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Multiphase semiclassical approximation of an electron in a one-dimensional crystalline lattice – III. From ab initio models to WKB for Schrödinger–Poisson

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Dedicated to the memory of Frédéric Poupaud (1961–2004)

Abstract

This work is concerned with the semiclassical approximation of the Schrödinger–Poisson equation modeling ballistic transport in a 1D periodic potential by means of WKB techniques. It is derived by considering the mean-field limit of a N-body quantum problem, then K-multivalued solutions are adapted to the treatment of this weakly nonlinear system obtained after homogenization without taking into account for Pauli's exclusion principle. Numerical experiments display the behaviour of self-consistent wave packets and screening effects.

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1. Introduction

This article is the third and last part of a numerical study of semiclassical approximation of the motion of electrons in short-scale periodic potentials. We have now in mind to take into account also

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for the self-consistent interaction potential, which leads to a *weak nonlinearity*. More precisely, we are about to focus onto the following Schrödinger–Poisson equation in one space dimension

$$\mathrm{i}\hbar\partial_t\psi + \frac{\hbar^2}{2m}\partial_{xx}\psi = e(V_{\mathrm{ions}}(x) + V_{\mathrm{ext}}(x) + eV_{\mathrm{P}}(t,x))\psi, \quad -\epsilon_0\partial_{xx}V_{\mathrm{P}} = |\psi|^2; \ x \in \mathbb{R} \tag{1}$$

with $\hbar$ the Planck's constant, ϵ_0 the dielectric permittivity of the medium (it will be set to $\epsilon_0 \equiv 1$ throughout the whole paper), m and e the electronic mass and charge and $V_{\mathrm{ion}} \in \mathbb{R}$ the periodic potential modeling the interaction with a lattice of ionic cores. The smooth and slowly-varying external potential V_{ext} stands usually for an applied electric field, a confining potential or a doping term.

In order to shed complete light on the derivation and the qualitative properties of the simplified model (1), we first start from the exact Hamiltonian for a neutral system constituted of N atoms with Z electrons each in $\mathbb{R}^3$:

$$\mathbf{H} = \sum_{\alpha=1}^{N}\left\{\frac{\mathbf{P}_\alpha^2}{2M} + \sum_{i=1}^{Z}\frac{\mathbf{p}_{\alpha_i}^2}{2m} + \sum_{\beta(\neq\alpha)=1}^{N}\left[\frac{1}{2}\frac{(Ze)^2}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|} + \sum_{i=1}^{Z}\left(-\frac{Ze^2}{|\mathbf{x}_{\beta_i} - \mathbf{X}_\alpha|} + \frac{1}{2}\sum_{j=1}^{Z}\frac{e^2}{|\mathbf{x}_{\alpha_i} - \mathbf{x}_{\beta_j}|}\right)\right]\right\}. \tag{2}$$

The notations have been chosen as follows: M, $\mathbf{P}_\alpha$, $\mathbf{X}_\alpha$ stand for the mass, momentum and position of the nuclei while $m, \mathbf{p}_{\alpha_i}, \mathbf{x}_{\alpha_i}$ refer to those of the electrons in the αth atom. All in all, this constitutes a system of $N(Z+1)$ charged particles interacting with each other via Coulombian forces (the atomic cores are lumped into a unique particle in this model). Ab initio computations will therefore refer to the ones involving this full Hamiltonian (2) which can be considered as exact in nonrelativistic quantum mechanics.

However, even for moderate values of N, Z, such ab initio computations become quickly almost impossible in terms of complexity. Hence, several simplifications are usually in order:

- The Born–Oppenheimer assumption states that the nuclei's motion decouples adiabatically because $M \gg m$; it can be neglected or at least treated classically.
- One can safely restrict (2) to vN valence and conduction electrons. All the others can generally be considered as tightly tied to the cores and confined inside the inner shells.

At this level, we have reduced our original system to a collection of N ions with v valence/conduction electrons. So the Hamiltonian (2) boils down to $\mathscr{H}_{\mathrm{ions}} + \mathscr{H}_{e^-}$ with

$$\mathscr{H}_{\mathrm{ions}} = \sum_{\alpha=1}^{N}\left\{\frac{\mathbf{P}_\alpha^2}{2M} + \frac{1}{2}\sum_{\beta(\neq\alpha)=1}^{N}\frac{(ve)^2}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|}\right\}, \quad \mathscr{H}_{e^-} = \sum_{i=1}^{vN}\left\{\frac{\mathbf{p}_i^2}{2m} + V_{\mathrm{ions}}(\mathbf{x}_i) + \frac{1}{2}\sum_{j(\neq i)=1}^{vN}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}\right\}. \tag{3}$$

The ionic potential $V_{\mathrm{ions}}(x) = \sum_{\alpha=1}^{N} V_{ps}(|x - X_\alpha|)$ where V_{ps} is a smoothered "pseudo-potential" originating from both Coulomb attraction and screening effects from inner shells electrons; it is referred to as the "effective core potential" in quantum chemistry. In the simplest Bohr–Oppenheimer framework, one assumes the $\mathbf{X}_\alpha$ to be constant and $\mathbf{P}_\alpha \equiv 0$ thus remains only $\mathscr{H}_{e^-}(\mathbf{x}, \mathbf{p})$ which can nonetheless constitute a delicate *quantum many-body problem*, especially in case $N \in \mathbb{N}$ is big.

A common way out lies in the *mean-field approximation* that we shall present in Section 2.1; roughly speaking, it consists in deriving self-consistently an average potential in place of the Coulomb interaction by letting $N \to \infty$ with a convenient scaling. Within this framework, electrons move as independent particles submitted to an overall mean electric field. The Pauli exclusion for fermions can be included or not in the derivation; Hartree or Hartree–Fock models are obtained accordingly. We shall choose to ignore it; hence we somehow consider an electron cloud treated as a *condensate*, that is a system endowed with the property that all its components share the *same one-particle state* described by a unique wave function