

Mass dispersion in transfer reactions with a stochastic mean-field theory

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Nucleon transfer in symmetric heavy-ion reactions at energies below the Coulomb barrier is investigated in the framework of a microscopic stochastic mean-field theory. Although mean field alone is known to significantly underpredict the dispersion of the fragment mass distribution, a considerable enhancement of the dispersion is obtained in the stochastic mean-field theory. The variance of the fragment mass distribution deduced from the stochastic theory scales with the number of exchanged nucleons. Therefore, the new approach provides the first fully microscopic theory consistent with the phenomenological analysis of the experimental data.

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The mean-field theory, otherwise known as the time-dependent Hartree-Fock (TDHF) model [1–6], has been widely used in describing reaction dynamics at low energies in nuclear collisions and other many-body systems. It is well known that the mean-field theory provides a good description of mean values of one-body observables in low energy reactions. However, it completely fails in the description of the dynamics of fluctuations of one-body observables. During the past decades, much effort has been devoted to overcoming this difficulty and to developing transport theories that are able to describe not only mean values but also fluctuations (for a review, see Refs. [7,8]). Among them, the variational principle proposed by Balian and Vénéroni (BV) appears as one of the most promising methods [9–11]. However, even nowadays it remains difficult to apply [12,13]. More than 30 years after the first application of TDHF, the absence of a practical solution to include fluctuations beyond mean field in a fully microscopic framework strongly restricts applications of mean-field-based theories.

There are mainly two mechanisms for density fluctuations: (i) collisional fluctuations generated by two-body collisions and (ii) one-body mechanisms or mean-field fluctuations. At low bombarding energies, the mean-field fluctuations provide the dominant mechanism for fluctuations of collective motion and collisional effects could be neglected. Restricting the treatment at low energies, recently, a stochastic mean-field (SMF) approach was proposed for nuclear dynamics [14]. It was demonstrated that the approach incorporates the one-body dissipation and associated fluctuation mechanism in accordance with the quantal dissipation-fluctuation relation. Furthermore, in the limit of small amplitude fluctuations, the SMF approach gives the same result for the dispersion of one-body observables as that of the formula derived from the BV approach [9,10]. Therefore, the SMF approach provides a powerful tool for describing low energy nuclear processes including induced fission, heavy-ion fusion near barrier energies, deep-inelastic collisions, and spinodal decomposition of nuclear matter [15]. In this work, by extending the previous work [16], we study nucleon exchange in low energy nuclear collisions and calculate the dispersion of the fragment mass distribution [2–4,6,17]. Diffusion coefficients for nucleon

exchange as well as for momentum transfer extracted from the SMF approach have the same structure as the result familiar from the phenomenological nucleon exchange model.

The SMF approach is based on a very appealing stochastic model proposed for describing deep-inelastic heavy-ion collisions and sub-barrier fusion [18–20]. In that model, the dynamics of relative motion is coupled to collective surface modes of colliding ions and treated in a classical framework. The initial quantum zero-point fluctuations are incorporated into the calculations in a stochastic manner by generating an ensemble of events according to the initial distribution of collective modes. In the mean-field evolution, couplings of relative motion with all other collective and noncollective modes are automatically taken into account. In the stochastic extension of the mean-field approach, the zero-point (and thermal) fluctuations of the initial state are taken into account in a stochastic manner, which is similar to the spirit presented in Refs. [18–20]. The initial fluctuations are simulated by considering an ensemble of initial single-particle density matrices. In this manner, the single Slater determinantal description is replaced by a superposition of Slater determinants. A member of the ensemble, indicated by event label λ , can be expressed as

$$\rho^\lambda(\mathbf{r}, \mathbf{r}', t) = \sum_{ij\sigma\tau} \Phi_{i\sigma\tau}^*(\mathbf{r}, t; \lambda) \rho_{ij}^\lambda(\sigma\tau) \Phi_{j\sigma\tau}(\mathbf{r}', t; \lambda), \quad (1)$$

where summations i and j run over a complete set of single-particle states $\Phi_{i\sigma\tau}(\mathbf{r}, t; \lambda)$, and σ and τ denote spin and isospin quantum numbers. According to the description of the SMF approach [14], the elements of density matrices $\rho_{ij}^\lambda(\sigma\tau)$ are assumed to be time-independent random Gaussian numbers with mean value $\overline{\rho_{ij}^\lambda(\sigma\tau)} = \delta_{ij} n_i^{\sigma\tau}$ and the variance of the fluctuating part $\delta\rho_{ij}^\lambda(\sigma\tau)$ is specified by

