A δf Drift-Kinetic Simulation for Off-Diagonal Neoclassical Transport Coefficients in Quasi-Symmetric Toroidal Configurations

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By explicitly excluding the Pfirsch-Schlüter diffusion and Spitzer terms from the perturbed distribution functions in δf drift-kinetic Monte Carlo simulations, off-diagonal neoclassical transport coefficients for quasi-symmetric toroidal plasmas can be calculated properly, ensuring the constancy of the geometric factor in the exact axisymmetric limit.

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Neoclassical transport studies in nonsymmetric toroidal plasmas require numerical solutions of the linearized drift-kinetic equations [1]. For this purpose, various numerical schemes such as δf Monte Carlo methods [2–7] have been developed. To efficiently use numerical solutions, several authors [8–10] have presented moment formalisms that facilitate the evaluation of the neoclassical viscosity, diffusion, and bootstrap current from the solutions of the drift-kinetic equations with the pitch-angle scattering approximation. What is interesting in these literature is that we can find three different expressions of the linearized drift-kinetic equations. The first (denoted by DKE1) was recently derived by Sugama and Nishimura [9], the second one (denoted by DKE2) is used in the well-known DKES code [11], and the third one (denoted by DKE3) is that used, e.g., in Beidler *et al.* [1] and in Hirshman *et al.* [12]. Although DKE2 and DKE3 were studied previously (see Ref. [7]), direct numerical solutions of DKE1 have not yet been evaluated. In this letter, by δf Monte Carlo methods, we investigate how the choice of drift-kinetic equation affects the neoclassical transport coefficients evaluated. DKE1 is shown to have advantages in applications to quasi-symmetric stellarators [13].

In the coordinate system $(\boldsymbol{x}, v, \xi)$, where $\boldsymbol{x}$ is the guiding-center position, v is the particle velocity, and $\xi \equiv v_\parallel/v$ is the pitch variable, DKE1 is written as

- DKE1:

$$(\partial_t + V_\parallel - C^{\mathrm{PAS}}) \begin{bmatrix} g_u \\ g_x \end{bmatrix} = \begin{bmatrix} \sigma_u \\ \sigma_x \end{bmatrix}, \tag{1}$$

$$\sigma_x \equiv -v^2 P_2(\xi) \frac{\boldsymbol{b} \cdot \nabla(B\tilde{U})}{2\Omega}, \tag{2}$$

$$\sigma_u \equiv -V_\parallel(mv\xi B) = -mv^2 P_2(\xi) \boldsymbol{B} \cdot \nabla \ln B. \tag{3}$$

Here, $P_2(\xi) = \frac{3}{2}\xi^2 - \frac{1}{2}$, $B \equiv |\boldsymbol{B}|$, $\boldsymbol{b} = \boldsymbol{B}/B$, $\Omega \equiv eB/m$, and

$$V_\parallel = v\xi \boldsymbol{b} \cdot \nabla - \frac{1}{2} v(1-\xi^2)(\boldsymbol{b} \cdot \nabla \ln B) \frac{\partial}{\partial \xi}, \tag{4}$$

$$C^{\mathrm{PAS}} = \frac{\nu_{\mathrm{D}}}{2} \frac{\partial}{\partial \xi}(1-\xi^2) \frac{\partial}{\partial \xi}. \tag{5}$$

We employ the contravariant and covariant representations of $\boldsymbol{B}$ in Boozer coordinates (s, θ, ζ): $\boldsymbol{B} = \psi' \nabla s \times \nabla\theta + \chi' \nabla\zeta \times \nabla s = B_s \nabla s + B_\theta \nabla\theta + B_\zeta \nabla\zeta$, where θ and ζ are the poloidal and toroidal angles, s represents an arbitrary surface label, and the prime denotes the derivative with respect to s; $2\pi\chi$ and $2\pi\psi$ are the poloidal and toroidal fluxes, respectively. In Eq. (1), the function $\tilde{U}$ is the Pfirsch-Schlüter flow function defined in [9]. It can be written as

$$\tilde{U}(s, \theta, \zeta) = \frac{V'}{4\pi^2 B} \boldsymbol{B} \times \nabla s \cdot \nabla G(s, \theta, \zeta), \tag{6}$$

where $V(s)$ denotes the volume enclosed by the flux surface, while $G(s, \theta, \zeta)$ is obtained from $\psi'(\partial G/\partial\zeta) + \chi'(\partial G/\partial\theta) = \langle B^2 \rangle / B^2 - 1$. The effect of $\boldsymbol{E} \times \boldsymbol{B}$ drift is not considered in this work. For comparison, we also solved the two other drift-kinetic equations, DKE2 and DKE3, which are written as

