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Stimming

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# On the time evolution of Wigner measures for Schrödinger equations

Rémi Carles, Clotilde Fermanian-Kammerer, Norbert J. Mauser,  
and Hans Peter Stimming

**ABSTRACT.** In this survey, our aim is to emphasize the main known limitations to the use of Wigner measures for Schrödinger equations. After a short review of successful applications of Wigner measures to study the semi-classical limit of solutions to Schrödinger equations, we list some examples where Wigner measures cannot be a good tool to describe high frequency limits. Typically, the Wigner measures may not capture effects which are not negligible at the pointwise level, or the propagation of Wigner measures may be an ill-posed problem. In the latter situation, two families of functions may have the same Wigner measures at some initial time, but different Wigner measures for a larger time. In the case of systems, this difficulty can partially be avoided by considering more refined Wigner measures such as two-scale Wigner measures; however, we give examples of situations where this quadratic approach fails.

## CONTENTS

1. Introduction	2
1.1. Setting of the problem	2
1.2. Some successful applications of Wigner measures: scalar case	5
1.3. Some successful applications of Wigner measures: the case of systems	7
2. Limitations of Wigner measures in the scalar case	8
2.1. Ill-posedness in the linear case: wave packets	9
2.2. Caustic crossing and ill-posedness in a nonlinear case	10
2.3. WKB analysis and weak perturbations	12
2.4. Supercritical WKB régime	14
3. Limitation of the Wigner measures in the case of systems	17
3.1. When one needs a second microlocalization	19
3.2. When the quadratic approach fails.	20
References	23

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## 1. Introduction

In this survey, we briefly review some successful applications of the Wigner measures for *classical limits* of Schrödinger equations, and discuss in more detail the limitations of this tool. Although most of the material presented is essentially known, we feel that a survey presenting the dis-advantages of Wigner measures in a clear unified picture is timely and useful.

Wigner measures are a very valuable tool for describing high frequency and homogenization limits for oscillatory PDEs, possibly with periodic coefficients. The Wigner measure is a phase space measure that allows to describe weak limits of quadratic quantities (the *observables*) of a (solution) family of functions which only converges weakly itself. The basic idea goes back to E. Wigner who used such a phase space approach in quantum mechanics for semi-classical approximations in 1932 [68]. In the 90's, Wigner functions and their limiting measures aroused the interest of mathematicians in the USA (e.g. [63]) and, independently, in Europe. As a variant of  $L^2$  defect measures (see [66, 38]) such objects were used as a technicality in proofs in the frame of the analysis of ergodic properties of eigenfunctions for the Dirichlet problem (see [64, 69, 22, 49]), with more systematic studies of *semiclassical measures* by P. Gérard and É. Leichtnam (see [37, 41]), or the survey of N. Burq, [4]). The term “Wigner measure” was used first in the French work “Sur les mesures de Wigner” of P.-L. Lions and T. Paul [54].

Adaptations to the case of Schrödinger operators with periodic coefficients and applications of the method to general problems were given by P. Gérard, P. Markowich, N.J. Mauser and the late F. Poupaud [37], [58], notably their joint paper [42], where a general theory of the use of Wigner measures for homogenization limits of energy densities for several wide classes of dispersive linear PDEs is laid out. In the context of our work we also want to mention the more recent use of Wigner measure for proving resolvent estimates ([5, 50, 51, 35]) following an idea of proof by contradiction of [53].

The method of Wigner measures allows to treat some (weakly) nonlinear equations, for example the semiclassical limit of the coupled Schrödinger–Poisson system, first done in '93 in [54] and [57], both works using “smoothed Wigner functions” as a technical step to prove the non-negativity of the limiting measure and both crucially depending on the use of mixed states — an assumption that could only be lifted in 1D so far [73]. The case of the inclusion of the additional difficulty of a periodic crystal potential was solved in [3], where the general theory of Wigner series, as Wigner measures in the context of a Bloch decomposition of  $L^2$ , was laid out.