$$\begin{aligned} & \overline{\delta\rho_{ij}^\lambda(\sigma\tau) \delta\rho_{j'i'}^\lambda(\sigma'\tau')} \\ &= \frac{1}{2} \delta_{jj'} \delta_{ii'} \delta_{\sigma\tau} \delta_{\sigma'\tau'} [n_i^{\sigma\tau} (1 - n_j^{\sigma\tau}) + n_j^{\sigma\tau} (1 - n_i^{\sigma\tau})]. \end{aligned} \quad (2)$$

Here, $n_i^{\sigma\tau}$ denotes the average single-particle occupation factor. At zero temperature occupation factors are 0 and 1, and at finite temperature they are determined by the

Fermi-Dirac distribution. The great advantage of the SMF theory is that each Slater determinant λ evolves independently from each other following the time evolution of its single-particle wave functions in its self-consistent mean-field Hamiltonian, denoted by $h(\rho^\lambda)$, according to

$$i\hbar \frac{\partial}{\partial t} \Phi_{i\sigma\tau}(\mathbf{r}, t; \lambda) = h(\rho^\lambda) \Phi_{i\sigma\tau}(\mathbf{r}, t; \lambda). \quad (3)$$

Following Refs. [21,22], we project the mean-field evolution on a collective degree of freedom associated with nucleon transfer. For the projection, it is useful to introduce the Wigner distribution for the event λ defined as a partial Fourier transform of the density matrix,

$$\begin{aligned} f^\lambda(\mathbf{r}, \mathbf{p}, t) &= \int d^3s \exp\left(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{s}\right) \\ &\times \sum_{ij\sigma\tau} \Phi_{j\sigma\tau}^* \left(\mathbf{r} + \frac{\mathbf{s}}{2}, t; \lambda\right) \rho_{ji}^\lambda(\sigma\tau) \\ &\times \Phi_{i\sigma\tau} \left(\mathbf{r} - \frac{\mathbf{s}}{2}, t; \lambda\right). \end{aligned} \quad (4)$$

In this work, we focus on the particular case of head-on collisions along the x axis. We indicate the position of the separation plane between the two collision partners at $x = x_0$. Then, the mass number of the projectile-like fragment in the event λ is defined by

$$A_P^\lambda(t) = \int \frac{d^3r d^3p}{(2\pi\hbar)^3} \theta(x - x_0) f^\lambda(\mathbf{r}, \mathbf{p}, t). \quad (5)$$

Other macroscopic variables such as the separation distance between fragments and the associated momentum can be defined in a similar manner (see Ref. [22]). In the diffusion model, time evolution of the mass number of the projectile-like fragment A_P^λ is described by a Langevin equation [23],

$$\frac{d}{dt} A_P^\lambda = v(A_P^\lambda, t) + \xi_A^\lambda(t), \quad (6)$$

where $v(A_P^\lambda, t)$ denotes the drift coefficient for nucleon transfer. Ignoring memory effects, we consider the quantity $\xi_A^\lambda(t)$ as a Gaussian white noise, which is determined with zero mean value $\overline{\xi_A^\lambda(t)} = 0$ and a correlation function,

$$\overline{\xi_A^\lambda(t) \xi_A^\lambda(t')} = 2\delta(t - t') D_{AA}, \quad (7)$$

where D_{AA} is the diffusion coefficient associated with nucleon exchange. To extract the diffusion coefficient, we calculate the rate of change of A_P^λ employing the SMF equations. The rate of change of A_P^λ involves only the kinetic part of the mean-field Hamiltonian and it can be expressed in terms of the reduced Wigner distribution on the window as

$$\frac{d}{dt} A_P^\lambda = - \int \frac{dp_x}{2\pi\hbar} \frac{p_x}{m} f^\lambda(x, p_x, t)|_{x=x_0}, \quad (8)$$

where the reduced Wigner distribution $f^\lambda(x, p_x, t)$ is obtained by integrating over the phase-space variables y, z, p_y , and p_z according to

$$f^\lambda(x, p_x, t) = \iint dy dz \frac{dp_y dp_z}{(2\pi\hbar)^2} f^\lambda(\mathbf{r}, \mathbf{p}, t). \quad (9)$$