- DKE2:

$$(\partial_t + V_\parallel - C^{\mathrm{PAS}}) \begin{bmatrix} g_1 \\ g_3 \end{bmatrix} = \begin{bmatrix} \sigma_1 \\ \sigma_3 \end{bmatrix}, \tag{7}$$

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$$\sigma_1 = -\boldsymbol{v}_\mathrm{d}\cdot\nabla s = -\frac{2v^2}{3\Omega}\left[1+\frac{1}{2}P_2(\xi)\right]\boldsymbol{b}\times\nabla\ln B\cdot\nabla s, \quad (8)$$

$$\sigma_3 = V_\parallel(Bv\xi/\nu_\mathrm{D}) = \frac{v^2}{\nu_\mathrm{D}}P_2(\xi)\boldsymbol{B}\cdot\nabla\ln B. \quad (9)$$

- DKE3:

$$(\partial_t + V_\parallel - C^\mathrm{PAS})\begin{bmatrix} g_1 \\ g_e \end{bmatrix} = \begin{bmatrix} \sigma_1 \\ \sigma_e \end{bmatrix}, \quad (10)$$

$$\sigma_e = Bv\xi. \quad (11)$$

For Eqs. (1), (7), and (10), the following identities hold if one assumes the steady-state solutions as $\partial_t g_i \equiv 0$ [9, 11]:

$$g_1 = -g_x - \frac{B}{\Omega}v\xi\tilde{U} + \frac{\nu_\mathrm{D}B}{\Omega}\int^l \tilde{U}\mathrm{d}l, \quad (12)$$

$$g_3 = -g_u/(m\nu_\mathrm{D}), \quad (13)$$

$$g_e = -g_3 + Bv\xi/\nu_\mathrm{D}, \quad (14)$$

where $\int^l \mathrm{d}l$ denotes the integral along the field line. The relationships among the microscopic fluxes σ_i can be written as

$$\sigma_3 = -\sigma_u/(m\nu_\mathrm{D}), \quad (15)$$

$$\sigma_1 = -\sigma_x - V_\parallel(Bv\xi\tilde{U}/\Omega). \quad (16)$$

The second and third terms of Eq. (12) are related to Pfirsch-Schlüter diffusion, while the second term of Eq. (14) indicates the classical Spitzer distribution, which is the solution of $-C^\mathrm{PAS}g_S = Bv\xi$. Noted that these terms do not contribute to off-diagonal elements of the neoclassical transport matrix, such as the bootstrap current coefficients, but contributes only to diagonal ones such as the Pfirsch-Schlüter diffusion and electrical conductivity coefficients. We emphasize that DKE1 *explicitly* removes these terms, which are irrelevant to off-diagonal transport coefficients, from the perturbed distribution functions that drive neoclassical transport.

Using the solutions of DKE1, DKE2, and DKE3, elements of the neoclassical transport matrix for each pair of indices, (x, u), $(1, 3)$, or $(1, e)$, can be evaluated as

$$D_{ij} = (\sigma_i, g_j), \quad (17)$$

where the parentheses denote the inner product operation $(\alpha,\beta) \equiv \frac{1}{2}\int_{-1}^{1}\mathrm{d}\xi\langle\alpha\beta\rangle$ with surface averaging $\langle\cdots\rangle$. The common properties of DKE1, DKE2, and DKE3 are the antisymmetry of $V_\parallel$ and the symmetry of C^PAS with respect to the inner product operation. These can be written as

$$(\alpha, V_\parallel\beta) = -(V_\parallel\alpha,\beta), \quad (\alpha, C^\mathrm{PAS}\beta) = (C^\mathrm{PAS}\alpha,\beta). \quad (18)$$

Using Eq. (18), the Onsager symmetry of the transport matrix can be formally shown for DKE1 and 2 such that

$$(\sigma_i, g_j) = (\sigma_j, g_i) \quad \text{for} \quad (1,3), \text{ or } (x,u). \quad (19)$$

For DKE3, $D_{e1} = -D_{1e}$ because of the odd parity of σ_e, but $|D^*_{xu}| = |D^*_{31}| = |D^*_{e1}|$, where asterisks denote the appropriate normalization following that of Ref. [9]. We note that the accuracy of $D_{ij} = D_{ji}$ for $i \neq j$ depends on the phase space resolution of δf Monte Carlo methods because Eq. (18) can be realized only in the limit of a large number of test particles as $N \to \infty$, which is normally inaccessible in particle simulations.