In general however, Wigner measure methods are not suitable for treating nonlinear problems and even their use for linear problems has severe limitations. The main aim of this paper is to list some (rather explicit) examples where the use of Wigner measures is not appropriate and thus unveil in a clear and concise way the inherent strengths and shortcomings of the Wigner measure approach for the semiclassical limit of time-dependent Schrödinger equations.

**1.1. Setting of the problem.** The semi-classical limit of the Schrödinger equation can be seen as a model problem for the kind of homogenization limits studied by this method. The rigorous mathematical development of Wigner measures was motivated by this problem. By semi-classical limit we mean the limit of

the (scaled) Planck constant tending to 0 in the Schrödinger equation, which reads

$$(1.1) \quad i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(x) \psi^\varepsilon \quad x \in \mathbb{R}^d, t \in \mathbb{R}$$

$$(1.2) \quad \psi^\varepsilon|_{t=0} = \psi_I^\varepsilon, \quad t \in \mathbb{R}.$$

Here  $\varepsilon$  stands for the scaled Planck constant,  $\psi^\varepsilon = \psi^\varepsilon(t, x) \in \mathbb{C}$  is the wave function, and  $V(x) \in \mathbb{R}$  is a given potential. The wave function may be vector-valued and the potential then is an Hermitian matrix: in this situation, (1.1) is a system. Clearly, this limit is a high frequency limit and can only exist in some weak sense.

From the viewpoint of physics, the main interest is not on  $\psi^\varepsilon$  itself, but in quantities which are quadratic expressions in  $\psi^\varepsilon$ , e. g. the *position density*

$$(1.3) \quad n^\varepsilon(t, x) = |\psi^\varepsilon(t, x)|^2.$$

Of course, this quadratic operation does not commute with the weak  $\varepsilon \rightarrow 0$  limit of  $\psi^\varepsilon$ . The importance of getting limits of quadratic quantities like (1.3) and the prevalence of the distinct scale  $\varepsilon$  of oscillations in the solutions of (1.1) make Wigner measures the “good” tool for this problem and generally for the homogenization of energy densities of time dependent PDEs with a scale of oscillations.

The Wigner transform of a function  $f \in L^2(\mathbb{R}^d)$  is defined by

$$(1.4) \quad w^\varepsilon[f](x, \xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} f\left(x - \varepsilon \frac{\eta}{2}\right) \overline{f}\left(x + \varepsilon \frac{\eta}{2}\right) e^{i\eta \cdot \xi} d\eta.$$

In this definition,  $\varepsilon$  is an arbitrarily introduced parameter, the scale of the Wigner transform.  $w^\varepsilon[f](x, \xi)$  is real-valued, but in general not positive. Now let  $w^\varepsilon(t, x, \xi)$  be the Wigner transform of  $\psi^\varepsilon(t, x)$ , then for  $n^\varepsilon(t, x)$  defined by (1.3) it holds that

$$(1.5) \quad n^\varepsilon(t, x) = \int_{\mathbb{R}_\xi^d} w^\varepsilon(t, x, \xi) d\xi, \quad x \in \mathbb{R}^d$$

Other quadratic quantities in  $\psi^\varepsilon$  can be obtained by taking (higher) moments in the  $\xi$ -variable of  $w^\varepsilon(t, x, \xi)$ . In the case of vector-valued  $f$ , the Wigner transform is matrix-valued: the product of  $f$  and  $\overline{f}$  is replaced by a tensor product in (1.4). One still has (1.5) provided one takes the trace of  $w^\varepsilon$ .

