Onsager Relations and Hydrodynamic Balance Equations in 2D Quantum Wells

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Abstract

In this letter we clarify the role of heat flux in the hydrodynamic balance equations in 2D quantum wells, facilitating the formulation of an Onsager relation within the framework of this theory. We find that the Onsager relation is satisfied within the framework of the 2D hydrodynamic balance equation transport theory at sufficiently high density. The condition of high density is consonant with the requirement of strong electron-electron interactions for the validity of our balance equation formulation.

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The Lei-Ting balance equation transport theory \[1,2\] has achieved much success in hot-electron transport of homogeneous semiconductors. This theory was subsequently generalized to deal with weakly nonuniform, inhomogeneous systems \[3\]. The resulting hydrodynamic balance equations consist of continuity equation, momentum balance equation, and energy balance equation. A salient feature of this hydrodynamic approach is that it includes a microscopic description of scattering in the form of a frictional force function due to electron-impurity and electron-phonon scattering, as well as an electron energy loss rate function due to electron-phonon interaction. These hydrodynamic balance equations have recently been applied to device simulations \[4–6\] and they have been further developed to include phonon-drag effects \[7\] and applied to discussion of thermoelectric power under both linear \[7\] and nonlinear \[8\] transport conditions.

Until recently, the important issue concerning the capability of this theory to lead to the correct form of Onsager relations \[9\] and/or how to determine Onsager relations within the framework of this theory has not been addressed. There is even some misunderstanding that the energy flux predicted by this theory is zero. It is well known that the Onsager relation is a manifestation of microscopic irreversibility for any statistical system near thermal equilibrium. Therefore any properly formulated statistical physics model should satisfy this relation. It is very easy to verify this relation in the framework of Kubo linear response theory. Moreover, if one can determine the distribution function from the Boltzmann equation, it is also straightforward to verify the Onsager relation by calculating the pertinent moments of the distribution function. However, for the traditional hydrodynamic model, \[10–21\] which is derived from Boltzmann equation, verification has been elusive. In fact, in a very recent article \[22\], it has been argued that the Onsager relation breaks down in this model.

Recently we \[23\] clarified the role of heat flux in this theory, and, by introducing the fourth balance equation, \textit{i.e.}, energy flux balance equation, we were able to show how to generate Onsager relations within the framework of this theory. Moreover, we closely checked the Onsager relation predicted by this theory for bulk semiconductors and found, that for
any temperature, when electron density is sufficiently high, the balance equation theory satisfies Onsager relations exactly. To our knowledge, this is the first set of hydrodynamic equations which has been shown to obey Onsager relation exactly.

The purpose of the present letter is to clarify the role of heat flux in hydrodynamic balance equations in quantum wells (and other 2D systems), facilitating the formulation of an Onsager relation within the framework of this theory, and to verify the validity of this theory in regard to the Onsager relation.

Following the procedure set forth in Ref. [23], the hydrodynamic balance equations which describe a weakly inhomogeneous electron system under the influence of an electron $E$ and a small lattice temperature gradient $\nabla T$ in two dimensional (2D) quantum wells can be written as

$$\frac{\partial n}{\partial t} + \nabla \cdot (nv) = 0 \tag{1},$$

$$\frac{\partial}{\partial t} \langle J \rangle + \nabla \cdot (\langle J \rangle v) = -\frac{1}{m} \nabla u + \frac{f}{m} \tag{2},$$

$$\frac{\partial u}{\partial t} + \nabla \cdot \langle J_H \rangle = v \cdot \nabla u + \frac{1}{2} mv^2 \nabla \cdot (nv) + \frac{1}{2} mnv \cdot \nabla v^2 - w - v \cdot f \tag{3},$$

