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Bloch Electrons in Constant Electric Field

F. Bentosela*

Department of Physics, Princeton University, Princeton, NJ 08540, USA

Abstract. The motion of a conduction electron of a crystal in a constant electric field is studied. It is shown that the modulus of the wave function in p-representation is well approximated by a periodic function for times smaller than several hundred periods.

The aim of this paper is to study the evolution of a wave packet describing a Bloch electron under the influence of a constant electric field, as a first step to understand from first principles, the electrical conductivity of crystals.

Contrarily, to the free case, in which the momentum average of the particle grows linearly in time as we can easily see from the expression: $e^{-i(p^2+e\mathscr{E}x_1)t} = e^{-ie^2\mathscr{E}^2t^3/3}e^{-ie\mathscr{E}x_1t}e^{ie\mathscr{E}pt^2}e^{-itp^2}$, we find that in the presence of a periodic potential, $V(x)$, the particle moves to a certain extent, periodically in the crystal.

More precisely, the probability the particle has a momentum in the infinitesimal volume $[\bar{p}, \bar{p}+d\bar{p}]$ is at times t, $t+T$, $t+2T$, almost the same, as $\psi_t(\mathbf{p})$ can be divided in three parts $\psi_t(\mathbf{p}) = \psi_t^{(1)}(\mathbf{p}) + \psi_t^{(2)}(\mathbf{p}) + \psi_t^{(3)}(\mathbf{p})$ and it exists $T = \left|\frac{2\pi}{a_1}\right| \hbar \frac{1}{e\mathscr{E}}$ such that:

$$|\psi_{nT}^{(1)}(\mathbf{p})| = |\psi_0^{(1)}(\mathbf{p})|, \quad n \in \mathbb{Z}^+, \tag{1}$$

$$\|\psi_t^{(2)}\| \leqq vt, \tag{2}$$

$$\|\psi_t^{(3)}\| \leqq \alpha. \tag{3}$$

α and v are such that $\alpha + vT$ is much smaller than 1. This result confirms the heuristic approach of the problem, given by the solid state physicists [1–3] when they suggest to replace the classical Newton law $\frac{d\mathbf{p}}{dt} = e\mathscr{E}$ by $\frac{d\mathbf{k}}{dt} = e\mathscr{E}$ where $\mathbf{k}$, the crystal momentum, is an element of a torus.

* On leave from Department of Physics, Luminy, Université d'Aix-Marseille II, and Centre de Physique Théorique, CNRS, Marseille, France

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