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Correlation Functions of Infinite System of Interacting Brownian Particles; Local in Time Evolution Close to Equilibrium

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The time-dependent correlation functions of infinite nonequilibrium systems of interacting diffusing particles are obtained in the thermodynamic limit in the case when the initial correlation functions coincide with the equilibrium correlation functions of the Gibbs system in an external field.

KEY WORDS: n-particle diffusion equation; stable integrable monotone potential; diffusion hierarchy; thermodynamic limit.

1. INTRODUCTION

Evolution of Brownian particles interacting via a pair potential ϕ may be described by a gradient system of stochastic differential equations

$$dx_j(t) = \sum_{\substack{i=1 \\ i\neq j}}^{n} (\nabla\phi)(x_i - x_j) + \beta^{-1/2} dw_j(t) \tag{1.1}$$

where $x_j(t)$ is a three-dimensional position vector of a particle labeled by j, $\{w_j(t)\}_{j=1}^{n}$ is a sequence of independent d-dimensional Wiener processes, and β is the inverse temperature,

$$(\nabla\phi)(x) = \frac{\partial\phi(x)}{\partial x} = \left(\frac{\partial\phi(x)}{\partial x^1}, \frac{\partial\phi(x)}{\partial x^2}, \frac{\partial\phi(x)}{\partial x^3}\right)$$

The solution of (1.1) can be obtained for bounded smooth potential by standard methods of probability theory.

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An important problem of statistical mechanics of nonequilibrium systems is to construct solutions of (1.1) in the limit of an infinite system ($n \to \infty$).

The first results concerning the problem was obtained by R. Lahg[1] for smooth, short-range potentials.

Evolution of n-particle system of interacting Brownian particles can also be described by the Smoluchowski equation which is the forward Kolmogorov equation for (1.1) for the probability density

$$\frac{\partial \rho_0(x_1, \ldots, x_n, t)}{\partial t} = \sum_{j=1}^{n} \frac{\partial}{\partial x_j} \left\{ \beta^{-1} \frac{\partial \rho_0(x_1, \ldots, x_n, t)}{\partial x_j} + \rho_0(x_1, \ldots, x_n, t) \sum_{\substack{i=1 \\ i \neq j}}^{n} (\nabla \phi)(x_i - x_j) \right\} \tag{1.2}$$

This equation approximates evolution of a mechanical system of two kinds of particles.[3] A discussion of rigorous results concerning the diffusion approximations can be found in Refs. 4 and 5.

To evolution of an infinite system there corresponds a hierarchy of equations for correlation functions

$$\frac{\partial \rho(x_1, \ldots, x_m, t)}{\partial t} = \sum_{j=1}^{m} \frac{\partial}{\partial x_j} \left\{ \beta^{-1} \frac{\partial \rho(x_1, x_m, t)}{\partial x_j} + \rho_0(x_1, x_m, t) \sum_{\substack{i=1 \\ i \neq j}}^{n} (\nabla \phi)(x_i - x_j) + \int_{\mathbb{R}^3} (\nabla \phi)(x_j - x_{m+1}) \rho(x_1, \ldots, x_{m+1}, t)\, dx_{m+1} \right\} \tag{1.3}$$

The hierarchy plays the role of the forward Kolmogorov equation for the infinite stochastic gradient system and it was derived in Ref. 6 for thermodynamic limit of a sequence of canonical correlation functions.

A natural candidate for a solution of (1.3) is thermodynamic limit of a sequence of grand canonical correlation functions $\rho^{\Lambda}(x_1, \ldots, x_m, t)$ of a system enclosed in a compact domain Λ.

These functions have the following representation:

$$\rho^{\Lambda}(x_1, \ldots, x_m, t) = \Xi_{\Lambda}^{-1} \sum_{n \geqslant 0} \frac{1}{n!} \int_{\Lambda^n} dx_{m+1} \ldots dx_{m+n} \rho_0(x_1, \ldots, x_{m+n}, t) \tag{1.4}$$

$$\Xi_{\Lambda} = \sum_{n \geqslant 0} \frac{1}{n!} \int_{\Lambda^n} dx_1 \cdots dx_n \rho_0(x_1, \ldots, x_n, t)$$

where $\rho_0(x_1, \ldots, x_n, t)$ is a bounded solution of (1.2) in $\mathbb{R}^{3n}$.

To simplify the matter we do not demand that $\rho_0(x_1, \ldots, x_n, t)$ satisfies a boundary conditions at the boundary of Λ.

In this paper we consider the problem of thermodynamic limit for the correlation functions $\rho^{\Lambda}(x_1, \ldots, x_m, t)$ when initial correlation functions $\rho_0(x_1, \ldots, x_n)$ corresponds to the equilibrium state with a polynomially decreasing potential $\phi(x)$ perturbed by an external field $\varphi(x)$ (see also Ref. 7). A similar problem was considered for one-dimensional mechanical systems in (8, 9).

We obtain for $\rho^{\Lambda}(x_1, \ldots, x_m, t)$ a series in powers of the activity $\mathscr{Z}$, prove that the series converges in a domain independent of Λ and perform the thermodynamic limit $(\Lambda \to \mathbb{R}^3)$ in every order of the perturbation series.

We start from a simple fact that (1.2) is connected with a heat equations, i.e., a parabolic equation whose right side contains a sum of derivatives of the second order (the $3n$-dimensional Laplacian) and a multiplicative term which can be interpreted as a potential energy with a pair and a three-body potentials. To get a solution of (1.2) one has to multiply a solution of the heat equation by an exponent of minus one half a potential.