which describe continuity, momentum balance and energy balance respectively. In these equations, the carrier drift velocity $v$, the electron temperature $T_e$, the average relative electron energy $u$, the carrier density $n$ and the chemical potential $\mu$, together with the particle flux $\langle J \rangle$ and energy flux $\langle J_H \rangle$ are all field quantities weakly dependent on the spatial coordinate, such that their spatial gradients are small and therefore are retained only to first order in Eqs. (1-3). The energy flux $\langle J_H \rangle$ appearing in Eq. (3) is just the energy flux predicted by hydrodynamic balance equation theory. It relation to the other field quantities in 2D case can be derived following Ref. [23] and be written as

$$\langle J_H(R) \rangle = 2u(R)v(R) + \frac{1}{2} mnv^2(R)vv(R). \tag{4}$$

Substituting this relation, together with the relation of density flux

$$\langle J(R) \rangle = n(R)v(R), \tag{5}$$
into Eqs. (2) and (3), one arrives at the original hydrodynamic balance equations [24].

In order to obtain the Onsager relation in the framework of balance equation theory, we need first derive the energy-flux balance equation [3]. This in the case of 2D electrons in quantum wells, is given as

$$
\frac{\partial}{\partial t} \langle J_{H} \rangle + \nabla \cdot \langle A \rangle = \langle B \rangle + \frac{2}{m} e u E + e n E \cdot v v + \frac{1}{2} e n v^2 E + \frac{1}{2} v^2 f - w v .
$$

(6)

The expression of $\langle B \rangle$ is composed of two parts. One is due to collisions with impurities ($\langle B_i \rangle$), and the other is due to interaction with phonons ($\langle B_{ph} \rangle$). They are given by

$$
\langle B_i \rangle = 2 \pi n_i \sum_{kq} |u(q)|^2 |F(q, z_0)|^2 (\varepsilon_{k+q} - \varepsilon_k) \frac{k + q/2}{m} \delta(\varepsilon_{k+q} - \varepsilon_k + q \cdot v) 
\times \left[ f\left( \frac{\varepsilon_k - \mu}{T_e} \right) - f\left( \frac{\varepsilon_{k+q} - \mu}{T_e} \right) \right] 
+ 2 \pi n_i \sum_{kq} |u(q)|^2 |F(q, z_0)|^2 (q \cdot v \frac{k + q}{m} + k \cdot v) \frac{q}{m} \delta(\varepsilon_{k+q} - \varepsilon_k + q \cdot v) 
\times \left[ f\left( \frac{\varepsilon_k - \mu}{T_e} \right) - f\left( \frac{\varepsilon_{k+q} - \mu}{T_e} \right) \right] 
+ \pi n_i \sum_{kq} |u(q)|^2 |F(q, z_0)|^2 (\varepsilon_{k+q} + \varepsilon_k) \frac{q}{m} \delta(\varepsilon_{k+q} - \varepsilon_k + q \cdot v) 
\times \left[ f\left( \frac{\varepsilon_k - \mu}{T_e} \right) - f\left( \frac{\varepsilon_{k+q} - \mu}{T_e} \right) \right],
$$

(7)

and

$$
\langle B_{ph} \rangle = -4 \pi \sum_{kQ} |M(Q, \lambda)|^2 |I(iq_z)|^2 (\varepsilon_{k+q} - \varepsilon_k) \frac{k + q/2}{m} \delta(\varepsilon_{k+q} - \varepsilon_k + \Omega Q \lambda - q \cdot v) 
\times \left[ f\left( \frac{\varepsilon_k - \mu}{T_e} \right) - f\left( \frac{\varepsilon_{k+q} - \mu}{T_e} \right) \right] 
\times \left[ n\left( \Omega Q \lambda / T \right) - n\left( \Omega Q \lambda - q \cdot v / T \right) \right] 
- 4 \pi \sum_{kQ} |M(Q, \lambda)|^2 |I(iq_z)|^2 (q \cdot v \frac{k + q}{m} + k \cdot v) \frac{q}{m} \delta(\varepsilon_{k+q} - \varepsilon_k + \Omega Q \lambda - q \cdot v) 
\times \left[ f\left( \frac{\varepsilon_k - \mu}{T_e} \right) - f\left( \frac{\varepsilon_{k+q} - \mu}{T_e} \right) \right] 
\times \left[ n\left( \Omega Q \lambda / T \right) - n\left( \Omega Q \lambda - q \cdot v / T \right) \right] 
- 2 \pi \sum_{kQ} |M(Q, \lambda)|^2 |I(iq_z)|^2 (\varepsilon_{k+q} + \varepsilon_k) \frac{q}{m} \delta(\varepsilon_{k+q} - \varepsilon_k + \Omega Q \lambda - q \cdot v) 
\times \left[ f\left( \frac{\varepsilon_k - \mu}{T_e} \right) - f\left( \frac{\varepsilon_{k+q} - \mu}{T_e} \right) \right] 
\times \left[ n\left( \Omega Q \lambda / T \right) - n\left( \Omega Q \lambda - q \cdot v / T \right) \right].
$$

