A metamaterial-inspired effective-medium theory for electron waves in graphene and semiconductor superlattices

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Abstract

It is demonstrated that ideas previously developed under the context of electromagnetic metamaterials can be extended to a wide class of physical systems whose dynamics is described by a Hamiltonian. An effective-medium approach that enables characterizing the propagation of electron waves in graphene and semiconductor superlattices is outlined. In our framework, the time evolution of *macroscopic states*, as well as the electronic band structure, can be exactly determined by an effective Hamiltonian.

1. Introduction

Effective-medium theories are of key importance in the study of "low energy" physical phenomena since they enable reducing the inherent microscopic complexity of a physical system to a few effective parameters. Particularly, in the context of electromagnetic media, such a homogenization of the physical response is possible when the wavelength of the radiation is much longer than the characteristic building blocks of the material (atoms, molecules, etc), so that the intrinsic granularity of the system can be neglected, and the structure can be regarded as a continuous effective medium. Typically, the macroscopic response of a conventional medium is described simply with two parameters: a permittivity function and a permeability function [1].

With the emergence of electromagnetic metamaterials – composites whose electromagnetic response is mainly determined by artificially built-in features and not directly by the chemical composition – these ideas have been greatly extended. The built-in features in a metamaterial effectively define a new length scale in the system (typically determined by the period a), and this can enable the emergence of novel exotic physical phenomena such as negative refraction and artificial magnetism [2]. Because the period a is typically several orders of magnitude larger than the atomic scale, the electromagnetic response of the "meta-atoms" can be characterized using conventional macroscopic electrodynamics. For excitations such that the wavelength of radiation is much larger than a, the metamaterial may itself be regarded as a continuous medium. The process of determination of the effective parameters of the metamaterial may thus be described as a *second level* of homogenization of matter.

Several homogenization methods have been proposed over the years to characterize the macroscopic response of composite electromagnetic media, e.g. [3-7]. In particular, some time ago a self-consistent

ISBN 978-952-67611-2-1

homogenization method was put forward to characterize periodic metamaterials formed by dielectric or metallic particles of arbitrary shapes and material parameters, taking into account both the effects of frequency and spatial dispersion [3-4]. Within this framework, the macroscopic response of the metamaterial is modeled by an effective dielectric function of the form $\overline{\overline{\varepsilon}}_{ef}(\omega,\mathbf{k})$ with $\mathbf{k} \leftrightarrow -i\nabla$ the wave vector and ω the frequency. Thus, in general the dielectric function may depend on the spatial derivatives, $\nabla = (\partial_x, \partial_y, \partial_z)$, because of spatial dispersion. The effective dielectric response is defined in such a manner that for an arbitrary *external macroscopic excitation* described by an external current density $\mathbf{j}_{ext}$, the induced macroscopic polarization vector $\mathbf{P}_g$ is exactly related to the macroscopic electric field $\mathbf{E}$ in the spectral domain by $\mathbf{P}_g = \left(\overline{\overline{\varepsilon}}_{ef}(\omega,\mathbf{k}) - \varepsilon_0 \mathbf{I}\right)\cdot\mathbf{E}$. By definition, we say that $\mathbf{j}_{ext}$ is a macroscopic current density if it is not more localized in space than the characteristic period of the metamaterial. More recently [4], it was shown that $\overline{\overline{\varepsilon}}_{ef}(\omega,\mathbf{k})$ can also be determined without formally introducing an external excitation ($\mathbf{j}_{ext}$). Specifically, within the framework of a time-domain formulation it is possible to define $\overline{\overline{\varepsilon}}_{ef}(\omega,\mathbf{k})$ as the response function that guarantees that for any *initial time macroscopic* field distribution for the microscopic electromagnetic fields the corresponding macroscopic fields satisfy $\mathbf{P}_g = \left(\overline{\overline{\varepsilon}}_{ef}(\omega,\mathbf{k}) - \varepsilon_0 \mathbf{I}\right)\cdot\mathbf{E}$ in the spectral domain. The objective of this work is to prove that these ideas can be extended in a straightforward manner to a wide range of physical systems whose dynamics is described by a Hamiltonian.

2. Hamiltonian formulation of the effective medium problem

To begin with, we show that in the electromagnetic case the effective medium problem can be formulated using a Hamiltonian formalism. The starting point is to note that the Maxwell's equations in a continuous medium can be written as,

$$\begin{pmatrix} 0 & i\nabla\times \\ -i\nabla\times & 0 \end{pmatrix}\mathbf{f} = i\frac{\partial \mathbf{g}}{\partial t}, \quad \text{with} \quad \mathbf{f} = \begin{pmatrix} \mathbf{e} \\ \mathbf{h} \end{pmatrix} \text{ and } \mathbf{g} = \begin{pmatrix} \mathbf{d} \\ \mathbf{b} \end{pmatrix} = \mathbf{M}\cdot\mathbf{f} = \begin{pmatrix} \varepsilon & 0 \\ 0 & \mu_0 \end{pmatrix}\cdot\mathbf{f}\,. \tag{1}$$