The property of the neoclassical transport matrix D_{ij} in the axisymmetric limit of magnetic field geometry plays an important role in this work. As derived in Ref. [14], for DKE1, the microscopic flux σ_x can be analytically decomposed into two parts; $\sigma_x \equiv \sigma_x^\mathrm{(sym)} + \sigma_x^\mathrm{(asym)}$, where

$$\sigma_x^\mathrm{(sym)} \equiv -\frac{\sigma_u}{2e\chi'\psi'}\left[\frac{\psi' B_\zeta - \chi' B_\theta}{\langle B^2\rangle} + \frac{V'}{4\pi^2}H_2\right], \quad (20)$$

$$\sigma_x^\mathrm{(asym)} \equiv \frac{m}{2e\chi'\psi'}\frac{B}{\langle B^2\rangle}v^2P_2(\xi)\left[\chi'(1-H_2)\frac{\partial B}{\partial\theta} - \psi'(1+H_2)\frac{\partial B}{\partial\zeta}\right] + \frac{m}{e}\frac{B}{\langle B^2\rangle}v^2P_2(\xi) \times\left[\frac{\partial G}{\partial\zeta}\frac{\partial B}{\partial\theta} - \frac{\partial G}{\partial\theta}\frac{\partial B}{\partial\zeta}\right]. \quad (21)$$

The function H_2 is given by [15]

$$H_2 \equiv \frac{\langle(\chi'\partial B/\partial\theta_\mathrm{H})^2 - (\psi'\partial B/\partial\zeta_\mathrm{H})^2\rangle}{\langle(\chi'\partial B/\partial\theta_\mathrm{H} + \psi'\partial B/\partial\zeta_\mathrm{H})^2\rangle}, \quad (22)$$

where θ_H and ζ_H are the poloidal and toroidal angles in Hamada coordinates. With this decomposition, one can show that for axisymmetric plasmas, σ_x becomes proportional to σ_u. Note that $\sigma_x = \sigma_x^\mathrm{(sym)} = F_u\sigma_u$ with the surface quantity $F_u = -B_\zeta/[e\chi'\langle B^2\rangle]$, defined by Eq. (20) because $\sigma_x^\mathrm{(asym)} \equiv 0$. The linearity of Eq. (1) leads to $g_x = g_x^\mathrm{(sym)} = F_u g_u$. According to this property, the transport matrix D_{ij} $(i, j = x, u)$ for axisymmetric plasmas substantially degenerates to single elements D_{uu}. For diagonal elements, $D_{xx} = F_u^2 D_{uu}$, while for off-diagonal elements, the Onsager relation holds exactly without invoking the symmetric properties of Eq. (18) as

$$(\sigma_x, g_u) = (\sigma_u, g_x) = F_u D_{uu}. \quad (23)$$

It is worth noting that this degeneracy in axisymmetric tokamaks is related to vanishing toroidal viscosity. To ensure the Onsager relation for DKE2 and 3 in the axisymmetric limit, we also need to impose the symmetric properties of Eq. (18) and the orthogonality conditions, namely $(\alpha,\beta) = 0$. However, these properties and conditions are not exact. They depend on the phase space resolution. For instance, $(Bv\xi\tilde{U}/\Omega, \sigma_3) \approx 0$ is an approximate expression with large finite N. In what follows, we demonstrate the above consideration regarding the Onsager relation in axisymmetric systems by performing δf drift-kinetic simulations.

To solve the linearized drift-kinetic equations, we used the linearized δf Monte Carlo weighting scheme