(8)

The tensor $A$ can be expressed as

$$
\langle A \rangle = \frac{1}{2} \left[ S(R) + w v^2 |I + 3 u v v + \frac{1}{2} m n v^2 v v, \right]
$$

(9)
$S(R) = 2 \sum_k \frac{k^4}{2m^3} f(\frac{\varepsilon_k - \mu}{T_e}) \cdot \tag{10}$

In these equations $\varepsilon_k = k^2/2m$, and $f(x) = 1/(e^x + 1)$ represent the energy dispersion of 2D electrons and Fermi distribution function separately, and $\mathcal{I}$ stands for the unit tensor.

The Onsager relation [25] is concerned with the linear response of the particle current $\langle J \rangle$ and the heat flux $\langle J_Q \rangle$ near thermal equilibrium, which flow as a result of generalized forces $X_i$ on the system:

$$\langle J \rangle = L^{11} X_1 + L^{12} X_2, \tag{11}$$
$$\langle J_Q \rangle = L^{21} X_1 + L^{22} X_2, \tag{12}$$

with $X_1 = -\frac{1}{T} \nabla (\mu + e\phi)$ and $X_2 = \nabla (1/T)$. The Onsager relation states that

$$L^{12} = L^{21}. \tag{13}$$

The heat flux $\langle J_Q \rangle$ relates to the energy flux in Eq. (4) through

$$\langle J_Q \rangle = \langle J_H \rangle - \mu \langle J \rangle. \tag{14}$$

The fluxes $\langle J \rangle$ and $\langle J_H \rangle$ have already been defined by Eqs. (3) and (4). Our task is to express them in terms of linear response in the form of Eqs. (11) and (12). To this end, we consider electron transport in a quantum well which is grown along $z$-direction), in the presence of a small lattice temperature gradient and a small electric field along the $x$ direction: $\nabla T = (\nabla_x T, 0, 0)$ and $E = (E_x, 0, 0)$ respectively. Therefore $T_e = T$, and $v = (v_x, 0, 0)$ is also small. The system is near equilibrium. Following the same steps as in Ref. [23], we can derive the first relation (11) from the momentum balance equation (2) and the second relation (12) from the energy-flux balance equation (3), by treating Eqs. (2) and (3) to first order in the small quantities $E_x$, $\nabla_x T$ and $v_x$, and have

$$L^{11} = \frac{T}{\rho e^2}, \tag{15}$$

with
\[ L^{12} = \frac{T^2}{\rho e^2} \left[ \frac{2 F_1(\zeta)}{F_0(\zeta)} - \zeta \right], \]  
(16)
\[ L^{21} = \frac{T^2}{\rho e^2} \left[ -\frac{\tau \rho e^2}{m} \frac{2 F_1(\zeta)}{F_0(\zeta)} - \zeta \right], \]  
(17)
\[ L^{22} = -\frac{\tau T^3}{m} \left[ \frac{3 F_2(\zeta)}{F_0(\zeta)} - 2 \zeta \frac{F_1(\zeta)}{F_0(\zeta)} \right] - \zeta T^3 \frac{2 F_1(\zeta)}{F_0(\zeta)} - \zeta \right]. \]  
(18)