It is known that the Cauchy problem for the heat equation is solved by the Feynman–Kac formula. Since the initial distribution is taken by us to be a Gibbs distribution characterized by a pair potential and an external field we obtain a solution of (1.2) as an integral over the Wiener measure concentrated on path starting from $(x_1, \ldots, x_n)$ of an exponent of two terms. The first term has a structure of a potential energy with a pair potential and the second has a structure of a positive potential energy with a three-body potential. The potential is stable if both $\phi(x)$ and $(-\Delta\phi)(x)$ are stable. We assume that the last condition is satisfied. As a consequence we have

$$\rho_0(x_1, \ldots, x_n, t) \leqslant \xi^n(t) \tag{1.5}$$

As a next step we introduce a sequence of new three-dimensional paths and a complex pair potential representing an exponent of the three-body term as a characteristic functional of the Wiener measure concentrated on $3n$-dimensional paths starting from the origin. The obtained expression for correlation functions resembles an expression for grand canonical density matrics of quantum systems.[10] By analogy with an algebraic technique[10,11] valid only for such systems with a pair potential we derive our perturbation series for correlation functions and obtain the necessary estimates.

2. MAIN CONDITIONS AND FORMULATIONS OF THE RESULT

We assume through our paper that the potential $\phi(x)$ satisfies the following conditions:

(C.1) The function ϕ is bounded and it has bounded partial derivatives up to the third order.

(C.2) The functions ϕ, $-\Delta\phi$ satisfy the stability conditions

$$\sum_{1\leqslant i<j\leqslant n} \phi(x_i - x_j) \geqslant -Bn, \qquad \sum_{1\leqslant i<j\leqslant n} (-\Delta\phi)(x_i - x_j) \geqslant -bn, \quad \Delta = \nabla^2$$

(C.3) There exists a bounded, monotone, integrable in $\mathbb{R}^3$ function $\omega(|x|)$ such that $\omega(|x|) \geqslant (1 + |x|)^{-4}$ and

$$|\phi(x)| \leqslant c\omega(|x|), \qquad |(\nabla\phi)(x)| \leqslant c\omega(|x|), \qquad |\Delta\phi(x)| \leqslant c\omega(|x|)$$

It is clear that (C.1) and (C.2) are satisfied if the Fourier transform $\hat{\phi}(k)$ of the function ϕ is positive and it belongs to $L^2(\mathbb{R}^3, |k|^3\,dk)$.

We shall also consider the solutions of (1.2) that in the initial moment look like the following:

(C.4) $\rho_0(x_1, \ldots, x_n) = \exp\{-\beta U(x_1, \ldots, x_n) - \beta \sum_{j=1}^{n} \varphi(x_j)\} \mathscr{Z}^n$ where $U(x_1, \ldots, x_n) = \sum_{1\leqslant i<j\leqslant n} \phi(x_i - x_j)$ and the external field $\varphi(x)$ is a bounded below measurable function: $\varphi(x) \geqslant -\varphi_0$.

Theorem. If the potential ϕ in (1.2) satisfies (C.1)–(C.3) and the initial distribution ρ_0 satisfies (C.4), then there exist a bounded continuous function $\rho_t(x_1, \ldots, x_m \mid x_1, \ldots, x_n')$ and positive entire function $k(t)$ such that $k(t) \xrightarrow[t\to\infty]{} \infty$,

$$\sup_{x_j\in\mathbb{R}^3} \int_{\mathbb{R}^{3n}} |\rho_t(x_1, \ldots, x_m \mid x_1', \ldots, x_n')|\, dx_1' \ldots dx_n' \leqslant n! \exp\{(m + n)k(t)\} \tag{2.1}$$

$$\rho^\Lambda(x_1, \ldots, x_m, t) = \sum_{n\geqslant 0} \frac{\mathscr{Z}^{n+m}}{n!} \int_{\Lambda^n} dx_1' \ldots dx_n'\, \rho_t(x_1, \ldots, x_m \mid x_1', \ldots, x_n') \tag{2.2}$$

Corollary. The correlation function $\rho^\Lambda(x_1, \ldots, x_m, t)$ is an analytic function of the activity in the domain $|\mathscr{Z}| < \exp\{-k(t)\}$.

The associated infinite volume correlation functions

$$\rho(x_1, \ldots, x_m, t) = \sum_{n \geqslant 0} \frac{\mathscr{Z}^n}{n!} \int_{\mathbb{R}^{3n}} dx'_1, \ldots, dx'_n \, \rho_t(x_1, \ldots, x_m \mid x'_1, \ldots, x'_n) \tag{2.3}$$

are analytic functions of the activity in the domain $|\mathscr{Z}| < \exp\{-k(t)\}$

