

## A Gauge-Invariant Wigner Equation for General Electromagnetic Fields

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Wigner quantum mechanics is standardly formulated in near electrostatic conditions with a scalar potential  $\phi$  gauge used to define the Wigner potential  $V_w$ . Theories, aiming to generalize this picture for the case of magnetic field  $\mathbf{B}$  usually involve the choice of a particular gauge. The latter enters the Wigner function  $f_w$  via the canonical momentum  $\mathbf{p}$ , obtained from the Weyl map of  $\hat{\mathbf{p}} = -i\hbar\nabla$ . In contrast, the kinetic momentum  $\mathbf{P} = \mathbf{p} - e\mathbf{A}(\mathbf{r})$ , where  $\mathbf{A}$  is the vector potential, is a physical quantity and thus is gauge-invariant. Furthermore averages of generic physical quantities depend on the kinetic momentum and thus can be easily obtained from  $f_w(\mathbf{P})$ . This inspired some theories [1],[2], where a variable change is performed to obtain  $f_w$  in terms of  $\mathbf{P}$ . Alternative theories involve the transform

$$f(\mathbf{P}, \mathbf{x}) = \int \frac{d\mathbf{s}}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}\mathbf{s}\cdot\mathbf{P}} e^{-\frac{i}{\hbar}\frac{e}{2}\mathbf{s}\cdot\int_{-1}^1 d\tau\mathbf{A}(\mathbf{x}+\frac{\mathbf{s}\tau}{2})} \rho\left(\mathbf{x} + \frac{\mathbf{s}}{2}, \mathbf{x} - \frac{\mathbf{s}}{2}\right) \quad (1)$$

which generalizes the Weyl map to obtain a kinetic momentum quantum theory directly from the density operator [3],[4]. The transform, which can be obtained by using the Baker-Campbell-Hausdorff formula, has been introduced six decades ago [5] by Stratonovich using an intuitive approach involving the characteristic function of the momentum. The corresponding evolution equations for  $f_w$  derived in the framework of these theories depend on the electromagnetic fields (EM), but not on the potentials. However, these fields appear as pseudo-differential operators: The position dependence of  $\mathbf{E}$  and  $\mathbf{B}$  is replaced by an expression containing the  $\nabla_{\mathbf{p}}$  operator. This gives rise to compact mathematical forms, but is a serious computational problem, as e.g the order of the equation with respect to the momentum derivatives varies with the position dependence of the EM fields, hampering any numerical approach. We derive an equation for general, inhomogeneous, and time-dependent EM conditions, which has an explicit mathematical structure with clearly defined differential and integral operations. The equation depends on the EM fields only, but in a nonlocal way: terms such as  $\int_{-1}^1 d\tau(\mathbf{s}\mathbf{B})_F(\mathbf{P}, \mathbf{x}, \tau)$  where  $(\mathbf{s}\mathbf{B})_F$  is the Fourier transform  $e^{-(i/\hbar)\mathbf{s}\cdot\mathbf{P}}$  of  $(\mathbf{s} \times \mathbf{B}(\mathbf{x} + \mathbf{s}\tau/2))$  (and similarly for  $\mathbf{E}$ ) act as integral operators on the  $f_w$  in the same way as  $V_w$ . For homogeneous magnetic fields the equation simplifies to a local action of  $\mathbf{B}$ :

$$\left[ \frac{\partial}{\partial t} + \frac{\mathbf{P}}{m} \cdot \frac{\partial}{\partial \mathbf{r}} + e \frac{\mathbf{P}}{m} \times \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{P}} \right] f_w(\mathbf{r}, \mathbf{P}, t) = \int d\mathbf{P}' V_w(\mathbf{P} - \mathbf{P}', \mathbf{r}) f_w(\mathbf{r}, \mathbf{P}', t) \quad (2)$$

Here, the potential  $V$  which defines  $V_w$  is determined by  $\mathbf{E}$ . As a generic application we repeat the emblematic simulations of magnetic field governed tunneling through a single barrier [6]. The ViennaWD stochastic simulator based on the signed particle approach [7] has been modified to account for accelerating forces and applied for obtaining the simulation data. In the experiment coherent electrons are injected from the bottom boundary towards the barrier marked by the blue lines, Figure 1.

Classical particle simulation results are conveniently used as a reference frame for the quantum effects, analyzed in the figure captions. The derived equation presents a computationally feasible task for the important case of homogeneous magnetic fields ( $\mathbf{B} = \text{const}$ ). The inhomogeneous terms imply presence of non-local effects.