In deriving these equations, we have used the relations

\[ n = 2 \sum_k f[(\varepsilon_k - \mu)/T_e] = \frac{2m}{\pi} TF_0(\zeta), \]  
(19)

and

\[ u = 2 \sum_k \varepsilon_k f[(\varepsilon_k - \mu)/T_e] = \frac{2m}{\pi} T^2 F_1(\zeta), \]  
(20)

with \( \zeta \equiv \mu/T \) and \( F_\nu(y) = \int_0^\infty x^\nu [\exp(x - y) + 1]^{-1} dx \). Here,

\[ \rho = -\frac{f_x}{n^2 e^2 v_x} = -\frac{f_x}{n e^2 \langle J_x \rangle} \]  
(21)

is the resistivity and independent of \( v_x \) (\( \langle J_x \rangle \)). The expression of it can be found in Ref. [2]. Further,

\[ 1/\tau = \frac{\langle B_z \rangle}{n(\langle J_x \rangle)} \]  
(22)

is also independent of \( v_x \) (therefore \( \langle J_x \rangle \)). Comparing Eq. (16) with Eq. (17), we find that the condition under which the Onsager relation holds is given by

\[ I \equiv -\frac{\tau \rho e^2}{m} = 1 \]  
(23)

We have closely examined Eq. (23) for a GaAs-based (10 nm well width along the \( z \)-direction) quantum well structure. (We have also considered other quantum wells of different well width and found that the tendency of \( I \) approaching to “1” is not very sensitive on the width of quantum well.) We only take the lowest subband occupation into account. Both \( \rho \) and \( \langle B_z \rangle \) are composed of contributions due to electron-impurity, electron–LO-phonon, and electron–acoustic-phonon scatterings (with the electron–acoustic-phonon scatterings due to
longitudinal mode acoustic phonons via deformation potential and piezoelectric interactions, and transverse mode via piezoelectric interaction). We have examined each scattering contribution in detail to check Eq. (23) separately for each interaction. It is clear that if \( I_i \equiv -e^2 \rho_i / m \) (1/\( \tau_i \)) = 1 is satisfied for each interaction, we have \(-e \sum_i \rho_{ii} / m \tau_i = 1\). Moreover, this procedure is advantageous in that each \( I_i \) is independent of impurity concentration and parameters of the electron-phonon interaction matrixes.

The expressions for \( I \) obtained from the balance equations are given by

\[
I_{ei} = \frac{\sum_q q^2 |u(q)|^2 |F(q, z_0)|^2 [\frac{\partial}{\partial \omega} \Pi_2(q, \omega)]\big|_{\omega=0}}{2(\frac{\pi}{n}) \sum_q q^2 |u(q)|^2 |F(q, z_0)|^2 [\frac{\partial}{\partial \omega} \Pi_2(q, \omega)]\big|_{\omega=0}},
\]

due to electron-impurity scattering; and

\[
I_{e-\text{ph}}(\lambda) = \frac{\sum_Q |M(Q, \lambda)|^2 |I(iq_z)|^2 \Omega_{Q\lambda} (\varepsilon_q + \Omega_{Q\lambda}) n'(\frac{\Omega_{Q\lambda}}{T}) \Pi_2(q, \Omega_{Q\lambda})}{2(\frac{\pi}{n}) \sum_q |M(Q, \lambda)|^2 |I(iq_z)|^2 \Omega_{Q\lambda} n'(\frac{\Omega_{Q\lambda}}{T}) \Pi_2(q, \Omega_{Q\lambda})} + \frac{-\sum_Q |M(Q, \lambda)|^2 |I(iq_z)|^2 \Omega_{Q\lambda} n'(\frac{\Omega_{Q\lambda}}{T}) \Pi_2(-\Omega_{Q\lambda})}{2(\frac{\pi}{n}) \sum_q |M(Q, \lambda)|^2 |I(iq_z)|^2 \Omega_{Q\lambda} n'(\frac{\Omega_{Q\lambda}}{T}) \Pi_2(q, \Omega_{Q\lambda})},
\]

