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LETTER TO THE EDITOR

Force-balance equations in a single-band subspace for electrons in a periodic potential

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Abstract. The previous failure to directly derive a momentum-balance equation for N electrons in a periodic potential stems from an excessive reliance on the validity of the commutation relation $[R^\alpha, P^\beta] = \mathrm{i}\delta_{\alpha\beta}$ $(\alpha, \beta = x, y, z)$ between the centre-of-mass position operator $\boldsymbol{R} = N^{-1}\sum_j \boldsymbol{r}_j$ and the total momentum operator $\boldsymbol{P} = \sum_j \boldsymbol{p}_j$ ($\boldsymbol{r}_j$ and $\boldsymbol{p}_j$ are the position and momentum of the jth electron). I point out that this commutation relation may no longer hold true if electrons are limited to moving within a single energy band. By evaluating the rate of change of the total momentum from the Heisenberg equation of motion and using the accurate commutation relation in the single-band subspace, we obtain the momentum-balance equation that I and my co-workers had given previously for a general energy band, without invoking the effective Hamiltonian. By considering the rate of change of the total lattice momentum we arrive at the modified Büttiker–Thomas force-balance equation having a reduction factor due to Bragg scattering.

The success of the balance-equation approach [1] in simplifying complex transport calculations, and the recent developments in superlattice miniband conduction [2–4], have stimulated quite a few investigations into developing an effective-force-balance equation capable of dealing with extremely nonparabolic systems. Several different schemes have been proposed [5–10]. Among them, there are essentially two different effective-force-balance equations which are able to give rise to bulk negative differential mobility of the Esaki–Tsu [11] type in superlattice vertical transport, i.e. the force-balance equation of Büttiker and Thomas [5] and the acceleration-balance equations that I and my co-workers proposed [2, 7]. It has been shown that these equations can be obtained as the moment equations from the Boltzmann transport equation [10], or as the rates of change of the velocity and momentum from the Heisenberg equation of motion with an effective Hamiltonian for Bloch electrons [7, 12]. Attempts to directly derive these equations without utilizing the effective Hamiltonian were, however, unsuccessful [6, 8, 13]. In this letter I point out that the reason for this failure stems from an excessive reliance on the validity of the commutation relations between the centre-of-mass position operator $\boldsymbol{R}$ and the total momentum operator $\boldsymbol{P}$: $[R^\alpha, P^\beta] = \mathrm{i}\delta_{\alpha\beta}(\alpha, \beta = x, y, z)$. This commutation relation certainly holds true in the full electron space, but may no longer be valid when electrons are limited to moving within a single energy band. By evaluating the rate of change of the total momentum from the Heisenberg equation of motion and using accurate commutation relations in the single-band subspace, we obtain the momentum-balance equation as given in [7], for a general energy band, without invoking the effective Hamiltonian. Considering

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the rate of change of the total crystal momentum we arrive at the modified Büttiker–Thomas (B–T) force-balance equation [5] having a reduction factor due to Bragg scattering.

We consider a system of N electrons moving in a periodic potential $U(\boldsymbol{r})$ subject to a uniform electric field $\boldsymbol{E}$ and impurity and phonon scatterings H_I. The Hamiltonian of this system is generally written as ($\hbar = 1 = k_B$) $H = H_e + H_E + H_I$. Here

$$H_e = \sum_j h_j \qquad h_j = \frac{p_j^2}{2m_e} + U(\boldsymbol{r}_j) \tag{1}$$

where $\boldsymbol{r}_j$ and $\boldsymbol{p}_j$ are the position and momentum of the jth electron and m_e is the free-electron mass, and

$$H_E = -Ne\boldsymbol{E}\cdot\boldsymbol{R} \tag{2}$$

is the electric field potential, with

$$\boldsymbol{R} = \frac{1}{N}\sum_j \boldsymbol{r}_j \tag{3}$$

being the centre-of-mass (CM) position operator. The total momentum of the system defined by

$$\boldsymbol{P} = \sum_j \boldsymbol{p}_j \tag{4}$$

has the following well-known commutation relation with $\boldsymbol{R}$:

$$[R^\alpha, P^\beta] = \mathrm{i}\delta_{\alpha\beta} \qquad (\alpha, \beta = x, y, z). \tag{5}$$

