Comment on "Time evolution of Bloch electrons in a homogeneous electric field"

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A gauge transformation connecting two approaches to the problem of a Bloch electron in an electric field is discussed. It is shown that the criticism of the Houston functions in a recent paper by Krieger and Iafrate [Phys. Rev. B 33, 5494 (1986)] is unfounded.

In a recent Physical Review paper[1] Krieger and Iafrate claim to have presented "a new derivation" for the dynamics of a Bloch electron in a homogeneous electric field. In particular, the authors of Ref. 1 claim that their "new treatment avoids all the basic assumptions of the conventional derivations," e.g., they avoid the Houston method and, correspondingly, their work does not assume that "an expansion of periodic functions is a solution of a nonperiodic Hamiltonian."

In this Comment we show that it does not seem to be so easy to avoid the conventional assumptions in the classical problem of a Bloch electron in an electric field that has been around from the beginning of the quantum theory of solids.[2] It certainly cannot be done as easily as suggested in Ref. 1 by just changing the representation of the electric field from the usual scalar potential to a vector potential. As the authors of Ref. 1 have themselves pointed out this change of representation is achieved by the well-known elementary gauge transformation.[3,4] It would be very surprising if this transformation actually removed all the difficulties and objections in the monumental problem of the Bloch electron in an electric field. What we show in this Comment is that this is not so and that the claim of the authors of Ref. 1 that their new treatment avoids all the basic assumptions of the conventional derivations is not correct.

An important contribution to the understanding of the dynamics of the Bloch electron in the presence of an electric field was made by Houston by the introduction of Houston functions (for simplicity we treat a one-dimensional problem for a homogeneous and constant electric field E)

$$\psi_n^{(H)}(x,t)=\exp\left[-\frac{i}{\hbar}\int_0^t \varepsilon_n(k(t'))dt'\right]\phi_{n,k(t)}(x) \; . \tag{1}$$

Here $\phi_{nk}(x)$ is a Bloch function corresponding to the band with energy $\varepsilon_n(k)$ and $k(t)$ satisfies the acceleration theorem $\dot{k}(t)=eE$ (e is the electron charge). The Houston function (1) has the physical significance of being a solution in the single-band approximation of the time-dependent Schrödinger equation for a Bloch electron in an electric field

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{p^2}{2m}+V(x)-eEx\right] . \tag{2}$$

In Eq. (2), $V(x)$ is the periodic potential with period a, and the electric field is presented by the scalar potential $-eEx$. In Ref. 1 the authors prefer to work with functions $\phi_i'(x,t)$ which are connected with the Bloch functions $\phi_{n,k(t)}(x)$ by a gauge transformation

$$\phi_i'(x,t)=\exp\left[-\frac{i}{\hbar}eExt\right]\phi_{n,k(t)}(x) \; . \tag{3}$$

$\phi_i'(x,t)$ is a solution of the equation

$$\left[\frac{(p+eEt)^2}{2m}+V(x)\right]\phi_i'(x,t)=\varepsilon_n(k(t))\phi_i'(x,t) \; , \tag{4}$$

in which the electric field is represented by the vector potential $A(t)=-cEt$, and where $k(t)$ satisfies according to Ref. 1 the relation

$$-\frac{1}{\hbar}eEt+k=\frac{l}{N}G \; . \tag{5}$$

Here l is an integer not exceeding N, the number of unit cells in the crystal, and $G=2\pi/a$ (the constant of the reciprocal lattice). The reason the functions $\phi_i'(x,t)$ are preferred in Ref. 1 over the Houston functions (1) is because the Hamiltonian of Eq. (4) is translationally invariant (in the space coordinate). It is clear that this is not the case with the Hamiltonian of Eq. (2) which is not translationally invariant. From here the authors of Ref. 1 come to the conclusion that by expanding in $\phi_i'(x,t)$ one can avoid the difficulties one encounters by using an expansion in Houston functions as done in the classical work by Houston.[5,6] In particular, the authors of Ref. 1 claim that, unlike Houston's method, in their work they do not assume that "an expansion of periodic functions is a solution of a nonperiodic Hamiltonian." That this is actually done in the Houston theory is true, but the authors of Ref. 1 have not removed this difficulty. As we are going to prove shortly, the only thing the authors of Ref. 1 have managed to accomplish is to shift this difficulty from the space domain to the domain of time, but they have certainly not removed it. In order to see it let us first point out that in Eq. (5) k can be chosen without any loss of generality to be $k=(1/\hbar)eEt$ (the constant can be absorbed into the vector potential). With this in mind the functions (3) become

$$\phi_i'(x,t)=u_{n,k(t)}(x) \; , \tag{6}$$

where $u_{nk}(x)$ is the periodic part of the Bloch function $\phi_{nk}(x)$, $u_{nk}(x+a)=u_{nk}(x)$. From Eqs. (5) and (6) it follows that

$$\phi_i'(x,t+T)=\exp\left[-i\frac{2\pi}{a}x\right]\phi_i'(x,t)\ , \tag{7}$$

where $T=2\pi\hbar/eEa$ is the period of an oscillating Bloch electron in the single-band approximation. What this means is that the functions $\phi_i'(x,t)$ are periodic in t with the period T at all the lattice points $x=sa$, $s=0,\pm1,\pm2,\ldots$. In Ref. 1 it was claimed that the Houston functions are not suitable as an expansion basis because they are periodic on the boundaries while the Hamiltonian of Eq. (2) is not translationally invariant in space. But as we have just shown the functions $\phi_i'(x,t)$ that were used in Ref. 1 have exactly the same deficiency: they are periodic in t at all points of the lattice while the Hamiltonian (4) in the gauge of the vector potential is not translationally invariant in time. To claim therefore that the functions $\phi_i'(x,t)$ are preferable over the classical Houston functions as an expansion basis for the Bloch electron in an electric field is unfounded.

From what we have shown it follows that the Houston functions [Eq. (1)] and the functions used in Ref. 1 [Eq. (3)] are completely equivalent as expansion bases and that the latter remove no difficulties of the former. It is therefore not surprising that the authors of Ref. 1 have arrived at well-known results. What is unfortunate, however, is that having mistakingly assumed that their "new treatment" is correct the authors of Ref. 1 criticize a number of other papers on the subject.[7-12] Since it is shown in this Comment that the new treatment of Ref. 1 is incorrect and since the criticism is based on this incorrect treatment we find this criticism completely unfounded.

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