For standard isotropic non-dispersive magneto-dielectrics, the microscopic electric and magnetic fields, $\mathbf{e}$ and $\mathbf{h}$, are linked to the microscopic electric displacement and induction fields, $\mathbf{d}$ and $\mathbf{b}$, by the standard constitutive relations $\mathbf{g} = \mathbf{M}\cdot\mathbf{f}$ where the material matrix $\mathbf{M}$ is written in terms of the "microscopic" permittivity and permeability as shown in Eq. (1). Hence, the dynamics of the "microscopic" electromagnetic fields (i.e. before any form of averaging on the scale of the unit cell of the metamaterial) can be described by a Schrödinger type equation of the form $\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi$ where $\psi \leftrightarrow \mathbf{g}$ is a six-component vector, and the operator $\hat{H}$ is given by:

$$\hat{H} = \hbar\begin{pmatrix} 0 & i\nabla\times \\ -i\nabla\times & 0 \end{pmatrix}\cdot\mathbf{M}^{-1}. \tag{2}$$

Evidently, this Hamiltonian does not represent the energy of the system, but is simply an operator that describes the dynamics of the classical electromagnetic field. The time evolution of the system is completely determined by the initial state $\psi_{t=0} = \mathbf{g}_{t=0}$.

Let us consider now an electromagnetic metamaterial, for which $\mathbf{M} = \mathbf{M}(\mathbf{r})$ is a periodic function of space. The objective is to determine an effective Hamiltonian $\hat{H}_{ef}$ that describes the dynamics of the *envelope wavefunction* $\Psi \equiv \langle\psi\rangle$, where $\langle . \rangle$ represents a suitable spatial-averaging operator. In our case, Ψ can be identified with the macroscopic electromagnetic field. We say that a state is macroscopic if it remains invariant after spatial averaging: $\psi = \langle\psi\rangle$. We define the effective Hamiltonian in

ISBN 978-952-67611-2-1

such a manner that $\hat{H}_{ef}\Psi = \langle \hat{H}\psi \rangle$ for any $t > 0$ and for any ψ whose time evolution is determined by an initial time macroscopic state ($\psi_{t=0} = \langle \psi_{t=0} \rangle$). This is analogous to the formulation of Ref. [4], where the effective dielectric response is determined by the time evolution of initial-time field distributions that are macroscopic. A detailed analysis shows that in the electromagnetic case the effective Hamiltonian in the *spectral domain* is given by:

$$\hat{H}_{ef} = \hbar \begin{pmatrix} 0 & -\mathbf{k}\times \\ \mathbf{k}\times & 0 \end{pmatrix} \cdot \mathbf{M}_{ef}^{-1}(\omega, \mathbf{k}), \qquad \text{where} \quad \mathbf{M}_{ef}(\omega, \mathbf{k}) = \begin{pmatrix} \overline{\overline{\varepsilon}}_{ef} & 0 \\ 0 & \mu_0 \end{pmatrix}, \tag{3}$$

and $\overline{\overline{\varepsilon}}_{ef}(\omega, \mathbf{k})$ is defined precisely as in our previous works [3-4]. It can be proven that the photonic band structure of the metamaterial is *exactly* determined by $\hat{H}_{ef}$, and can be obtained by solving $\det\left(\hat{H}_{ef}(\omega, \mathbf{k}) - \hbar\omega\mathbf{I}\right) = 0$.

The remarkable point here is that these ideas can be readily extended to any periodic system whose dynamics is described by a Hamiltonian, particularly to the field of electronics where semiconductor and graphene superlattices may be regarded as the counterpart of electromagnetic metamaterials [8]. Superlattices were proposed by Esaki and Tsu more than forty years ago [9], who suggested that by either periodically doping a monocrystalline semiconductor or by varying the composition of the alloy, quantum mechanical effects may be observed in a new physical scale. Typically, the electronic structure of superlattices and related heterostructures is described using perturbation theory methods, such as the $k \cdot p$ method or Bastard's envelope function approximation.

At the conference, we will show that our effective medium approach (extended to electronics in the context of the one-body Schrödinger equation) provides an alternative way for describing the effective response of graphene and III-V and II-VI semiconductor superlattices, and enables establishing straightforward analogies with electromagnetic metamaterials. In particular, for the case of one-dimensional graphene superlattices, such that the electrostatic potential is a stepwise continuous periodic function (Kronig-Penney type model) [8], we will show that the low-energy physics in these structures can be characterized simply in terms of an energy dependent effective potential and an anisotropy tensor that characterizes the pseudospin. Based on this effective-medium model, we predict a novel perfect tunneling effect in graphene superlattices [8], showing that electron waves with a specific energy can be perfectly tunneled through a nanomaterial with specific properties, analogous to the perfect lens proposed for electromagnetic metamaterials [2], but based on entirely new physical principles.

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ISBN 978-952-67611-2-1