Small fluctuations of the mass number are connected to small amplitude fluctuations of the Wigner distribution according to

$$\frac{d}{dt} \delta A_P^\lambda = - \int \frac{dp_x}{2\pi\hbar} \frac{p_x}{m} \delta f^\lambda(x, p_x, t)|_{x=x_0} = \xi_A^\lambda(t). \quad (10)$$

In Ref. [16], we derived an expression for the correlation function of the reduced Wigner distribution in the semiclassical approximation. Employing the result derived in that reference, we have the following expression for the nucleon diffusion coefficient,

$$\begin{aligned} D_{AA}(t) &= \int \frac{dp_x}{2\pi\hbar} \frac{|p_x|}{m} \frac{1}{2} \\ &\times \sum_{\sigma\tau} \{ f_P^{\sigma\tau}(x_0, p_x, t) [1 - f_T^{\sigma\tau}(x_0, p_x, t)/\Omega(x_0, t)] \\ &+ f_T^{\sigma\tau}(x_0, p_x, t) [1 - f_P^{\sigma\tau}(x_0, p_x, t)/\Omega(x_0, t)] \}. \end{aligned} \quad (11)$$

Here $\Omega(x_0, t)$ is the phase-space volume over the window and

$$\begin{aligned} f_{P/T}^{\sigma\tau}(x_0, p_x, t) &= \iint dy dz \int ds_x \exp\left(-\frac{i}{\hbar} p_x s_x\right) \\ &\times \sum_{i \in P/T} \Phi_{i\sigma\tau}^* \left(x + \frac{s_x}{2}, y, z, t\right) n_i^{\sigma\tau} \\ &\times \Phi_{i\sigma\tau} \left(x - \frac{s_x}{2}, y, z, t\right) \end{aligned} \quad (12)$$

is the averaged value of the reduced Wigner distribution associated with single-particle wave functions originating from the projectile/target. Details on the determination of $\Omega(x_0, t)$ can be found in Ref. [16].

We note that the expression of the diffusion coefficient has the same form as that given by the phenomenological nucleon exchange model in Ref. [24]. We also note that diffusion coefficients not only for nucleon exchange but also associated with other macroscopic variables are evaluated in terms of the average evolution specified by the standard TDHF evolution. In computations, to employ fully quantum mechanical expression for the reduced Wigner distribution does not provide a consistent description because the diffusion coefficient is derived in the semiclassical approximation. A semiclassical form of the reduced Wigner distribution can be obtained by approximating the s_x dependence of the integrand of Eq. (4) by a Gaussian. The mean value and the second moment of this Gaussian are determined by carrying out a Taylor expansion of the integrand up to second order in s_x .

We carry out calculations for head-on collisions of symmetric $^{40}\text{Ca} + ^{40}\text{Ca}$, $^{56}\text{Ni} + ^{56}\text{Ni}$, and $^{90}\text{Zr} + ^{90}\text{Zr}$ systems at energies just below the Coulomb barrier. Calculations are performed using the three-dimensional TDHF code developed by P. Bonche and co-workers with the SLy4d Skyrme effective force [25]. For technical details, see Ref. [21]. Colliding ions approach each other, exchange a number of nucleons, and then re-separate. In symmetric collisions by TDHF, there is no net nucleon transfer; i.e., drift is zero. According to the Langevin equation, the variance $\sigma_{AA}^2(t) = \overline{\delta A_P^\lambda \delta A_P^\lambda}$ of fragment mass distribution, neglecting contributions from the drift term, is