In order to study the convergence properties of  $w^\varepsilon$ , in [54] the following space was introduced:

$$\mathcal{A} = \left\{ \varphi \in C_0(\mathbb{R}_x^d \times \mathbb{R}_\xi^d) \mid (\mathcal{F}_\xi \varphi)(x, \eta) \in L^1(\mathbb{R}_\eta^d; C_0(\mathbb{R}_x^d)) \right\},$$

$$\text{with } \|\mathcal{F}_\xi \varphi\|_{L_\eta^1(C_x)} = \int_{\mathbb{R}_\eta^d} \sup_x |\mathcal{F}_\xi \varphi|(x, \eta) d\eta,$$

where the Fourier transform is defined as follows:

$$(1.6) \quad \mathcal{F}f(\xi) = \widehat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^d} e^{-ix \cdot \xi} f(x) dx.$$

It is easy to verify that  $\mathcal{A}$  is an algebra of test functions and a separable Banach algebra containing  $\mathcal{S}(\mathbb{R}_x^d \times \mathbb{R}_\xi^d)$ . This space immediately allows for a uniform estimate on the Wigner function :

**PROPOSITION 1.1.** *Let  $\psi^\varepsilon$  be a sequence uniformly bounded in  $L^2(\mathbb{R}^d)$ . Then the sequence of Wigner transforms  $w^\varepsilon[\psi^\varepsilon]$  is uniformly bounded in  $\mathcal{A}'$ .*

It follows that, after selection of a subsequence,

$$(1.7) \quad w^\varepsilon[\psi^\varepsilon](x, \xi) \xrightarrow{\varepsilon \rightarrow 0} w^0(x, \xi) \quad \text{in } \mathcal{A}'.$$

It can be shown that  $w^0(x, \xi)$  is a non-negative measure on the phase space: the semi-classical or Wigner measure of the sequence  $\psi^\varepsilon$ , which is not necessarily unique. Note that the Wigner transform  $w^\varepsilon$  is in general real, but may also

have negative values, whereas the limit  $w^0$  is non-negative, thus justifying the term “Wigner measure”. In the vector-valued situation, one uses matrices of test functions and  $w^0$  is a non-negative hermitian matrix of measures, which means that  $w^0 = (w_{i,j}^0)$  with  $w_{ii}^0$  non-negative measure and  $w_{ij}^0$  absolutely continuous with respect to  $w_{ii}^0$  and  $w_{jj}^0$ .

We could work also with uniform bounds and convergence in the distribution space  $\mathcal{S}'$  as the dual of the Schwartz space, as it was done e.g. in [42] without recourse to the space  $\mathcal{A}'$ .

In the scalar case, when applying the Wigner transform to equation (1.1), a kinetic transport equation will result, the so-called “Wigner equation”. The formal limit under  $\varepsilon \rightarrow 0$  of this transport equation leads to the following Vlasov equation for the Wigner measure  $w^0$ :

$$(1.8) \quad \partial_t w^0 + \xi \cdot \nabla_x w^0 - \nabla_x V(x) \cdot \nabla_\xi w^0 = 0$$

If this limit can be made rigorous, and the above equation is well posed as an initial value problem, the Wigner measure of  $\psi^\varepsilon(t, x)$  at a positive time can be obtained by solving the equation with the initial Wigner measure as data: the Wigner measure is constant along the Hamiltonian trajectories  $(x(t, y, \eta), \xi(t, y, \eta))$

$$\begin{cases} \partial_t x(t, y, \eta) = \xi(t, y, \eta) & ; \quad x(0, y, \eta) = y, \\ \partial_t \xi(t, y, \eta) = -\nabla_x V(x(t, y, \eta)) & ; \quad \xi(0, y, \eta) = \eta. \end{cases}$$

For describing the limit in the position density  $n^\varepsilon$ , the following definition will be necessary:

DEFINITION 1.2. *A sequence  $\{f^\varepsilon\}_\varepsilon$  uniformly bounded in  $L^2$ , is called  $\varepsilon$ -oscillatory if, for every continuous and compactly supported function  $\phi$  on  $\mathbb{R}^d$ ,*

$$(1.9) \quad \overline{\lim}_{\varepsilon \rightarrow 0} \int_{|\xi| \geq R/\varepsilon} \left| \widehat{\phi f^\varepsilon}(\xi) \right|^2 d\xi \xrightarrow{R \rightarrow \infty} 0.$$

