Investigation of the Buttiker-Thomas momentum balance equation from the Heisenberg equation of motion for Bloch electrons

1995 J. Phys.: Condens. Matter 7 L429

(http://iopscience.iop.org/0953-8984/7/32/002)

J. Phys.: Condens. Matter 7 (1995) L429–L434. Printed in the UK

LETTER TO THE EDITOR

Investigation of the Büttiker–Thomas momentum balance equation from the Heisenberg equation of motion for Bloch electrons

X L Lei

China Centre of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China
Shanghai Institute of Metallurgy, Chinese Academy of Sciences, 865 Changning Road, Shanghai 200050, People's Republic of China

Received 14 June 1995, in final form 3 July 1995

Abstract. Using an appropriate momentum function for Bloch electrons moving in a single energy band, we are able to obtain the effective force balance equation with the Büttiker–Thomas reduction factor by calculating the rate of change of the total momentum from the Heisenberg equation of motion.

For a system consisting of N electrons subject to a uniform electric field $\boldsymbol{E}$ and subject to impurity and phonon scatterings, the universal momentum theorem, i.e. the rate of change of the total momentum of a system equals the total force exerted on it, is usually expressed as

$$\mathrm{d}\boldsymbol{P}/\mathrm{d}t = Ne\boldsymbol{E} + \boldsymbol{F}_{\mathrm{sc}} \tag{1}$$

where $\boldsymbol{P}$ is the total momentum, e is the electron charge and $\boldsymbol{F}_{\mathrm{sc}}$ stands for the total force due to impurity and phonon scatterings. Such an expression of the momentum theorem, however, may not be valid when these electrons are moving in a crystal or in a superlattice, where the existence of the periodic potential results in additional momentum change that can not be fully included by modifying $\boldsymbol{F}_{\mathrm{sc}}$ only. Büttiker and Thomas (BT) [1, 2] pointed out that the Bragg momentum loss at the Brillouin zone boundary reduces the effect of the field acceleration, leading to a reduction factor of $Ne\boldsymbol{E}$. From the viewpoint of the Boltzmann equation, this reduction factor stems from the nonzero surface integral in the momentum equation for an energy band of finite width [3]. In this letter we show that the BT reduction factor and the necessary modification of $\boldsymbol{F}_{\mathrm{sc}}$ for a general energy band can be derived from the Heisenberg equation of motion with an effective Hamiltonian for Bloch electrons, when the appropriate momentum function is used in the calculation of the momentum change.

We consider an interacting electron system which consists of N electrons moving within a single energy band under the influence of a uniform electric field $\boldsymbol{E}$ and being scattered by phonons and by randomly distributed impurities. The Hamiltonian of the system can be written in the form ($\hbar = 1 = k_{\mathrm{B}}$)

$$H = H_e + H_E + H_{et} + H_{ep}. \tag{2}$$

Here

$$H_E = -e\boldsymbol{E} \cdot \sum_j \boldsymbol{r}_j \tag{3}$$

0953-8984/95/320429+06$19.50

is the electric potential of the uniform field, in which r_j represents the spatial position of the jth electron and e the electron charge. H_{ei} and H_{ep} are, respectively, electron–impurity and electron–phonon interactions,

$$H_{ei} = \sum_{q,a} u(q) e^{iq \cdot R_a} \rho_q \tag{4}$$

$$H_{ep} = \sum_{q,\lambda} M(q, \lambda) \phi_q \rho_q \tag{5}$$

where R_a stands for the impurity position, $u(q)$ and $M(q, \lambda)$ are the Fourier representations of the impurity potential and electron–phonon coupling matrix element, $\phi_q = b_{q\lambda} + b^{\dagger}_{-q\lambda}$ is the phonon field operator, and

$$\rho_q = \sum_j e^{iq \cdot r_j} \tag{6}$$

is the Fourier representation of the electron density operator. The electron Hamiltonian H_e is composed of a single-particle part plus the electron–electron Coulomb interaction:

$$H_e = H_0 + H_{ee} \tag{7}$$

where

$$H_{ee} = \sum_{i \neq j} v_c(r_i - r_j) = \frac{1}{2V} \sum_q v_c(q) \rho_q \rho_{-q} \tag{8}$$