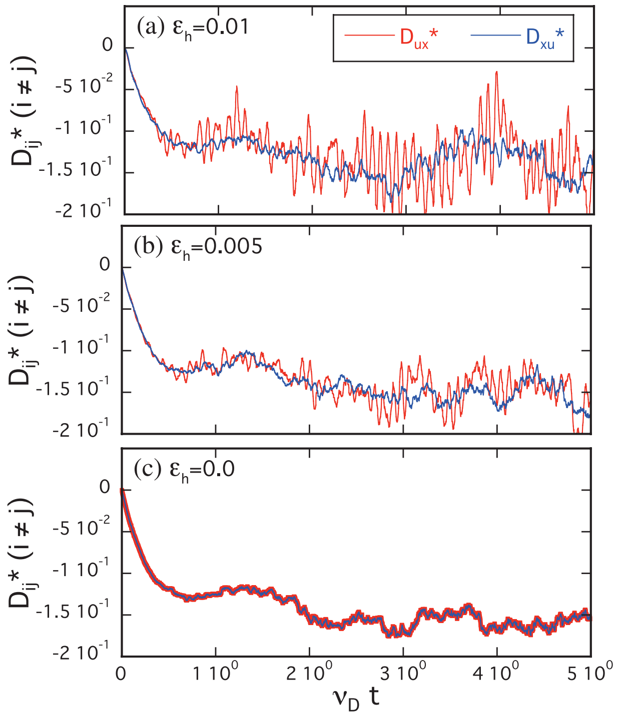

Fig. 1 Time history of off-diagonal transport coefficients D^*_{xu} and D^*_{ux} calculated with DKE1 for three different ϵ_h (where $\epsilon_t = 0.1$). The collisionality is $\nu_D/v = 3 \times 10^{-2}$. The number of particles used is $N = 3000$.

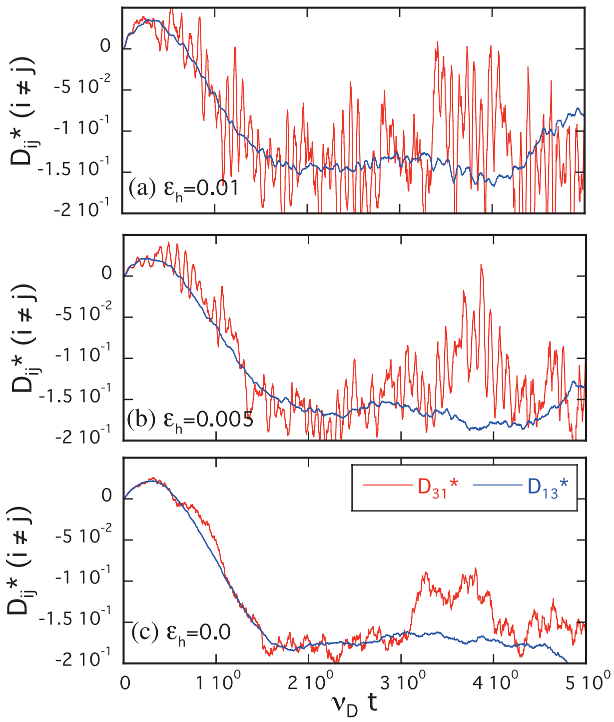

Fig. 2 Time history of off-diagonal transport coefficients D^*_{31} and D^*_{13} calculated with DKE2 for three different ϵ_h (where $\epsilon_t = 0.1$). The collisionality is $\nu_D/v = 3 \times 10^{-2}$. The number of particles used is $N = 3000$.

(e.g., as discussed in Ref. [3]), which is suitable for determining local transport coefficients as functions of the surface label without causing particle loss from the computational region. The lowest-order guiding-center motion (i.e., the parallel motion along the field lines) is solved by the fourth-order Runge Kutta method, and the pitch-angle scattering operator is implemented in the manner of Boozer and Kuo-Petravic [16]. The magnetic field used here is the single-helicity model $B = B_0[1 - \epsilon_t \cos\theta - \epsilon_h \cos(2\theta - 10\zeta)]$, whose configuration parameters are those listed in Ref. [7].

To examine the Onsager relations numerically, we calculated normalized off-diagonal elements $D^*_{ij}\,(i \neq j)$ with DKE1 in exact ($\epsilon_h = 0$) and in nearly axisymmetric ($\epsilon_h = 0.005$ and 0.01) systems. Figure 1 shows the time history of a pair of off-diagonal elements D^*_{xu} and D^*_{ux} for the collisionality $\nu_D/v = 3 \times 10^{-2}$ (located between the plateau and Pfirsch-Schlüter regimes for $\epsilon_h = 0$). The results obtained with DKE1 clearly indicate that the difference $|D^*_{xu} - D^*_{ux}|$ between off-diagonal elements, which is a measure of the numerical error in the Onsager relation, monotonically decreases with the reduction of the helical perturbation. In the limit of axisymmetry, the Onsager relation holds regardless of time $\nu_D t$ as the relation $\sigma_x \propto \sigma_u$ suggests. Similar calculations performed with DKE2, however, uncovered an important difference. As shown in Fig. (2), $|D^*_{13} - D^*_{31}|$ calculated with DKE2 decreased with ϵ_h but did not vanish, even in the axisymmetric limit.