due to electron-phonon scattering, for phonons of mode \( \lambda \). \( I_{e-\text{ph}}(\lambda) \) is further composed of contributions due to electron–LO-phonon scattering, \( I_{e-LO} \); due to electron–longitudinal acoustic phonons by deformation potential coupling, \( I_{ed} \); and by piezoelectric interaction, \( I_{ep} \); and due to electron–transverse acoustic phonons by piezoelectric interaction, \( I_{ept} \). In these equations, \( \Omega_{Q\lambda} \) is the phonon frequency of wave vector \( Q \equiv (q_x, q_y, q_z) \) and mode \( \lambda \); \( u(q) \), the electron-impurity interaction potential; and \( M(q, \lambda) \), the electron-phonon interaction matrix element. \( F(q, z_0) \) and \( I(iq_z) \) are form factors of electron-impurity and electron-phonon interaction respectively, with \( z_0 \) standing for the position of impurity. \( n(x) = (e^x - 1)^{-1} \) stands for the Bose distribution. \( \Pi_2(q, \lambda) \) denotes the imaginary part of electron density-density correction function. \( \Pi_2 \) is defined by

\[
\Pi_2(q, \omega) = 2\pi \sum_k \varepsilon_k \delta(\varepsilon_k + q - \varepsilon_k + \omega) \left[ f \left( \frac{\varepsilon_k - \mu}{T} \right) - f \left( \frac{\varepsilon_k + q - \mu}{T} \right) \right].
\]

For the LO phonon, \( \Omega_{Q,LO} = \Omega_0 = 35.4 \) meV, and the Fröhlich matrix element is \( |M(Q, LO)|^2 = e^2 (\kappa^{-1} - \kappa^{-1}) \Omega_0 / (2\varepsilon_0 Q^2) \propto 1/Q^2 \). (Since the constants in the matrix elements cancel in Eq. (25), in the following we only specify their relation to \( Q \).)
matrix element due to longitudinal deformation potential coupling is $|M(\mathbf{Q}, dl)|^2 \propto Q$, that due to longitudinal piezoelectric interaction is $|M(\mathbf{Q}, pl)|^2 \propto (q_x q_y q_z)^2/Q^7$, and for the two branches of independent transverse piezoelectric interaction: $\sum_{j=1,2} |M(\mathbf{Q}, pt_j)|^2 \propto (q_x^2 q_y^2 + q_y^2 q_z^2 + q_z^2 q_x^2 - (3q_x q_y q_z)^2/Q^2)/Q^5$. For acoustic phonons $\Omega_{Q\lambda}$ can be written as $v_s Q$, with the longitudinal sound speed $v_s$ being $5.29 \times 10^3$ m/s, and the transverse sound speed being $2.48 \times 10^3$ m/s. The effective mass of electron is $0.07 m_e$, with $m_e$ denoting the free electron mass.

We present the results of our numerical calculations in Fig. 1 to Fig. 4, where contributions to $I$ due to the various interactions discussed above are plotted against electron density for several different temperatures (the results of $I_{epd}$ are similar to those of $I_{ept}$, so we only plot one as representative). As it is generally believed that the contribution of acoustic phonons is important only at low temperature, while the contribution of LO phonons is dominant at high temperature, our temperatures are chosen as 10, 20, and 40 K for the former, and 50, 300, 500, and 1000 K for the latter. Impurity scattering is present at all temperature, so we take $T = 10, 50, 100, 300, and 1000$ K in Fig. 1. From these figures it is evident that, for any temperature, when electron density is sufficiently high $I$ is exactly unity, indicating that the Onsager relation holds. This is consistent with the understanding that the Lei-Ting balance equation theory holds only for strong electron-electron interaction.