($v_c(r_i - r_j) = e^2/[8\pi\epsilon_0(r_i - r_j)]$, $v_c(q) = e^2/(\epsilon_0 q^2)$, and V is the volume of the system), and $H_0 = \sum_j h_j$,

$$h_j = -\frac{\nabla_j^2}{2m_e} + V(r_j) \tag{9}$$

being the single-particle Hamiltonian for an electron with mass m_e in the presence of the lattice periodic potential $V(r)$. Restricting our discussion to electrons in a *single* energy band, we can describe the electron state by a lattice wave vector k within the Brillouin zone (BZ) (together with a spin index σ), with eigen-wave function $\psi_{k\sigma}(r)$ and eigenenergy $\varepsilon(k)$:

$$h\psi_{k\sigma}(r) = \varepsilon(k)\psi_{k\sigma}(r). \tag{10}$$

It is convenient to use a periodic zone scheme, i.e. to allow lattice vector k to extend beyond the BZ such that k has a continuous spectrum covering the entire three-dimensional space but with the convention that, for any reciprocal lattice vector G, k and $k+G$ represent the same electron state. A physical quantity, which must be a function of the electron state, is a periodic function of k in the periodic zone scheme. It is now well established [4] that, with the energy function extended this way, $\varepsilon(k) = \varepsilon(k + G)$, when limiting electron motion within this single band one can use the following operator function:

$$\varepsilon(-i\nabla_j) \equiv \varepsilon(\hat{k}_j) \tag{11}$$

as an effective Hamiltonian to replace h_j of equation (9). Here $\hat{k}_j = -i\nabla_j$ is *the lattice momentum operator* of the jth electron. In the periodic zone scheme, $\psi_{k\sigma}(r)$ can be treated as the eigenstate of operator $\hat{k}$ with eigenvalue k. We have the commutation relation ($\alpha, \beta = x, y, z$)

$$[r_{i\alpha}, \hat{k}_{j\beta}] = i\delta_{\alpha\beta}\delta_{ij} \tag{12}$$

between this lattice momentum operator and the spatial coordinate of the electron.

Let $p(k)$ be the momentum of an electron in the state k. $p(k)$ is a function of state. Therefore it must be a periodic function of k in the periodic zone scheme:

$$p(k) = p(k + G). \tag{13}$$

Inside the BZ, we should have

$$p(k) = k. \tag{14}$$

The momentum function $p(k)$ is thus uniquely determined by these two relations. Unlike the velocity function

$$v(k) \equiv \nabla\varepsilon(k) \tag{15}$$

which is a periodic and continuous function of k (because the energy function $\varepsilon(k)$ is a periodic and continuous function), the momentum function $p(k)$ is not a continuous function in the periodic zone scheme but has a jump of a reciprocal lattice momentum at the BZ boundary. The physical meaning of this discontinuity is the Bragg scattering: an electron reaching (due to some kind of driving force or scattering) the BZ boundary from inside will suffer a momentum loss equal to a reciprocal lattice momentum. This discontinuity of the $p(k)$ function at the BZ boundary gives rise to an additional term in the momentum equation, as shown in the following.

The operator of the total momentum of the electron system is

$$\hat{P} = \sum_j p(\hat{k}_j) = \sum_{k\in\mathrm{BZ},\sigma} p(k)\, c^\dagger_{k\sigma} c_{k\sigma}. \tag{16}$$

Here $c^\dagger_{k\sigma}$ and $c_{k\sigma}$ stand for the creation and annihilation operators of the single-electron state $\psi_{k\sigma}$ and the sum on the right-hand side of equation (16) runs over the entire electron states in a single band, i.e. $k \in$ BZ should cover a semiclosed BZ: the whole interior of the zone and half of the zone boundary. The rate of change of the total momentum is given by the Heisenberg equation of motion for the operator $\hat{P}$

$$\frac{\mathrm{d}\hat{P}}{\mathrm{d}t} = -\mathrm{i}[\hat{P}, H] = -\mathrm{i}[\hat{P}, H_0 + H_{ee} + H_E + H_{ei} + H_{ep}]. \tag{17}$$

It is easily seen that $[\hat{P}, H_0] = 0$ and

$$\begin{aligned}[\hat{P}, H_{ee}] &= \sum_{l,i\neq j}[p(\hat{k}_l), v_c(r_i - r_j)] = \sum_{i\neq j}[p(\hat{k}_i) + p(\hat{k}_j), v_c(r_i - r_j)] \\ &= \sum_{i\neq j}\left[p\left(-\mathrm{i}\frac{\partial}{\partial(r_i - r_j)}\right) + p\left(\mathrm{i}\frac{\partial}{\partial(r_i - r_j)}\right), v_c(r_i - r_j)\right] = 0.\end{aligned} \tag{18}$$

In writing the last equality we have made use of the fact that for $i \neq j$

$$\hat{k}_i = -\mathrm{i}\frac{\partial}{\partial r_i} = -\mathrm{i}\frac{\partial}{\partial(r_i - r_j)} \qquad \hat{k}_j = -\mathrm{i}\frac{\partial}{\partial r_j} = \mathrm{i}\frac{\partial}{\partial(r_i - r_j)} \tag{19}$$

and the momentum function $p(k)$ satisfies

$$p(k) = -p(-k). \tag{20}$$

The calculation of the third term on the right-hand side of equation (17) yields

$$-\mathrm{i}[\hat{P}, H_E] = -\mathrm{i}eE \cdot \sum_{i,j}[r_i, p(\hat{k}_j)] = eE \cdot \sum_j \nabla p(\hat{k}_j) = eE \cdot \sum_{k\in\mathrm{BZ},\sigma} \nabla p(k)\, c^\dagger_{k\sigma} c_{k\sigma}. \tag{21}$$