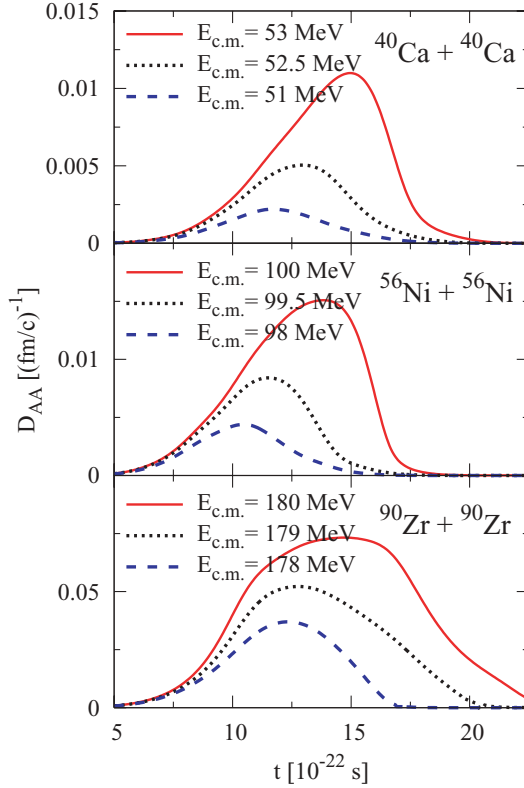


FIG. 1. (Color online) Evolution of diffusion coefficients calculated in the SMF approach for $^{40}\text{Ca} + ^{40}\text{Ca}$ (top), $^{56}\text{Ni} + ^{56}\text{Ni}$ (middle), and $^{90}\text{Zr} + ^{90}\text{Zr}$ (bottom) collisions at different center-of-mass energies.

related to the diffusion coefficient according to [23,26]

$$\sigma_{AA}^2(t) \simeq 2 \int_0^t D_{AA}(s) ds = N_{\text{exc}}(t). \quad (13)$$

In this expression $N_{\text{exc}}(t)$ denotes the accumulated total number of exchanged nucleons until time t . The relation $\sigma_{AA}^2(t) = N_{\text{exc}}(t)$ follows from the nucleon exchange model and it was often used to analyze the experimental data. In the SMF model, we can calculate both sides of this relation independently.

Figure 1 illustrates the dependence of diffusion coefficients for collisions of three different symmetric systems at different center-of-mass energies. The Coulomb barrier energies, which are obtained in the frozen density approximation [27], are 54.7, 103, and 184 MeV for the ^{40}Ca , ^{56}Ni , and ^{90}Zr systems, respectively. The magnitude of the diffusion coefficient essentially depends on the size of the window, the larger the window the larger the rate of change of nucleon exchange [26]. At a given center-of-mass energy, the diffusion coefficient becomes maximum at the turning point where the size of the window is the largest. Also, as seen from the figure, because of increasing overlap of the projectile and the target, the magnitude of the diffusion coefficient increases with energy.

Figure 2 illustrates the variances of the fragment mass distributions as a function of time for the same symmetric systems at the same center-of-mass energies as those in Fig. 1. Lines are the results obtained by the integration

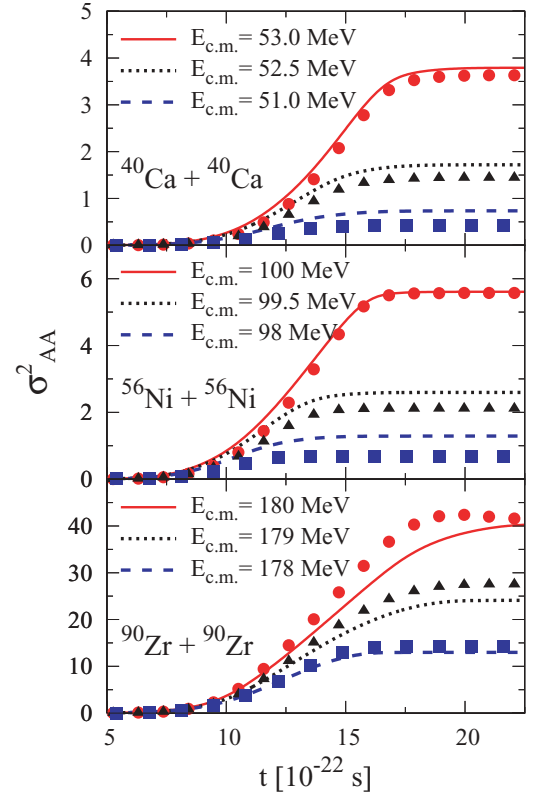


FIG. 2. (Color online) Evolution of σ_{AA}^2 calculated in the SMF approach for $^{40}\text{Ca} + ^{40}\text{Ca}$ (top), $^{56}\text{Ni} + ^{56}\text{Ni}$ (middle), and $^{90}\text{Zr} + ^{90}\text{Zr}$ (bottom) collisions at different center-of-mass energies. Number of exchanged nucleons is superimposed by the solid circles, solid triangles, and solid squares from high to low energies.