3. CONSTRUCTION OF $\rho_t(x_1, \ldots, x_m \mid x'_1, \ldots, x'_n)$

It can be easily checked that the function $\sigma(X_n, t) = \exp\{(\beta/2)U(X_n)\}$ $\rho_0(X_n, t)$ (by a capital letter indexed by n we denote an element of $\mathbb{R}^{3n}$) satisfies the heat equation

$$\frac{\partial \sigma(X_n, t)}{\partial t} = \beta^{1}\left(\sum_{j=1}^{n} \Delta_j \sigma(X_n, t) + V(X_n)\sigma(X_n, t)\right) \tag{3.1}$$

where

$$V(X_n) = \frac{\beta}{2} \sum_{j=1}^{n} \Delta_j U(X_n) - \frac{\beta^2}{2} \sum_{j=1}^{n} (\nabla_j U)^2(X_n)$$

$$\Delta_j = \sum_{\nu=1}^{3} \frac{\partial^2}{\partial (x_j^\nu)^2}, \qquad \nabla_j = \left(\frac{\partial}{\partial x_j^1}, \frac{\partial}{\partial x_j^2}, \frac{\partial}{\partial x_j^3} \right), \qquad (\nabla_j U)^2 = \sum_{\nu=1}^{3} \frac{\partial U}{\partial x_j^\nu} \frac{\partial U}{\partial x_j^\nu}$$

The heat equation (3.1) is solved by the Feynman–Kac formula. Hence this formula permits to solve (1.2).

Proposition (3.1). Let $P_X(dZ)$ be the Wiener measure on the space Ω_3 of three-dimensional paths. If the potential satisfies (C.1) and the initial distribution ρ_0 satisfies (C.4) then the unique solution to the classic Cauchy problem of the Smoluchowski equation (1.2) is given by

$$\rho(X_n, t) = \mathscr{Z}^n \int_{\Omega_3^n} P_{X_n}(dZ_n) \exp\left\{ -\beta U_t(X_n, Z_n) - \beta \sum_{j=1}^{n} \varphi\big(z_j(\beta^{-1}t)\big)\right\} \tag{3.2}$$

where

$$P_{X_n}(dZ_n) = \prod_{j=1}^{n} P_{x_j}(dz_j)$$

$$U_t(X_n, Z_n) = \sum_{1 \leqslant i < j \leqslant n} \phi_t(x_i - x_j, z_i - z_j) + \frac{\beta}{4} \sum_{j=1}^{n} \int_0^{t\beta^{-1}} (\nabla_j U)^2(Z_n(\tau))\, d\tau \tag{3.3}$$

$$\phi_t(x, z) = \tfrac{1}{2}\left[\phi(x) + \phi\big(z(\beta^{-1})\big)\right] + \int_0^{t\beta^{-1}} (-\Delta\phi)(z(\tau))\, d\tau = \sum_{j=1}^{3} \phi_{t,j}(x, 2)$$

The "potential" $\phi_t(x,z)$ satisfies the stability condition

$$\sum_{1\leqslant i<j\leqslant n} \phi_t(x_i - x_j, z_i - z_j) \geqslant -nB_t, \qquad B_t = B + t\beta^{-1}b \tag{3.4}$$

From (3.4) we get (1.5).

The last term at the right side of (3.3) has a three-body structure. Now let us transform the Gibbs factor containing this term as

$$\exp\left\{ -\frac{\beta^2}{4}\sum_{j=1}^{n}\int_0^{t\beta^{-1}} (\nabla_j U)^2(Z_n(\tau))\,d\tau \right\}$$
$$= \int_{\Omega_3^n} P(dQ_n)\exp\left\{ \frac{i}{2}\beta\sum_{j=1}^{n}\int_0^{t\beta^{-1}} (\nabla_j U)(Z_n(\tau))\,dq_i(\tau) \right\}$$

where $P(dQ_n) = \prod_{j=1}^{n} P(dq_j)$ is the Wiener measure on Ω_3 concentrated on the paths starting from the origin, the differential $dq(\tau)$ of the Wiener path $q(\tau)$ defines a stochastic measure.

As a result we obtain for $\rho_0(X_n, t)$ the following representation:

$$\rho_0(X_n, t) = \mathscr{Q}^n \int_{\Omega_3^{2n}} P_{X_n}(dZ_n)\,P(dQ_n)\exp\{-\beta U_t(X_n, Z_n, Q_n)\}$$
$$\times \exp\left\{ -\beta\sum_{j=1}^{n}\varphi\big(z_j(\beta^{-1}t)\big)\right\} \tag{3.5}$$

where

$$U_t(X_n, Z_n, Q_n) = \sum_{1\leqslant k<j\leqslant n} \phi_t(x_k - x_j, z_k - z_j \mid q_k, q_j)$$

$$\phi_t(x,z\mid q,q') = \phi_t(x,z) + \frac{i}{2}\int_0^{t\beta^{-1}} (\nabla\phi)(z(\tau))\,(dq(\tau) - dq'(\tau))$$
$$= \phi_t(x,z) + \phi_{t,4}(x,z\mid q,q'),$$
$$(\nabla\phi)(z(\tau))\,dq(\tau) = \sum_{\nu=1}^{3}\frac{\partial\phi}{\partial z^\nu}\,dq^\nu(\tau)$$

Now the correlation functions $\rho^\Lambda(X_m, t)$ look like

$$\rho^\Lambda(X_m, t) = \int_{\Omega_3^{2m}} P_{X_m}(dZ_m)\,P(dQ_m)\,\rho_t^\Lambda(Z_m, Z_m, Q_m)$$
$$\rho_t^\Lambda(X_m, Z_m, Q_m) = \Xi_\Lambda^{-1}\sum_{n\geqslant 0}\frac{\mathscr{Q}^{n+m}}{n!}\int_{\Lambda^n} dX_n\int_{\Omega_3^{2n}} P_{X_n'}(dZ_n')\,P(dQ_n')$$
$$\times \exp\left\{ -\beta U(X_mX_n', Z_mZ_n', Q_mQ_n') \right.$$
$$\left. -\beta\sum_{j=1}^{m}\varphi\big(z_j(\beta^{-1}t)\big) - \beta\sum_{j=1}^{n}\varphi\big(z_j'(\beta^{-1}t)\big)\right\} \tag{3.6}$$

The function $\rho_t^\Lambda(X_m, Z_m, Q_m)$ has the structure of a grand canonical correlation function of a Gibbs system with a complex two-body potential.

