Long-Time Tail in an Electric Conduction System

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The long-time behavior of the velocity autocorrelation function in a classical two-dimensional electric conduction system is studied by the molecular dynamics simulation. In equilibrium, the effect of coexistence of many-body interactions and a random potential is investigated. A crossover from a positive tail proportional to $t^{-1}$, to a negative tail proportional to $-t^{-2}$ is observed as the strength of the random potential increases. In nonequilibrium, the positive tail is enhanced whereas the negative tail appears at earlier times as an electric field increases.

§1. Introduction

The long-time tail was first discovered by Alder and Wainwright\cite{1} for the velocity autocorrelation function (VACF) in a hard-core fluid system. This tail is positive and proportional to $t^{-d/2}$ (hereafter called the fluid-type tail).\cite{2, 7} Here, $d$ is the dimension of the system. As a result the self-diffusion coefficient $D$ in this system is logarithmically divergent in terms of the system size $L$ for $d = 2$.

Another system which has a long-time tail is the Lorentz model, which describes the motion of a single particle in a disordered system. In this system the tail of the VACF is negative and proportional to $-t^{-(d+2)/2}$ (called the Lorentz-type tail hereafter).\cite{8, 13} Although $D$ is not divergent even for $d = 2$, this tail might cause an algebraically $L$-dependent term in $D$.

In the hard-core fluid only a many-body interaction exists and in the Lorentz model only a random potential exists. Hence a question occurs: How does the long-time tail change when a many-body interaction and a random potential coexist? A typical system which has both a many-body interaction and a random potential is an electric conduction system. In this system electron-electron ($e-e$) interaction corresponds to a many-body interaction and electron-impurity ($e-i$) interaction to a random potential.

In studies of the long-time tails in the hard-core fluid and the Lorentz model the equilibrium states have mainly been investigated. Regarding electric conduction systems, another interesting question arises: How does the long-time tail change under a nonequilibrium condition?

In this paper we report the results of the molecular dynamics (MD) simulations on a model of a two-dimensional electric conduction system to answer these two questions.\cite{14}

§2. Model and its physical meanings

We use a model of electric conduction proposed in Ref. 15). We here explain its physical meanings in more detail.

The model is a two-dimensional classical system, the size of which is $L_x \times L_y$. 
In the system are three sorts of particles, which we call electrons, phonons and impurities.\(^*\) An external electric field \(E\) is applied in the \(x\)-direction, which acts only on electrons. The boundary condition in the \(x\)-direction is periodic, and those in the \(y\)-direction are potential walls for electrons and thermal walls with temperature \(T\) for phonons. Moreover we assume that short-range interactions are present among all these particles. The charge of an electron is denoted by \(e\) (see the footnote \(*\) on this page). The mass, radius, number density of the electrons (phonons) are denoted by \(m_e\) \((m_p)\), \(R_e\) \((R_p)\) and \(n_e\) \((n_p)\), respectively. The impurities are immobile and play the role of a random potential. The radius and number density of the impurities are denoted by \(R_i\) and \(n_i\), respectively. In this study we control the strength of the random potential by changing \(n_i\). The configuration of the impurities is given by an almost uniform distribution except for the restriction that the distance between any pair of the impurities is larger than \(2(R_e + R_i)\). The initial positions of the electrons and phonons are randomly arranged not to overlap with the other particles, and their initial velocities are given by the Maxwell distribution with temperature \(T\).

We can control the frequencies of the \(e-e\) and \(e-i\) collisions by changing \(n_e\) and \(n_i\). Thus we can investigate independently the effects of the many-body interactions \((e-e, e-p\) and \(p-p\) interactions\) and that of the random potential \((e-i\) interaction\) on the long-time behavior of the VACF. It should be also noted that the situation where \(n_i = 0\) corresponds to the hard-disk fluid and that the situation without \(e-e\) interaction corresponds to the (non-overlapping) Lorentz model.

A typical system corresponding to this model is a two-dimensional electron system in a doped semiconductor at room temperature. Since the Fermi energy is smaller than room temperature in such a system, electrons can be treated as classical particles. Furthermore, we can treat them as being confined in a two-dimensional plane because the temperature is lower than the exciting energy between the ground and the second subbands\(^**\) of an electron.