This definition is presented here in the form that is used in [42], following [37] and [41]; in [54] the equivalent condition that  $1/\varepsilon^d \left| \widehat{f^\varepsilon}(\xi/\varepsilon) \right|^2$  is a relatively compact sequence in  $\mathcal{M}(\mathbb{R}^d)$  is used instead. Heuristically this means that the wavelength of oscillations of  $f^\varepsilon$  is at least  $\varepsilon$ . A sufficient condition for (1.9) is

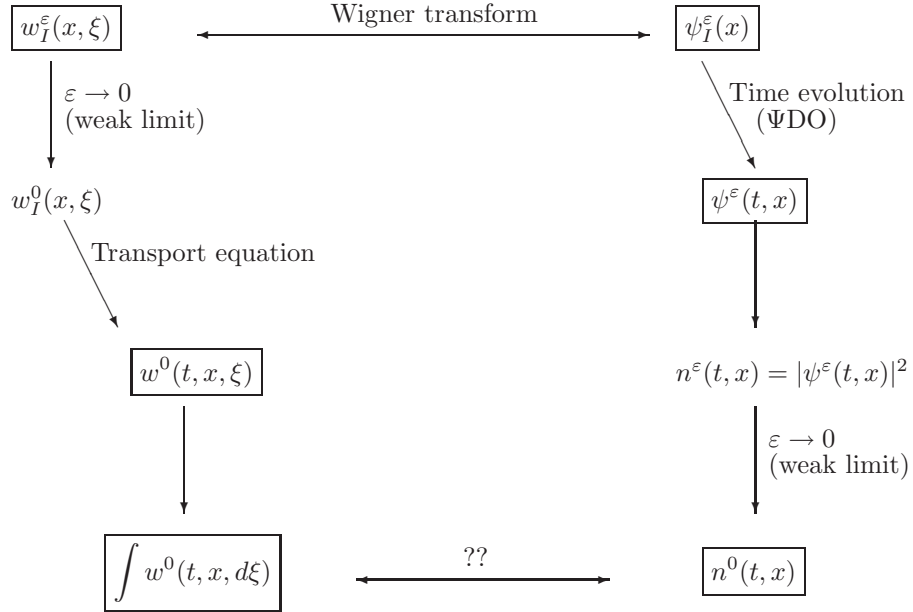
$$\exists \kappa > 0 \quad \text{such that} \quad \varepsilon^\kappa D^\kappa f^\varepsilon \text{ is uniformly bounded in } L_{loc}^2.$$

If  $\psi^\varepsilon$  is  $\varepsilon$ -oscillatory, it is possible to pass to the limit in (1.5), and we find

$$(1.10) \quad \int_{\xi \in \mathbb{R}^d} w^0(x, d\xi) = (w-) \lim_{\varepsilon \rightarrow 0} n^\varepsilon(x) = n^0(x) \quad \text{in } \mathcal{D}'.$$

If now the Wigner measure at a positive time  $t > 0$  can be obtained in an appropriate sense by the evolution equation (1.8), this identity serves to get the desired limit in the density. In the context of quantum mechanics the strength of the method lies in the fact that the transport equation of the Wigner measure (1.8) is identical to the transport equation from classical statistical physics. So according to the “correspondence principle” the quantum problem converges to a classical problem in the limit where the “quantum parameter”  $\varepsilon$  vanishes.

The following diagram gives a schematic sketch of the method used to obtain homogenization limits of quadratic quantities by Wigner measures.



If it is possible to do the operations on the left hand side of this diagram, the limit of  $n^\epsilon$  can be found by applying (1.5) to the Wigner measure at a positive time  $t > 0$ . So it is necessary

- to have a unique Wigner measure of the data,
- that the transport equation for  $w^0$  is a well-posed problem such that a solution exists up to a relevant time  $t > 0$ ,
- the  $\xi$ -integral (zero-th moment) of  $w^0$  at  $t > 0$  must be equal to the limit  $n^0(t, x)$ .

