Calculation of neoclassical diffusion and viscosity coefficients for stellarator/heliotron devices by the Green-Kubo approach*

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Introduction

The toroidal viscosity induced by magnetic field asymmetry dominates plasma transport in stellarator/heliotron devices. In neoclassical transport theory, the viscosity-flow relations, which constitute a closure of moment equations, are written in terms of a transport matrix as[1]

$$\begin{bmatrix} \langle \mathbf{B}_P \cdot (\nabla \cdot \Pi_a) \rangle \\ \langle \mathbf{B}_P \cdot (\nabla \cdot \Theta_a) \rangle \\ \langle \mathbf{B}_T \cdot (\nabla \cdot \Pi_a) \rangle \\ \langle \mathbf{B}_T \cdot (\nabla \cdot \Theta_a) \rangle \end{bmatrix} = \begin{bmatrix} M_{a1PP} & M_{a2PP} & M_{a1PT} & M_{a2PT} \\ M_{a2PP} & M_{a3PP} & M_{a2PT} & M_{a3PT} \\ M_{a1PT} & M_{a2PT} & M_{a1TT} & M_{a2TT} \\ M_{a2PT} & M_{a3PT} & M_{a2TT} & M_{a3TT} \end{bmatrix} \begin{bmatrix} \langle u_a^\theta \rangle / \chi' \\ \frac{2}{5p_a} \langle q_a^\theta \rangle / \chi' \\ \langle u_a^\zeta \rangle / \psi' \\ \frac{2}{5p_a} \langle q_a^\zeta \rangle / \psi' \end{bmatrix}, \qquad (1)$$

where one assumes $\varepsilon \equiv \rho_p / L \ll 1$; ρ_p is the poloidal gyroradius and L is the radial scale length. All the elements of the transport matrix in Eq. (1) are necessary for a complete theoretical description of neoclassical transport in stellarator/heliotrons although this matrix degenerates in tokamaks owing to axisymmetry. Recently, several authors[1, 2] have been proposed methods to evaluate this matrix numerically, in which the calculation of the 4×4 viscosity matrix is reduced to that of 2×2 energy-dependent transport matrix by moment expansions of gyro-averaged distribution functions[3].

The purpose of this paper is to present a new algorithm to calculate the required energy-dependent transport matrix using a guiding-center particle simulation. While the previous works [1, 2] consider the drift-kinetic equations, our theoretical starting point is on the linear response theory. The correspondence between linear response and kinetic theories may be apparent, but the numerical implementation, e.g., of Green-Kubo relations in neoclassical transport is non-trivial. It is worth to note that the present approach has been employed in molecular dynamics simulations to calculate a self-diffusion coefficient, shear and bulk viscosities, and thermal conductivity, which determine a closure of Navier-Stokes equations[4].

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Theory and Simulations

We employ two standard methods to calculate the transport matrix in molecular dynamics simulations, namely Green-Kubo and Einstein relations. These two relations describe the relaxation of thermodynamic fluctuation according to a linear hydrodynamical law with essentially identical but with different formulas. In linear response theory, the transport matrix is regarded as being related to the admittance of the equilibrium system to external forces. According to the Green-Kubo relations, the transport matrix requried here can be calculated by the integration of time-correlation functions of microscopic fluxes such that

$$D_{ij} = \int_0^\infty d\tau R_{ij}(\tau), \quad R_{ij}(t) = \langle \sigma_i(t)\sigma_j(0)\rangle, \tag{2}$$

where the bracket represents ensemble averages with respect to an equilibrium distribution. The expressions for microscopic fluxes are specified by $\sigma_{Xa} \equiv -v^2 P_2(\xi)\mathbf{b}\cdot\nabla(B\tilde{U})/(2\Omega_a)$ and $\sigma_{Ua} \equiv -m_a v^2 P_2(\xi)\mathbf{B}\cdot\nabla \ln B$, where $P_2(\xi)$ is the second-order Legendre polynomial of the pitch variable ξ, $\Omega_a = e_a B/m_a$ is the gyrofrequency, and $\tilde{U}$ can be expressed by a generating function of Hamada coordinates. With the choice of *time-reversal symmetric* microscopic fluxes σ_{Xa} and σ_{Ua}, the Onsager reciprocal relation $D_{ij} = D_{ji}\,(i \neq j)$ can be formally assumed. Next, assuming that the correlation functions $R_{ij}(t)\,(i,j = X,U)$ are invariant under a time-translation in the steady state, and using the symmetry of the functions, we can derive another formula, which are often referred to as the Einstein relations[5],

