Implications of the Coherence Length on the Discrete Wigner Potential

P. Ellinghaus, M. Nedjalkov, and S. Selberherr
Institute for Microelectronics, TU Wien, Gußhausstraße 27–29/E360, 1040 Wien, Austria
E-mail: {ellinghaus | nedjalkov | selberherr}@iue.tuwien.ac.at

We investigate how a finite coherence length influences the calculation of the Wigner potential (WP) in terms of momentum resolution and computational aspects, in addition to the physical meaning attributed to it. Firstly, we define the semi-discrete WP:

$$\begin{aligned} V_W(\mathbf{r},\mathbf{P}) &\equiv \frac{1}{i\hbar\mathbf{L}}\int_{-\mathbf{L}/2}^{\mathbf{L}/2} d\mathbf{s}\, e^{-i2\mathbf{P}\Delta\mathbf{k}\cdot\mathbf{s}}\delta V \\ \delta V(\mathbf{s};\mathbf{r}) &\equiv V(\mathbf{r}+\mathbf{s}) - V(\mathbf{r}-\mathbf{s}), \end{aligned} \tag{1}$$

where the position vectors, $\mathbf{r}$ and $\mathbf{s}$, are bounded by the (active) device length, $\mathbf{L}_{dev}$, and the coherence length, $\mathbf{L}$, respectively. The momentum vector, $\mathbf{P}\Delta k$, is discretized in steps of $\Delta k = \frac{\pi}{\mathbf{L}}$, which makes the full discretization of (1) akin to a discrete Fourier transform (DFT) of the potential difference.

From a computational point of view, the coherence length affects the momentum resolution Δk, therefore, $\mathbf{L}$ must be chosen sufficiently large to resolve the spectral content of the device profile. Fig. 1 shows different potential profiles, with their corresponding WP, for a fixed position, in Fig. 2. The potential profiles were chosen to have known spectral components ($\mathbf{P}$-values) that should appear within bins 1 and 2 only. Therefore, the values at higher bins are not attributable to the physical profile, but rather the 'spectral leakage' effects inherent, when applying the DFT to a non-periodic function. The WP is normalized to represent a probability distribution for the generation of particles with a given momentum offset $\mathbf{P}$ (negative values of V_w represent a negative offset; $-V_w(\cdot,\mathbf{P}) = V_w(\cdot,-\mathbf{P})$). To attain a distribution which better represents the physical profiles, we apply a Tukey window [1] to smooth (only) the sharp edges of the potential profile. Fig. 3 shows that by applying the Tukey window the (unphysical) higher bin values are suppressed, while the actual spectral components of the profile, at bins 1 and 2, remain pronounced. This results in a relative change of the probability distribution (Fig. 4), which better reflects the physical situation in the device, by highlighting the bins the actual potential influences.

Several physical viewpoints are possible when choosing the coherence length: If decoherence effects are not modelled through the choice of $\mathbf{L}$ itself [2] – e.g. [3] considers an exponential damping which essentially reduces $\mathbf{L}$ to model decoherence – the coherence length should be chosen to (at least) cover the extent of the device at every point where the WP is calculated; this implies $\mathbf{L} \geq 2\mathbf{L}_{dev}$. However, under the physical assumption that no coherence exists between contacts, we must adopt $\mathbf{L} = \mathbf{L}_{dev}$. Nonetheless, when calculating (1) at any point other than the centre of the device, i.e. $V_W\left(\mathbf{r} \neq \frac{\mathbf{L}}{2},\cdot\right)$, the boundaries of the device are exceeded and therefore the potential is unknown. Two limiting approaches to treat this situation are to i) regard any point outside the device to be in a contact region and extend the potential value at the boundary as a constant, or to ii) assume no coherence exists between the device and the region outside, and progressively reduce the coherence length as the boundary is approached. Fig. 5 reveals that the difference between these two approaches is significant. Approach ii) implies a decreasing value of Δk as the boundary is approached. To efficiently interpolate the values onto the fixed, finer, momentum grid, the potential difference in (1) is zero-padded at the front and back.

We have highlighted some of the implications a finite coherence length has on numerical simulation along with possible treatments, but, ultimately, the choice of the boundary conditions reflects the adopted physical interpretation and remains a challenging research topic [4].

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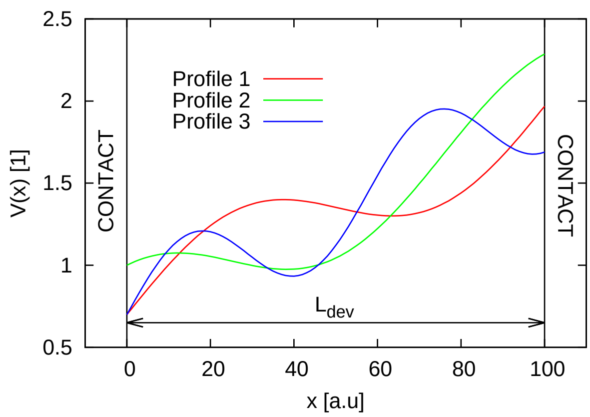

Fig. 1. Various potential profiles with known spectral content, reflecting a 1.3 V bias between the left and the right contacts.