With the help of the standard algebraic technique we obtain for $\rho^\Lambda(X_m, t)$ a formal perturbation series (2.4) with $\rho_t(X_m \mid X_n')$ given by

$$\rho_t(X_m \mid X_n') = \int_{\Omega_3^{2(m+n)}} P_{X_m}(dZ_m)\, P(dQ_m)\, P_{X_n'}(dZ_n')\, P(dQ_n')$$
$$\times \rho_t(X_m, Z_m, Q_m \mid X_n', Z_n', Q_n')$$
$$\times \exp\left\{ -\beta \sum_{j=1}^{m} \varphi\big(z_j(\beta^{-1}t)\big) - \beta \sum_{j=1}^{n} \varphi\big(z_j'(\beta^{-1}t)\big) \right\}, \quad (3.7)$$

where $\rho_t(X_m, Z_m, Q_m \mid X_n', Z_n', Q_n')$ satisfies the relation

$$\rho_t(X_m, Z_m, Q_m \mid X_n', Z_n', Q_n')$$
$$= \exp\left\{ -\beta \sum_{\substack{k=i \\ i\neq j}}^{m} \phi_t(x_j - x_k, z_j - z_k \mid q_k, q_j) \right\}$$
$$\times \sum_{\{s\}\in(1,n)} K(X_j, Z_j, Q_j \mid X'_{\{s\}}, Z'_{\{s\}}, Q'_{\{s\}})$$
$$\times \rho_t(X_{m(j)} X'_{\{s\}}, Z_{m(j)} Z'_{\{s\}}, Q_{m(j)} Q'_{\{s\}} \mid X'_{\{n\setminus s\}}, Q'_{\{n\setminus S\}}) \quad (3.8)$$

$$\rho_t(X_m, Z_m, Q_m \mid \phi) = \exp\{ -\beta U(X_m, Z_m, Q_m) \}$$

The summation in (3.8) is performed over all subsequences $\{s\}$ of the sequence $(1, \dots, n)$, $\{n\setminus s\} = (1, \dots, n)\setminus\{s\}$, $m(j) = (1, j-1, j+1, \dots, m)$, a capital letter indexed by $\{s\}$ denotes a sequence of three-dimensional variables indexed by the elements of the sequence $\{s\}$,

$$K(x, z, q \mid X_n', Z_n', Q_n') = \prod_{j=1}^{n} \left(\exp\{ -\beta\phi_t(x - x_j', z - z_j' \mid q, q_j')\} - 1\right)$$

Lemma. If the conditions (C.1), (C.2), (C.4) are satisfied then there holds the inequality

$$\sup_{x_j\in\mathbb{R}^3} \int_{\mathbb{R}^{3n}} dX_n'\, \rho_t(X_m \mid X_n')$$
$$\leqslant n! \left[\exp\{4\beta B_t + 2\beta\psi_0\} \sum_{p=0}^{n} \frac{2^{p+1}}{(p!)^2} \left(\sup_{x\in\mathbb{R}^3} \int_{\mathbb{R}^{3p}} dX_p\, K(X_p \mid x) \right)^2 \right]^{(m+n)/2} \quad (3.9)$$

where

$$K^2(X_p \mid x) = \int_{\Omega_3^2} P_X(dZ)\, P(dq) \prod_{j=1}^{n} \int_{\Omega_3^2} P_{X_j}(dZ_j)\, P(dQ_j) \times \left|\exp\{-\beta_t^{\phi}(x - x_j, z - z_j \mid q, q_j)\} - 1\right|^2$$

Proof. Let us put

$$|\rho_t|_n(X_m, Z_m, Q_m) = \int_{\mathbb{R}^{3n}} dX'_n \int_{\Omega_3^{2n}} P_{X'_n}(dZ'_n)\, P(dQ'_n) \times |\rho_t(X_m, Z_m, Q_m \mid X'_n, Z'_n, Q'_n)|,$$

$$|\rho_t|_{n,2}^2(X_m, Z_m, Q_m \mid X_{\{k\setminus m\}}) = \int_{\Omega_3^{k-m}} P_{X_{\{k\setminus m\}}}(dZ_{\{k\setminus m\}})\, P(dQ_{\{k\setminus m\}}) \times |\rho_t|_n^2(X_k, Z_k, Q_k), \qquad k \geqslant m$$

$$\|\rho_t\|_{m,n}^2 = \sup_{x_j \in \mathbb{R}^3} \int_{\Omega_3^m} P_{X_m}(dZ_m)\, P(dQ_m)\, |\rho_t|_n^2(X_m, Z_m, Q_m)$$

From (3.7) (C.4) and the Schwartz inequality it follows it is sufficient to prove the following inequality:

$$\|\rho_t\|_{m,n}^2 \leqslant n! \left\{ \exp\{4B_t\} \sum_{p=0}^{n} \frac{2^{p+1}}{(p!)^2} \left(\sup_{x \in \mathbb{R}^{3p}} \int_{\mathbb{R}^{3p}} dX'_p\, K(X'_p \mid x) \right)^2 \right\}^{m+n} \tag{3.10}$$