of the diffusion coefficient in Eq. (13). In each case, the corresponding evolution of the number of exchanged nucleons is superimposed by the solid circles, solid triangles, and solid squares from high to low energies. We also calculate the variances of fragment mass distribution using standard TDHF approach. In Table I, for the same systems at the same energies, the asymptotic values $\sigma_{\text{TDHF}}^2(+\infty)$ of the variances obtained from TDHF is compared with the asymptotic values $\sigma_{AA}^2(+\infty)$ calculated in the SMF approach. In the same table,

TABLE I. Asymptotic values of the fragment mass variances for $^{40}\text{Ca} + ^{40}\text{Ca}$, $^{56}\text{Ni} + ^{56}\text{Ni}$, and $^{90}\text{Zr} + ^{90}\text{Zr}$ collisions in SMF (σ_{AA}^2) and TDHF (σ_{TDHF}^2). Asymptotic values of the number of exchanged nucleons are also given in the last column.

Reaction	$E_{\text{c.m.}}$ (MeV)	$\sigma_{\text{TDHF}}^2(+\infty)$	$\sigma_{AA}^2(+\infty)$	$N_{\text{exc}}(+\infty)$
$^{40}\text{Ca} + ^{40}\text{Ca}$	51.0	0.004	0.730	0.432
	52.5	0.008	1.718	1.441
	53.0	0.008	3.790	3.634
$^{56}\text{Ni} + ^{56}\text{Ni}$	98	0.024	1.288	0.667
	99.5	0.088	2.594	2.111
	100	0.142	5.606	5.567
$^{90}\text{Zr} + ^{90}\text{Zr}$	178	0.774	12.98	14.19
	179	1.046	24.09	27.51
	180	1.085	40.40	41.56

the asymptotic values of the number of exchanged nucleons $N_{\text{exc}}(+\infty)$ are also given.

The semi-empirical relation $\sigma_{AA}^2(t) \simeq N_{\text{exc}}(t)$ has been extensively used to analyze experimental data [28,29]. As seen in Table I, the mass variance estimated from the SMF approach is consistent with this relation. Looking at the asymptotic values, in all cases, the TDHF results $\sigma_{\text{TDHF}}^2(+\infty)$ for the variance are much smaller than the results $\sigma_{AA}^2(+\infty)$ obtained in the SMF approach and are also much smaller than the results $N_{\text{exc}}(+\infty)$. The failure of TDHF on the description of variances of the fragment mass distribution has been recognized for a long time as a major limitation of the mean-field theory. It appears that the SMF approach cures this shortcoming of the mean-field theory. As seen from Fig. 2, both the asymptotic value of σ_{AA}^2 and the entire time evolution are very close to the evolution of $N_{\text{exc}}(t)$. The small differences may arise from the estimation of the phase-space volume on the window and/or from the Gaussian approximation for the reduced Wigner distribution.

In summary, we investigate the variances of fragment mass distributions in heavy-ion collisions at energies near the Coulomb barrier by employing the microscopic SMF approach. By projecting the SMF equation on the mass-asymmetry macroscopic variable, we deduce the diffusion coefficient associated with nucleon exchange. The expression of the diffusion coefficient has a structure similar to that of

those familiar from the phenomenological nucleon exchange model. Comparison between the calculated variance and the number of exchanged nucleons supports a strong confirmation for the fact that the SMF approach provides a realistic description of dissipation and fluctuation dynamics at low energies. The stochastic extension of the mean-field theory provides a practical solution to the estimate of fluctuations of observables at low energies. We have shown here that fluctuations comparable with macroscopic models can be recovered using the SMF approach. A quantitative comparison with experimental data requires that our work be extended to off-central collisions. In the continuation of this work, we plan to carry out calculations for grazing deep-inelastic collisions of symmetric and nonsymmetric heavy ions, for which plenty of experimental data are available for comparison. It can be applied not only to nuclear dynamics but also to the description of fluctuating dynamics of many-body problems in other areas of physics.

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