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A REVIEW OF DISPERSIVE LIMITS OF (NON)LINEAR SCHRÖDINGER-TYPE EQUATIONS

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Abstract. In this review paper we present the most important mathematical properties of dispersive limits of (non)linear Schrödinger type equations. Different formulations are used to study these singular limits, e.g., the kinetic formulation of the linear Schrödinger equation based on the Wigner transform is well suited for global-in-time analysis without using WKB-(expansion) techniques, while the modified Madelung transformation reformulating Schrödinger equations in terms of a dispersive perturbation of a quasilinear symmetric hyperbolic system usually only gives local-in-time results due to the hyperbolic nature of the limit equations. Deterministic analogues of turbulence are also discussed. There, turbulent diffusion appears naturally in the zero dispersion limit.

1. Introduction

It has been known since the early days of quantum mechanics that the **linear** Schrödinger equation can be written in hydrodynamical form. In this formulation, the **linear** Schrödinger equation is replaced by a system of **nonlinear** equations which are formally analogous to the equations of motion of a classical fluid. They are called quantum hydrodynamics equations (QHD equations). More precisely, the QHD equations originate from the classical way of rewriting the single state Schröd- inger equation in terms of the particle density and velocity [18]. Mathematically, these models are dispersively

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regularized hydrodynamic models, where the square of the (scaled) Planck constant $\hbar$ plays the role of the dispersivity.

Very similar model equations have been used for quite a while in other areas of theoretical and computational physics, namely in superfluidity [23, 24] and in superconductivity [10].

A different way of deriving QHD-models is analogous to the derivation of the gas-dynamics Euler equation from the Boltzmann equation, namely based on the so-called moment method. Taking the zeroth, first and second order velocity moments of the quantum Boltzmann equation (or, in the collisionless case, Wigner transport equation) [11] results in a hydrodynamical model which then has to be "closed" in an approximate way, i.e., a reasonable macroscopic approximation for the quantum heat flow tensor has to be derived by using additional (quantum) physical properties of the particle ensembles. Also small mean-free-path asymptotics have been used to derive QHD-models in the case of high electric fields. The obtained models have linear quantum corrections [27].

It is a fundamental principle in quantum mechanics that, when the time and distance scales are large enough relative to the Plank constant $\hbar$, the system will approximately obey the laws of classical, Newtonian mechanics. This is usually rephrased in a colloquial form as: in the limit as $\hbar \to 0$ quantum mechanics becomes Newtonian mechanics. The asymptotics of quantum variables as $\hbar \to 0$ are known as "semiclassical", which expresses this limiting behavior.

The quantum-mechanical pressure becomes negligible in the "semiclassical limit" or WKB limit, when ∇_x and ∂_t scale like ε as $\varepsilon \to 0$ (ε is the scaled Planck constant), and the initial condition has the form $\phi(x,0) = \phi_I(x)e^{iS_I(x)/\varepsilon}$. In this limit, the Euler equation for an isentropic compressible flow is formally recovered from the nonlinear Schrödinger equation. This was proven rigorously by Jin, Levermore and McLaughlin [16, 17] for the one-dimensional integrable case using the inverse scattering technique and by Grenier [15] for higher dimensions in situations where no vortices are involved (i.e., time locally).

The semiclassical limit of the general modified nonlinear Schrödinger (GMNLS for short) equation can be discussed in the similar strategy as Grenier's [15], but the GMNLS equation has a space derivative in the nonlinear term which causes the so-called *derivative loss.* Thus the GMNLS equation does not possess parity and Galilean invariance and therefore the canonical momentum is not conserved. To overcome this difficulty, we introduce the *noncanonical momentum*, which is indeed *the* conservative quantity of the GMNLS equation, and represent it as a dispersive perturbation of the modified Euler system.

Based on Schrödinger's original idea on reformulation of the quantum mechanics in terms of a pair of time-reflection-invariant macroscopic equations, Schrödinger type equations can be represented as a dispersive perturbation of a quasilinear symmetric hyperbolic system. In this case, the amplitude of the wave function must be interpreted as a complex-valued function. However, due to the hyperbolic nature of the limiting system, this approach only works before the shocks occur. After the breaking-time the conserved densities can be expected to have only weak limits.

2. Hydrodynamics of Dispersive Equations

As mentioned in the introduction there are different ways to derive QHD-equations. Here we deal first with a derivation starting from a quantum mechanical single or mixed state described by one or, resp., a sequence of Schrödinger equations, and secondly we present the connection to the usual derivation using the moment method for the Wigner equation.

We start with a single state Schrödinger equation in $\mathbb{R}^d$:

$$i\varepsilon\psi_t^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V^\varepsilon\psi^\varepsilon, \quad x \in \mathbb{R}^d, \quad t \in \mathbb{R} \tag{2.1a}$$

subject to the initial condition

$$\psi^\varepsilon(x, t = 0) = \psi_I^\varepsilon(x), \quad x \in \mathbb{R}^d. \tag{2.1b}$$

The scaled Planck constant is here denoted by ε. The superscript ε in the wave function $\psi^\varepsilon(x, t)$ indicates the ε-dependence. The potential V^ε is assumed to be given or to be described self-consistently by Poisson's equation

$$-\lambda^2\Delta V^\varepsilon = n^\varepsilon - C, \tag{2.2}$$

where the particle density n^ε is defined by

$$n^\varepsilon(x, t) = \bar{\psi}^\varepsilon(x, t)\psi^\varepsilon(x, t) \tag{2.3}$$

("$^-$" denotes complex conjugation). In semiconductor applications the function $C = C(x)$ denotes the doping profile. In general, it describes a fixed background charge. λ is the scaled Debye length. Introducing the (scaled) phase S^ε of the wave function

$$\psi^\varepsilon(x, t) = \sqrt{n^\varepsilon(x, t)}\exp\left(\frac{i}{\varepsilon}S^\varepsilon(x, t)\right) \tag{2.4}$$

and separating real and imaginary parts in the Schrödinger equation (2.1a), the following irrotational flow equations

$$n_t^\varepsilon + \mathrm{div}(n^\varepsilon \nabla S^\varepsilon) = 0, \tag{2.5a}$$

$$S_t^\varepsilon + \frac{1}{2}\Big|\nabla S^\varepsilon\Big|^2 + V - \frac{\varepsilon^2}{2}\frac{1}{\sqrt{n^\varepsilon}}\Delta\sqrt{n^\varepsilon} = 0 \tag{2.5b}$$

are obtained [18].

The definition of the current density

$$J^\varepsilon(x,t) = \varepsilon \mathrm{Im}\Big(\bar{\psi}^\varepsilon(x,t)\nabla\psi^\varepsilon(x,t)\Big) \tag{2.6a}$$

gives

$$J^\varepsilon = n^\varepsilon \nabla S^\varepsilon \,. \tag{2.6b}$$

Taking the gradient of equation (2.5b), multiplying it by n^ε and using (2.5a), we obtain QHD flow equations for the density n^ε and the current density J^ε:

$$n_t^\varepsilon + \mathrm{div} J^\varepsilon = 0, \tag{2.7a}$$

$$J_t^\varepsilon + \mathrm{div}\left[\frac{J^\varepsilon \otimes J^\varepsilon}{n^\varepsilon}\right] + n^\varepsilon \nabla V^\varepsilon = \frac{\varepsilon^2}{2} n^\varepsilon \nabla\left[\frac{1}{\sqrt{n^\varepsilon}}\Delta\sqrt{n^\varepsilon}\right] \tag{2.7b}$$

(the symbol $\otimes$ denotes the tensor product of vectors) with irrotational initial conditions

$$n^\varepsilon(x, t=0) = n_I^\varepsilon(x) \geq 0, \quad J^\varepsilon(x,t=0) = n_I^\varepsilon(x)\nabla S_I^\varepsilon(x), \tag{2.7c}$$

which are associated to the initial wave function

$$\psi_I^\varepsilon(x) = \sqrt{n_I^\varepsilon(x)}\exp\Big(\frac{i}{\varepsilon}S_I^\varepsilon(x)\Big). \tag{2.8}$$

The equations (2.7) represent a fluid dynamic formulation of the linear Schrödinger equation and are known as Madelung's fluid equations [23, 24]. The difference between the classical zero temperature Euler equations and the equations (2.7) lies in the quantum correction term of order ε^2 in the current equation (2.7b). This density-dependent term can be interpreted either as internal self-potential

$$Q^\varepsilon = -\frac{\varepsilon^2}{2}\frac{1}{\sqrt{n^\varepsilon}}\Delta\sqrt{n^\varepsilon} = -\frac{\varepsilon^2}{2}\frac{\Delta|\psi^\varepsilon|}{|\psi^\varepsilon|}, \tag{2.9}$$

the so-called Bohm potential, or, using

$$n^\varepsilon \nabla\left[\frac{1}{\sqrt{n^\varepsilon}}\Delta\sqrt{n^\varepsilon}\right] = \frac{1}{2}\operatorname{div}\left[n^\varepsilon(\nabla\otimes\nabla)\ln n^\varepsilon\right],$$

as nondiagonal quantum pressure tensor

$$p^\varepsilon = -\frac{\varepsilon^2}{4}n^\varepsilon(\nabla\otimes\nabla)\ln n^\varepsilon. \tag{2.10}$$