To prove this inequality we utilize the geometric mean of (3.8)

$$\begin{aligned} &\rho_t(X_m, Z_m, Q_m \mid X'_n, Z'_n, Q'_n) \\ &\quad = \exp\{-2\beta U_t(X_m, Z_m, Q_m)\} \\ &\quad\quad \times \prod_{j=1}^{m} \Bigg\{ \sum_{\{s\} \subset (t, \ldots, n)} K(x_j, z_j, Q_j \mid X'_{\{s\}}, Z'_{\{s\}}, Q'_{\{s\}}) \\ &\quad\quad\quad \times \rho_t(X_{m(j)} X'_{\{s\}}, Z_{m(j)} Z'_{\{s\}}, Q_{m(j)} Q'_{\{s\}} \mid \\ &\quad\quad\quad\quad X'_{\{n\setminus s\}}, Z'_{\{n\setminus s\}}, Q'_{\{n\setminus s\}}) \Bigg\}^{1/m} \end{aligned} \tag{3.11}$$

We shall prove (3.10) with the help of induction. Assume, that (3.10) holds for $m + n = k$. Now we are going to prove that the same inequality holds for $m + n = k + 1$.

By integrating (3.11) and applying the Holder and the Schwartz inequalities we get

$$|\rho_t|_n(X_m, Z_m, Q_m)$$

$$\leqslant \exp\{2\beta B_t\}$$

$$\times \prod_{j=1}^{m} \left\{ \sum_{p=0}^{n} \frac{n!}{p!\,(n-p)!} \right.$$

$$\times \int_{\mathbb{R}^{3p}} dX'_p \int_{\Omega_3^{2p}} P_{X_p}(dZ'_p)\, P(dQ'_p)\, |K(x_j, z_j, q_j \mid X'_p, Z'_p, Q'_p)|$$

$$\left. \times |\rho_t|_{n-p}(X_{m(j)} X'_p, Z_{m(j)} Z'_p, Q_{m(j)} Q'_p) \right\}^{1/m}$$

$$\leqslant \exp\{2\beta B_t\} \prod_{j=1}^{m} \left\{ \sum_{p=0}^{n} \frac{n!}{p!\,(n-p)!} \int_{\mathbb{R}^{3p}} dX'_p\, K(x_j, z_j, q_j \mid X'_p) \right.$$

$$\left. \times |\rho_t|_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X'_p) \right\}^{1/m}$$

$$K(x, z, q \mid X'_p) = \prod_{s=1}^{p} K(x, z, q \mid X'_s)$$

$$K^2(x, z, q \mid x) = \int_{\Omega_3^2} P_{X'}(dz')\, P(dq')\, |\exp\{-\beta\phi_t(x - x', z - z' \mid q, q')\} - 1|^2$$

From elementary inequalities it follows that

$$|\rho|_n^2(X_m, Z_m, Q_m) \leqslant \exp\{4\beta B_t\}$$

$$\times \prod_{j=1}^{m} \left\{ \sum_{p=0}^{n} \left(\frac{n!\, 2^{(p+1)/2}}{p!\,(n-p)!} \right)^2 \right.$$

$$\times \left[\int_{\mathbb{R}^{3p}} dX'_p\, K(x_j, z_j, q_j \mid X'_p) \right.$$

$$\left. \left. \times |\rho_t|_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X'_p) \right]^2 \right\}^{1/m}$$

Applying once more the Hölder and the Schwartz inequalities we obtain $|\rho_t|^2_{n,2}(X_m)$

$$\leqslant \exp\{4\beta B_t\} \prod_{j=1}^{m} \left\{ \sum_{p=0}^{n} \left(\frac{n!\, 2^{(p+1)/2}}{p!\,(n-p)!} \right)^2 \int_{\Omega_3^{2m}} P_{X_m}(dZ_m)\, P(dQ_m) \times \left[\int_{\mathbb{R}^{3p}} dX'_p\, K(x_j, z_j, q_j \mid X'_p) \times |\rho_t|_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X'_p) \right]^2 \right\}^{1/m}$$

$$\leqslant \exp\{4\beta B_t\} \prod_{j=1}^{m} \left\{ \sum_{p=0}^{n} \left(\frac{n!\, 2^{(p+1)/2}}{p!\,(n-p)!} \right)^2 \int_{\mathbb{R}^{6p}} dX'_p\, dX''_p \int_{\Omega_3^2} P_{X_j}(dz_j)\, P(dQ_j) \times K(x_j, z_j, q_j \mid X'_p) K(x_j, z_j, q_j \mid X''_p) \times \int_{\Omega_3^{2(m-1)}} P_{X_{m(j)}}(dZ_{m(j)})\, P(dQ_{m(j)}) \times |\rho_t|_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X'_p) \times |\rho_t|_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X''_p) \right\}^{1/m}$$