It is well-known that in a uniform solid (such as our model), the motion of the electron system can be separated into the collective oscillations and the individual motions, and that the long-range effects of the Coulomb force are adequately incorporated in the collective oscillations.\(^15\) Moreover the collective oscillations do not play the central role in the electric conduction. [It is worth mentioning here that for non-uniform systems, such as a conductor connected to electron reservoirs,\(^16\) \(^17\) the long-range effects should be treated more carefully as discussed in Refs. 17) and 18).] For these reasons, we can treat the electrons as individual particles interacting through a short-range force when discussing transport properties of conductors. We can roughly estimate the range (the screening length) of the effective interaction

\(^*\) We set the charge of the electrons positive. As usual in the solid state physics, the background charge (negative in this case) is included in the system, which ensures the charge neutrality of the system.

\(^**\) In a real two-dimensional electron system, electron motion in the confined \((z)\) direction is quantized. In each quantized level \(n = 1, 2, \cdots\), a conduction electron moves freely in the \(x-y\) plane, and thus a small band is formed which is called a subband. The conduction band therefore splits into subbands which are labeled by \(n\). Conduction electrons can be well regarded as two-dimensional electrons when only the ground subband is occupied.
among electrons by the Debye length, \((k_B T/4\pi n e^2)^{1/2}\), in such a classical system. The potential produced by an impurity is also screened and its effective potential range is also estimated by the Debye length. Therefore the interaction ranges of e-e and e-i interactions are comparable.

In real solids phonons are the oscillation modes of the crystal lattice in the conductors. Therefore the total number of phonons does not conserve. However, because almost all the possible modes of phonons are excited in semiconductor at room temperature, the number density of phonons is so high that the non-conservation of the phonon number would be irrelevant. Moreover, the energy-momentum dispersion relations of phonons are complicated in real solids. This would be also irrelevant, however, when discussing general nonequilibrium properties, which are independent of the details of the materials, of electric conduction. In this study, therefore, it is sufficient to model phonons as classical particles\(^*\) whose number conserves and whose mass is constant, which corresponds to parabolic dispersion relation. Note that if one wants to reproduce the \(T\)-dependence of conductivity, such as the famous linear-\(T\) dependence, then the number of phonons should be varied as a function of \(T\). In this paper, however, we are not interested in the \(T\)-dependence of conductivity.

This model contains what we believe to be essential elements of electric conduction in the context of nonequilibrium statistical physics. These elements are the following: (i) A driving force which induces electric current: *electric field*. (ii) Careers which transfer heat to outside the conductor: *phonons*. In real physical systems (i.e., in experiments), a conductor is surrounded by a large insulating material, which works as the heat bath. The energy supplied from an external electric field to electrons is dissipated as the Joule heat transferring into the heat bath through the walls of the conductor to keep the system in a steady state. The heat flow *across* the walls of the conductor is mediated not by electrons but by phonons, while the heat flow *in* the conductor is mediated by both of them. Therefore the electron-phonon interactions and heat contact of phonons at the walls are essential to realize a nonequilibrium steady state. (iii) Objects which break the microscopic translational invariance in the bulk region: *impurities*. Although the conductor is macroscopically uniform, the microscopic translation invariance is violated by the imperfections of the conductor (impurities, defects and so on). This defines the rest frame of the electrons at equilibrium, and thereby eliminates any possible anomalies which may arise from the translational invariance. (iv) Many-body interactions: *short-range interactions among all particles*. (v) A nonequilibrium steady state is

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\(^*\) One might be suspicious about treating waves as particles. However, it can be shown that a classical mixture (mixed state), such as the one treated here, of many extended quantum modes (plane waves) is identical to a classical mixture of localized quantum wavepackets. A wavepacket can be treated as a classical particle in a classical regime. Furthermore, in a doped semiconductor at room temperature the average wavelength of phonons is shorter than that of conduction electrons because width of the phonon band \(\sim k_B T \ll\) width of the conduction band. Hence, the size of a wavepacket of a phonon is shorter than that of an electron. It is well-known that at room temperature an electron can be treated as a classical particle (with respect to the motion in the \(x-y\) (non-confining) plane for the case of two-dimensional electron systems). Therefore, a phonon can also be treated as a classical particle. The difference of the statistics (fermion versus boson) is not important at such a high temperature.
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Fig. 1. Average velocities of an electron for (a) $n_i = 0.0004$ and (b) $n_i = 0.04$, plotted against $E$.

uniquely determined by a small number of macroscopic parameters: $T$ and $E$.