In the interior of the BZ, $p(k) = k$ such that $\nabla p(k) = \mathcal{I}$ (unit tensor), leading to a contribution

$$eE \cdot \mathcal{I} \sum_{k\in \mathrm{BZ},\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} = NeE \tag{22}$$

where

$$N = \sum_{k\in \mathrm{BZ},\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} \tag{23}$$

is the total number of electrons in the volume V. In addition to the contribution of equation (22), because of the jump in the $p(k)$ function, $\nabla p(k)$ yields a term with a δ-function, $-\hat{n}G\,\delta(k_n - k_{bn})$, around the BZ boundary position k_b, where $\hat{n}$ stands for the unit vector of the normal direction of the boundary surface around k_b, $k_n = k \cdot \hat{n}$ and $k_{bn} = k_b \cdot \hat{n}$, and G is the reciprocal lattice vector connecting the boundary position k_b and the position k'_b on the opposite side of the BZ boundary: $G = k_b - k'_b$. In the vicinity of the half of the BZ boundary that contributes, one can write the k-summation in the form of a volume integral

$$\begin{aligned} -\frac{V}{4\pi^3}\, eE \cdot \int_{S/2} \mathrm{d}s \int \mathrm{d}k_n\, \hat{n}G\,\delta(k_n - k_{bn}) c^{\dagger}_{k\sigma}\, c_{k\sigma} \\ = -\frac{V}{4\pi^3}\, eE \cdot \int_{S/2} \mathrm{d}s\, G\, c^{\dagger}_{k\sigma} c_{k\sigma} = -\frac{V}{4\pi^3}\, eE \cdot \int_{S/2} (\mathrm{d}s\, k_b + \mathrm{d}s'\, k'_b)\, c^{\dagger}_{k\sigma} c_{k\sigma} \\ = -\frac{V}{4\pi^3}\, eE \cdot \oint_{S_{\mathrm{BZ}}} \mathrm{d}s\, k_b\, c^{\dagger}_{k\sigma} c_{k\sigma}. \end{aligned} \tag{24}$$

Here $S/2$ stands for the contributing half of the BZ boundary area S_{BZ}, $\mathrm{d}s = n\,\mathrm{d}s$, and $\mathrm{d}s' = -\mathrm{d}s$ is the vector area element at k'_b on the opposite side of the BZ boundary.

Putting contributions of equations (22) and (24) together we obtain

$$-\mathrm{i}[\hat{P}, H_E] = NeE \cdot \hat{\mathcal{R}} \tag{25}$$

where the tensor operator is given by

$$\hat{\mathcal{R}} = \mathcal{I} - \frac{1}{4\pi^3 n} \oint_{S_{\mathrm{BZ}}} \mathrm{d}s\, k\, c^{\dagger}_{k\sigma} c_{k\sigma} \tag{26}$$

and $n = N/V$ is the electron number density.

The last two terms of the right-hand side of equation (17) are resistive forces due to impurity and phonon scatterings respectively,

$$-\mathrm{i}[\hat{P}, H_{ei}] = \hat{F}_i = -\mathrm{i} \sum_{k\in \mathrm{BZ},q,a} u(q) \mathrm{e}^{\mathrm{i}q\cdot R_a} [p(k+q) - (k)]\, \rho_{kq} \tag{27}$$

$$-\mathrm{i}[\hat{P}, H_{ep}] = \hat{F}_p = -\mathrm{i} \sum_{k\in \mathrm{BZ},q,\lambda} M(q,\lambda) \phi_{q\lambda} [p(k+q) - p(k)]\, \rho_{kq}. \tag{28}$$

Here

$$\rho_{kq} = \sum_{\sigma} g(k,q)\, c^{\dagger}_{k+q\sigma} c_{k\sigma} \tag{29}$$

and $g(k,q)$ is a form factor related to the wave function of the Bloch electron [5, 6].