$$\leqslant \exp\{4\beta B_t\} \prod_{j=1}^{n} \left\{ \sum_{p=0}^{n} \left(\frac{n!\, 2^{(p+1)/2}}{p!\,(n-p)!} \right)^2 \int_{\mathbb{R}^{6p}} dX'_p\, dX''_p \times \left\{ \int_{\Omega_3^2} P_{X_j}(dZ_j)\, P(dQ_i)\, K^2(x_j, z_j, q_j \mid X'_p) \times \int_{\Omega_3^2} P_{x_j}(dz_j)\, P(dq_j)\, K^2(x_j, z_j, q_j \mid X''_p) \times \int_{\Omega_3^{2(m-1)}} P_{X_{m(j)}}(dZ_{m(j)})\, P(dQ_{m(j)}) \times |\rho|^2_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X'_p) \times \int_{\Omega_3^{2(m-1)}} P_{X_{m(j)}}(dZ_{m(j)})\, P(dQ_{m(j)}) \times |\rho|^2_{n-p,2}(X_{m(j)}, Z_{m(j)}, Q_{m(j)} \mid X''_p) \right\}^{1/2} \right\}^{1/m}$$

$$\leqslant \exp\{4\beta B_t\}(n!)^2 \sum_{p=0}^{n} \left(\frac{2^{(p+1)/2}}{p!\,(n-p)!} \right)^2$$
$$\times \left\{ \sup_x \int_{\mathbb{R}^{3p}} dX_p \left[\int_{\Omega_3^2} P_x(dz)\, P(dq)\, K^2(x,z,q \mid X_p) \right]^{1/2} \right\}^2$$
$$\times \|\rho_t\|^2_{n-p,m+p-1}$$

Thus (3.10) holds for $m + n = k$ if it holds for $m + n = k + 1$.

4. MAIN ESTIMATES; DEFINITION OF $K(t)$

Let us consider $K(X_p \mid x)$. From the Hölder inequality and the equality

$$\exp\left\{ -\beta \sum_{j=1}^{4} \phi_{t,j} \right\} = \sum_{j=1}^{4} (\exp\{-\beta\phi_{t,j}\} - 1)\exp\left\{ -\beta \sum_{k=j+1}^{4} \phi_{t,k} \right\}$$

we get [the functions $\phi_{t,j}$ are defined by (3.3) and (3.5)]

$$K(X_n \mid x) \leqslant \exp\left\{ n\left(\frac{\beta}{2} |\phi|_0 + t|\Delta\phi|_0 \right) \right. \sum_{\substack{\{n_1\} \ldots \{n_4\} \\ \cup\{n_j\} = (1, \ldots, n)}} \prod_{j=1}^{4} K_j^{1/3}(X_{\{n_j\}} \mid x), \tag{4.1}$$

$$K_j(X_n \mid x) = \int_{\Omega_3^2} P_x(dz)\, P(dq) \prod_{j=1}^{n} \int_{\Omega_3^2} P_{X_j}(dZ_j)\, P(dq_j) |\exp\{-\beta\phi_{t,j}\} - 1|^6 \tag{4.2}$$

Proposition (4.1). There exists a constant $\omega_0 > 1$ such that

$$K_2(X_n \mid x) \leqslant \left(\frac{\beta}{2} c\omega_0 \exp\left\{ \frac{\beta}{2} |\phi|_0 + \frac{1}{3} t\beta^{-1} \right\} \right)^{6n} \mathscr{K}(X_n - x)$$
$$\mathscr{K}(X_n) = \int_{\Omega_3} P(dz) \prod_{j=1}^{n} \omega^6\left(\frac{|z(t\beta^{-1}) - x_j|}{2} \right) \tag{4.3}$$

$$K_3(X_n \mid x) \leqslant \left(\beta c\omega_0 \exp\left\{ t|\Delta\phi|_0 + \frac{1}{3} t\beta^{-1} \right\} \right)^{6n} t^{5n} \mathscr{R}(X_n - x)$$
$$\mathscr{R}(X_n) = n! \int_{0 \leqslant \tau_1 \leqslant \cdots \leqslant t} d\tau_1 \ldots d\tau_n \int_{\Omega_3} P(dz) \prod_{j=1}^{n} \omega^6\left(\frac{|z(\tau_j) - x_j|}{2} \right) \tag{4.4}$$

$$K_4(X_n \mid x) \leqslant 2\left(\beta\sqrt{3}\, 6c\omega_0 \exp\left\{ \frac{1}{3} t\beta^{-1} \right\} \right)^{6n} t^{2n} n^{3n} \mathscr{R}(X_n - x) \tag{4.5}$$

Proof. The inequalities (4.3) and (4.4) follow from (C.3) and the inequalities (4.6),

$$|\exp\{x\} - 1| \leqslant |x|\exp\{|x|\}, \qquad \left(\int_0^t \psi(\tau)\,d\tau\right) \leqslant t^{p-1}\int_0^t \psi^p(\tau)\,d\tau$$

Applying the Hölder inequality and the inequalities $|\exp\{ix\} - 1| \leqslant \sqrt{2}\,|x|$, $(a+b)^n \leqslant 2^n(a^n + b^n)$ we obtain

$$K_4(X_n \mid x) \leqslant \beta^{6n}\int_{\Omega_3} P_x(dz) \prod_{j=1}^n \int_{\Omega_3} P_{X_j}(dz_j)$$

$$\times \left\{ \int_{\Omega_3^2} P(dq)\,P(dq_j)\,|\phi_{t,4}(z - z_j \mid q, q_j)|^{6n} \right\}^{1/n}$$

$$\leqslant (2\beta)^{6n}2\int_{\Omega_3^2} P_x(dz) \prod_{j=1}^n \int_{\Omega_3} P_{x_j}(dz_j)$$

$$\times \left\{ \int_{\Omega_3} P(dq)\left(\frac{1}{2}\int_0^{t\beta^{-1}} (\nabla\phi)(z(\tau) - z_j(\tau))\,dq(\tau)\right)^{6n} \right\}^{1/n}$$