For the third step to be valid,  $\psi^\epsilon(t, x)$  has to be  $\epsilon$ -oscillatory as stated above, which means that there must be no oscillations at faster scales than  $\epsilon$ . If the  $\epsilon$ -oscillatory property is imposed on the data, it will be preserved by (1.1) for positive times. The second step, existence and uniqueness of a global solution to the transport equation of the Wigner measure, is known to hold for a large class of linear scalar problems, but it turns out to be much more complicated for systems (see Section 3); however in nonlinear settings this point is a mostly open question.

Note that in the nonlinear case the non-uniqueness of the Wigner measure of the sequence of solutions  $\psi^\epsilon(t, x)$  somewhat corresponds to the non-uniqueness of the (weak) solution  $w^0(t, x)$  of the limiting nonlinear Vlasov equation; clearly, we are not able to pick one particular solution of the ill-posed PDE by a semiclassical limit of the unique solution of the nonlinear Schrödinger equation.

## 1.2. Some successful applications of Wigner measures: scalar case.

For  $\epsilon$ -independent potentials, as in (1.1), the convergence of the Wigner function to a Wigner measure as a solution of a Vlasov equation was systematically described in [54]. If the potential  $V$  is sufficiently smooth ( $C^{1,1}$ ), then the Wigner measure for  $(\psi^\epsilon)_\epsilon$  is given in terms of the Hamiltonian flow associated to  $|\xi|^2/2 + V(x)$ . On the other hand, if  $V$  is not sufficiently smooth, uniqueness for the Hamiltonian flow fails, and the above mentioned convergence is not guaranteed; see [54] for an exhaustive list of examples and results.

Note that actually the first mathematical study of “semiclassical measures” for linear Schrödinger equations was done by P. Gérard [37] in the context of the

setting in a crystal, where Bloch waves are considered.

$$(1.11) \quad i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon \quad ; \quad \psi^\varepsilon(0, x) = \psi_0\left(\frac{x}{\varepsilon}\right),$$

where  $V_\Gamma$  is lattice-periodic. In the independent later work [58] the names ‘‘Wigner Bloch functions’’ and ‘‘Wigner series’’ for their limits were coined, phase space objects that are essentially obtained via the definition (1.4) by replacing the Fourier integral by a Fourier sum, keeping the position variable  $x$  in whole space and restricting the kinetic variable to the torus (the Brillouin zone) as the dual of the lattice.

Wigner measures have also proven successful in the study limits of quadratic quantities of the Schrödinger–Poisson system:

$$(1.12) \quad i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V_{NL}^\varepsilon\psi^\varepsilon \quad ; \quad \psi^\varepsilon|_{t=0} = \psi_I^\varepsilon,$$

for a potential  $V_{NL}^\varepsilon = V_{NL}^\varepsilon(|\psi^\varepsilon|^2)$  which depends on  $n^\varepsilon = |\psi^\varepsilon|^2$ . The main problem in applying the Wigner measure method to this equation is the low regularity of  $w^0$ , which generally is only in  $\mathcal{A}'$ . This means that the transport equation for  $w^0$  can only be fulfilled in a rather weak sense, so in general a nonlinear expression in  $w^0$  will have no meaning.

The applications of Wigner measures to nonlinear problems which are available so far hold for Hartree type nonlinearities, where the nonlinear potential  $V_{NL}^\varepsilon$  is given by

$$(1.13) \quad V_{NL}^\varepsilon = \int U(x-y)n^\varepsilon(y)dy$$

for some suitable  $U$  and  $n^\varepsilon$  given by (1.3). For the Schrödinger–Poisson system, one usually considers  $U(x) = 1/|x|$  when  $d = 3$  (and in the absence of background ions). The semiclassical limit results for nonlinear cases in [54] and [57] are possible only for the case of a so-called ‘‘mixed state’’, i.e. by considering infinitely many Schrödinger equations. In this case convergence can take place in a stronger sense since a uniform  $L^2$ -bound on the initial Wigner transform can be imposed by choosing very particular initial states (see [59] for a comprehensive discussion).