Defining the kinetic energy density tensor E_K^ε as

$$E_K^\varepsilon = \frac{1}{2}\frac{J^\varepsilon\otimes J^\varepsilon}{n^\varepsilon} \tag{2.11}$$

and using (2.7), we obtain the 'classical' energy density tensor equation

$$\begin{aligned}(E_{Kls}^\varepsilon)_t + \frac{\partial}{\partial x_m}\Big(\frac{J_m^\varepsilon}{n^\varepsilon}E_{Kls}^\varepsilon\Big) + \frac{1}{2}\Big(J_l^\varepsilon\frac{\partial}{\partial x_s}(V^\varepsilon + Q^\varepsilon)\\ + J_s^\varepsilon\frac{\partial}{\partial x_l}(V^\varepsilon + Q^\varepsilon)\Big) = 0.\end{aligned} \tag{2.12}$$

(The indices l, s, m denote the lth, sth, mth component of the corresponding vector or tensor. Also, the Einstein summation convention is used.) Obviously, the equation (2.12) is superfluous, since E_K^ε is a function of n^ε and J^ε only. If we define the energy density tensor E^ε by

$$E^\varepsilon = \frac{1}{2}\frac{J^\varepsilon\otimes J^\varepsilon}{n^\varepsilon} - \frac{\varepsilon^2}{8}n^\varepsilon(\nabla\otimes\nabla)\ln n^\varepsilon, \tag{2.13}$$

then the corresponding energy density tensor equation reads

$$\begin{aligned}(E_{ls}^\varepsilon)_t + \frac{\partial}{\partial x_m}\left[\frac{J_m^\varepsilon}{n^\varepsilon}E_{ls}^\varepsilon + \frac{1}{2}\Big(\frac{J_l^\varepsilon}{n^\varepsilon}p_{sm}^\varepsilon + \frac{J_s^\varepsilon}{n}p_{lm}^\varepsilon\Big)\right]\\ + \frac{1}{2}\Big(J_l^\varepsilon\frac{\partial}{\partial x_s}V^\varepsilon + J_s^\varepsilon\frac{\partial}{\partial x_l}V^\varepsilon\Big) - \frac{\varepsilon^2}{8}\frac{\partial}{\partial x_m}\Big(n^\varepsilon\frac{\partial^2}{\partial x_l\partial x_s}\Big(\frac{J_m^\varepsilon}{n^\varepsilon}\Big)\Big) = 0.\end{aligned} \tag{2.14}$$

The expression

$$q_{lsm}^\varepsilon := -\frac{\varepsilon^2}{8}n^\varepsilon\frac{\partial^2}{\partial x_l\partial x_s}\left(\frac{J_m^\varepsilon}{n^\varepsilon}\right) \tag{2.15}$$

plays the role of a quantum heat flux tensor. The scalar equation for the energy density $W^\varepsilon = \operatorname{tr}(E^\varepsilon)$ follows:

$$\begin{aligned}(W^\varepsilon)_t + \frac{\partial}{\partial x_m}\left[\frac{J_m^\varepsilon}{n^\varepsilon}W^\varepsilon + \frac{J_l^\varepsilon}{n^\varepsilon}p_{lm}^\varepsilon\right] + J_l^\varepsilon\frac{\partial}{\partial x_l}V^\varepsilon\\ - \frac{\varepsilon^2}{8}\frac{\partial}{\partial x_m}\left[n^\varepsilon\Delta\left(\frac{J_m^\varepsilon}{n^\varepsilon}\right)\right] = 0.\end{aligned} \tag{2.16}$$

These considerations on energy density equations become important below when passing from a single state to a mixed state in which additional quantities like (classical) pressure or temperature are introduced.

We also mention the equivalence of the nonlinear Schrödinger equation

$$i\varepsilon\psi_t^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + \Big(V^\varepsilon + h(\bar{\psi}^\varepsilon\psi^\varepsilon)\Big)\psi^\varepsilon \tag{2.17}$$

and the (irrotational) flow equations

$$n_t^\varepsilon + \mathrm{div} J^\varepsilon = 0, \tag{2.18a}$$

$$J_t^\varepsilon + \mathrm{div}\left[\frac{J^\varepsilon \otimes J^\varepsilon}{n^\varepsilon} + p(n^\varepsilon)\right] + n^\varepsilon\nabla V^\varepsilon = \frac{\varepsilon^2}{2}n^\varepsilon\nabla\left[\frac{1}{\sqrt{n^\varepsilon}}\Delta\sqrt{n^\varepsilon}\right], \tag{2.18b}$$

in which the density dependent pressure $p(n^\varepsilon)$ and the enthalpy $h(n^\varepsilon)$ are related by

$$p'(n^\varepsilon) = n^\varepsilon h'(n^\varepsilon). \tag{2.19}$$

The equivalence, which is obtained in the same way as in the case of the linear Schrödinger equation (2.1a) by using (2.3) and (2.6), does not represent a physical derivation of the isothermal ($p(n) = n$) or isentropic ($p(n) = n^\gamma, 1 < \gamma < 3$) QHD equations, since a physical interpretation of the nonlinear term in the Schrödinger equation is still intricate. Heuristically, $h(n^\varepsilon)$ can be considered as a self-interaction potential. Nevertheless, the nonlinear Schrödinger equation (2.17) is very helpful for the mathematical analysis of the isentropic irrotational QHD-system [14, 16, 17, 35].

A similar hydrodynamical structure holds for general modified nonlinear Schrö dinger equations (GMNLS for short)in one space dimension ($d = 1$):

$$i\varepsilon\,\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\partial_x^2\psi^\varepsilon - i\frac{\varepsilon}{2}\partial_x\big(\Phi'(|\psi^\varepsilon|^2)\psi^\varepsilon\big) + h(|\psi^\varepsilon|^2)\psi^\varepsilon. \tag{2.20}$$

By using the ansatz (2.3) for the wave function ψ^ε, we obtain the system of two equations for the so-called *Madelung fluid* (which is equivalent to the GMNLS equation (2.20)):

$$\partial_t n^\varepsilon + \partial_x\left(n^\varepsilon S_x^\varepsilon + n^\varepsilon\Phi'(n^\varepsilon) - \frac{1}{2}\Phi(n^\varepsilon)\right) = 0, \tag{2.21a}$$

$$\partial_t S^\varepsilon + \frac{1}{2}(S_x^\varepsilon)^2 + \frac{1}{2}\Phi'(n^\varepsilon)S_x^\varepsilon + h(n^\varepsilon) = \frac{\varepsilon^2}{2}\frac{1}{\sqrt{n^\varepsilon}}\left(\sqrt{n^\varepsilon}\right)_{xx}. \tag{2.21b}$$

These equations are the continuity equation and Hamilton-Jacobi equation for the "quantum fluid", respectively. It follows immediately from (1.8a,b) that the current density J^ε defined by (2.6) satisfies the differential equation

$$\begin{aligned}\partial_t J^\varepsilon + \partial_x \left(\frac{(J^\varepsilon)^2}{n^\varepsilon} + \frac{1}{2} J^\varepsilon \Phi'(n^\varepsilon) + p(n^\varepsilon) \right) + J^\varepsilon \Phi''(n^\varepsilon) \partial_x n^\varepsilon \\ = \frac{\hbar^2}{4} \partial_x (n^\varepsilon \partial_x^2 \log n^\varepsilon),\end{aligned} \tag{2.22}$$

which is not a conservation law except when $\Phi''(n^\varepsilon) = 0$. This is due to the *derivative loss* caused by the space derivative nonlinear term, $i\frac{\varepsilon}{2}\partial_x\big(\Phi'(|\psi^\varepsilon|^2)\psi^\varepsilon\big)$. The continuity equation (2.21a) gives

$$\begin{aligned}\partial_t \Phi(n^\varepsilon) + \partial_x \Big(\Phi(n^\varepsilon) u^\varepsilon \Big) + \Big(n^\varepsilon \Phi'(n^\varepsilon) - \Phi(n^\varepsilon) \Big) \partial_x u^\varepsilon \\ + \partial_x \Big(\frac{1}{2} n^\varepsilon (\Phi'(n^\varepsilon))^2 \Big) = 0\end{aligned} \tag{2.23}$$

with the fluid velocity $u^\varepsilon := (S^\varepsilon)_x$. As in [6], we introduce the noncanonical current density

$$M^\varepsilon \equiv J^\varepsilon + \Phi(n^\varepsilon). \tag{2.24}$$

Even if the fluid velocity vanishes, i.e., $u^\varepsilon = 0$, the flow has a background momentum with characteristic speed. This implies that solitons of derivative nonlinear Schrödinger equations have nontrivial static limit. In the field theoretical language, we can say that the spectrum of excitations has always a gap (like in superfluidity). We have the local conservation laws associated with the GMNLS equation (2.20):

$$\partial_t n^\varepsilon + \partial_x \left(M^\varepsilon + n^\varepsilon \Phi' - \frac{3}{2} \Phi \right) = 0, \tag{2.25a}$$

$$\begin{aligned}\partial_t M^\varepsilon + \partial_x \left[\frac{M^\varepsilon}{n^\varepsilon} \Big(M^\varepsilon + n^\varepsilon \Phi' - \frac{3}{2}\Phi + \frac{1}{2}(n^\varepsilon \Phi' - \Phi) \Big) \right] \\ + \partial_x \left[\frac{1}{n^\varepsilon} (n^\varepsilon \Phi' - \Phi) \left(\frac{1}{2} n^\varepsilon \Phi' - \Phi \right) \right] + \partial_x p(n^\varepsilon) = \frac{\hbar^2}{4} \partial_x (n^\varepsilon \partial_x^2 \log n^\varepsilon).\end{aligned} \tag{2.25b}$$

