substantial wave function penetration in the barrier while a large number of subbands is still present, allowing for wave functions that oscillate many times over the typical SR deviation length (see Fig. 1). However, this type of approximation allows for a replacement of the SR deviation by its auto-correlation function (ACF), leading to an analytical expression of the absolute value squared of the matrix element that appears in the collision term of the BTE [3].

The SR integral can still be solved analytically for the finite potential well with averaging over the SR if an appropriate SR distribution function $f(S,S')$ is chosen, with $S,S'$ the SR deviations at different positions on a wire boundary. We propose to use a distribution functions on a finite domain ($-\sqrt{3}\Delta \leq S,S',\leq \sqrt{3}\Delta$) and give two variants below:

$$f_{\mathrm{I}}\left(S,S'\right) \equiv \frac{1}{12\Delta^2}\left\{1+\frac{4}{3}C\left[\theta\left(SS'\right)-\theta\left(-SS'\right)\right]\right\},$$

$$f_{\mathrm{II}}\left(S,S'\right) \equiv \frac{(1-C)}{12\Delta^2}+\frac{C\delta\left(S-S'\right)}{\sqrt{12}\Delta}.$$

with $\Delta$ the SR standard deviation, $C$ the correlation of the SR at the different positions, provided by a given ACF (here Gaussian) and $\theta$ the step function.

We compare the resistivity results with the bivariate normal SR distribution function, that was recently proposed by Lizzit et al., for a one subband toy model in Fig. 2 [4]. The distribution functions have different disadvantages ($f_I$: negative weights when $C > 3/4$, $f_{II}$: Dirac delta peak for $S = S'$, bivariate normal: non-zero probability for SR crossing the opposite wire boundary) but mutually agree quite well, while the PN result is incorrect. The finite domain models allow for fast and accurate simulations due to their analytic expression, while the bivariate normal model requires numerical treatment. Hence with the latter approach simulations are much slower (see Fig. 3) and we were unable to study metal wires with larger diameters.

For larger diameter simulations the first order approximation and finite domain models agree well on the diameter scaling trend, but the predicted resistivity values differ up to a factor of 2 (see Fig. 4). The PN model works much better than for the one subband model and in certain cases even better than the first order approximation, however this is believed to be coincidental.

A large resistivity drop is observed for $D \approx 3.25$ nm for all methods and appears when the bottom of all subbands is as far below the Fermi level as possible. In this case back-scattering of the Fermi level states is suppressed and the current is protected. The predicted resistivity values for this drop are in good agreement for the finite domain models, while the approximate methods deviate substantially.

## References

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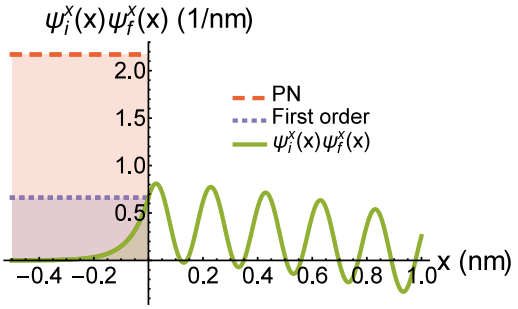
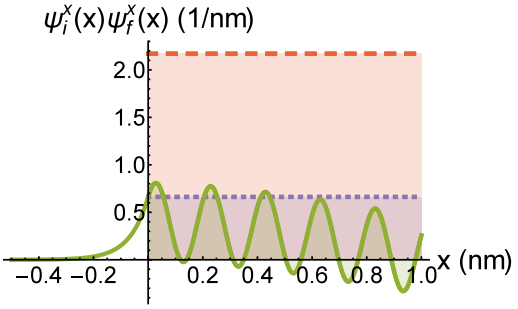
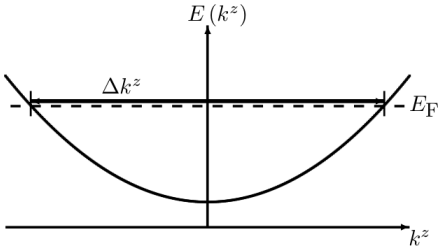