The complete set of the Bloch functions, $\{|n\boldsymbol{k}\rangle\}$ (n is the band index and $\boldsymbol{k}$ is the lattice vector), which are eigenfunctions of the single-particle Hamiltonian h, $h|n\boldsymbol{k}\rangle = \varepsilon_n(\boldsymbol{k})|n\boldsymbol{k}\rangle$, spans the whole space for electrons in the periodic potential. In the second-quantization representation of Bloch states the Hamiltonian H_e, the CM coordinate $\boldsymbol{R}$ and the total momentum $\boldsymbol{P}$ are expressed respectively as

$$H_e = \sum_{n,\boldsymbol{k},\sigma} \varepsilon_n(\boldsymbol{k}) c^\dagger_{n\boldsymbol{k}\sigma} c_{n\boldsymbol{k}\sigma} \tag{6}$$

$$\boldsymbol{R} = \frac{1}{N}\sum_{n,n',\boldsymbol{k},\boldsymbol{k}',\sigma} [\mathrm{i}\delta_{nn'}\,\boldsymbol{\nabla}\delta(\boldsymbol{k}-\boldsymbol{k}') + \boldsymbol{x}_{nn'}(\boldsymbol{k})\,\delta(\boldsymbol{k}-\boldsymbol{k}')] c^\dagger_{n\boldsymbol{k}\sigma} c_{n'\boldsymbol{k}'\sigma} \tag{7}$$

and

$$\boldsymbol{P} = \sum_{n,n',\boldsymbol{k},\sigma} [\boldsymbol{k}\delta_{nn'} + \boldsymbol{p}_{nn'}(\boldsymbol{k})] c^\dagger_{n\boldsymbol{k}\sigma} c_{n'\boldsymbol{k}\sigma}. \tag{8}$$

Here $c^\dagger_{n\boldsymbol{k}\sigma}$ and $c_{n'\boldsymbol{k}\sigma}$ are electron creation and annihilation operators corresponding to the Bloch state $|n\boldsymbol{k}\rangle$ and spin σ, and

$$\boldsymbol{p}_{nn'}(\boldsymbol{k}) = -\mathrm{i}\int u^*_n(\boldsymbol{k},\boldsymbol{r})\,\boldsymbol{\nabla}_{\boldsymbol{r}} u_{n'}(\boldsymbol{k},\boldsymbol{r})\,\mathrm{d}^3 r$$

and

$$\boldsymbol{x}_{nn'}(\boldsymbol{k}) = \mathrm{i}\int u^*_n(\boldsymbol{k},\boldsymbol{r})\,\boldsymbol{\nabla}_{\boldsymbol{k}} u_{n'}(\boldsymbol{k},\boldsymbol{r})\,\mathrm{d}^3 r$$

are integrals over the unit cell in conjunction with the cell function $u_n(\boldsymbol{k},\boldsymbol{r})$ associated with the Bloch state $|n\boldsymbol{k}\rangle$ [14].

In the presence of a slowly varying external electric field, i.e. when effects such as interband (Zener) tunnelling are negligible (e.g. in the case of superlattice miniband

transport), it is a good approximation to assume that electrons move entirely among the states of a single energy band [15]. Restricting electrons to the energy band of index n, having energy $\varepsilon_n(\boldsymbol{k}) = \varepsilon(\boldsymbol{k})$ (for brevity the band index n will be neglected hereafter), we are in fact dealing with a system which is described by the Hamiltonian $H^s = H_e^s + H_E^s + H_I^s$, rather than H. Here