Equation (2.25b) is derived by adding (2.22) and (2.23) together. This equation also tells us that the space derivative nonlinear term, $i\frac{\varepsilon}{2}\partial_x\big(\Phi'(|\psi^\varepsilon|^2)\psi^\varepsilon\big)$, not only affects the momentum but also the pressure from the hydrodynamical point of view except when Φ is a linear function. Indeed, if we have $n^\varepsilon \Phi'(n^\varepsilon) - \Phi(n^\varepsilon) = 0$, then $\partial_x\big[\frac{1}{n^\varepsilon}(n^\varepsilon\Phi' - \Phi)(\frac{1}{2}n^\varepsilon\Phi' - \Phi)\big] = 0$. Equations

(2.25a) and (2.25b) correspond to the mass and momentum (or current) conservation laws.

We now return to the linear Schrödinger equation with given potential $V = V(x)$. A mixed quantum mechanical state consists of a sequence of single states with occupation probabilities λ^l, $l = 0, 1, \ldots,$ for the lth single state described by

$$i\varepsilon\psi_t^l = -\frac{\varepsilon^2}{2}\Delta\psi^l + V\psi^l, \tag{2.26a}$$

$$\psi^l(x, t=0) = \psi_I^l(x) = \sqrt{n_I^l(x)}\exp\left(\frac{i}{\varepsilon}S_I^l(x)\right) \tag{2.26b}$$

(for convenience we drop the superscript ε), or, equivalently, by

$$n_t^l + \operatorname{div} J^l = 0, \tag{2.27a}$$

$$J_t^l + \operatorname{div}\left[\frac{J^l \otimes J^l}{n^l}\right] + n^l\nabla V = \frac{\varepsilon^2}{2}n^l\nabla\left[\frac{1}{\sqrt{n^l}}\Delta\sqrt{n^l}\right], \tag{2.27b}$$

$$n^l(x, t=0) = n_I^l(x), \quad J^l(x, t=0) = n_I^l(x)\nabla S_I^l(x). \tag{2.27c}$$

The occupation probabilities satisfy

$$\sum_{l=0}^{\infty}\lambda^l = 1. \tag{2.28}$$

The charge density n, the current J, the energy density tensors E_K, E of the mixed state are given by

$$n(x,t) = \sum_{l=0}^{\infty}\lambda^l n^l(x,t), \tag{2.29a}$$

$$J(x,t) = \sum_{l=0}^{\infty}\lambda^l J^l(x,t), \tag{2.29b}$$

$$E_K(x,t) = \sum_{l=0}^{\infty}\lambda^l E_K^l(x,t), \tag{2.29c}$$

$$E(x,t) = \sum_{l=0}^{\infty}\lambda^l E^l(x,t). \tag{2.29d}$$

E_K^l, E^l are defined as in (2.11) and (2.13) for the lth single state. Note that the flow generated by the mixed state is in general not irrotational anymore.

The definitions of the "current velocities" $u_c = \frac{J}{n}, u_c^l = \frac{J^l}{n^l}, l = 0, 1, 2, \ldots,$ of the "osmotic velocities" $u_{os} = \frac{\varepsilon}{2}\frac{\nabla n}{n}, u_{os}^l = \frac{\varepsilon}{2}\frac{\nabla n^l}{n^l}, l = 0, 1, 2, \ldots,$ and the relations

$$u_c = \sum_{l=0}^{\infty} \Big(\lambda^l \frac{n^l}{n}\Big) u_c^l \tag{2.30a}$$

$$u_{os} = \sum_{l=0}^{\infty} \Big(\lambda^l \frac{n^l}{n}\Big) u_{os}^l \tag{2.30b}$$

allow the definition of a discrete velocity distribution

$$b^l(x,t) = \lambda^l \frac{n^l(x,t)}{n(x,t)}. \tag{2.31}$$

In analogy to the classical kinetic theory, we call the covariance tensors

$$T_c = \sum_{l=0}^{\infty} b^l (u_c^l - u_c) \otimes (u_c^l - u_c), \tag{2.32a}$$

$$T_{os} = \sum_{l=0}^{\infty} b^l (u_{os}^l - u_{os}) \otimes (u_{os}^l - u_{os}) \tag{2.32b}$$

current and osmotic temperature, respectively. Multiplication of (2.27a), (2.27b) by λ^l and summation over l give

$$n_t + \operatorname{div} J = 0, \tag{2.33a}$$

$$J_t + \operatorname{div}\Big[\frac{J \otimes J}{n} + nT - \frac{\varepsilon^2}{4} n (\nabla \otimes \nabla) \ln n\Big] + n\nabla V = 0 \tag{2.33b}$$

with the total temperature $T = T_c + T_{os}$. By (2.32), the constitutive relation reads

$$E = \frac{1}{2}\Big[\frac{J \otimes J}{n} + nT - \frac{\varepsilon^2}{4} n (\nabla \otimes \nabla) \ln n\Big].$$

Multiplying the energy density tensor equation (2.11) by λ^l and summing over l lead to

$$\begin{aligned}(E_{ls})_t + &\frac{\partial}{\partial x_m}\Big[\frac{J_m}{n} E_{ls} + \frac{1}{2}(J_l T_{sm} + J_s T_{lm}) \\ &-\frac{\varepsilon^2}{8}\Big(J_l \frac{\partial^2}{\partial x_s \partial x_m} \ln n + J_s \frac{\partial^2}{\partial x_l \partial x_m} \ln n\Big)\Big] \\ &+\frac{1}{2}\Big(J_l \frac{\partial}{\partial x_s} V + J_s \frac{\partial}{\partial x_l} V\Big) + \frac{\partial}{\partial x_m} q_{mls} = 0.\end{aligned} \tag{2.33c}$$

Obviously, the heat flux tensor q for the mixed state cannot (in general) be expressed in terms of n, J and T only.

In classical fluid dynamics, additional assumptions are made in order to obtain a closed set of equations. One is to consider that the temperature is a scalar (times identity tensor) and another one is to ignore the heat conduction or, if heat conduction phenomena can be expected to be important in the system, to set

$$q = \kappa \nabla T. \tag{2.34}$$

(κ denotes the heat conductivity.) Note that under the constitutive assumption of a scalar temperature it suffices to consider a scalar energy density equation with heat flux vector instead of an energy density tensor equation with heat flux tensor. The Fourier term (2.34) was also used for the QHD-equations (2.33) in semiconductor applications [11, 12]. Other closure conditions for the QHD-equations are not known to the authors.

Now, let us consider the Wigner function [22, 28]

$$w^\varepsilon(x,v,t) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d_\eta} \bar{\psi}^\varepsilon\Big(x + \frac{\varepsilon}{2}\eta, t\Big) \psi^\varepsilon\Big(x - \frac{\varepsilon}{2}\eta, t\Big) e^{i\eta\cdot v}\, d\eta, \tag{2.35}$$

where the wave function $\psi(x,t)$ solves the single state Schrödinger equation (2.1). $w^\varepsilon(x,v,t)$ satisfies the so-called Wigner equation

$$w^\varepsilon_t + v\cdot\nabla_x w^\varepsilon - \theta^\varepsilon[V]w^\varepsilon = 0, \qquad x, v \in \mathbb{R}^d, \quad t \in \mathbb{R}, \tag{2.36a}$$

$$w^\varepsilon(x,v,t=0) = w^\varepsilon_I(x,v), \tag{2.36b}$$

where $\theta^\varepsilon[V]$ is the pseudo-differential operator

$$\theta^\varepsilon[V]w^\varepsilon = \frac{i}{(2\pi)^d} \int_{\mathbb{R}^d_{v'}} \int_{\mathbb{R}^d_\eta} \frac{V(x+\frac{\varepsilon}{2}\eta) - V(x-\frac{\varepsilon}{2}\eta)}{\varepsilon} \\ w^\varepsilon(x,v',t) e^{i(v-v')\cdot\eta}\, d\eta\, dv'$$

and w^ε_I is the Wigner transform of the initial state ψ^ε_I given by (2.8):

$$\begin{aligned} w^\varepsilon_I(x,v) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d_\eta} & \sqrt{n^\varepsilon_I\Big(x+\frac{\varepsilon}{2}\eta\Big) n^\varepsilon_I\Big(x-\frac{\varepsilon}{2}\eta\Big)} \\ & \exp\left\{ \frac{i}{\varepsilon}\Big(S^\varepsilon_I\Big(x+\frac{\varepsilon}{2}\eta\Big) - S^\varepsilon_I\Big(x-\frac{\varepsilon}{2}\eta\Big)\Big) + i\eta\cdot v \right\}\, d\eta. \end{aligned} \tag{2.37}$$

