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Dispersive Transport Equations and Multiscale Models

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Dispersive Transport Equations and Multiscale Models

With 113 Illustrations

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Douglas N. Arnold, Director of the IMA

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FOREWORD

This IMA Volume in Mathematics and its Applications

DISPERSIVE TRANSPORT EQUATIONS AND MULTISCALE MODELS

along with the accompanying volume, "Transport in Transition Regimes" which will be published as IMA Volume 135 contains papers presented at three one-week workshops. The first workshop "Dispersive Corrections to Transport Equations" which took place on May 1–5, 2000 was organized by Anton Arnold (Universitaet Muenster), Naoufel Ben Abdallah (Université Paul Sabatier), C. David Levermore (University of Maryland), and Ken T.-R. McLaughlin (University of Arizona). The second workshop "Simulation of Transport in Transition Regimes" was held on May 22–26, 2000. The organizers were Pierre Degond (Université Paul Sabatier), Irene M. Gamba (University of Texas at Austin), and Philip Roe (University of Michigan). Leonard J. Borucki (Motorola, Inc.) and Christian Ringhofer (Arizona State University) were the organizers of the third workshop "Multiscale Models for Surface Evolution and Reacting Flows" which took place on June 5–9, 2000. The three workshops were integral parts of the 1999-2000 IMA program on "REACTIVE FLOW AND TRANSPORT PHENOMENA."

We would like to thank the organizers and all the participants for making the events successful. We also appreciate the organizers for their vital role as editors of the two proceedings.

We take this opportunity to thank the National Science Foundation, whose financial support of the IMA made the annual program possible.

Series Editors

Douglas N. Arnold, Director of the IMA

Fadil Santosa, Deputy Director of the IMA

PREFACE

IMA Volumes 135: Transport in Transition Regimes and 136: Dispersive Transport Equations and Multiscale Models are the compilation of papers presented in 3 related workshops held at the IMA in the spring of 2000. The focus of the program was the modeling of processes for which transport is one of the most complicated components. This includes processes that involve a wide range of length scales over different spatio-temporal regions of the problem, ranging from the order of mean-free paths to many times this scale. Consequently, effective modeling techniques require different transport models in each region.

In some cases the underlying kinetic description is relatively well understood, such as is the case for the Boltzmann equation for rarified gases, or the transport equation for radiation. In such cases the main issue is one of economy, a fully resolved kinetic simulation being impractical. One therefore develops homogenization, stochastic, or moment based subgrid models. This was the focus of two of the workshops: "Model Hierarchies for the Evolution of Surfaces under Chemically Reacting Flows" and "Transport Phenomena in Transition Regimes."

In other cases there is considerable disagreement about the underlying kinetic description, especially when dispersive effects become macroscopic, for example due to quantum effects in semiconductors and superfluids. These disagreements are the focus of the workshop: "Dispersive Corrections to Transport Equations."

Workshop on "Dispersive Corrections to Transport Equations," May 1–5, 2000 (Organized by D. Levermore, A. Arnold, N. Ben Abdallah, K. McLaughlin)

Dispersive corrections to classical and semiclassical transport equations arise from the rudimentary incorporation of quantum effects into macroscopic flow descriptions. These models play an increasing role in the study of nanometer scale electronic devices and of fluids at extremely low temperatures. One of the advantages of dispersively corrected transport equations is that they allow for a more classical coupling of the quantum system to the environment than the fully quantum mechanical descriptions. The main topics of this workshop were, on one hand, the mathematical derivation of dispersive correction terms, and, on the other hand, the computational issues raised by the interplay between nonlinear and dispersive effects in quatum dots and wires, superfluids and dispersive phenomena in nonlinear optics.

Workshop on "Simulation of Transport in Transition Regimes," May 22–26. 2000 (Organized by P. Degond, I. Gamba, P. Roe, R. Glassey)

Technology is increasingly advancing into regimes in which particle mean-free paths are comparable to the length scales of interest, whereby traditional transport models breakdown. For example, drift-diffusion models of electron-hole transport break down for submicron semiconductors, while Navier-Stokes approximations of fluid dynamics break down in outer planetary atmospheres or hypersonic flight. The cost of particle simulations is usually much larger than that of fluid simulations. This makes the simulation of problems in which transition regimes coexist with fluid regimes particularly difficult. This difficulty is compounded when the geometry of the problem is complex or even random. This workshop explored advanced moment based models, both deterministic and stochastic in origin, in the context of the simulation of high-altitude flight, charged particles in outer planetary atmospheres, electron and holes in submicon semiconductor devices, and radiation through inhomogenous media, together with hybrid numerical schemes that properly match transition regimes.