To clarify the nonvanishing errors $|D^*_{ij} - D^*_{ji}|\,(i \neq j)$ for nonaxisymmetric runs in Fig. 1, we examined the convergence properties of the Onsager relation for small but finite ϵ_h. In Fig. 3, by changing the number of particles N used, we illustrate how the time history of the pair of off-diagonal elements D^*_{xu} and D^*_{ux} calculated with DKE1 is affected. One can see a clear reduction in the error associated with the Onsager symmetry with increasing N in the simulations. In Fig. 4, the dependences of the errors $|D^*_{ij} - D^*_{ji}|$ $(i \neq j)$ on N are compared for the three drift-kinetic equations. Note that $|D^*_{e1} + D^*_{1e}|$ has been evaluated for $(1, e)$ because of odd parity. From Fig. 4, we see that the errors $|D^*_{ij} - D^*_{ji}|$ $(i \neq j)$ have Monte-Carlo convergences of $1/\sqrt{N}$ for all the pairs. Although $|D^*_{ij} - D^*_{ji}|$ were comparable with any choices of the drift-kinetic equation for the lower collisionality $\nu_D/v = 10^{-3}$, the smaller error was observed with DKE1 in the plateau and Pfirsch-Schlüter regimes, where the Pfirsch-Schlüter diffusion and Spitzer terms in Eqs. (12) and (14) become significant.

The degeneracy of σ_x to σ_u in the axisymmetric limit is physically interpreted by the fact that the banana-plateau fluxes become proportional to the parallel viscosity. In such systems, the geometric factor $G^{(\mathrm{BS})}$ is always constant such that $G^{(\mathrm{BS})} = -e\langle B^2\rangle D_{xu}/D_{uu} = B_\zeta/\chi'$. We have confirmed this by a numerical experiment estimating the geo-

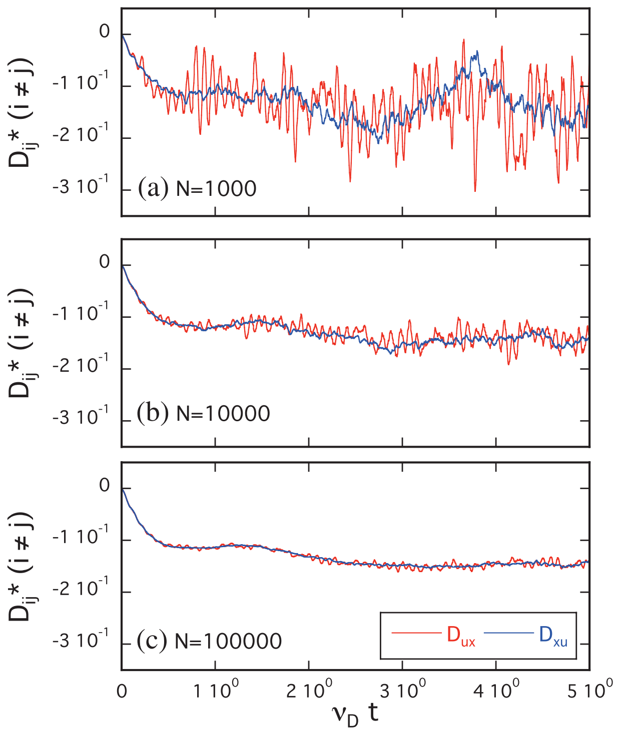

Fig. 3 Time history of off-diagonal transport coefficients D^*_{xu} and D^*_{ux} calculated with DKE1 for three different numbers of particles N, where $\epsilon_h = 0.01$ and $\epsilon_t = 0.1$. The collisionality is $\nu_D/v = 3 \times 10^{-2}$.