We perform the time-step-driven MD on this model (using Gear’s fifth-order predictor-corrector method). We set $R_e, m_e, k_B T$ and $e$ to unity, and take $L_x = 2000$, $L_y = 125$, $R_p = 1$, $R_i = 0.5$ and $m_p = 1$ in these units.\(^\dagger\) The number densities of the electrons and phonons are fixed to $n_e = 0.04$ and $n_p = 0.002$. Since $n_e$ is taken larger than that in our previous study,\(^\dagger\) the long-time tails are more clearly observed. In this study we employ the Hertzian interaction $U_{jk}^{\text{int}} = Y(\max\{0, d_{jk}\})^{5/2}$ as the interaction potential between any pair of the particles. Here, $Y$ is a constant (fixed to 4000 in the simulation), and $d_{jk} = R_j + R_k - |r_j - r_k|$ is the overlap of the potential ranges of the $j$-th and $k$-th particles ($R_j$ is the radius of the $j$-th particle and equals $R_e, R_p$ or $R_i$. $r_j$ is the position of the $j$-th particle, see the footnote on this page).

We previously confirmed that this model shows good properties of steady states.\(^\ddagger\) For example, as shown in Fig. 1, we observe linear response of $v_x$ to $E$ near equilibrium and nonlinear response far from equilibrium, where $v_x$ is the component of electron’s velocity in the $x$-direction (parallel to $E$). We also observed that the Kramers-Kronig relation of the complex admittance as well as the fluctuation-dissipation theorem\(^\ddagger\) holds at all frequencies in the equilibrium states.

\section{3. Results}

We calculate the VACF,

$$C(t) = \frac{\langle (v_x(t) - \langle v_x \rangle)(v_x(0) - \langle v_x \rangle) \rangle}{\langle (v_x - \langle v_x \rangle)^2 \rangle},$$

(3.1)

of an electron in steady states under various conditions.

\(^{\dagger}\) Note that $R_e, R_p$ and $R_i$ are not the real radii but the effective lengths of the interaction ranges.
Fig. 2. A double logarithmic plot of the absolute value of the VACF in the equilibrium states for various values of \( n_i \). The open and closed symbols correspond to positive and negative values of the VACF, respectively. The dotted and dashed lines are reference lines proportional to \( t^{-1} \) and \( t^{-2} \), respectively.

Table I. Exponents \( \alpha \) and signs of \( A \) of the tails (fitted with \( At^{\alpha} \)) for various values of \( n_i \), which we show in Fig. 2.

| \( n_i \)   | exponent \( \alpha \) | sign of \( A \) |
|------------|------------------------|---------------|
| 0          | -1.17(2)               | positive      |
| \( 4 \times 10^{-4} \) | -1.26(2)               | positive      |
| \( 2 \times 10^{-3} \) | -1.70(5)               | positive      |
| \( 4 \times 10^{-3} \) | -2.9(1)                | positive      |
| \( 2 \times 10^{-2} \) | -2.01(4)               | negative      |
| \( 4 \times 10^{-2} \) | -2.21(5)               | negative      |

3.1. Equilibrium case

First we show the results of the VACF in the equilibrium states. We calculate the VACFs with \( n_e \) and \( n_p \) fixed, and \( n_i \) varied from 0 to 0.04. In this case, we can investigate the effect of the random potential introduced into the fluid system. Figure 2 displays the results. We observe power-law tails of the VACFs at longer times. We estimate the exponents of the tails by fitting the data of the VACFs in regions of power-law decay with a function, \( At^{\alpha} \). In Table I we show the exponents \( \alpha \) and the signs of \( A \). When \( n_i = 0 \) the tail is positive and the exponent is nearly equal to \(-1,^*\) which is the result for the fluid system. As \( n_i \) increases, this positive tail becomes weaker (that is, \(|\alpha|\) becomes larger), and eventually it disappears. Instead,