Workshop on "Multiscale Models for Surface Evolution and Reacting Flows," June 5–9, 2000 (Organized by L. Borucki and C. Ringhofer)

Multilayered compound materials with microscopically structured surfaces play a key role in semiconductor manufacturing. These structures are produced by a variety of processes, such as the deposition of thin films, etching techniques and controlled crystal growth. The topic of this workshop was the integration of different models describing these processes on different spatial and temporal scales. Well-developed models exist for each stage of the above processes on the microscopic-atomistic and macroscopic-fluid scale. However, in order to describe completely the whole process, it is necessary to link these models via an appropriate mathematical description of the transition regimes. This involves a mixture of boundary layer and homogenization techniques as well as a mathematical analysis of the transition process from the atomistic description of the early stages of thin film growth to the evolution of continuous films. Computational issues covered by this workshop were the deterministic and probabilistic representation of film surfaces and numerical methods for the transitional models.

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CONTENTS

ON THE DERIVATION OF NONLINEAR SCHRÖDINGER AND VLASOV EQUATIONS

CLAUDE BARDOS*, FRANÇOIS GOLSE†, ALEX GOTTLIEB‡, AND NORBERT J. MAUSER§

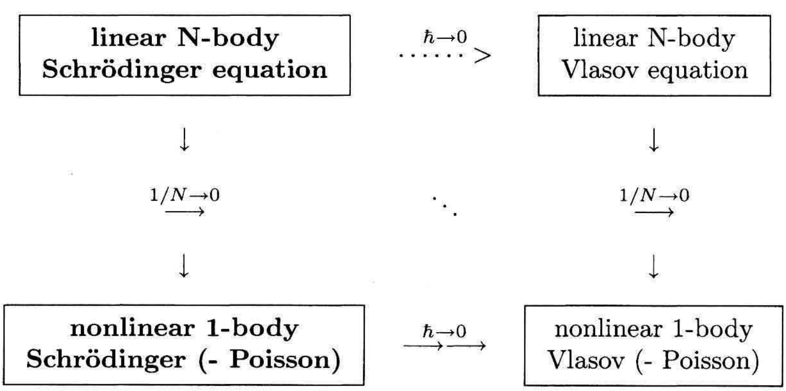
Abstract. We present and discuss derivations of nonlinear 1-particle equations from linear N-particle Schrödinger equations with pair interaction in the time dependent case.

We regard both the "classical" limit of vanishing Planck constant $\hbar \to 0$ which leads to Vlasov type equations and the "weak coupling" limit $1/N \to 0$ which leads to nonlinear 1 particle equations.

We use an approach to weak coupling limits where the so-called "finite Schrödinger hierarchy" and the limiting "(infinite) Schrödinger hierarchy" play a central role. Convergence of solutions of the first to solutions of the second is established using "physically relevant" estimates (L^2 and energy conservation) under very general assumptions on the interaction potential, including in particular the Coulomb potential.

The goal of this work is to give an overview of the existing results, including some minor improvements, and clearly state the open problems.

1. Introduction. In this work we give a survey of the derivation of nonlinear 1-particle Schrödinger and Vlasov equations starting from the linear N-particle Schrödinger equation. We regard both the "classical" limit of vanishing Planck constant $\hbar \to 0$ which leads to Vlasov type equations and the "weak-coupling" limit $1/N \to 0$ which leads to nonlinear 1-particle equations. The relevant particle systems and limits are illustrated in the following (presumably commutative) diagram:



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The vertical arrows represent the weak-coupling limits and the horizontal arrows represent the classical limits. The diagonal limit, i.e., the classical + weak-coupling limit corresponding to letting $\hbar \to 0^+$ and $N \to \infty$ (simultaneously) shall also be considered in the present contribution.

The vertical limit from the linear N-particle Schrödinger equation to a nonlinear 1-particle Schrödinger equation has been given by Spohn in [Sp1], with recent minor improvements in [BGM1]; both contributions assuming bounded potentials.