$$H_e^s = \sum_{\boldsymbol{k},\sigma} \varepsilon(\boldsymbol{k}) c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma} \tag{9}$$

and

$$H_E^s = -Ne\boldsymbol{E} \cdot \boldsymbol{R}_s \tag{10}$$

where $\boldsymbol{R}_s$ stands for CM position of electrons moving in the single band:

$$\boldsymbol{R}_s = \frac{\mathrm{i}}{N} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} [\boldsymbol{\nabla}\delta(\boldsymbol{k} - \boldsymbol{k}')] c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}'\sigma} + \frac{1}{N} \sum_{\boldsymbol{k},\sigma} \boldsymbol{x}(\boldsymbol{k}) c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma}. \tag{11}$$

Meanwhile, when these electrons reside only in this single band, the total momentum is expressed as [16]

$$\boldsymbol{P}_s = \sum_{\boldsymbol{k},\sigma} \langle \boldsymbol{k}|\boldsymbol{p}|\boldsymbol{k}\rangle c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma} = m_e \sum_{\boldsymbol{k},\sigma} \boldsymbol{v}(\boldsymbol{k}) c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma} \tag{12}$$

where $\boldsymbol{v}(\boldsymbol{k}) \equiv \boldsymbol{\nabla}\varepsilon(\boldsymbol{k})$ is the velocity function. For the expression for H_I^s in the second-quantization representation please refer to [7]. Thus what we are dealing with is not the full space of the electrons in the periodic potential but a subspace of it, which we may call the single-band subspace. In the single-band subspace the commutation relations among physical quantities may be different from those in the full electron space. For instance, we have

$$[H_e^s, \boldsymbol{P}_s] = 0 \tag{13}$$

while in the full electron space $[H_e, \boldsymbol{P}] \neq 0$. Furthermore, in the single-band subspace the total momentum operator $\boldsymbol{P}_s$ and the CM position operator $\boldsymbol{R}_s$ do not obey a commutation relation like equation (5). In fact, it is easily verified from equations (11) and (12) that $\boldsymbol{R}_s$ and $\boldsymbol{P}_s$ obey the following commutation relation ($\alpha, \beta = x, y, z$):

$$\begin{aligned}
[R_s^\alpha, P_s^\beta] &= \frac{\mathrm{i}m_e}{N} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\sigma,\sigma_1} [\boldsymbol{\nabla}\delta(\boldsymbol{k} - \boldsymbol{k}')] v_\beta(\boldsymbol{q}) [c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}'\sigma}, c_{\boldsymbol{q}\sigma_1}^\dagger c_{\boldsymbol{q}\sigma_1}] \\
&= \frac{\mathrm{i}m_e}{N} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} [\boldsymbol{\nabla}\delta(\boldsymbol{k} - \boldsymbol{k}')][v_\beta(\boldsymbol{k}) - v_\beta(\boldsymbol{k}')] c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}'\sigma} \\
&= \frac{\mathrm{i}m_e}{N} \sum_{\boldsymbol{k},\sigma} \left(\frac{\partial^2 \varepsilon(\boldsymbol{k})}{\partial k_\alpha \, \partial k_\beta} \right) c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma} \equiv \mathrm{i}m_e \hat{\mathcal{K}}_{\alpha\beta}
\end{aligned} \tag{14}$$

where $\hat{\mathcal{K}}_{\alpha\beta}$ stands for the $\alpha\beta$-component of the tensor $\hat{\mathcal{K}}$. Equation (14) may be drastically different from commutation relation (5) unless the energy band discussed is parabolic.