The Wigner equation is a quantum mechanical equivalent of the classical Vlasov equation. Easy calculations show that the lowest-order moments of the Wigner equation are

$$\int_{\mathbb{R}_v^d} w^\varepsilon(x,v,t)\,dv = n^\varepsilon(x,t), \tag{2.38a}$$

$$\int_{\mathbb{R}_v^d} v w^\varepsilon(x,v,t)\,dv = J^\varepsilon(x,t), \tag{2.38b}$$

$$\begin{aligned}\int_{\mathbb{R}_v^d} v\otimes v w^\varepsilon(x,v,t)\,dv = {} & \frac{J^\varepsilon(x,t)\otimes J^\varepsilon(x,t)}{n^\varepsilon(x,t)} \\ & -\frac{\varepsilon^2}{4} n^\varepsilon(x,t)(\nabla\otimes\nabla)\ln n^\varepsilon(x,t) = 2E^\varepsilon\end{aligned} \tag{2.38c}$$

and that

$$W^\varepsilon(x,t) = \frac{1}{2}\int_{\mathbb{R}_v^d} |v|^2 w^\varepsilon(x,v,t)\,dv, \tag{2.38d}$$

$$\begin{aligned}-\frac{\varepsilon^2}{8} n^\varepsilon(x,t)\Delta\left(\frac{J_l^\varepsilon(x,t)}{n^\varepsilon(x,t)}\right) = {} & \frac{1}{2}\int_{\mathbb{R}_v^d}\left(v_l - \frac{J_l^\varepsilon(x,t)}{n^\varepsilon(x,t)}\right) \\ & \left|v - \frac{J^\varepsilon(x,t)}{n^\varepsilon(x,t)}\right|^2 w^\varepsilon(x,v,t)\,dv\end{aligned} \tag{2.38e}$$

hold for the energy density and the heat flux vector. Therefore, multiplying the Wigner equation (2.36a) by $1, v, v\otimes v, |v|^2$ and integrating over $\mathbb{R}^d$ we obtain the continuity, momentum, energy tensor and scalar energy equations (2.7a), (2,7b), (2.14) and (2.16), respectively.

Similar considerations can be made as far as the mixed state is concerned. The mixed state Wigner function reads

$$w(x,v,t) = \sum_{l=0}^{\infty} \lambda^l w^l(x,v,t), \tag{2.39}$$

in which $w^l(x,v,t)$ denotes the Wigner function of the lth single state. Using (2.31) and (2.39) it is easy to see that

$$\int_{\mathbb{R}_v^d} w(x,v,t)\,dv = n(x,t), \tag{2.40a}$$

$$\int_{\mathbb{R}_v^d} vw(x,v,t)\,dv = J(x,t), \tag{2.40b}$$

$$\int_{\mathbb{R}_v^d} v \otimes vw(x,v,t) = \frac{J(x,t)\otimes J(x,t)}{n(x,t)} + n(x,t)T(x,t) - \frac{\varepsilon^2}{4} n(x,t)(\nabla \otimes \nabla)\ln n(x,t) = 2E, \tag{2.40c}$$

$$\frac{1}{2}\int_{\mathbb{R}_v^d} |v|^2 w(x,v,t)\,dv = W = \mathrm{tr}(E), \tag{2.40d}$$

$$\frac{1}{2}\int_{\mathbb{R}_v^d} \left(v_i - \frac{J_i(x,t)}{n(x,t)}\right)\left(v_j - \frac{J_j(x,t)}{n(x,t)}\right)\left(v_k - \frac{J_k(x,t)}{n(x,t)}\right) w(x,v,t)\,dv = q_{ijk}(x,t). \tag{2.40e}$$

Thus, even in the mixed state the QHD equations (2.33) are the lowest-order moment equations of the Wigner equation.

In classical kinetic theory, the same procedure allows the derivation of the Euler equations as moment equations of the Vlasov equation. Special assumptions on the (classical) space distribution function give scalar temperature and vanishing centered third-order moment. The main ingredient in the closure assumptions in classical kinetic theory is the explicit knowledge of an equilibrium solution of the Boltzmann collision operator. In quantum kinetics this is not the case.

3. Global-in-Time Analysis of the Linear Schrödinger Equation

In the following we investigate the classical limit $\varepsilon \to 0$ of the zero temperature QHD equations (2.7). Here we only present the general outline; for details see [13]. From the previous section we know that the QHD equations (2.7) are formally equivalent to the single state Schrödinger equation (2.1). In [13] we have shown rigorously that every solution ψ^ε of the Schrödinger equation (2.1) generates with

$$n^\varepsilon = \bar{\psi}^\varepsilon \psi^\varepsilon, \qquad J^\varepsilon = \varepsilon \mathrm{Im}(\bar{\psi}^\varepsilon \nabla \psi^\varepsilon),$$

a weak solution (in the sense of distributions) of the zero temperature QHD equations (2.7). This result holds even for the nonlinear Schrödinger equation (2.17) and the associated (isothermal or isentropic) QHD equations (2.21a,b).

Now, assume the ε-independent irrotational initial conditions

$$n_I^\varepsilon(x) = n_I(x) \geq 0, \qquad J_I^\varepsilon(x) = n_I(x)u_I(x) = n_I(x)\nabla S_I(x) \tag{3.1}$$

for the QHD equations (2.6). The classical limit analysis $\varepsilon \to 0$ consists of two major points. In a first step, we have to ascertain the existence of a limiting density $n(x,t)$ and a limiting current density $J(x,t)$ of the solutions $n^\varepsilon(x,t)$ and $J^\varepsilon(x,t)$ of (2.6) with initial conditions (3.1) as $\varepsilon \to 0$. Secondly, we have to verify whether the limits $n(x,t)$ and $J(x,t)$ satisfy the formal limit equations of (2.6)

$$n_t + \mathrm{div} J = 0, \tag{3.2a}$$

$$J_t + \mathrm{div}\left[\frac{J \otimes J}{n}\right] + n\nabla V = 0, \tag{3.2b}$$

$$n(t=0) = n_I, \qquad J(t=0) = J_I. \tag{3.2c}$$

In the case of the Korteweg deVries equation, the zero dispersion limit was performed by Lax and Levermore using inverse scattering theory [21]. The same method, the so-called Lax-Levermore procedure, was used by Shan Jin, Levermore and McLaughlin to establish the semiclassical limit of the one-dimensional defocusing cubic nonlinear Schrödinger (NLS) equation in [16, 17]. The integrability is exploited to obtain the complete global characterization of the weak limits of the entire NLS hierarchy of conserved densities as the field evolves from reflectionless initial data under all the associated commuting flows. In this case, all the infinite conserved densities can be represented in terms of derivatives of a potential $\varepsilon^2 \log \tau(x,t)$, where the so-called τ-function is a certain $N \times N$ determinant. For the zero-dispersion limit of the KdV equation [21] and the semiclassical limit of the defocusing NLS hierarchy [16, 17], the τ-function $\tau(x,t)$ is the determinant of a matrix $I + G(x,t)$, where $G(x,t)$ is Hermitian and positive definite. If $\tau(x,t)$ is then written as a sum of the principal minors of $G(x,t)$, it is evidently a sum of positive terms. It can then be shown that the largest term dominates in the limit, leading to a variational theory of the semiclassical limits of many integrable equations.

For the one-dimensional focusing cubic nonlinear Schrödinger problem which is integrable, the matrix $G(x,t)$ is not Hermitian positive definite, and determining the leading contribution to $\tau(x,t)$ in the semiclassical limit remains an open problem. Furthermore, unlike in the defocusing case, the macroscopic dynamics seem to be governed by elliptic partial differential equations. For general initial data, except for analytic initial data, the initial value problem is ill-posed. Thus the semiclassical limit of a sequence of well-posed initial value problems is an ill-posed initial value problem. For numerical experiments we refer to [31].