The vertical limit from the linear N-particle Vlasov equation to a nonlinear 1-particle Vlasov equation has been given by Braun and Hepp in [BH], assuming bounded and regular potentials.

The diagonal limit from the linear N-particle Schrödinger equation to a nonlinear 1-particle Vlasov equation is given by Narnhofer and Sewell in [NS] for the case of a bounded, real analytic interaction potential.

The lower horizontal limit has been given by Lions and Paul in [LP], and Markowich and Mauser in [MM] thus deriving the Vlasov-Poisson from the Schrödinger-Poisson system.

Validating the upper horizontal limit, from the linear N-particle Schrödinger equation to the linear N-particle Vlasov equation, is still an open problem for the case of Coulomb interaction.

The three succeeding sections of this article investigate the three non-horizontal limits just mentioned. Our ultimate goal is to prove the existence and uniqueness of solutions to an *infinite hierarchy* of equations associated to the relevant N-particle dynamics and scaling. Existence and uniqueness of solutions to the infinite hierarchy easily implies the limits with which we are concerned. Uniqueness can be shown to hold if the 2-body potential satisfies strong enough conditions, like boundedness, but existence is easier to establish (cp. [BGM1]. Solutions to the infinite hierarchy are obtained as accumulation points of the finite-particle dynamics, in a suitable topology. This convergence does not require boundedness of the interparticle potential. Since we have in mind the case of the Coulomb potential, which leads to the Schrödinger-Poisson system, we value the existence theorems announced below because their hypotheses accommodate unbounded potentials.

The weak-coupling limit of N-particle quantum systems is the tool for the derivation of a time-dependent Hartree equation, as indicated by the left vertical "$1/N$ arrow" in the diagram above. However, the same technique seems not to work for deriving a (local approximation of) time dependent Hartree-Fock equation based on Pauli's exclusion principle. As shown in Section 5, the weak limit of the density matrix is vanishing in this "fermion case".

How to derive a nonlinear 1-body time-dependent Schrödinger equation for fermions in the infinite-particle limit (but not *classical* limit) is not known. The following diagram outlines an approach to this problem in the stationary case which is outside the scope of this article. For the stationary case indeed rigorous results are available (see e.g. [BM] and references therein), for the time dependent case a heuristic model is given in [M6].

linear N-body Schrödinger equation

↓

Hartree Fock ansatz
minimization of total energy

↓

Hartree-Fock system

↓

local approximation of exchange term
$N \to \infty$

↓

Schrödinger - Poisson-$X\alpha$ equation

2. The weak coupling limit of the linear N Schrödinger equation. The starting point is the Schrödinger equation for the wave function $\Psi_N = \Psi_N(x_1, x_2, ..., x_N, t)$ of N interacting particles, which reads

$$(1) \qquad i\hbar\partial_t\Psi_N = -\frac{\hbar^2}{2}\sum_{1\le j\le N}\Delta_{x_j}\Psi_N + \frac{1}{N}\sum_{1\le j<k\le N} V(|x_j - x_k|)\Psi_N =: H_N\Psi_N$$

$$(2) \qquad \Psi_N(t=0) = \Psi_N^I(x_1, x_2, ..., x_N).$$

The factor $1/N$ in front of the potential V is the standard weak-coupling scaling, as discussed e.g. by Spohn in [Sp2]. It corresponds to assuming that collective effects of order 1 can be observed over a unit length of the macroscopic time scale.

The potential V is assumed to be real-valued and bounded from below, but no assumption is made as to its sign. In other words, attractive as well as repulsive interactions are amenable to the methods presented in this paper.