Calculating the rate of change of the total momentum from the Heisenberg equation of motion

$$\mathrm{d}\boldsymbol{P}_s/\mathrm{d}t = \mathrm{i}[H_e^s, \boldsymbol{P}_s] + \mathrm{i}[H_E^s, \boldsymbol{P}_s] + \mathrm{i}[H_I^s, \boldsymbol{P}_s] \tag{15}$$

in which the first term on the right-hand side vanishes, the second term, according to (14), becomes

$$[H_E^s, \boldsymbol{P}_s] = -\mathrm{i}m_e Ne\boldsymbol{E} \cdot \hat{\mathcal{K}} \tag{16}$$

and the third term is the frictional force

$$\hat{\boldsymbol{F}} \equiv \mathrm{i}[H_I^s, \boldsymbol{P}_s] \tag{17}$$

we have

$$\mathrm{d}\boldsymbol{P}_s/\mathrm{d}t = m_e N e \boldsymbol{E} \cdot \hat{\mathcal{K}} + \hat{\boldsymbol{F}}. \tag{18}$$

Or, by defining $\hat{\boldsymbol{v}}_d \equiv \boldsymbol{P}_s/Nm_e$ and $\hat{\boldsymbol{A}} \equiv \hat{\boldsymbol{F}}/Nm_e$, we can write

$$\mathrm{d}\hat{\boldsymbol{v}}_d/\mathrm{d}t = e\boldsymbol{E} \cdot \hat{\mathcal{K}} + \hat{\boldsymbol{A}}. \tag{19}$$

This is exactly the operator equation for acceleration balance derived in [7] with the help of the effective Hamiltonian for electrons in a single band. Taking the statistical average of equation (19) with respect to an appropriate density matrix $\boldsymbol{\rho}_0$ which is diagonal in the lattice wavevector, we obtain the acceleration-balance equation as given in [7]. The present derivation indicates that this equation is just the balance equation for the total momentum of the system.

On the other hand, in the single-band subspace we may define the total lattice momentum operator of electrons as

$$\hat{\boldsymbol{P}}_\ell = \sum_{\boldsymbol{k},\sigma} \boldsymbol{p}(\boldsymbol{k})\, c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} \tag{20}$$

where the function $\boldsymbol{p}(\boldsymbol{k})$ represents the 'lattice momentum' of an electron in the $\boldsymbol{k}$-state: $\boldsymbol{p}(\boldsymbol{k}) = \boldsymbol{k}$ if $\boldsymbol{k}$ is located in the interior of the Brillouin zone (BZ), and it is a periodic function if $\boldsymbol{k}$ is allowed to go beyond the BZ in the periodic zone scheme: $\boldsymbol{p}(\boldsymbol{k}) = \boldsymbol{p}(\boldsymbol{k} + \boldsymbol{G})$. In equation (20) the summation runs over all of the electron states in the single band, i.e. $\boldsymbol{k}$ should cover a semiclosed BZ: the whole interior of the zone and a half of the zone boundary. We have the commutation relation

$$\begin{aligned}[\boldsymbol{R}_s, \boldsymbol{P}_\ell] &= \frac{\mathrm{i}}{N} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\sigma,\sigma_1} [\boldsymbol{\nabla}\delta(\boldsymbol{k} - \boldsymbol{k}')]\boldsymbol{p}(\boldsymbol{q})[c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}'\sigma}, c^\dagger_{\boldsymbol{q}\sigma_1} c_{\boldsymbol{q}\sigma_1}] \\ &= \frac{\mathrm{i}}{N} \sum_{\boldsymbol{k},\sigma} [\boldsymbol{\nabla}\boldsymbol{p}(\boldsymbol{k})] c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} \equiv \mathrm{i}\hat{\mathcal{R}}. \end{aligned} \tag{21}$$

Here the tensor operator $\hat{\mathcal{R}}$ is given by

$$\hat{\mathcal{R}} = \mathcal{I} - \frac{1}{4\pi^3 n} \oint_{S_{\mathrm{BZ}}} \mathrm{d}\boldsymbol{s}\ \boldsymbol{k}\, c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}. \tag{22}$$

The first term (the unit tensor) on the right-hand side of equation (22) comes from the sum over the interior of the BZ where $\boldsymbol{p}(\boldsymbol{k}) = \boldsymbol{k}$ such that $\boldsymbol{\nabla}\boldsymbol{p}(\boldsymbol{k}) = \mathcal{I}$. The second term with a closed-area integral over the BZ boundary results from the jump of the $\boldsymbol{p}(\boldsymbol{k})$-function at the BZ boundary [12]. Here n is the electron density.