Note however that even in the case of such strong assumptions that is possible only if we replace the one pure state Schrödinger equation by infinitely many mixed state Schrödinger equations, the results are not strong enough for obtaining a limit that satisfies the conditions for ensuring unique classical solutions of the Vlasov–Poisson system (see [75]). The theory of global weak/strong solutions of the Vlasov equations is laid out, for example, in [26, 55] and [18, 36]), with famous non-uniqueness results notably for measure valued initial data in [74].

For the Schrödinger–Poisson system

$$(1.14) \quad \begin{cases} i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V_{NL}^\varepsilon\psi^\varepsilon, \\ -\Delta V_{NL}^\varepsilon = |\psi^\varepsilon|^2 - b, \end{cases}$$

with  $b = b(x) \in L^1(\mathbb{R}^d)$ , the Wigner measure associated to  $\psi^\varepsilon$  was computed in [72] for WKB-type initial data

$$\psi^\varepsilon(0, x) = \sqrt{\rho_0^\varepsilon(x)}e^{i\phi_0(x)/\varepsilon}.$$

It was proven that the Wigner measure is given in terms of the solution to an Euler–Poisson system, before the solution to the latter develops a singularity. We will see in §2 that in this special case, more can be said on the semi-classical limit

of  $\psi^\varepsilon$ . In particular, its pointwise behavior can be described, showing phenomena that the Wigner measures do not capture.

In the special case of only one space dimension, a *global in time* description of the Wigner measure without any mixed state setting and the corresponding strong assumptions on the initial data is given [73]. Consider

$$(1.15) \quad \begin{cases} i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \partial_x^2 \psi^\varepsilon + V_{NL}^\varepsilon \psi^\varepsilon, & x \in \mathbb{R}, \quad t > 0, \\ -\partial_x^2 V_{NL}^\varepsilon = b^\varepsilon(x) - |\psi^\varepsilon|^2, \\ \psi^\varepsilon|_{t=0} = \psi_I^\varepsilon, & x \in \mathbb{R}, \end{cases}$$

in the case where  $b^\varepsilon \geq 0$  is the mollification of a function  $b \in L^1 \cap L^2$ , and  $\psi_I^\varepsilon$  is the mollification (with the same mollifier) of a sequence  $\varphi_\varepsilon$  bounded in  $L^2(\mathbb{R})$ . Then the Wigner transform of  $\psi^\varepsilon$  converges to a weak solution of the Vlasov–Poisson system

$$(1.16) \quad \begin{cases} \partial_t f + \xi \partial_x f - E \partial_\xi f = 0, & f|_{t=0} = f_I. \\ \partial_x E = b(x) - \int_{\mathbb{R}} f d\xi, & x \in \mathbb{R}, \quad t \geq 0. \end{cases}$$

Following [56] we denote by *weak solution* on the interval  $[0, T]$  any pair  $(E, f)$  consisting of  $E \in (BV \cap L^\infty)([0, T] \times \mathbb{R})$  and  $f \in L^\infty(\mathbb{R}^+, \mathcal{M}^+(\mathbb{R}^2))$  such that

$$(1) \quad \forall \phi \in C_c^\infty([0, T] \times \mathbb{R}^2), \exists q_\phi \in BV([0, T] \times \mathbb{R}),$$

$$\int_{\mathbb{R}} \phi(t, x, \xi) f(t, x, \xi) d\xi = \partial_x q_\phi.$$

$$(2) \quad E(t, x) = \int_{-\infty}^x (b(y) - \int_{\mathbb{R}} f(t, y, \xi) d\xi) dy \text{ a. e.},$$