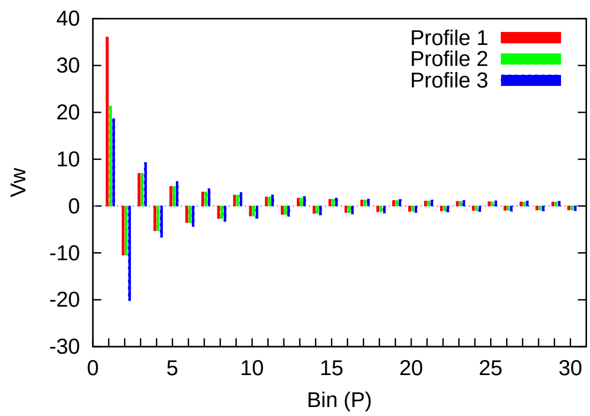

Fig. 2. Wigner potential at a fixed position, V_W $(x = 50, P)$, for the profiles in Fig. 1, calculated with a coherence length of $\mathbf{L} = \mathbf{L}_{dev}$.

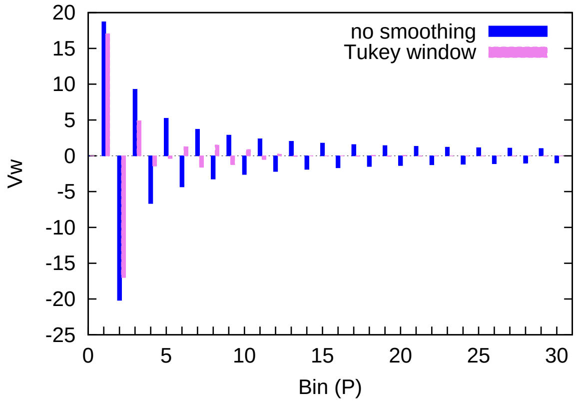

Fig. 3. The unnormalized WP, V_W $(x = 50, P)$, calculated at the centre of the device with and without the application of a smoothing Tukey window ($\alpha = 0.2$), using Profile 3 (blue) in Fig. 1, and a coherence length of $\mathbf{L} = \mathbf{L}_{dev}$.

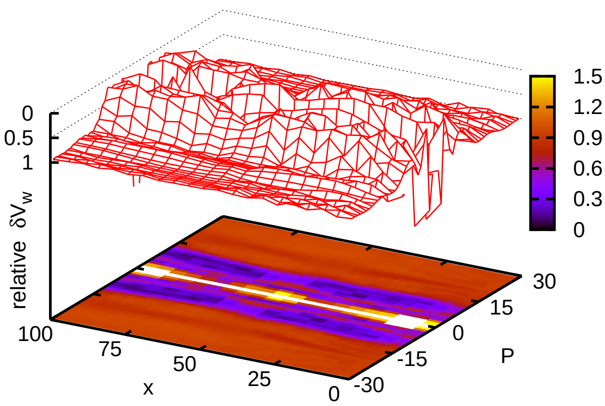

Fig. 4. The relative absolute difference of the probability distributions (normalized WPs) calculated with and without the application of a smoothing Tukey window ($\alpha = 0.2$), using Profile 3 (blue) in Fig. 1. A coherence length of $\mathbf{L} = \mathbf{L}_{dev}$ is used, along with boundary approach i) discussed in the text.

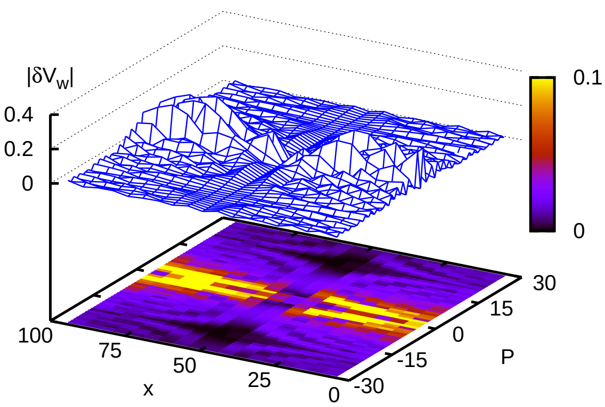

Fig. 5. The absolute value of the difference of the (normalized) WPs corresponding to the different boundary treatments (discussed in text), using Profile 3 (blue) in Fig. 1.