$$D_{ij} = \sum_{t\to\infty} \frac{t}{2}\langle \bar{\sigma}_i(t)\bar{\sigma}_j(t)\rangle, \quad \bar{\sigma}_i(t) = \frac{1}{t}\int_0^t d\tau\, \sigma_i(\tau), \tag{3}$$

where $\bar{\sigma}_i(t)$ represents the time averages of the microscopic fluxes, which can be regarded as those of microscopic fluctuations driven by thermodynamic forces. Equation (3) generalizes the concept of mean-square displacements for self-diffusion coefficients.

In our guiding-center particle simulation, we calculated the trajectories of test particles from numerical solutions of Itô-type Langevin equations in Boozer coordinates. The probability distribution of these particles obeys the Fokker-Planck equation equivalent to the zeroth-order drift-kinetic equation. The time integrations appearing in the Green-Kubo and the Einstein relations of Eqs. (2) and (3) are evaluated along the trajectories of test particles in phase space, similarly to δf particle simulations[2]. An output from the simulation is the 2×2 transport matrix $D_{ij}\,(i,j = X,U)$ as a function of collisionality ν/v. We here note that the reciprocal relation $D_{XU} = D_{UX}$ of this matrix is guaranteed explicitly for the Einstein relations in Eq. (3).

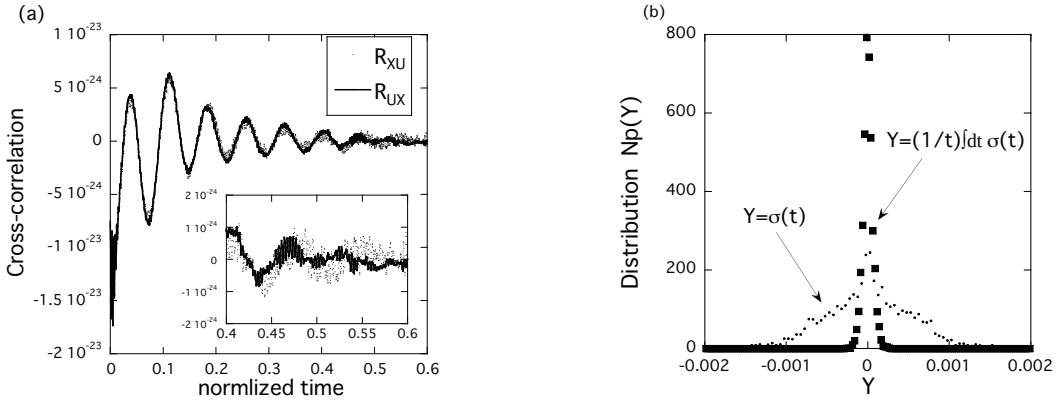

Figure 1: Linear relaxation observed in (a) the Green-Kubo and (b) the Einstein relations for $\nu/v = 1\times10^{-3}$ with $\varepsilon_t = 0.1$ and $\varepsilon_h = 0.01$. Figure 1 (a) shows time evolution of the cross-correlations, where we have also plotted enlarged one for the range from $\nu t = 0.4$ to 0.6. In Fig. (b), the instantaneous (small circles) and time-averaged distributions (squares) of the microscopic flux σ_{Xa} at $\nu t = 2.59$ are displayed.