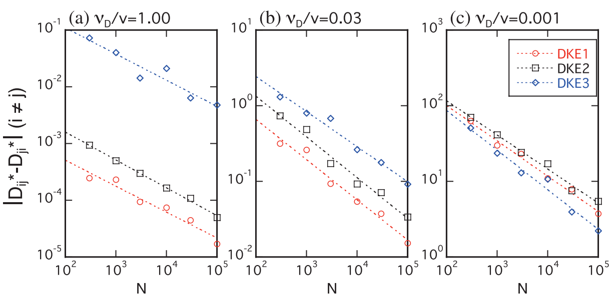

Fig. 4 Dependence of $|D^*_{ij} - D^*_{ji}|$ $(i \neq j)$ on the number of test particles N for three different drift-kinetic equations (DKE1, DKE2, and DKE3), where $\epsilon_h = 0.01$ and $\epsilon_t = 0.1$. The errors $|D^*_{ij} - D^*_{ji}|$ shown are the maximum (upper bound) in time. The collisionalities are (a) $\nu_D/v = 1 \times 10^0$, (b) 3×10^{-2}, and (c) 1×10^{-3}, respectively.

metric factor "dynamically" in terms of the time-dependent transport coefficients as

$$G^{(\mathrm{BS})}(t) = -\frac{\langle B^2 \rangle \bar{D}^*_{ij}(t)}{(\nu_D/v) D^*_{uu,\,\mathrm{or}\,33}(t)}, \tag{24}$$

where $\bar{D}^*_{ij}(t) = \frac{1}{2}[D^*_{ij}(t) + D^*_{ji}(t)]$ for $i \neq j$. Note that $D^*_{uu}(t) = D^*_{33}(t)$. Figure 5 shows the time history of $G^{(\mathrm{BS})}(t)$ for quasi-axisymmetric systems with DKE1 and DKE2. We have also plotted the $G^{(\mathrm{BS})}$ given in Ref. [9] (calculated with the DKES code) for finite ϵ_h cases. As shown

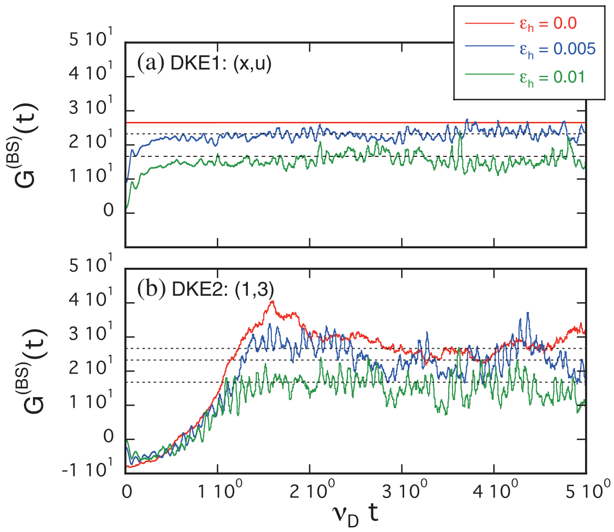

Fig. 5 "Dynamical" estimation of the geometric factor $G^{(\mathrm{BS})}(t)$ with (a) DKE1 and (b) DKE2 for nearly axisymmetric systems with $\epsilon_h = 0, 0.005$, and 0.01, where $\epsilon_t = 0.1$. Dashed lines indicate the numerical value obtained from the DKES code in Ref. [9]. The collisionality is $\nu_D/v = 3 \times 10^{-2}$; 3000 particles are employed.

in Fig. 5, DKE1 can properly reproduce $G^{(\mathrm{BS})} = B_\zeta/\chi'$ in the axisymmetric case because of the degeneracy $\sigma_x \propto \sigma_u$. Simulation results obtained with DKE1 converged to results from the DKES code faster than those with DKE2.

In summary, we have shown that DKE1 can appropriately treat numerical solutions of the drift-kinetic equations in axisymmetric systems by explicitly excluding the Pfirsch-Schlüter diffusion and Spitzer terms. These terms are irrelevant to the off-diagonal neoclassical transport coefficients and cause additional "numerical noise" that breaks the Onsager relations. Theoretically, the importance of excluding these collisional contributions can be explained by the the formal decomposition of the entropy-production rate [17] with the banana-plateau and with the Pfirsch-Schlüter fluxes, which was derived by Sugama and Horton [17]. The numerically realized constancy of the geometric factor obtained with DKE1 in the exact symmetric limit would be useful for simulation studies of quasi-symmetric stellarators.

We here investigated the numerical accuracy of the Onsager relations for nonaxisymmetric toroidal plasmas as well. Although many authors [17–21] have discussed the Onsager symmetry with respect to neoclassical transport by analytical treatments, we showed that the Onsager relations for nonaxisymmetric systems inherently depend on the phase space resolution, which has been demonstrated by the $1/\sqrt{N}$ scaling of Fig. 4. To our knowledge, such numerical confirmation of $D_{ij} = D_{ji}$ for $i \neq j$ with Monte Carlo methods has not been reported so far.

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