$$(3) \quad \forall \phi \in C_c^\infty((0, T) \times \mathbb{R}^2),$$

$$\int_0^T \int_{\mathbb{R}^2} (\phi_t f + \phi_x \xi f) dx dt - \int_0^T \int_{\mathbb{R}} \tilde{E} \int_{\mathbb{R}} \phi_\xi f(d\xi) dx dt = 0,$$

where  $\tilde{E}(t, x)$  is Vol’pert’s symmetric average:

$$\tilde{E}(t, x) = \begin{cases} E(t, x), & \text{if } E \text{ is approximately continuous at } (t, x), \\ \frac{1}{2}(E_l(t, x) + E_r(t, x)) & \text{if } E \text{ has a jump at } (t, x), \end{cases}$$

where  $E_l(t, x)$ ,  $E_r(t, x)$  denote the left and right limits of  $E$  at  $(t, x)$ .

$$(4) \quad \exists s > 0, f \in C^{0,1}([0, T], H_{loc}^{-s}(\mathbb{R}^2)) \text{ and } f(0, x, \xi) = f_I(x, \xi) \text{ in } H_{loc}^{-s}(\mathbb{R}^2).$$

We refer to [73] for precise statement of the weak convergence result. We point out that the existence of weak solutions is proved in [74], but the difficulty is that there is no uniqueness of these solutions: a counterexample is given in [56]. We close the section by pointing out that this latter result applies in particular to initial data which are  $\varepsilon$ -independent or of the WKB form  $\varphi^\varepsilon(x) = \rho(x)e^{iS(x)/\varepsilon}$ , with  $\rho \in L^2(\mathbb{R})$ .

**1.3. Some successful applications of Wigner measures: the case of systems.** In the nonlinear case, several results are available in the case of the Schrödinger–Poisson system

$$(1.17) \quad \begin{cases} i\varepsilon \partial_t \psi_j^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi_j^\varepsilon + V_{NL}^\varepsilon \psi_j^\varepsilon, & j \in \mathbb{N}, \quad x \in \mathbb{R}^d, \quad t > 0, \\ V_{NL}^\varepsilon = U * \rho^\varepsilon, \\ \psi_j^\varepsilon|_{t=0} = \phi_j^\varepsilon, & j \in \mathbb{N}, \quad x \in \mathbb{R}^d, \end{cases}$$

where the total position density is defined as

$$(1.18) \quad \rho^\varepsilon = \sum_{j=1}^{\infty} \lambda_j^\varepsilon |\psi_j^\varepsilon|^2$$



with  $\lambda_j^\varepsilon \in \mathbb{R}_+$ ,  $\sum_{j=1}^\infty \lambda_j^\varepsilon = 1$ . The Wigner transform for mixed states is defined, in analogy to (1.4), as

$$(1.19) \quad w^\varepsilon(t, x, \xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-i\xi \cdot y} z^\varepsilon \left( t, x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2} \right) dy,$$

where  $z^\varepsilon(t, r, s)$  is the so-called *mixed state density matrix* defined by

$$(1.20) \quad z^\varepsilon(t, r, s) = \sum_{j=1}^\infty \lambda_j^\varepsilon \psi_j^\varepsilon(t, r) \overline{\psi_j^\varepsilon(t, s)}, \quad r, s \in \mathbb{R}^d.$$

Note that  $z^\varepsilon(t, r, s)$  is the integral kernel of the density operator  $\widehat{\rho}^\varepsilon$  in  $L^2$ , which is trace class with  $\text{Tr}(\widehat{\rho}^\varepsilon) = \sum_{j=1}^\infty \lambda_j^\varepsilon = 1$ . For more details we refer to [54, 57]. A crucial property of the mixed state is the fact that a uniform  $L^2$ -bound on  $w_j^\varepsilon(x, \xi)$  holds if

$$(1.21) \quad \frac{1}{\varepsilon^3} \sum_{j=1}^\infty (\lambda_j^\varepsilon)^2 \leq C.$$

This makes it possible to improve the sense of convergence for  $w^\varepsilon(t, x, \xi)$  to weak- $L^2$ .