Simulation Results

We used a simple magnetic-field model such that $B = B_0[1-\varepsilon_t\cos\theta - \varepsilon_h\cos(l\theta - m\zeta)]$, where $l = 2$, $m = 10$, and $B_0 = 1.0$. In Fig. 1, we illustrate what observed by the Green-Kubo and the Einstein relations, respectively. Figure 1 (a) shows that the auto and cross-correlation functions exponentially decay in about an effective collision time $\nu_{\rm eff}^{-1}$ because the test particle behavior is purely diffusive in our simulation. Figure 1 (b) shows distributions of instantaneous and time-averaged fluxes calculated with the Einstein relations. For an equilibrium system, time averages of statistically independent fluxes $\sigma_i(t)$ are expected to approach Gaussian distributions according to the central limit theorem. Therefore, the rate of this relaxation of the distribution of $\bar{\sigma}_i(t)$ to a Gaussian in long-time limit, where short-time correlations of $\sigma_i(t)$ may be neglected, gives the transport coefficient corresponding to that defined by the Green-Kubo relations[5].

An interesting observation in Fig. 1 (a) is that the time correlations R_{XU} and R_{UX} exhibit different levels of numerical noise. Although the reciprocal relation in Eq. (2) was verified reasonably for axisymmetric cases, but was less satisfactory for nonaxisymmetric cases, $\varepsilon_h \neq 0$. In general, particle simulations for nonaxisymmetric 3D systems suffer significant numerical noise compared to those for 2D tokamaks. (In this work, we use $N \simeq 10^3$ test particles.) The transport coefficients given by the Einstein relations, however, satisfy the reciprocal relation explicitly; it thus allows us to avoid the numerical ambiguity occurred in Eq. (2). Because of this feature with regard to the reciprocal relation, the Einstein relations of Eq. (3) would be preferable. Figure 2 shows a part of benchmarking results which verify the calculation with

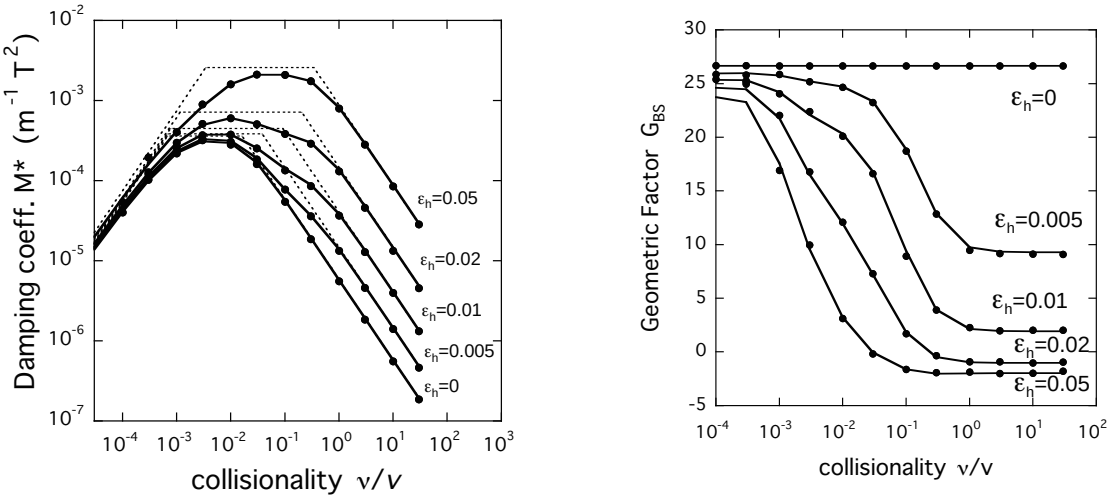

Figure 2: Parallel viscosity coefficients M^* (left) and the geometric factor (right) calculated by the Einstein relations. Solid lines show the reference DKES results[3], and dashed lines show asymptotic values of M^* for characteristic collisionality regimes.

the Einstein relations. According to Ref. 1, the results are displayed in the form of viscosity and diffusion coefficients M^*, L^*, and the geometric factor G_{BS}. The results in Fig. 2 are in reasonable agreement with those obtained by the kinetic approach (the DKES code[6]).

In summary, the algorithm based on the linear response theory to calculate the neoclassical transport for stellarator/heliotron devices has been investigated. We have implemented the two approaches based on the Green-Kubo and the Einstein relations, and showed that the latter can be used as a reliable technique for our purpose. While we have mainly focused on the theoretical aspects, our numerical code combined with the moment-equation approach[1] would be a useful tool to predict neoclassical toroidal and poloidal flows in stellarator/heiotron devices as future applications.

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