\(^*\) When the packing fraction of the fluid particles is high, the exponent deviates slightly from \(-1\) for hard-disk fluid. See Ref. 20).
we observe another tail which is negative and whose exponent is approximately −2. That is, the long-time behavior of the VACF is a crossover from the fluid-type tail to the Lorentz-type tail as \( n_i \) becomes larger. According to phenomenological theories,\(^2,4)−7,12,13\) the origin of the long-time tail in a fluid is the mode coupling of the momentum field and the density field (because of the conservation of the total momentum and total number of the particles) while that in the Lorentz model is the coupling of the density field and a static mode generated by the configuration of the impurities. From these theories, we have a qualitative explanation of the crossover from the fluid-type tail to the Lorentz-type tail. When \( n_i \) is small, the momentum conservation is approximately valid and we can regard the system as a fluid. Then the momentum field can contribute to the hydrodynamic mode and we observe the fluid-type tail. As \( n_i \) increases, the violation of the momentum conservation becomes larger and simultaneously the static mode by the impurity configuration becomes more relevant. Then the fluid-type tail disappears and the Lorentz-type tail appears.

A necessary condition to treat the electron system as a fluid is that the mean number \( \bar{N}_e \) of the electrons in an area among the impurities is sufficiently large. Because the mean area per impurity is \( 1/n_i \), \( \bar{N}_e \) is estimated as \( \bar{N}_e = n_e/n_i \). Therefore we can use the ratio of the electron and impurity density as a criterion for the long-time behavior of the VACF. From Fig. 2 the crossover value \( (n_e/n_i)_c \) is evaluated as \( 2 \lesssim (n_e/n_i)_c \lesssim 10 \) [the fluid-type tail appears when \( n_e/n_i > (n_e/n_i)_c \) and the Lorentz-type tail appears when \( n_e/n_i < (n_e/n_i)_c \)].

3.2. Nonequilibrium case

Next, we show the results of the VACF when electric current is flowing. We calculate the VACFs for \( n_e/n_i \gg (n_e/n_i)_c \) and \( n_e/n_i \ll (n_e/n_i)_c \), with varying \( E \). In Fig. 3, we show the long-time behavior of the VACFs of the steady states including the states in the nonlinear response regimes as well as those in equilibrium and in the linear response regimes. When \( n_i = 0.0004 \) \([n_e/n_i \gg (n_e/n_i)_c]\), we observe that the amplitude of the fluid-type tail gets enhanced as \( E \) increases. Because \( C(t) \) is normalized by \( \langle (v_x - \langle v_x \rangle)^2 \rangle \) to be \( C(0) = 1 \), this enhancement is not simply due to the rise of the kinetic temperature of the electrons. This result implies that a “temperature” is different among different time scales in nonequilibrium states. For the system with \( n_i = 0.04 \) \([n_e/n_i \ll (n_e/n_i)_c]\), the Lorentz-type tail appears at earlier times as \( E \) becomes larger. One of the reasons for the early appearance of the Lorentz-type tail would be that the duration time of the e-i collision becomes shorter as \( E \) increases.

§4. Concluding remarks

In summary, we have investigated the long-time behavior of the VACF in a system where many-body interactions and a random potential coexist. In equilibrium, we have observed a crossover from the fluid-type tail to the Lorentz-type tail as the impurity density increases. We have interpreted that this crossover occurs because the system cannot be regarded as a fluid when the impurity density becomes large. The ratio of the electron and impurity densities is a criterion quantity for this
crossover. In nonequilibrium, as an electric field increases we have observed that the fluid-type tail is enhanced for $n_e/n_i \gg (n_e/n_i)_c$ and that the Lorentz-type tail appears at earlier times for $n_e/n_i \ll (n_e/n_i)_c$.

Finally, we list some issues related to this study.

(1) The long-time tails in equilibrium states induce system-size dependence of $D$. In an electric conduction system $D$ can be translated into the electrical conductivity $\sigma$ in the linear response regime by the Einstein relation. Thus some system-size dependence of $\sigma$ should be observed in experiments. To our knowledge, however, no experiment has been reported which observed a system-size dependence of $\sigma$ for uniform two-dimensional electron systems at room temperature.\(^*\) This might be because the amplitude of the system-size dependent term in $\sigma$ is too small to detect in comparison with the system-size independent term, or because phonon scattering would introduce a system-size independent cutoff.