The following notations will be used constantly in the sequel

$$(3) \qquad \begin{array}{lll} X_N := (x_1, x_2, ..., x_N), & X_n := (x_1, x_2, ..., x_n), & X_N^n := (x_{n+1}, ..., x_N) \\ Y_N := (y_1, y_2, ..., y_N), & Y_n := (y_1, y_2, ..., y_n), & Y_N^n := (y_{n+1}, ..., y_N) \\ Z_N := (z_1, z_2, ..., z_N), & Z_n := (z_1, z_2, ..., z_n), & Z_N^n := (z_{n+1}, ..., z_N) \\ V_N := (v_1, v_2, ..., v_N), & V^n := (v_1, v_2, ..., v_n), & V_N^n := (v_{n+1}, ..., v_N). \end{array}$$

The state of the N-particle system can also be described (see for example [LL3]) by the density operator $\rho_N(t)$ acting on $L^2(I\!R^3)^N$ or equivalently by its integral kernel, known as the density matrix $\rho_N(X_N, Y_N, t)$. For a general "mixed state" we have

$$\rho_N(X_N, Y_N, t) = \sum_{k \in I\!N} \lambda_k \Psi_{N,k}(X_N, t)\overline{\Psi_{N,k}(Y_N, t)}\,, \tag{4}$$

where $\lambda_k > 0$ are the "occupation probabilities" satisfying $\sum_k \lambda_k = 1$. However, the N-particle Schrödinger equation is linear, so that we can assume without loss of generality that the density matrix is that of a "pure state":

$$\begin{aligned} \rho_N(X_N, Y_N, t) &= \rho_N(x_1, x_2, ..., x_N, y_1, y_2, ..., y_N, t) \\ &= \Psi_N(X_N, t)\overline{\Psi_N(Y_N, t)}. \end{aligned} \tag{5}$$

This density matrix $\rho_N(X_N, Y_N, t)$ is the integral kernel of the density operator $\rho_N(t)$, the time evolution of which is given by

$$\rho_N(t) = e^{-i\frac{tH_N}{\hbar}} \rho_N(0) e^{i\frac{tH_N}{\hbar}} \tag{6}$$

i.e. the density operator $\rho_N(t)$ satisfies the "von Neumann equation":

$$i\hbar\partial_t\rho_N = H_N\rho_N - \rho_N H_N\,. \tag{7}$$

Equivalently, the density matrix must satisfy

$$\begin{aligned} i\hbar\partial_t\rho_N(X_N, Y_N, t) &= -\frac{\hbar^2}{2}[\Delta_{X_N} - \Delta_{Y_N}]\rho_N(X_N, Y_N, t) \\ +\frac{1}{N} &\sum_{1\le j<k\le N} [V(|x_j - x_k|)dis - V(|y_j - y_k|)]\rho_N(X_N, Y_N, t)\,. \end{aligned} \tag{8}$$

The operator ρ_N is of trace class, its trace being given by:

$$\begin{aligned} \mathrm{Tr}\rho_N(t) &= \int \rho_N(X_N, X_N, t)dX_N = \int |\Psi_N(X_N, t)|^2 dX_N \\ &= \int |\Psi_N^I(X_N)|^2 dX_N = 1 \end{aligned} \tag{9}$$

after normalization.

The "marginal distributions" or "partial traces" are introduced according to the formula:

$$\rho_{N,n}(t) := \mathrm{Tr}_{[n+1,N]}\rho_N(t) = \int \rho_N(X_n, Z_N^n, Y_n, Z_N^n, t)dZ_N^n\,. \tag{10}$$

We further assume that the initial data satisfy the relation

$$\begin{aligned} &\rho_N(x_1, x_2, ..., x_n, y_1, y_2, ..., y_n, 0) = \\ &\qquad \rho_N(x_{\sigma(1)}, x_{\sigma(2)}, ..., x_{\sigma(n)}, y_{\sigma(1)}, y_{\sigma(2)}, ..., y_{\sigma(n)}, 0) \end{aligned} \tag{11}$$

for any permutation σ of the set $\{1,2,3,...,N\}$. This encodes the fact that we are considering the statistics of undistinguishable particles. This property is preserved by the time evolution of the von Neumann equation, so that (11) implies that

$$\rho_N(x_1,x_2,...,x_n,y_1,y_2,...,y_n,t) = \rho_N(x_{\sigma(1)},x_{\sigma(2)},...,x_{\sigma(n)},y_{\sigma(1)},y_{\sigma(2)},...,y_{\sigma(n)},t) \tag{12}$$

holds for all $t \in \mathbb{R}$.

