

Floquet projections of a Gaussian Wigner function in a Kronig-Penney potential

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Abstract. In this contribution, we apply the multiband model developed in [1] to a Kronig-Penney potential and calculate the Floquet projections of a Gaussian Wigner function in phase space. The Bloch functions are calculated numerically and then used in the expressions of the Wigner projections.

1. Introduction

The Wigner-function approach is a commonly used method in the study of electron transport properties in semiconductors and in the description of their physical properties. [2, 3, 4]. All the relevant and realistic applications of this approach, however, have considered until now only those processes which can be adequately described within the single-parabolic-band approximation. This formalism cannot be applied to those processes which involve non-parabolicity of the band profiles or multi-band transitions. The latter ones, for example, play a significant role in determining the flow of current in interband devices (e.g., the Resonant Interband Tunneling Diode [5]). Therefore, the Wigner-function approach needs to be extended; the definition of the Wigner function should include the populations of all bands involved in the transport processes and the evolution equation should take into account possible non-parabolicity effects. A general model of multiband, non-parabolic transport by the Wigner-function approach was developed in [1], where a multi-band Wigner function was introduced by using a straightforward expansion of the wave functions in Bloch states and a Bloch-state representation of the density matrix. This multi-band model is probably the most general way of using the Wigner-function approach in the context of multi-band model problems; other formulations, such as the envelope function model and the Kane model, have recently been explored in the literature [6, 7, 8, 9].

While the effects of non-parabolicity are easy to include in Wigner-function models (see [10]), the description of multiband transitions requires the knowledge of the energy bands and of the Bloch functions of the periodic potential, which enter the expressions of the Floquet projections of the Wigner function. The calculation of these projections is an essential intermediate step towards the numerical solution of the equation which governs the time evolution of the Wigner function, and have not been obtained until now. In this work, we show the Floquet projections of a Gaussian Wigner function in a one-dimensional Kronig-Penney potential.

2. Multiband Wigner function

By using the completeness of the Bloch functions, we express the Wigner function as a sum over the components onto the Floquet band subspaces:

$$f(x, p) = \sum_{mn} f_{mn}(x, p) \quad (1)$$

with

$$f_{mn}(x, p) = \frac{1}{2\pi} \int \int_{B^2} \frac{dk' dk''}{|B|^2} \rho_{mn}(k, k') \phi_{mn}(k, k', x, p) \quad (2)$$

where B is the Brillouin zone and $|B|$ its volume, the ρ_{mn} 's are the elements of the density matrix in the Bloch-state representation, the coefficients ϕ_{mn} are given by

$$\phi_{mn}(k, k', x, p) = \int_{\mathbb{R}} \Psi_{mk}(x + \eta/2) \Psi_{nk'}^*(x - \eta/2) e^{-i p \eta} d\eta$$

and $\Psi_{mk}(x) = u_{mk}(x) e^{i k x}$ is the Bloch function of the m -th band of the periodic potential. The diagonal projections f_{mm} are real, while the off-diagonal ones are complex conjugates, $f_{mn} = f_{nm}^*$. After some steps, we find

$$\begin{aligned} f_{mn}(x, p) &= \sum_{m'n'} \sum_{m''n''} e^{i(m'-n')x} \Theta(\alpha_{m'n'}(p)) \int_{-\alpha_{m'n'}(p)}^{\alpha_{m'n'}(p)} e^{i\tau x} \\ &U_{mm'} \left(K_{m'n'} + \frac{\tau}{2} \right) U_{nn'}^* \left(K_{m'n'} - \frac{\tau}{2} \right) U_{mm''}^* \left(K_{m'n'} + \frac{\tau}{2} \right) U_{nn''} \left(K_{m'n'} - \frac{\tau}{2} \right) \\ &\hat{f} \left(\tau + m'' - n'', K_{m'n'} + \frac{m'' + n''}{2} \right) d\tau \end{aligned} \quad (3)$$

where we have indicated by $\hat{f}(\lambda, p)$ the Fourier transform of $f(x, p)$ with respect to x . Here, the $U_{mm'}(k)$ are the m' -th Fourier coefficients of the periodic part of the Bloch functions. Also, $K_{mn}(p) = p - (m+n)/2$, $\alpha_{mn}(p) = 1 - 2|K_{mn}(p)|$ and Θ is the Heaviside function. In order to obtain analytical or numerical data for the $U_{mm'}(k)$'s, we consider a Kronig-Penney potential of period 2π , given by