We use a completely different approach in order to carry out the classical limit $\varepsilon \to 0$ for the zero temperature QHD equations (2.6) with initial conditions (3.1). From the previous section we know that the single state Schrödinger equation (2.1) is equivalent to the Wigner equation (2.29) for the Wigner function w^ε defined in (2.28). It can be seen easily from (2.28) that the initial Wigner function $w_I^\varepsilon(x,v)$ associated to the ε-independent initial conditions (3.1) converges to the measure

$$w_I(x,v) = n_I(x)\delta(v - \nabla S_I(x)) \tag{3.3}$$

as $\varepsilon \to 0$. It is known from the classical limit analysis of the Wigner equation [22, 26] that the Wigner function $w^\varepsilon(x,t)$ converges to a positive measure $w(x,v,t)$, which solves the limiting Vlasov equation

$$w_t + v \cdot \nabla_x w - \nabla_x V \cdot \nabla_v w = 0 \tag{3.4}$$

with initial condition

$$w(x,v,t=0) = w_I(x,v). \tag{3.5}$$

Even the lowest-order moments $n^\varepsilon(x,t)$ and $J^\varepsilon(x,t)$ of the Wigner function w^ε (see (2.38)) converge to the corresponding moments of the measure w:

$$n^\varepsilon(x,t) = \int_{\mathbb{R}_v^d} w^\varepsilon(x,v,t)\,dv \to n(x,t) = \int_{\mathbb{R}_v^d} w(x,v,t)\,dv, \tag{3.6a}$$

$$J^\varepsilon(x,t) = \int_{\mathbb{R}_v^d} v w^\varepsilon(x,v,t)\,dv \to J(x,t) = \int_{\mathbb{R}_v^d} v w(x,v,t)\,dv, \tag{3.6b}$$

if, say, the initial energy is uniformly bounded as $\varepsilon \to 0$ (see [13]). Under weak assumptions on the potential V, the Hamiltonian flow H_t,

$$H_t(x,v) = \Big(\tilde{x}(t;x,v), \tilde{v}(t;x,v)\Big), \tag{3.7}$$

where $\tilde{x}$ and $\tilde{v}$ solve

$$\dot{\tilde{x}} = \tilde{v}, \qquad \tilde{x}(0) = x, \tag{3.8a}$$

$$\dot{\tilde{v}} = -\nabla V(\tilde{x}), \quad \tilde{v}(0) = v, \tag{3.8b}$$

is globally defined and the relation

$$\int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} \begin{pmatrix} 1 \\ v_l \\ v_l v_m \end{pmatrix} \sigma\, dw(t) = \int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} \left(\begin{pmatrix} 1 \\ v_l \\ v_l v_m \end{pmatrix} \sigma \right) \circ H_t \, dw_I \tag{3.9}$$

holds for all bounded continuous functions σ on $\mathbb{R}_x^d \times \mathbb{R}_v^d$. This relation with the special form of w_I in (3.1) is used to evaluate the limiting density $n(x,t)$, current density $J(x,t)$ and energy density tensor

$$E(x,t) = \frac{1}{2}\int_{\mathbb{R}_v^d} v \otimes v w(x,v,t)\, dv$$

at every time $t > 0$. The first two moment equations of the Vlasov equation (3.4) are easily obtained

$$n_t + \operatorname{div} J = 0, \quad n(t=0) = n_I, \tag{3.10a}$$

$$J_t + \operatorname{div}(2E) + n\nabla V = 0, \quad J(t=0) = J_I. \tag{3.10b}$$

Introducing the Radon-Nikodym derivatives u and r of J and E respectively with respect to n, (3.10) reads

$$n_t + \operatorname{div}(un) = 0, \quad n(t=0) = n_I, \tag{3.11a}$$

$$(un)_t + \operatorname{div}(2rn) + n\nabla V = 0, \quad u(t=0) = u_I. \tag{3.11b}$$

Therefore, the limits n and J of n^ε and J^ε solve the formal limit equations (3.2) if $2r$ is equal to $u \otimes u$. We show the following result in [13]:

Theorem 3.1. *Let* $-\infty \le T_1 \le 0 \le T_2 \le \infty$. *Then* $n \in C_b(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}^d)w-\star)$, $u \in L^\infty(\mathbb{R}_t; L^1(\mathbb{R}^d; dn(t))^d)$ *with* $nu \in C_b(\mathbb{R}_t; \mathcal{M}(\mathbb{R}^d)^d w - \star)$ *solve*

$$(n\sigma(u))_t + \operatorname{div}_x(nu\sigma(u)) + n\nabla_x V \cdot \nabla_u \sigma(u) = 0, \tag{3.12a}$$

$$n(t=0) = n_I, \quad u(t=0) = u_I \tag{3.12b}$$

in

$$\begin{cases} \mathcal{D}'(\mathbb{R}_x^d \times (T_1,T_2)) & for \quad T_1 < 0 < T_2, \\ \mathcal{D}'(\mathbb{R}_x^d \times [0,T_2)) & for \quad T_1 = 0, \\ \mathcal{D}'(\mathbb{R}_x^d \times (T_1,0]) & for \quad T_2 = 0 \end{cases} \tag{3.13}$$

for every $\sigma = \sigma(v) \in C^1(\mathbb{R}^d;\mathbb{R})$ *with* $\sigma(v)/(1+|v|) \in L^\infty(\mathbb{R}^d)$ *and* $\nabla_v\sigma(v)/(1+|v|^2) \in L^\infty(\mathbb{R}^d)$ *iff the solution of* (3.1) *is given by*

$$w(x,v,t) = n(x,t)\delta(u(x,t) - v) \tag{3.14}$$

in

$$\begin{cases} \mathcal{D}'(\mathbb{R}^d_x \times (T_1, T_2)) & for \quad T_1 < 0 < T_2, \\ \mathcal{D}'(\mathbb{R}^d_x \times [0, T_2)) & for \quad T_1 = 0, \\ \mathcal{D}'(\mathbb{R}^d_x \times (T_1, 0]) & for \quad T_2 = 0. \end{cases}$$

Proof. Assume that $T_1 < 0 < T_2$ and choose $\omega = \omega(x,t) \in \mathcal{D}(\mathbb{R}^d_x \times (T_1, T_2))$. For given $\sigma \in \mathcal{D}(\mathbb{R}^d_u)$, the weak formulation of (3.12a,b) reads

$$\int_{T_1}^{T_2} \int_{\mathbb{R}^d_x} \sigma(u)\omega_t dn(t)dt + \int_{T_1}^{T_2} \int_{\mathbb{R}^d_x} \sigma(u) u \cdot \nabla_x \omega dn(t)dt$$

$$- \int_{T_1}^{T_2} \int_{\mathbb{R}^d_x} \nabla_x V \cdot \nabla_v \sigma(u) \omega dn(t)dt = 0.$$

This is exactly the weak formulation of the Vlasov equation (3.1) with the test function $\omega(x,t)\sigma(v)$, where w is given by (3.12). Now let $\sigma_l(v) \in \mathcal{D}(\mathbb{R}^d_v)$ be a sequence satisfying the conditions stated in the theorem and converging almost everywhere to $\sigma(v) \in C^1(\mathbb{R}^d)$ as $l \to \infty$. Lemma 3.3 below and the fact that the energy is bounded guarantees $|u|^2 \in L^\infty(\mathbb{R}_t; L^1(\mathbb{R}^d; dn(t)))$. Therefore, the dominated convergence theorem implies the assertion. ■

The equation (3.12a,b) is a renormalized formulation of (3.11a,b). In particular, (3.12a) is obtained by choosing $\sigma \equiv v_i$, $i = 1, \ldots, d$. Thus, the limit densities n and $J = nu$ of the quantum WKB-densities $n\varepsilon$ and J^ε satisfy (3.12) on a given time interval (T_1, T_2) if n, nu are renormalized solutions of (3.12) on (T_1, T_2) (in the sense defined in Theorem 3.1).

Theorem 3.1 yields

Corollary 3.2. *Let $u_I \in C^1_b(\mathbb{R}^d)$ and let $-\infty \leq T_1 \leq 0$ be an interval on which the Burger's equation* (3.15) *has a solution $u \in C^1_b(\mathbb{R}^d_x \times (T_1, T_2))$. Then the limits n, $J = nu$ of the densities n^ε, J^ε satisfy* (3.10) *on* (T_1, T_2) *with $2r = u \otimes u$. Also u is vortex free in (T_1, T_2).*

Proof. Let $\sigma \in C^1(\mathbb{R}^d; \mathbb{R})$, $\sigma(v)/(1 + |v|) \in L^\infty(\mathbb{R}^d)$, $\nabla_v \sigma(v)/(1 + |v|^2) \in L^\infty(\mathbb{R}^d)$ and multiply (3.18)(a) by $\sigma'(u)$:

$$\sigma(u)_t + u \cdot \nabla \sigma(u) + \nabla V \cdot \nabla_u \sigma(u) = 0.$$

Multiplication by the (regular) solution n of the continuity equation (3.13a) shows that (n, u) is a renormalized solution on (T_1, T_2). ■

If the field driven Burger's equation

$$u_t + (u \cdot \nabla)u + \nabla V = 0, \tag{3.15a}$$

$$u(x, t = 0) = u_I(x) \tag{3.15b}$$

has a classical solution on a certain time interval, then the limit equations (3.2) are satisfied by n and J.

The result we obtained in [13] is slightly more general, but it's formulation is lengthy and beyond the scope of this presentation. The breakdown of the classical solution of the Burger's equation is strictly related to the occurrence of caustics in the field of characteristic curves:

$$\dot{\hat{x}} = \hat{v}, \quad \hat{x}(t = 0, x) = x \tag{3.16a}$$

$$\dot{\hat{v}} = -\nabla V(\hat{x}), \quad \hat{v}(t = 0, x) = u_I(x). \tag{3.16b}$$

In [13], a characterization of the behavior of the limits n and J at the breakdown points of the classical solution is also given. In particular, concentration phenomena in the density n may occur (see examples below).