Calculating the rate of change of the total lattice momentum from the Heisenberg equation of motion

$$\mathrm{d}\boldsymbol{P}_\ell/\mathrm{d}t = \mathrm{i}[H_e^s, \boldsymbol{P}_\ell] + \mathrm{i}[H_E^s, \boldsymbol{P}_\ell] + \mathrm{i}[H_I^s, \boldsymbol{P}_\ell] \tag{23}$$

where the first term on the right-hand side vanishes,

$$[H_e^s, \boldsymbol{P}_\ell] = 0 \tag{24}$$

and the second term yields

$$[H_E^s, \boldsymbol{P}_\ell] = -\mathrm{i}Ne\boldsymbol{E} \cdot \hat{\mathcal{R}} \tag{25}$$

while the third term is denoted as the frictional force related to the lattice momentum

$$\hat{\boldsymbol{F}}^{\ell} \equiv \mathrm{i}[H_I^s, \boldsymbol{P}_\ell] \tag{26}$$

we have

$$\frac{\mathrm{d}\boldsymbol{P}_\ell}{\mathrm{d}t} = Ne\boldsymbol{E}\cdot\hat{\mathcal{R}} + \hat{\boldsymbol{F}}^{\ell} \tag{27}$$

or

$$\frac{\mathrm{d}\hat{\boldsymbol{p}}_\ell}{\mathrm{d}t} = e\boldsymbol{E}\cdot\hat{\mathcal{R}} + \hat{\boldsymbol{f}}^{\ell} \tag{28}$$

where $\hat{\boldsymbol{p}}_\ell \equiv \boldsymbol{P}_\ell/N$ is the lattice momentum per particle, and $\hat{\boldsymbol{f}}^{\ell} \equiv \hat{\boldsymbol{F}}^{\ell}/N$ is the lattice-momentum-related frictional force per particle. Taking the statistical average of equation (28) with respect to an appropriate density matrix, we arrive at

$$\frac{\mathrm{d}\boldsymbol{p}_d}{\mathrm{d}t} = e\boldsymbol{E}\cdot\mathcal{R} + \boldsymbol{f}^{\ell} \tag{29}$$

where $\boldsymbol{p}_d = \langle\hat{\boldsymbol{p}}_\ell\rangle$, $\mathcal{R} = \langle\hat{\mathcal{R}}\rangle$, and $\boldsymbol{f}^{\ell} = \langle\hat{\boldsymbol{f}}^{\ell}\rangle$. This is the force-balance equation first given by Büttiker and Thomas [5] with a reduction factor $\mathcal{R}$. The present derivation clarifies the fact that the 'momentum' $\boldsymbol{p}_d$, appearing in the Büttiker–Thomas equation, is the average lattice momentum (per particle) rather than the average (physical) momentum (per particle) discussed in equation (12):

$$\boldsymbol{p}_s = m_e\boldsymbol{v}_d. \tag{30}$$

Here $\boldsymbol{p}_s = \langle\boldsymbol{P}_s/N\rangle$ and $\boldsymbol{v}_d = \langle\hat{\boldsymbol{v}}_d\rangle$. No matter what density matrix is used for the statistical average, equation (30) cannot be a valid relation between the average lattice momentum and the average drift velocity, unless the energy band is parabolic. The previous *ansatz* used in [5], $\boldsymbol{p}_d = m_e\boldsymbol{v}_d$, should be abandoned. Furthermore, equation (26) enables us to obtain a generally valid expression for the lattice-momentum-related frictional force [12], allowing more accurate analysis of transport than the constant-relaxation-time approximation previously adopted [5].

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