Assuming that the initial N-particle distribution satisfies (11), we obtain from a rather straightforward computation that the marginal distributions $\rho_{N,n}(t)$ solve the system

$$\begin{aligned} i\hbar\partial_t\rho_{N,n}(X_n,Y_n,t) &= -\frac{\hbar^2}{2}[\Delta_{X_n}-\Delta_{Y_n}]\rho_{N,n}(X_n,Y_n,t) \\ &+\frac{1}{N}\sum_{1\le j<k\le n}[V(|x_j-x_k|)-V(|y_j-y_k|)]\rho_{N,n}(X_n,Y_n,t) \\ &+\frac{N-n}{N}\sum_{1\le j\le n}\int[V(|x_j-z|)-V(|y_j-z|)]\rho_{N,n+1}(X_n,z,Y_n,z,t)dz. \end{aligned} \tag{13}$$

Observe indeed that the missing term in (13) is the one corresponding to applying the partial trace $\mathrm{Tr}_{[n+1,N]}$ to the summation that appears as the last term in the right hand side of (8) restricted to the subset of indices $\{(j,k)\,|\,n+1\le j,k\le N\}$. Since this restricted sum involves only terms that obviously vanish on the set $\{(X_N,Y_N)\,|\,X_N^n = Y_N^n\}$, applying the partial trace $\mathrm{Tr}_{[n+1,N]}$ does not contribute any additional term in (13).

The system (13) is called the "N-particle (finite) Schrödinger hierarchy". Observe in particular that for $n=N$ one recovers the equation (8) for $\rho_{N,N}=\rho_N$.

Introducing the operators $\mathcal{C}_{n,n+1}$ mapping $n+1$-particle densities to n-particle functions formally defined by

$$\mathcal{C}_{n,n+1}(\rho_{N,n+1})(X_n,Y_n) = \sum_{1\le j\le n}\int[V(|x_j-z|)-V(|y_j-z|)]\rho_{N,n+1}(X_n,z,Y_n,z)dz\,, \tag{14}$$

the N-particle Schrödinger hierarchy is rewritten as:

$$\begin{aligned} i\hbar\partial_t\rho_{N,n}(X_n,Y_N,t) &= -\frac{\hbar^2}{2}[\Delta_{X_n}-\Delta_{Y_n}]\rho_{N,n}(X_n,Y_n,t) \\ &+\frac{1}{N}\sum_{1\le j<k\le n}[V(|x_j-x_k|)-V(|y_j-y_k|)]\rho_{N,n}(X_n,Y_n,t) \\ &+\frac{N-n}{N}(\mathcal{C}_{n,n+1}\rho_{N,n+1})(X_n,Y_n,t)\,,\quad \forall n=1,\dots,N\,, \end{aligned} \tag{15}$$

$$\rho_{N,n}(X_n, Y_n, t) = 0\,, \quad \forall n > N\,. \tag{16}$$

The "infinite Schrödinger hierarchy" is obtained from the N-particle (finite) Schrödinger hierarchy by letting $N \to +\infty$ while keeping $\hbar$ fixed and giving up the constraint (16). We denote by ρ_n the n-particle marginal distribution involved in the infinite Schrödinger hierarchy which of course differs from $\rho_{N,n}$, the n-th marginal distribution involved in the N-particle (finite) hierarchy. Letting formally $N \to +\infty$ in (13) leads to:

$$\begin{aligned} i\hbar\partial_t\rho_n(X_n, Y_n, t) &= -\frac{\hbar^2}{2}[\Delta_{X_n} - \Delta_{Y_n}]\rho_n(X_n, Y_n, t) \\ &+ \sum_{1\le j\le n}\int [V(|x_j - z|) - V(|y_j - z|)]\rho_{n+1}(X_n, z, Y_n, z, t)dz\,. \end{aligned} \tag{17}$$

A function ρ_n of the variables (X_n, Y_n) is henceforth said to be factorized if it is the n-th fold tensor power of a function $\rho \equiv \rho(x_1, y_1)$, i.e.