Lemma 3.3. $2r(\cdot, t) \geq u(\cdot, t) \otimes u(\cdot, t)$ $n(\cdot, t)$*-a.e. in the sense of positive semidefinite symmetric matrices.*

Proof. Take $\varphi \in C_b(\mathbb{R}^d)$. Then, by the definition of $u = (u_1, \ldots, u_d)$ we have

$$\int_{\mathbb{R}^d_x} u_i u_j \varphi dn = \int_{\mathbb{R}^{2d}_{x,v}} v_i u_j \varphi dw.$$

Thus, for $\gamma \in C_b(\mathbb{R}^d; \mathbb{R}^d)$ we obtain

$$\begin{aligned}
\int_{\mathbb{R}^d_x} \gamma^T u \otimes u \gamma dn &= \int_{\mathbb{R}^d_x} \sum_{i,j=1}^d u_i \gamma_i u_j \gamma_j dn = \int_{\mathbb{R}^{2d}_{x,v}} \sum_{i=1}^d v_i \gamma_i \sum_{j=1}^d u_j \gamma_j dw \\
&\leq \left(\int_{\mathbb{R}^{2d}_{x,v}} \left(\sum_{i=1}^d v_i \gamma_i \right)^2 dw \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^{2d}_{x,v}} \left(\sum_{j=1}^d u_j \gamma_j \right)^2 dw \right)^{\frac{1}{2}} \\
&= \left(\int_{\mathbb{R}^d_x} 2\gamma^T r \gamma dn \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^d_x} \gamma^T u \otimes u \gamma dn \right)^{\frac{1}{2}}.
\end{aligned}$$

■

Thus, we have just shown

$$2r(x, t) = u(x, t) \otimes u(x, t) + T(x, t)$$

holds, where T is a positive semidefinite (temperature) tensor. Obviously, $T \equiv 0$ in the regime of classical solutions. Note also that in case of classical solutions, the Burger's equation (3.15) can be obtained easily from the limit equations (3.2) by using the continuity equation and eliminating n from the momentum equation.

The following two examples give an idea of the theory presented above.

Example 3.4. Let $V(x) \equiv 0$ and $n_I(x) > 0$. We set

$$u_I = 1\!\!1_{(x<0)} + (1-x) 1\!\!1_{(0\le x<1)}.$$

We obtain the characteristics

$$\hat{x}(t,x) = (x+t) 1\!\!1_{(x<0)} + [x + (1-x)t]\, 1\!\!1_{(0\le x<1)} + x 1\!\!1_{(1\le x)}.$$

Up to time $t = 1$, they do not intersect. For $t > 1$, we have intersections in the region $1 < x \le t$. The Burger's equation has a smooth solution up to $t = 1$ and a shock with speed $s = 1/2$ starting at $t = 1$, $x = 1$ (as vanishing viscosity limit of the solutions of the viscous regularized Burger's equation).

Using (3.9), we obtain

$$n(x,t) = \begin{cases} n_I(x-t) 1\!\!1_{(x<t)} + \dfrac{1}{1-t} n_I\left(\dfrac{x-t}{1-t}\right) 1\!\!1_{(t\le x<1)} + n_I(x) 1\!\!1_{(1<x)} \\ \qquad\qquad \text{if} \quad t<1, \\ \displaystyle\int_0^1 n_I(y)dy\, \delta(x-1) + n_I(x-1) 1\!\!1_{(x<1)} + n_I(x) 1\!\!1_{(1<x)} \\ \qquad\qquad \text{if} \quad t=1, \\ n_I x - t) 1\!\!1_{(x\le 1)} + \left[n_I(x-t) + \dfrac{1}{t-1} n_I\left(\dfrac{x-t}{1-t}\right) + n_I(x) \right] \\ \quad 1\!\!1_{(1<x\le t)} + n_I(x) 1\!\!1_{(t<x)} \qquad \text{if} \quad t>1. \end{cases}$$

Easy calculations lead to

$$u(x,t) = \begin{cases} 1\!\!1_{(x<t)} + \dfrac{1-x}{1-t} 1\!\!1_{(t\le x<1)}, & t<1, \\ \dfrac{\int_0^1 n_I(y)(1-y)dy}{\int_0^1 n_I(y)dy} + 1\!\!1_{(x<1)}, & t=1, \\ 1\!\!1_{(x\le 1)} + \dfrac{n_I(x-t) + \frac{x-1}{(t-1)^2} n_I\left(\frac{x-t}{1-t}\right)}{n_I(x-t) + \frac{1}{t-1} n_I\left(\frac{x-t}{1-t}\right) + n_I(x)} 1\!\!1_{(1<x\le t)}, & t>1, \end{cases}$$

and

$$2r(x,t) = \begin{cases} \mathbb{1}_{(x<t)} + \left(\dfrac{1-x}{1-t}\right)^2 \mathbb{1}_{(t\le x<1)}, & t<1, \\ \dfrac{\int_0^1 n_I(y)(1-y)^2 dy}{\int_0^1 n_I(y)dy} + \mathbb{1}_{(x<1)} & t=1, \\ \mathbb{1}_{(x\le 1)} + \dfrac{n_I(x-t) + \frac{(x-1)^2}{(t-1)^3} n_I\left(\frac{x-t}{1-t}\right)}{n_I(x-t) + \frac{1}{t-1} n_I\left(\frac{x-t}{1-t}\right) + n_I(x)} \mathbb{1}_{(1<x\le t)}, & t>1. \end{cases}$$

As we see, $u(x,t)$ is a smooth solution of the Burger's equation up to $t=1$ but for $t>1$ it is not even a weak solution. For $t<1$, we have $2r(x,t) = u(x,t)^2$. At $t=1$, charge concentrates at $x=1$.

Characteristics of Example 3.4.

Characteristics of Example 3.5 in one space dimension.

Example 3.5. Let the potential $V = V(x) = |x|^2/2$ (harmonic oscillator), $u_I(x) = u_I =$ const. and $n_I(x) > 0$ (d space dimensions). The IVP (3.16) gives

$$\hat{x}(t,x) = x\cos t + u_I \sin t,$$
$$\hat{v}(t,x) = -x\sin t + u_I \cos t.$$

All characteristics intersect at time $t = ((2k+1)/2)\pi$, $k = \dots, -1, 0, 1, \dots$, at the point $x = u_I(-1)^{k+1}$. In-between the points $t = ((2k+1)/2)\pi$ and $t = ((2k+3)/2)\pi$, $k = \dots, -1, 0, 1, \dots$, we have no intersection and the map $x \mapsto \hat{x}(t,\cdot)$: $\mathbb{R}^d \to \mathbb{R}^d$ is an isomorphism. The relations (3.9) give

$$n(x,t) = \begin{cases} \dfrac{1}{|\cos t|^d}\, n_I\left(\dfrac{x - u_I \sin t}{\cos t}\right), & t \neq \dfrac{2k+1}{2}\pi, \\ \displaystyle\int_{-\infty}^{\infty} n_I(y)dy\, \delta(x - (-1)^k u_I), & t = \dfrac{2k+1}{2}\pi, \end{cases}$$

$$J(x,t) = \begin{cases} \dfrac{1}{|\cos t|^d} n_I \left(\dfrac{x - u_I \sin t}{\cos t} \right) \dfrac{u_I - x \sin t}{\cos t}, & t \neq \dfrac{2k+1}{2}\pi, \\ \displaystyle\int_{-\infty}^{\infty} n_I(y) y dy (-1)^{k+1} \delta(x - (-1)^k u_I), & t = \dfrac{2k+1}{2}\pi, \end{cases}$$

$$2E(x,t) = \begin{cases} \dfrac{1}{|\cos t|^d} n_I \left(\dfrac{x - u_I \sin t}{\cos t} \right) \left(\dfrac{u_I - x \sin t}{\cos t} \right) \otimes \left(\dfrac{u_I - x \sin t}{\cos t} \right), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad t \neq \dfrac{2k+1}{2}\pi, \\ \displaystyle\int_{-\infty}^{\infty} n_I(y) y \otimes y dy (-1)^{k+1} \delta(x - (-1)^k u_I), \quad t = \dfrac{2k+1}{2}\pi, \end{cases}$$

for $k = \ldots, -1, 0, 1, \ldots$ and therefore

$$u(x,t) = \begin{cases} \dfrac{u_I - x \sin t}{\cos t}, & t \neq \dfrac{2k+1}{2}\pi, \\ \dfrac{\int_{-\infty}^{\infty} n_I(y) y dy}{\int_{-\infty}^{\infty} n_I(y) dy} (-1)^{k+1}, & t = \frac{2k+1}{2}\pi, \end{cases}$$

$$2r(x,t) = \begin{cases} \left(\dfrac{u_I - x \sin t}{\cos t} \right) \otimes \left(\dfrac{u_I - x \sin t}{\cos t} \right), & t \neq \dfrac{2k+1}{2}\pi, \\ \dfrac{\int_{-\infty}^{\infty} n_I(y) y \otimes y dy}{\int_{-\infty}^{\infty} n_I(y) dy}, & t = \dfrac{2k+1}{2}\pi, \end{cases}$$

for $k = \ldots, -1, 0, 1, \ldots$. This is an example where the limit equations are satisfied by n and J even after the breakdown of the classical solution in the Burger's equation except at the points $t = ((2k+1)/2)\pi$, $k = \ldots, -1, 0, 1, \ldots$, of charge concentration.