(2) In §3.1 we have presented a possible scenario of a mode-coupling theory for the crossover from the fluid-type tail to the Lorentz-type tail in equilibrium. This should be explicitly shown by combining the mode-coupling theories for the

\(^*\) Note that although the weak (Anderson) localization effect causes a system-size dependence of $\sigma$ at low temperature, the origin of this dependence is different from the long-time tails in classical systems and this effect becomes weaker at room temperature. It is also an interesting problem how the effect of the long-time tail in a classical system and the weak localization effect in a quantum system on $\sigma$ are connected. A similarity between the fluid-type tail and the weak localization effect is pointed out in Ref. 7).
fluid\(^2\),\(^4\)–\(^7\) and for the Lorentz model.\(^{12},\(^13\)\)

(3) This crossover behavior would also be supported by a kinetic theory with a two-parameter \((n_e\text{ and } n_i)\) expansion, which combines the kinetic theory for the hard-core fluid \((n_e\text{-expansion})\)^3 and that for the Lorentz gas \((n_i\text{-expansion})\)^8.

(4) A crossover might occur from the fluid-type tail to the Lorentz-type tail, even in a system with lower density of impurities [that is, \(n_e/n_i > (n_e/n_i)_c\)], at longer times when the effect of the violation of the momentum conservation becomes relevant. If this is true, \(D\) is convergent\(^{\ast}\) in two-dimensional systems except when the impurity density vanishes. To demonstrate this, a larger-scale simulation with higher accuracy is necessary. This issue should also be studied by a mode-coupling theory and a kinetic theory.

(5) In §3.2 we have observed an enhancement of the fluid-type tail in a nonequilibrium steady state. This might be explained by a mode-coupling theory similar to the one recently developed in sheared fluids.\(^{21}\)

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References

1) B. J. Alder and T. E. Wainwright, Phys. Rev. A 1 (1970), 18.
2) M. H. Ernst, E. H. Hauge and J. M. J. van Leeuwen, Phys. Rev. Lett. 25 (1970), 1254.
3) J. R. Dorfman and E. D. G. Cohen, Phys. Rev. Lett. 25 (1970), 1257.
4) R. Zwanzig and M. Bixon, Phys. Rev. A 2 (1970), 2005.
5) K. Kawasaki, Phys. Lett. A 32 (1970), 379.
6) Y. Pomeau and P. Résibois, Phys. Rep. 19 (1975), 63.
7) T. R. Kirkpatrick, D. Belitz and J. V. Sengers, J. Stat. Phys. 109 (2002), 373.
8) M. H. Ernst and A. Weijland, Phys. Lett. A 34 (1971), 39.
9) C. Bruin, Phys. Rev. Lett. 29 (1972), 1670.
10) B. J. Alder and W. E. Alley, J. Stat. Phys. 19 (1978), 341.
11) B. J. Alder and W. E. Alley, Physica A 121 (1983), 523.
12) W. Götze, E. Leutheusser and S. Yip, Phys. Rev. A 23 (1981), 2634.
13) M. H. Ernst, J. Machta, J. R. Dorfman and H. van Beijeren, J. Stat. Phys. 34 (1983), 477.
14) T. Yuge and A. Shimizu, J. Phys. Soc. Jpn. 76 (2007), 093001 [Errata: 77 (2008), 028001].
15) T. Yuge, N. Ito and A. Shimizu, J. Phys. Soc. Jpn. 74 (2005), 1895.
16) D. Pines, Solid State Phys. 1 (1955), 367.
17) A. Shimizu and T. Miyadera, Physica B 249-251 (1998), 518.
18) A. Shimizu and H. Kato, “Nonequilibrium Mesoscopic Conductors Driven by Reservoirs”, in Low-Dimensional Systems — Interactions and Transport Properties, ed. T. Brandes (Springer, 2000), p. 3, cond-mat/9911333.
19) H. Nyquist, Phys. Rev. 32 (1928), 110.
20) M. Isobe, Phys. Rev. E 77 (2008), 021201.
21) M. Otsuki and H. Hayakawa, arXiv:0711.1421.

\(^{\ast}\) Some Burnett coefficients might diverge as in the Lorentz model.\(^{13}\)