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REFERENCES

[1] X.L. Lei and C.S. Ting, Phys. Rev. B 30, 4809 (1984); 32, 1112 (1985).

[2] X.L. Lei and N.J.M. Horing, Int. J. Mod. Phys. B 6, 805 (1992).

[3] X.L. Lei, J. Cai, and L.M. Xie, Phys. Rev. B 38, 1529 (1988).

[4] J. Cai, H.L. Cui, and N.J.M. Horing, and X.L. Lei, Mat. Res. Soc. Symp. Proc. 326, 215 (1994).

[5] J. Cai, H.L. Cui, N.J.M. Horing, X.L. Lei, E. Lenzing, and B.S. Perlman, Proc. 3rd Int. Workshop Comp. Electron., p. 127, 1994.

[6] J. Cai and H.L. Cui, J. Appl. Phys. 78, 6802(1995).

[7] M.W. Wu, N.J.M. Horing, and H.L. Cui, Phys. Rev. B 54, 1996.

[8] M.W. Wu, W. Sun, N.J.M. Horing, and H.L. Cui, Phys. Stat. Sol. (b) 196, 1996.

[9] L. Onsager, Phys. Rev. B 37, 405 (1931).

[10] Q. Lin, N. Goldsman, and G. Tai, Solid-State Electron. 37, 359 (1994).

[11] S. Ramaswamy and T. Tang, IEEE Trans. Ele. Dev. ED-41, 76 (1994)

[12] G.L. Gardner, SIAM J. Appl. Math. 54, 409 (1994).

[13] Y. Zhang and M. Nokali, Solid-State Electron. 36, 1689 (1993).

[14] J.R. Zhou, D. Vasileska, and D.K. Ferry, Solid-State Electron. 36, 1294 (1993).

[15] T. Tang, S. Ramaswamy, and J. Nam, IEEE Trans. Ele. Dev. 40, 1469 (1993).

[16] A. Majorana and G. Russo, COMPEL-Int. J. Comp. Math. Electrical and Electron. Eng. 12, 81 (1993).

[17] D.K. Ferry and J.R. Zhou, Phys. Rev. B 48, 7944 (1993).
[18] D.A. Teeter, J.R. East, RIK. Mains, and G.I. Haddad, IEEE Trans. Ele. Dev. **ED-40**, 837 (1993).

[19] J.R. Zhou and D.K. Ferry, IEEE Trans. Ele. Dev. **ED-40**, 421 (1993).

[20] K. Souissi, F. Odeh, H.H.K. Tang, A. Gnudi, and P.F. Lu, IEEE Trans. Ele. Dev. **ED-40**, 1501 (1993).

[21] W. Quade, E. Schöll, and M. Rudan, Solid-State Electron. **36**, 1493 (1993).

[22] A.M. Anile and O. Muscato, Phys. Rev. B **51**, 16728 (1995).

[23] M.W. Wu, H.L. Cui, and N.J.M. Horing, Phys. Rev. B **54**, 1996.

[24] X.L. Lei, J. Phys.: Condens. Matter **6**, L305 (1994).

[25] G.D. Mahan, *Many-Particle Physics*, (Plenum Press, New York 1981), p. 212.

[26] L.Y. Chen, C.S. Ting, and N.J.M. Horing, Phys. Rev. B **42**, 1129 (1990).

[27] L.Y. Chen, C.S. Ting, and N.J.M. Horing, Solid State Commun. **73**, 437 (1990).
FIGURES

FIG. 1. $I$ due to electron-impurity scattering is plotted as a function of electron density for several different temperatures.

FIG. 2. $I$ due to electron–LO-phonon scattering is plotted as a function of electron density for several different temperatures.

FIG. 3. $I$ due to electron–longitudinal acoustic-phonon scattering via deformation potential coupling is plotted as a function of electron density for several different temperatures.

FIG. 4. $I$ due to electron–transverse acoustic-phonon scattering via piezoelectric interaction is plotted as a function of electron density for several different temperatures.