Remark 3.6. Peter Lax initiated [19] the modern study of the zero-dispersion limit in the discrete setting. The Lax-Levermore theory [21] for the KdV equation has also been carried out on other integrable systems. The semi-classical limit of the one-dimensional defocusing cubic nonlinear Schrödinger equation (NLS) was the first to be treated after the KdV equation [16, 17]. Because that work introduced the hierarchical approach, it therefore includes the defocusing modified KdV (mKdV) equation, which is the next equation in the NLS hierarchy. Both the KdV and defocusing NLS hierarchies have self-adjoint Lax operator, so it was a surprise when a zero-dispersion limit for the focusing mKdV equation was the next to be treated [9]. In that case the Lax operator is nonselfadjoint Zakharov-Shabat operator. The continuum limit of the Toda lattice was the next [8]. It was the first discrete system to be so analyzed. Recently, a continuum limit for Ablowitz-Ladik lattice has been carried out [34].

4. Local-in-Time Analysis of (Nonintegrable) Nonlinear Schrödinger Equations

In this section we shall consider the semiclassical limit of nonintegrable nonlinear Schrödinger equations. At first we mention that a modified Madelung's transformation has been utilized in the short-time study of the semiclassical limit (WKB limit) of the NLS:

$$i\varepsilon\psi_t^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + h(\bar{\psi}^\varepsilon\psi^\varepsilon)\psi^\varepsilon \tag{4.1}$$

with initial data: $\psi^\varepsilon(x,t=0) = \sqrt{n_I(x)}e^{iS_I(x)/\varepsilon}$. Grenier [15] showed in particular that for n_I and S_I in $H^s(\mathbb{R}^d)$, $s > 2 + d/2$ and $h' > 0$, solutions ψ^ε exist on a small time interval $[0,T]$, T independent of ε. Moreover, $\psi^\varepsilon = \sqrt{n^\varepsilon(x,t)}e^{iS^\varepsilon(x,t)/\varepsilon}$, with n^ε and S^ε in $L^\infty([0,T];H^s)$ uniformly in ε, and $(n^\varepsilon, \nabla S^\varepsilon)$ converges to the solution (n,u) of the isentropic compressible Euler equation:

$$n_t + \operatorname{div}(nu) = 0, \tag{4.2a}$$

$$u_t + \nabla\left(\frac{|u|^2}{2} + h(n)\right) = 0. \tag{4.2b}$$

We can also rewrite (4.2) in terms of the density and momentum $(n, J = nu)$ as

$$n_t + \operatorname{div}(nu) = 0, \tag{4.3a}$$

$$J_t + \operatorname{div}\left(\frac{J\otimes J}{n}\right) + \nabla p(n) = 0, \tag{4.3b}$$

where $p(n) = nU'(n) - U(n)$ and $U(n) = \int h(n)dn$. The condition $h' > 0$ or equivalently $p'(n) = nU''(n) > 0$ which ensures the hyperbolicity of the Euler system (4.2) or (4.3) means that the pressure $p(n)$ must be a strictly increasing function of n. This implies that U must be a strictly convex function of n and thus corresponds to a *defocusing* NLS equation. In this context, a *focusing* nonlinear Schrödinger equation can be understood as a fluid whose pressure decreases when the mass density increases – a phenomenon leading to the development of mass concentration.

The above cited result is only correct as long as the solution of the Euler system (4.2) or (4.3) remains classical. In this case the limiting energy density will be given by

$$E = \frac{1}{2}\frac{|J|^2}{n} + U(n) \tag{4.4}$$

and satisfies

$$\partial_t E + \operatorname{div}\left(\frac{J}{n}(E + p(n))\right) = 0 \tag{4.5}$$

hence, playing the role of a Lax entropy for the Euler system (4.3). Moreover, the genuinely nonlinear nature of the Euler system ensures that its classical solution will develop singular behavior (an infinite derivative) for all but rarefaction initial data.

The same modified Madelung's transformation used by Grenier also applied to the derivative and modified nonlinear Schrödinger equations as well. More precisely, we look for solutions ψ^ε of the form

$$\psi^\varepsilon(x,t) = A^\varepsilon(x,t)\exp\left(\frac{i}{\varepsilon}S^\varepsilon(x,t)\right), \tag{4.6}$$

where the complex-valued function $A^\varepsilon = a^\varepsilon + ib^\varepsilon$ represents the amplitude and the real-valued S^ε represents the phase. Here we allow the phase function S^ε to depend on ε.

Now inserting (4.6) into the GMNLS equation (2.20) and then splitting into two parts, of order $O(1/\varepsilon)$ and $O(1)$ respectively, we obtain

$$S^\varepsilon_t + \frac{1}{2}(S^\varepsilon_x)^2 + \frac{1}{2}\Phi' S^\varepsilon_x + U' = 0, \tag{4.7}$$

$$iA^\varepsilon_t + \frac{i}{2}(A^\varepsilon S^\varepsilon_{xx} + 2A^\varepsilon_x S^\varepsilon_x) + \frac{i}{2}\Phi' A^\varepsilon_x + \frac{i}{2}A^\varepsilon \Phi'' \partial_x(|A^\varepsilon|^2) = -\frac{\varepsilon}{2}A^\varepsilon_{xx}. \tag{4.8}$$

The equations (4.7) are not the same as $(2.21a, b)$ where we split into the real and imaginary parts. The second-derivative term (the dispersive term) is highly nonlinear in (2.21a,b) but it is *linear* in (4.7). Hence the classical quasilinear hyperbolic theory can be applied to the local-in-time analysis of the semiclassical limit of Schrödinger-type equations. Considering the change of variable $w^\varepsilon = S^\varepsilon_x$ and using $A^\varepsilon = a^\varepsilon + ib^\varepsilon$, we have

$$a^\varepsilon_t + (w^\varepsilon + \frac{1}{2}\Phi')a^\varepsilon_x + \frac{1}{2}\Phi'' a^\varepsilon\left[(a^\varepsilon)^2 + (b^\varepsilon)^2\right]_x + \frac{1}{2}a^\varepsilon w^\varepsilon_x = -\frac{\varepsilon}{2}b^\varepsilon_{xx}, \tag{4.8a}$$

$$b_t^\varepsilon + (w^\varepsilon + \frac{1}{2}\Phi')b_x^\varepsilon + \frac{1}{2}\Phi'' b^\varepsilon \big[(a^\varepsilon)^2 + (b^\varepsilon)^2\big]_x + \frac{1}{2} b^\varepsilon w_x^\varepsilon = \frac{\varepsilon}{2} a_{xx}^\varepsilon, \tag{4.8b}$$

$$w_t^\varepsilon + (w^\varepsilon + \frac{1}{2}\Phi')w_x^\varepsilon + (\frac{1}{2}\Phi'' w^\varepsilon + U'')\big[(a^\varepsilon)^2 + (b^\varepsilon)^2\big]_x = 0. \tag{4.8c}$$

This system can be written in the form

$$V_t^\varepsilon + \mathcal{A}(V^\varepsilon)V_x^\varepsilon = \frac{\varepsilon}{2}\mathcal{L}(V^\varepsilon), \qquad V^\varepsilon = (a^\varepsilon, b^\varepsilon, w^\varepsilon)^t, \tag{4.9}$$

where

$$\mathcal{A}(V^\varepsilon) \equiv \begin{pmatrix} w^\varepsilon + \frac{1}{2}\Phi' + (a^\varepsilon)^2\Phi'' & a^\varepsilon b^\varepsilon \Phi'' & \frac{1}{2}a^\varepsilon \\ a^\varepsilon b^\varepsilon \Phi'' & w^\varepsilon + \frac{1}{2}\Phi' + (b^\varepsilon)^2\Phi'' & \frac{1}{2}b^\varepsilon \\ a^\varepsilon(w^\varepsilon\Phi'' + 2U'') & b^\varepsilon(w^\varepsilon\Phi'' + 2U'') & w^\varepsilon + \frac{1}{2}\Phi' \end{pmatrix} \tag{4.10}$$

and

$$\mathcal{L}(V^\varepsilon) = \begin{pmatrix} 0 & -\partial_x^2 & 0 \\ \partial_x^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a^\varepsilon \\ b^\varepsilon \\ w^\varepsilon \end{pmatrix} = \begin{pmatrix} -b_{xx}^\varepsilon \\ a_{xx}^\varepsilon \\ 0 \end{pmatrix} \tag{4.11}$$

is an antisymmetric matrix. The matrix $\mathcal{A}(V^\varepsilon)$ can be symmetrized by

$$\mathcal{S}(V^\varepsilon) = \begin{pmatrix} 2w^\varepsilon\Phi'' + 4U'' & 0 & 0 \\ 0 & 2w^\varepsilon\Phi'' + 4U'' & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{4.12}$$

which is symmetric and positive if $w^\varepsilon\Phi'' + 2U'' > 0$ for all V^ε. Thus, we wrote the general modified nonlinear Schrödinger equation (2.20) as a *linear* dispersive perturbation of a quasilinear symmetric hyperbolic system:

$$\mathcal{S}(V)V_t + \tilde{\mathcal{A}}(V)V_x = \frac{\varepsilon}{2}\tilde{\mathcal{L}}(V), \tag{4.13}$$

where $\tilde{\mathcal{A}} = \mathcal{S}\mathcal{A}$ is a symmetric matrix (we omit ε for convenience). The antisymmetric operator $(\varepsilon/2)\tilde{\mathcal{L}} = (\varepsilon/2)\mathcal{S}\mathcal{L}$ reflects the dispersive nature of the equations. Moreover, the classical energy estimate shows that this term contributes nothing to the estimate, i.e., the singular perturbation does not create energy. Therefore, the existence of the classical solutions and its semiclassical limit proceed along the lines of the classical theory of quasilinear symmetric hyperbolic systems (with some modifications). Indeed, we have the following theorems [6, 7].