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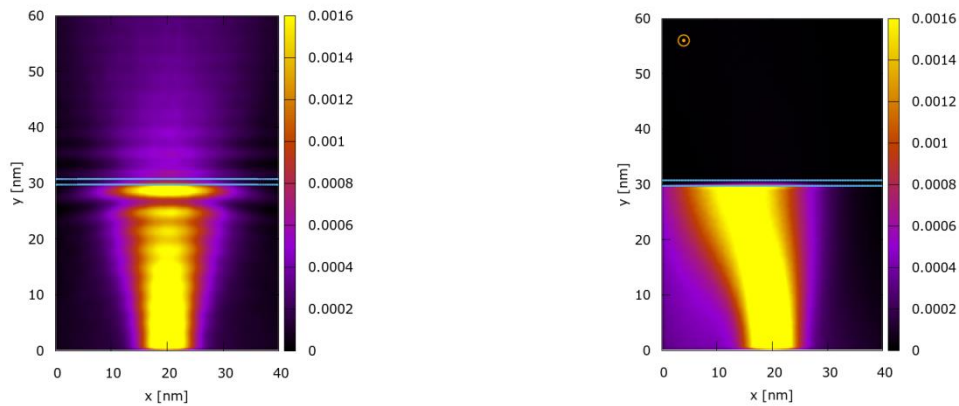


Fig.1: Electron density [a.u.] around a 0.2 eV barrier. The left picture shows the symmetry of the quantum density for  $\mathbf{B}=0$ . Two important properties are demonstrated: (i) interference effects reveal the wave nature of the evolution, in particular the finite density after the barrier is due to tunneling; (ii) the non-locality of the potential, which affects the electron density far before the barrier. In contrast, on the right picture, classical electrons with energy less than 0.2 eV (the here presented case) are back scattered locally by the barrier. The magnetic field of  $\mathbf{B} = 6\text{T}$  breaks the symmetry by bending the electron trajectory. In this case there is no wave-like transport and no tunneling; all particles are reflected back from the barrier.

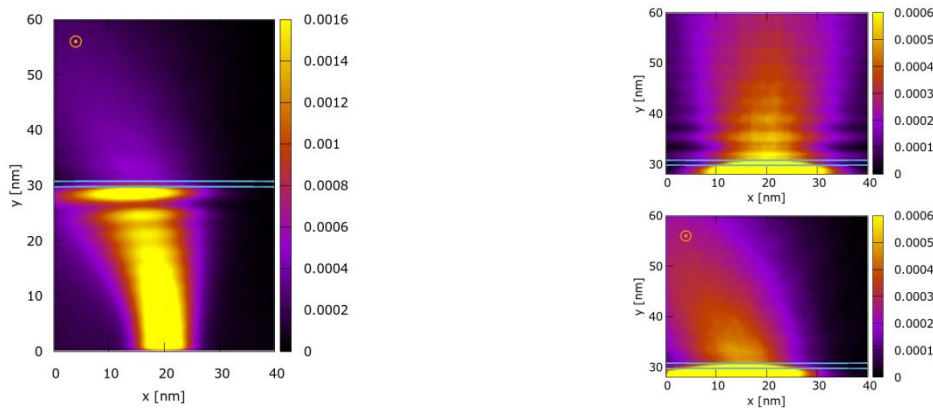


Fig.2: The quantum density [a.u.] for  $\mathbf{B}=6\text{T}$  (left) and the zoom of the density above the barrier with  $\mathbf{B}=6\text{T}$  (right, bottom) and without magnetic field (right, top) show that even if the electric field action is still non-local the coherence of the transport is affected by the magnetic field.

- [1] R. Kubo, J. Phys. Soc. Jpn. **19**, 2127 (1964)
- [2] I. B. Levinson, Sov. Phys. JETP **30**, 362 (1970)
- [3] O. T. Serimaa, J.Javanien S. Varro, Phys. Rev. A **33**, 2913 (1986)
- [4] H. Haug, A. P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, 2018)
- [5] R. Stratonovich, Dokl. Akad. Nauk SSSR **109**, 72 (1956)
- [6] N.C. Kluksdahl, A.M. Krivan, D.K. Ferry, Springer Series in Solid State Sciences **87**, 335 (1989)
- [7] P. Ellinghaus, Ph. D. Dissertation, Technische Universität Wien 2016.