$$V(x) = \begin{cases} V_0, & -b \leq x < 0 \\ 0, & 0 \leq x < c, \end{cases}$$

with $b+c = 2\pi$. In the equations above, we have used dimensionless variables. If a is the lattice period, we have scaled the space variable x , the energy E , the potential V , the Wigner momentum p and the wave function Ψ according to

$$2\pi \frac{x}{a} \rightarrow x \quad \frac{2ma^2}{(2\pi\hbar)^2} E \rightarrow E \quad \frac{2ma^2}{(2\pi\hbar)^2} V(x) \rightarrow V(x) \quad 2\pi \frac{a}{\hbar} p \rightarrow p \quad \sqrt{\frac{a}{2\pi}} \psi \rightarrow \psi.$$

For given values of the parameters b and V_0 , the eigenvalue problem for the Kronig-Penney potential can be solved completely, the Fourier coefficients $U_{mm'}$ can be evaluated and the Floquet projections (3) of the Wigner function can be calculated.

3. Numerical results

In this section, we calculate the projections of a Gaussian shaped Wigner function which, as is well known [11], results from the Wigner-Weyl transform of a Gaussian wave packet,

$$f(x, p) = \frac{1}{2\pi\sqrt{M}} e^{-\frac{\sigma_{02}(x-x_0)^2}{2M} - \frac{\sigma_{20}(p-p_0)^2}{2M} + \frac{\sigma_{11}(x-x_0)(p-p_0)}{M}}, \quad (4)$$

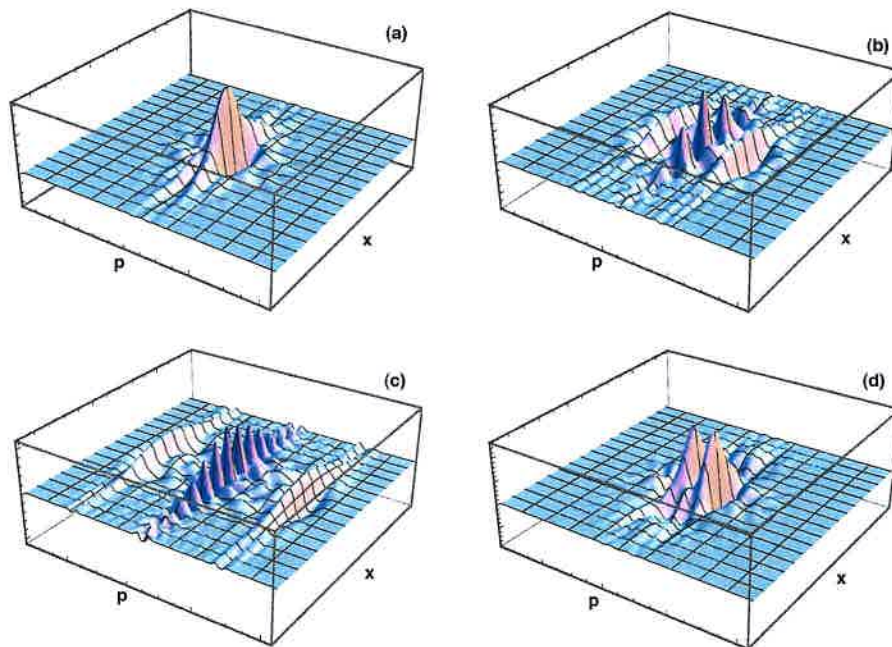


Figure 1. (a) $f_{00}(x, p)$, (b) $f_{22}(x, p)$, (c) $f_{44}(x, p)$ and (d) real part of $f_{01}(x, p)$ projections of the Gaussian Wigner function (4) for $p_0 = 0$.

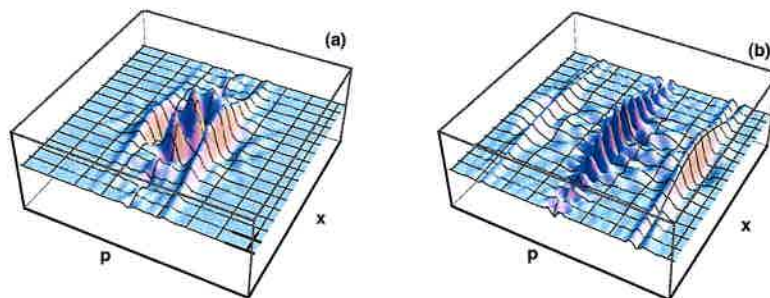


Figure 2. (a) $f_{11}(x, p)$ and (b) $f_{44}(x, p)$ projections of the Gaussian Wigner function (4) for $p_0 = 1$.