From the well-known formulas

$$\int_\Omega P(dq)\left(\int_0^t f(\tau)\,dq(\tau)\right)^{2n} = \frac{(2n)!}{n!}\left(\int_0^t f^2(\tau)\,d\tau\right)^n \qquad 3^{-n}n^n \leqslant n! \leqslant n^n$$

it follows that

$$K_4(X_n \mid x) \leqslant 2\beta^{6n}12^{3n}3^{6n}n^{3n}t^{2n}\int_{\Omega_3} P_x(dz) \prod_{j=1}^n \int_0^{t\beta^{-1}} d\tau$$

$$\times \int_{\Omega_3} P_{x_j}(dz_j)\,(\nabla\phi)^6(|z(\tau) - z_j(\tau)|)$$

To derive (4.5) it is sufficient to take into account the following inequality:

$$\int_{\Omega_3} P(dz)\,\omega^6(|z(\beta^{-1}t) - x|) = \int_{\mathbb{R}^3} P^{t\beta^{-1}}(|y|)\omega^6(|y - x|)\,dy$$

$$\leqslant \exp\{2t\beta^{-1}\}\omega_0^6\omega^6\left(\frac{|x|}{2}\right) \qquad (4.6)$$

Now let us prove (4.6).

The monotonicity of $\omega(|x|)$ and $\exp\{(-|x|^2/4t)\beta\}$ with (C.4) gives

$$(4\pi t)^{-3/2}\int_{\mathbb{R}^3} dy \exp\left\{-\frac{|x-y|}{45}\beta\right\}\omega^6(|y|)\,dy$$

$$\leqslant \exp\left\{-\frac{|x|^2}{32t}\beta\right\}\int_{|y|\leqslant|x|/2} dy\,(4\pi t)^{-3/2}\exp\left\{-\frac{|x-y|}{8t}\beta\right\}\underline{\omega^6(|y|)}$$

$$+\,\omega^6\left(\frac{|x|}{2}\right)\int_{|y|>|x|/2} dy\,(4\pi t)^{-3/2}\exp\left\{-\frac{|x-y|}{4t}\beta\right\}$$

$$\leqslant \omega^6\left(\frac{|x|}{2}\right)\left\{1+2^{3/2}|\omega|_0^6\left(\sup_{\rho\in\mathbb{R}^+}\exp\left\{-\frac{\rho^2}{32t}\beta+\frac{\rho}{2}\right\}\right)\right.$$

$$\left.\times\sup_{\rho\in\mathbb{R}'}\exp\left\{-\frac{\rho}{2}\right\}\left(1+\frac{\rho}{2}\right)^{24}\right\}$$

$$\leqslant\left(1+|\omega|_0 2^{17}\right)^6\exp\{2t\beta^{-1}\}\,\omega^6\left(\frac{|x|}{2}\right)$$

Proposition (4.2). There hold the inequalities

$$\int_{\mathbb{R}^{3n}} dX_n \mathscr{K}^{1/6}(X_n) \leqslant \left(2^6\|\omega\|\right)^n\omega_0\exp\left\{t\frac{\beta^{-1}}{3}\right\} \tag{4.7}$$

$$\int_{\mathbb{R}^{3n}} dX_n \mathscr{R}^{1/6}(X_n) \leqslant \left(2^{10}\|\omega\|\omega_0\right)^n t^n\omega_0\exp\left\{t\frac{\beta^{-1}}{3}\right\},\qquad \|\omega\|=\int_{\mathbb{R}^3}dx\,\omega(|k|) \tag{4.8}$$

Proof. Let us make the change of a variable $y - X_n = y'$ in the expression for $\mathscr{K}(X_n)$ and split $\mathbb{R}^3$ into two domains $|y| \leqslant |X_n - X_{n-1}|/2$, $|y| > |X_n - X_{n-1}|/2$. In the first domain $\omega^6(|y - X_{n-1} + X_n|/2) \leqslant \omega^6(|X_n - X_{n-1}|/4)$ and in the second domain $\omega^6(|y|/2) \leqslant \omega^6(|X_n - X_{n-1}|/4)$.

Taking into account these inequalities

$$\mathscr{K}(X_n) \leqslant \omega^6\left(\frac{|X_n - X_{n-1}|}{4}\right)\left\{\int_{|y|\leqslant|X_n-X_{n-1}|/2} dy\,\omega^6\left(\frac{|y|}{2}\right)\right.$$

$$\left.+\int_{|y|>|X_n-X_{n-1}|/2} dy\,\omega^6\left(\frac{|y-X_n-X_{n-1}|}{2}\right)\right\}$$

$$\times\prod_{j=1}^{n-2}\omega^6\left(\frac{|y-X_j+X_n|}{2}\right)P^{t\beta^{-1}}(|y|)$$

Integrating over $\mathbb{R}^3$ and making an inverse change of a variable $y + X_n = y'$, we get

$$\mathscr{K}(X_n) \leqslant \omega^6\left(\frac{|X_n - X_{n-1}|}{4}\right)(\mathscr{K}(X_{n-1}) + \mathscr{K}(X_{n-2}, X_n))$$

This inequality and the inequality (4.6) give (4.7).