(a) Rough boundary position: -0.5 nm

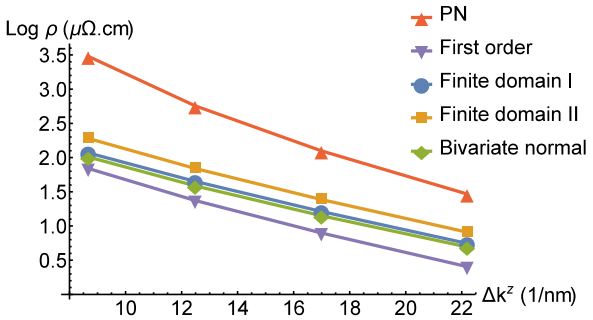



(b) Rough boundary position: 1 nm

Fig. 1. A product of wave functions for a wire with width of approximately 2.15 nm and the integral up to the rough boundary position are shown as a shaded area under the curve. The correct value in the SR matrix element of Ando's model should be the area under the wave function product, but the PN and the first order approximation replace this area by a rectangular box.




(a) One subband toy model




(b) Resistivity

Fig. 2. In (a) the dispersion relation of a one subband toy model is shown with the momentum gap $\Delta k^z$ indicated. The resistivity values obtained with the SR matrix elements of Ando's model are shown in (b), using the PN and the first order approximation, the two newly proposed variants: using $f_I$ and $f_{II}$, and the bivariate normal model [4].

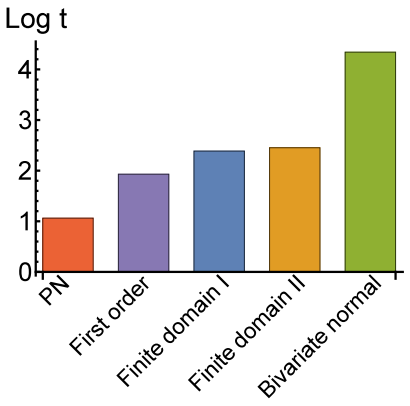
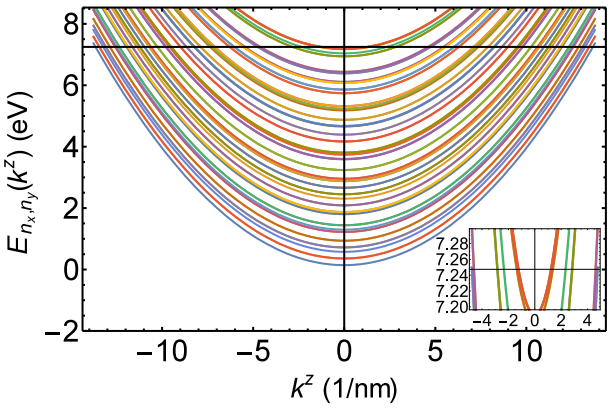
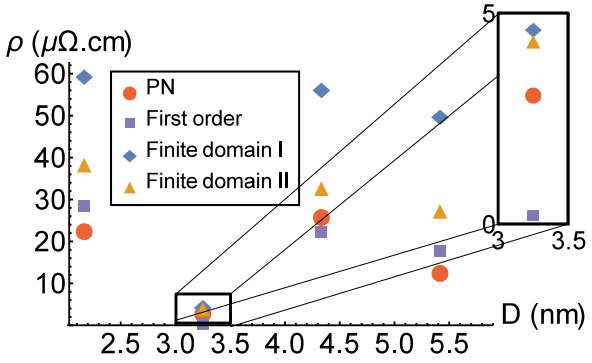



Fig. 3. The computation times ($t$) for the SR matrix elements are shown in a logarithmic scale for the different methods: the Prange-Nee approximation (*PN*), the first order approximation (*First order*), the approach with a finite domain distribution function using $f_I$ (*Finite domain I*) and $f_{II}$ (*Finite domain II*), and the bivariate normal distribution function (*Bivariate normal*). The timescale is in milliseconds and corresponds to the one subband toy model simulation shown in Fig. 2.




(a) Subbands




(b) Resistivity

Fig. 4. The resistivity for copper nanowires with square cross-section of equal sides $D$ ranging from 2 to 6 nm (SR standard deviation of $2a_{\mathrm{Cu}} \approx 0.7$ nm and correlation length of $5a_{\mathrm{Cu}} \approx 1.75$ nm) are shown in (b), using the different methods for Ando's model that are computationally feasible (same methods as in Fig. 3 without *Bivariate normal*). The subbands dropping below the Fermi level of the $D \approx 2.15$ nm wire are shown in (a).