(with $M = \sigma_{20}\sigma_{02} - \sigma_{11}^2$), in the Kronig-Penney potential introduced above. The results are shown in Figures 1 and 2. We have chosen $b = 0.2$ and $V_0 = 10$ as characteristic parameters of the Kronig-Penney potential, and $x_0 = 0$, $\sigma_{02} = 0.2$, $\sigma_{11} = 0$ and $\sigma_{20} = 0.3$, with $p_0 = 0$ (Figure 1) and $p_0 = 1$ (Figure 2).

The projection onto the $m = 0$ band space shows a maximum centered at $x = 0, p = 0$ surrounded by lower maxima and negative minima (not seen), due to interference effects. The projections onto the higher band subspaces show an oscillating structure along the $p = 0$ line, with two other peaks located symmetrically about $p = 0$; they are of equal height in the $p_0 = 0$ case (Figure 1), while in the $p_0 = 1$ case (Figure 2) the one at positive p is higher. The oscillating

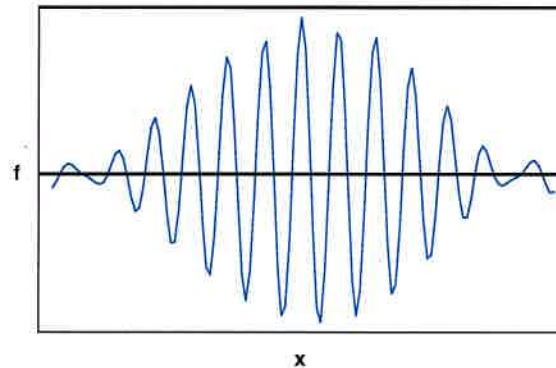


Figure 3. $f_{44}(x, p)$ at $p = 0$ as a function of x , for $p_0 = 1$.

structure at $p = 0$, shown in Figure 3, is due to the interference of different contributions to the sum in equation (3), which have an almost gaussian profile. This effect is similar the one observed in Schrödinger cat states.

4. Conclusions and outlook

We have calculated the Floquet projections of a Gaussian shaped Wigner function in a Kronig-Penney periodic potential. These are important intermediate results, needed in the study of the multiband dynamics of a group of carriers in a semiconductor by the Wigner-function approach. The algorithms and techniques for the calculation of these projections will be included in a large-scale numerical computation, which is underway, with the aim of describing a coherent interband transition by the Wigner-function approach.

References

- [1] L. Demeio, P. Bordone and C. Jacoboni, *Multi-band, non-parabolic Wigner-function approach to electron transport in semiconductors*, Transport Theory and Statistical Physics, **34**(7), 499-522 (2005).
- [2] E. Wigner, *On the Quantum Correction for Thermodynamic Equilibrium*, Phys. Rev **40**, 749-759 (1932).
- [3] W. R. Frensley, *Boundary conditions for open quantum systems driven far from equilibrium*, Rev. Modern Phys. **62**(3), 745-791 (1990).
- [4] C. Jacoboni, R. Brunetti, P. Bordone, and A. Bertoni, *Quantum transport and its simulation with the Wigner-function approach*, International journal of high speed electronics and systems, **11**(2), 387-423 (2001).
- [5] M. Sweeney and J. M. Xu, *Resonant Interband Tunneling Diodes*. Appl. Phys. Lett. **54**, 546-548 (1989).
- [6] O. Morandi and M. Modugno, *A multiband envelope function model for quantum transport in a tunneling diode*, Phys. Rev. B **71**, 235331(1-8) (2005).
- [7] O. Morandi and L. Demeio, *A Wigner-function approach to interband transitions based on the multiband-envelope-function model*, Transport Theory and Stat. Phys., **37**, 437-459 (2008).
- [8] L. Barletti, *Wigner Envelope Functions for Electron Transport in Semiconductor Devices*, Transport Theory Stat. Phys. **32**, 253-278 (2003).
- [9] G. Borgioli, G. Frosali, and P. F. Zweifel, *Wigner Approach to the Two-Band Kane Model for a Tunneling Diode*, Transport Theory Stat. Phys. **32**, 347-366 (2003).
- [10] L. Demeio, P. Bordone and C. Jacoboni, *Numerical simulation of an intervalley transition by the Wigner-function approach*, Semiconductor Science and Technology, **19**, 1-3 (2004).
- [11] W. Tatarskii, *The Wigner picture of quantum mechanics*, Sov. Journal Uspehi Phys. Sci. **139**, 587-619 (1983).