$$\rho_n(X_n, Y_n) = \prod_{1\le k\le n} \rho(x_k, y_k)\,. \tag{18}$$

Observe that if $\psi(x, t)$ is a solution of the (nonlinear) "self-consistent, 1-particle Schrödinger equation"

$$i\hbar\partial_t\psi(x, t) = -\frac{\hbar^2}{2}\Delta_x\psi(x, t) + \psi(x, t)\int V(|x - z|)|\psi(z, t)|^2 dz \tag{19}$$

then

$$\rho = \psi(x, t)\overline{\psi(y, t)} \tag{20}$$

is a solution of the "self-consistent von Neumann equation"

$$\begin{aligned} i\hbar\partial_t\rho(x, y, t) &= -\frac{\hbar^2}{2}[\Delta_x - \Delta_y]\rho(x, y, t) \\ &+\rho(x, y, t)\int [V(|x - z|) - V(|y - z|)]\rho(z, z, t)dz\,, \end{aligned} \tag{21}$$

while the (sequence of) factorized n-particle densities

$$\rho_n(X_n, Y_n, t) = \prod_{1\le k\le n} \rho(x_k, y_k, t) \tag{22}$$

is a solution of the (infinite) Schrödinger hierarchy. On the other hand, at $t = 0$ (cf (9)):

$$\begin{aligned} \rho_{N,n+1}(X_n, Y_n, 0) &= \prod_{1\le k\le n} \psi(x_k, 0)\overline{\psi(y_k, 0)} \prod_{n+1\le k\le N} \int |\psi(z_k)|^2 dz_k \\ &= \prod_{1\le k\le n} \psi(x_k, 0)\overline{\psi(y_k, 0)} = \prod_{1\le k\le n} \rho(x_k, y_k, 0). \end{aligned} \tag{23}$$

As a consequence a uniqueness result for the hierarchy (Corollary 2.1 below) implies that, with initial data factorized as in (18), the solution of the hierarchy is given by

$$\rho_n(x_n, y_n, t) = \prod_{1\le k\le n} \psi(x_k, t)\overline{\psi(y_k, t)} \tag{24}$$

with $\psi(x_k, t)$ solution of the self-consistent Schrödinger equation (19). The factorization, assumed at $t = 0$ for the finite hierarchy, will in general get lost at later times due to the presence of the interaction potential V; however it is recovered in the limit as $N \to +\infty$.

2.1. A priori estimates for the N-particle Schrödinger hierarchy. The starting point is a variant of the Cauchy-Schwarz inequality applied to the marginal distributions. While straightforward, it provides useful estimates.

PROPOSITION 2.1. *The marginal distributions satisfy the inequalities*

$$\iint |\rho_{N,n}(X_n, Y_n, t)|^2 dX_n dY_n \le 1 \tag{25}$$

and

$$\begin{aligned} &|\rho_{N,n+1}(X_n, z, Y_n, z, t)| \le \\ &\qquad \rho_{N,n+1}(X_n, z, X_n, z, t)^{\frac{1}{2}} \rho_{N,n+1}(Y_n, z, Y_n, z, t)^{\frac{1}{2}} \end{aligned} \tag{26}$$

for all $t \in \mathbb{R}$.

Another basic result is a $\hbar$-dependent estimate on the kinetic energy of the N-particle system.

PROPOSITION 2.2. *Assume that the interacting potential is of the form*

$$\begin{aligned} &V(|x|) = V_+(|x|) + V_-(|x|) \\ &\textit{with} \quad V_+(|x|) \ge 0\,,\ V_+ \in L^2(\mathbb{R}^3)\,,\ V_-(|x|)) \ge -C_{\text{pot}} > -\infty\,. \end{aligned} \tag{27}$$

Assume further that the initial data $\Psi_N^I(x_1, \dots, x_N)$ satisfies the assumption of undistinguishable particles (11) and has energy

$$\begin{aligned} \mathcal{E}_{N,\hbar} = \ &\frac{1}{2}\hbar^2 \sum_{1\le j\le N} \int |\nabla_{x_j} \Psi_N^I(X_N)|^2 dX_N \\ &+\frac{1}{N} \sum_{1\le j<k\le m} \int V(|x_j - x_k|)|\Psi_N^I(X_N)|^2 dX_N = O(N) \end{aligned} \tag{28}$$

as $N \to +\infty$.

Then, for any j such that $1 \le j \le n$, the solution Ψ_N of the N-particle Schrödinger equation satisfies

$$\sup_{1\le j\le N} \int |\nabla_{x_j} \Psi_N(X_N, t)|^2 dX_N \le C_{\text{pot}} \frac{N(N-1)}{N^2\hbar^2} + 2\frac{\mathcal{E}_{N,\hbar}}{N\hbar^2}\,. \tag{29}$$