Let us put now

$$\mathscr{R}_{n,p}(X_{k-1} \mid x)$$
$$= n! \int_{0 \leqslant \tau_1 \leqslant \cdots \leqslant t\beta^{-1}} \cdots \int d\tau_1 \ldots d\tau_n \exp\{2(\tau_n - \tau_{k-1})\beta^{-1}\}$$
$$\times \int_{\mathbb{R}^{3(k-1)}} dY_{k-1} P^{\tau_1}(|y_1|)\omega^6\left(\frac{|y - x_1|}{2}\right)$$
$$\times \prod_{j=2}^{k-1} P^{\tau_j - \tau_{j-1}}(|y_j - y_{j-1}|)\omega^6\left(\frac{|y_j - x_j|}{2}\right)\omega^6\left(\frac{|y_{x-1} - x|}{2^{PH}}\right)$$

Applying the same argument as in the case of $\mathscr{K}(X_n)$ we obtain

$$\mathscr{R}(X_n) \leqslant \omega_0^6 \mathscr{R}_{n,1}(X_{n-1} \mid X_n)$$

$$\mathscr{R}_{n,p}(X_{k-1} \mid x)| \leqslant \omega_0^6\left\{\omega^6\left(\frac{|X_{k-1} - x|}{2^{p+2}}\right)\mathscr{R}_{n,1}(X_{k-2} \mid X_{k-1}) + \omega^6\left(\frac{|X_{k-1} - x|}{4}\right)\mathscr{R}_{n,p+1}(X_{k-2} \mid x)\right\}$$

$$\mathscr{R}_{n,p}(X_1 \mid x) \leqslant \omega_0^6 \exp\{2t\beta^{-2}\}\left\{\omega^6\left(\frac{|x - x_1|}{2^{p+2}}\right) + \omega^6\left(\frac{|x - x_1|}{4}\right)\right\}t^n$$

Hence

$$\int_{\mathbb{R}^{3n}} dX_n \mathscr{R}^{1/6}(X_n) \leqslant \omega_0 \int_{\mathbb{R}^{3n}} dX_n \mathscr{R}_{n,1}^{1/6}(X_{n-1} \mid x_n)$$
$$\leqslant 4^3\omega_0^2\|\omega\|\left\{2^3 \int_{\mathbb{R}^{3(n-1)}} dX_{n-1} \mathscr{R}_{n,1}^{1/6}(X_{n-2} \mid X_{n-1}) + \int_{\mathbb{R}^{3(n-1)}} dX_{n-1} \mathscr{R}_{n,2}^{1/6}(X_{n-2} \mid X_{n-1})\right\}$$
$$\leqslant 4^6\omega_0^3\|\omega\|^2\left\{2 \cdot 2^6 \int_{\mathbb{R}^{3(n-2)}} dX_{n-2} \mathscr{R}_{n,1}^{1/6}(X_{n-3} \mid X_{n-3}) + 2^3 \int_{\mathbb{R}^{3(n-2)}} dX_{n-2} \mathscr{R}_{n,2}^{1/6}(X_{n-3} \mid X_{n-2}) + \int_{\mathbb{R}^{3(n-2)}} dX_{n-2} \mathscr{R}_{n,3}^{1/6}(X_{n-3} \mid X_{n-2})\right\}$$
$$\leqslant \cdots \leqslant 2^{10n}\omega_0^{n+1}\|\omega\|^n t^n \exp\left\{t\frac{\beta^{-1}}{3}\right\}$$

Thus from (4.3)–(4.5), (4.7), and (4.8) it follows that

$$\sup_{x\in\mathbb{R}^3}\int_{\mathbb{R}^{3n}} dX_n\, K_j^{1/6}(X_n\,|\,x) \leqslant (n!)^{1/2}\gamma^n\kappa_j^n(t)\exp\left\{\frac{t\beta^{-1}}{3}+\ln 4\omega_0\right\}$$

$$\gamma=\beta\omega_0^2c\|\omega\|\exp\left\{\frac{\beta}{2}|\phi|_0\right\},$$

$$\kappa_1=\frac{1}{2},\qquad \kappa_2=2^5\exp\left\{t\frac{\beta^{-1}}{3}\right\},\qquad \kappa_3=2^{10}t\exp\left\{t\frac{\beta^{-1}}{3}+t|\Delta\phi|_0\right\},$$

$$2^{11}g\sqrt{t}\exp\left\{t\frac{\beta^{-1}}{3}\right\}$$

Using the inequality

$$\left[\sum_{\{n_1\}\,\ldots\,\{n_4\}}\prod_{i=1}^{4}K_j^{1/3}(X_{\{n_j\}}\,|\,x)\right]^{1/2}\leqslant\sum_{\{n_1\}\,\ldots\,\{n_4\}}\prod_{j=1}^{4}K_j^{1/6}(X_{\{n_j\}}\,|\,x)$$

taking into account (3.9), (4.1), (4.9) and making trivial computations we derive the basic estimate

$$\sup_{x_j\in\mathbb{R}^3}\int_{\mathbb{R}^{3n}} dX_n'\,\rho t(X_m\,|\,X_n')\leqslant n!\exp\{(m+n)K(t)\}$$

where

$$2K(t)=\beta\varphi_0+2B_t+2\gamma^2\exp\{\beta|\phi|_0+2t\|\Delta\phi\|_0\}\left(\sum_{j=1}^{4}\kappa_j(t)\right)^2$$
$$+\frac{t\beta^{-1}}{3}+\ln 4\omega_0$$

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