Theorem 4.1. *Let $\Phi, U \in C^\infty(\mathbb{R}^+, \mathbb{R})$ with $\frac{\partial}{\partial x} S_I^\varepsilon \Phi''(n_I) + 2U''(n_I) > 0$. Let $s > 5/2$ be such that A_I^ε and $\partial_x S_I$ are uniformly bounded in H^s. Then a solution ψ^ε of the GMNLS equation* (2.20) *exists on a small time interval* $[0, T]$, *T independent of ε. Moreover, $\psi^\varepsilon(x,t) = A^\varepsilon(x,t)\exp((i/\varepsilon)S^\varepsilon(x,t))$ with A^ε and S_x^ε bounded in $L^\infty((0,T); H^s)$ uniformly in ε and limit points of $(A^\varepsilon, S_x^\varepsilon)$ are solutions of the modified Euler equation* (2.25a,b)

Theorem 4.2. *Let (n, M) be a solution of the quasilinear hyperbolic system* (2.25a,b) (*the modified Euler equations*) *for $0 \le t \le T$ with initial condition*

$$n_I(x) = n(x, t = 0) = |A_I(x)|^2,$$
$$M_I(x) = M(x, t = 0) = |A_I(x)|^2 \partial_x S_I(x) + \Phi(|A_I(x)|^2).$$

Then there exists a critical value of ε, ε_c, and a constant $C > 0$ such that under the hypotheses

(1) *$A_I^\varepsilon(x)$ converges strongly to A_I in H^s as ε tends to* 0,

(2) $\|n_I\|_{H^s} < \infty, \quad \|M_I\|_{H^s} < \infty, \quad s \ge 3,$

(3) $0 < \varepsilon < \varepsilon_c,$

the initial value problem for the GMNLS equation (2.20) *has a unique classical solution of the form $\psi^\varepsilon(x,t) = A^\varepsilon(x,t)\exp((i/\varepsilon)S^\varepsilon(x,t))$ on* $[0, T]$. *Moreover, A^ε and S_x^ε are bounded in $L^\infty((0,T); H^s)$ uniformly in ε.*

The question of how to analyze dispersive limits of nonintegrable nonlinear Schrödinger equations globally in time is widely open. Simple modulation theories have been worked out, and there have been some very preliminary analytical results, but the gaps are enormous to our knowledge.

5. Deterministic Analogue of Turbulence Via Zero Dispersion Limit

Some of the basic ideas of turbulence can be addressed in a deterministic setting instead of introducing random realizations of the fluid. In particular, the weak limits of oscillatory sequences of dispersive (quantum) compressible flows show a remarkable resemblance to the ensemble average of classical turbulence flow. Remarkably, the weak limit satisfies an equation with an extra diffusion, hence the name *turbulent diffusion* appears naturally. Following the program initiated by Peter D. Lax [20], the diffusive property of the limit was analyzed by C. Bardos, J-M Ghidaglia and S. Kamvissis in [5]. The specific problem under consideration is the defocusing 1-d cubic nonlinear Schrödinger equation given by

$$i\varepsilon\psi_t^\varepsilon + \frac{\varepsilon^2}{2}\psi_{xx}^\varepsilon + (1 - |\psi^\varepsilon|^2)\psi^\varepsilon = 0 \tag{5.1}$$

with the far-field boundary condition

$$\psi^\varepsilon(x,t) \sim \exp\Big(\pm \frac{i}{\varepsilon} S_\infty\Big) \qquad \text{as } x \to \pm\infty,$$

for some $S_\infty \in \mathbb{R}$, and the initial condition

$$\psi^\varepsilon(x,t=0) = \sqrt{n(x)}\exp\Big(\frac{i}{\varepsilon}S(x)\Big) \tag{5.2}$$

with smooth functions $n(x)$ and $S(x)$ which are independent of ε and consistent with the far-field boundary conditions. The defocusing NLS equation is equivalent to the system

$$n^\varepsilon_t + J^\varepsilon_x = 0, \tag{5.3a}$$

$$J_t + \Big(\frac{(J^\varepsilon)^2}{n^\varepsilon} + \frac{(n^\varepsilon)^2}{2}\Big)_x = \frac{\varepsilon^2}{4}(n^\varepsilon(\log n^\varepsilon)_{xx})_x. \tag{5.3b}$$

The equation (5.1) is time reversible and (5.3a,b) is a reversible perturbation of the usual isentropic compressible Euler equation. For ε going to zero the function n^ε and J^ε converge weakly (because of the uniform energy bound) to

$$\bar{n} = \text{weak-}\lim_{\varepsilon\to 0} n^\varepsilon, \tag{5.4a}$$

$$\bar{J} = \text{weak-}\lim_{\varepsilon\to 0} J^\varepsilon, \tag{5.4b}$$

respectively. The weak limit of the energy is given by

$$\bar{Q} = \text{weak-}\lim_{\varepsilon\to 0} Q(n^\varepsilon, J^\varepsilon) \equiv \text{weak-}\lim_{\varepsilon\to 0} \frac{(J^\varepsilon)^2}{n^\varepsilon} + \frac{(n^\varepsilon)^2}{2}. \tag{5.5}$$

The limit equation is

$$\bar{n}_t + \bar{J}_x = 0, \tag{5.6a}$$

$$\bar{J}_t + \Big(\frac{\bar{J}^2}{\bar{n}} + \frac{\bar{n}^2}{2}\Big)_x + \big(\bar{Q} - Q(\bar{n},\bar{J})\big)_x = 0. \tag{5.6b}$$

In the context of the semiclassical limit of the defocusing cubic nonlinear Schrödinger hierarchy, it is known [17] that the conserved densities converge in the weak-L^1_{loc} topology. In the prebreaking regime the weak-L^1_{loc} convergence can be strengthened to strong-L^1 convergence by using conservation of the densities and the convexity of the energy. Thus, in the region where strong convergence occurs one has

$$\bar{Q} - Q(\bar{n}, \bar{J}) = 0. \tag{5.7}$$

As expected, in these regions (5.6) is the compressible Euler equation for an isentropic fluid:

$$\bar{n}_t + \bar{J}_x = 0, \tag{5.8a}$$

$$\bar{J}_t + \left(\frac{\bar{J}^2}{\bar{n}} + \frac{\bar{n}^2}{2}\right)_x = 0. \tag{5.8b}$$

However, the strong convergence does not hold everywhere except in the pre-breaking regime. The regions where strong convergence fails are called the *Whitham regions*. Since the function $(n, J) \mapsto Q(n, J)$ is convex, the convexity argument implies

$$\bar{Q} - Q(\bar{n}, \bar{J}) > 0 \tag{5.9}$$

in the Whitham region. Define

$$\nu = \frac{\bar{Q} - Q(\bar{n}, \bar{J})}{\bar{J}_x}. \tag{5.10}$$

Then (5.6) become

$$\bar{n}_t + \bar{J}_x = 0, \tag{5.11a}$$

$$\bar{J}_t + \left(\frac{\bar{J}^2}{\bar{n}} + \frac{\bar{n}^2}{2}\right)_x + (\nu \bar{J}_x)_x = 0. \tag{5.11b}$$

The term $(\nu \bar{J}_x)_x$ plays the role of the *turbulent diffusion.* The existence of the turbulent model requires that ν be nonnegative, which is equivalent to the property

$$\nu = \frac{\bar{Q} - Q(\bar{n}, \bar{J})}{\bar{J}_x} \geq 0 \qquad \Longleftrightarrow \qquad \bar{J}_x > 0. \tag{5.12}$$

Since diffusive properties may appear on a larger time scale, it is natural to explore the properties (5.13) for large time. Assume that the initial datum $\sqrt{n(x)}$ is a single up-side-down positive bump with a unique minimum and a horizontal asymptotic of 1 as $|x| \to \infty$ which is also its upper bound. Then the scattering data for $\sqrt{n(x)}$ and $S(x)$ can be computed asymptotically for small ε in terms of the associated Riemann invariants using the semiclassical (WKB) method. Observe that the existence for large time of a diffusive regime would be given by $\bar{J}_x \geq 0$ in the Whitham region and with the conservation of mass (5.11a) this is equivalent to $\bar{n}_t \leq 0$. This can be discussed in detail with the help of the Weyl formula [17].

The above observation concerns the appearance of the positive turbulent viscosity in the limit equation satisfied by $(\bar{n}, \bar{J})$ for the NLS dispersive limit. This is clearly related to the appearance of irreversibility in the weak limit of reversible model [5].

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