Collecting the above results we obtain the operator equation for the rate of change of the total momentum

$$\frac{\mathrm{d}\hat{P}}{\mathrm{d}t} = NeE \cdot \hat{\mathcal{R}} + \hat{F}_i + \hat{F}_p. \tag{30}$$

Employing the density matrix in the nonparabolic method [5, 6] to carry out the statistical average over the above equation, we obtain the momentum balance equation for a general energy band:

$$\frac{\mathrm{d}p_d}{\mathrm{d}t} = eE \cdot \mathcal{R} + f \tag{31}$$

where p_d is the average electron momentum per carrier, $\mathcal{R}$ is a reduction factor associated with Bragg scattering

$$\mathcal{R} = \mathcal{I} - \frac{1}{4\pi^3 n} \oint_{S_{\mathrm{BZ}}} \mathrm{d}s\, k f(k). \tag{32}$$

The momentum balance equation having a reduction factor due to Bragg scattering was first given by Büttiker and Thomas [1]. The original BT equation takes a constant-relaxation-time *ansatz* for the force: $f = -\gamma_p p_d$. The present investigation yields the average frictional force due to impurity and phonon scatterings of the form

$$\begin{aligned} f = {} & \frac{n_i}{4\pi^2 n} \int_{\mathrm{BZ}} \mathrm{d}^3k \sum_q |u(q)|^2 |g(k,q)|^2 [p(k+q) - p(k)] \\ & \times \delta(\varepsilon(k+q) - \varepsilon(k))[f(k) - f(k+q)] \\ & + \frac{1}{2\pi^2 n} \int_{\mathrm{BZ}} \mathrm{d}^3k \sum_{q,\lambda} |M(q,\lambda)|^2 |g(k,q)|^2 \\ & \times [p(k+q) - p(k)]\delta(\varepsilon(k+q) - \varepsilon(k) + \Omega_{q\lambda}) \\ & \times \{n(\Omega_{q\lambda}/T)[f(k) - f(k+q)] - f(k)[1 - f(k+q)]\}. \end{aligned} \tag{33}$$

In the above equation

$$n = \frac{1}{4\pi^3} \int_{\mathrm{BZ}} \mathrm{d}^3k\, f(k) \tag{34}$$

is the electron density, and

$$f(k) = 1/\exp[(\varepsilon(k - p_d) - \mu)/T_e] + 1 \tag{35}$$

is an effective distribution function in the initial state [5, 6], including the average momentum per carrier p_d, the electron temperature T_e, and the chemical potential μ as parameters. The identification of p_d as the average momentum per carrier is justified by the identity

$$p_d \equiv \frac{1}{4\pi^3 n} \int_{\mathrm{BZ}} \mathrm{d}^3k\, k f(k). \tag{36}$$

Equation (31), which states the momentum theorem in a general energy band, is probably useful in its own right. Nevertheless, often it is ultimately the average velocity (or current) that is of more practical interest. In [1, 2] the carrier average velocity v_d is assumed to be proportional to the average momentum:

$$v_d = p_d/m \tag{37}$$

m being a constant. This relation, however, can not be justified for a nonparabolic system. A physically acceptable identification of the average carrier velocity for a general energy band should be

$$v_d \equiv \frac{1}{4\pi^3 n} \int_{\mathrm{BZ}} \mathrm{d}^3k\, v(k) f(k) \tag{38}$$

where $v(k)$ is the velocity function given by equation (15). For a tight-binding-type band in the z-direction (e.g. a superlattice miniband), $\varepsilon(k_z) = (\Delta/2)(1 - \cos k_z d)$, equation (38)

gives rise to a z-component of the average drift velocity v_d which is related to the z-direction average momentum p_d by $v_d \propto \sin(p_d d)$. Although this result depends on the specific form of the energy spectrum and the distribution function (35) used for the initial state, the carrier average velocity derived from equation (38) is always drastically different from equation (37) for a strongly nonparabolic system. Apparently, for an accurate analysis one should give up assumption (37) in a general energy band.

On the other hand, an acceleration balance equation can be derived if we directly calculate the rate of change of the average carrier velocity from the Heisenberg equation of motion [5]. The equation thus obtained describes the acceleration balance of a mass variable particle and is not formally identical to (31) and (34) in general [5]. However, since both sets of effective momentum balance equations include the full effects of the Bragg scattering and the frictional forces or accelerations due to scatterings, they are expected to yield quantitatively similar results if the average momentum and average velocity are calculated properly. This problem is under further investigation and the detailed results will be presented in a later publication.

The author thanks the National Natural Science Foundation of China and the National and Shanghai Municipal Commissions of Science and Technology of China for support of this work.

References

[1] Büttiker M and Thomas H 1977 *Phys. Rev. Lett.* **38** 78
[2] Büttiker M and Thomas H 1979 *Z. Phys.* B **33** 275; **34** 301
[3] Lei X L 1994 *J. Phys.: Condens. Matter* **6** 9189
[4] Anderson P W 1963 *Concepts in Solids* (New York: Benjamin) section 2c
[5] Lei X L 1992 *Phys. Status Solidi* b **170** 519
[6] Lei X L, Horing N J M and Cui H L 1991 *Phys. Rev. Lett.* **66** 3277