In [3], the case of the Schrödinger–Poisson system was considered, with an extra Bloch potential (as in (1.11)). Note however that the analysis does not allow band crossings. Indeed, the analysis in terms of Wigner measures of systems face several difficulties in presence of eigenvalue crossings.

The analysis of [42] for systems cover the case of matrix valued potentials with eigenvalues of constant multiplicity in (1.1). Let us denote by  $\lambda_j$  the eigenvalues of  $V$  and by  $\Pi_j$  the associated projectors,  $1 \leq j \leq N$ . Then any Wigner measure  $w^0$  of  $\psi^\varepsilon$  decomposes as  $w^0 = \sum_{j=1}^N w^{0,j}$  where the measures  $w^{0,j}$  satisfy  $\Pi_j w^{0,j} \Pi_j = w^{0,j}$  and transport equations in the distribution sense

$$\partial_t w^{0,j} + \xi \cdot \nabla_x w^{0,j} - \nabla_x \lambda_j \cdot \nabla_\xi w^{0,j} = [F_j(x, \xi), w^{0,j}]$$

(the matrix  $F_j$  depends on  $\Pi_j$ ,  $\lambda_j$ ,  $1 \leq j \leq N$ , see [42, 43] for precise formula). As soon as the eigenvalues are not of constant multiplicities, this analysis is no longer valid and there may happen energy transfers between the modes which cannot be calculated in terms of Wigner measures. Such a phenomenon has been well-known since the works of Landau and Zener in the 30's (see [52] and [70]). It has been discussed from Wigner measures point of view in the articles [33] and [29] for a larger class of systems. Eigenvalue crossings appear for Schrödinger systems in the frame of quantum chemistry where one can find a large variety of potentials presenting such features (see [27]). In Section 3, for

$$V(x) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix},$$

we explain how one can modify Wigner measure so that a quadratic approach still is possible and give examples where this approach fails.

This article is organized as follows: we first describe in Section 2 the limitation of Wigner measures in scalar situations for  $\varepsilon$  depending potential or nonlinear situations; then in Section 3, we focus on the case of systems.

## 2. Limitations of Wigner measures in the scalar case

The Wigner measure method is rather limited when nonlinear problems are treated, as can already be seen from the discussion of the above results. Note however that some limitations are present even in the linear case. We list below four

families of problems for which the loss of information due to the Wigner measure analysis is rather serious.

**2.1. Ill-posedness in the linear case: wave packets.** We first discuss a situation where this approach fails in a linear setting, by recalling a case where the Cauchy problem (1.8) is ill-posed. Such an example for scalar Schrödinger equation is given by F. Nier [61]. In that case, the potential is  $\varepsilon$ -dependent, as in (1.11), but is decaying instead of lattice-periodic. The problem is that the Wigner measure does not contain enough information on the properties of concentration of wave packets. Thus, Nier introduces in [62] a larger phase space, and a refined Wigner transform which takes into account the spread of the wave packets around the point of concentration involved. Similar ideas can be found in [60] and [28]. The quadratic approach does not fail once it is refined. The same kind of difficulties appear in systems with matrix-valued potentials presenting eigenvalues crossings (see Section 3).

As a particular case of [61, 62], consider the problem:

$$(2.1) \quad i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + U\left(\frac{x}{\varepsilon}\right) \psi^\varepsilon,$$

$$(2.2) \quad \psi^\varepsilon(0, x) = \frac{1}{\varepsilon^{n/2}} u_0\left(\frac{x}{\varepsilon}\right),$$

where  $U$  is a short range potential and  $u_0 \in \text{Ran } W_- = \text{Ran } W_+$ , the wave operators to the classical Hamiltonian  $-\frac{1}{2}\Delta + U$ :  $u_0 = W_- \mathcal{F}^{-1} \psi_- = W_+ \mathcal{F}^{-1} \psi_+$ . Introducing the solution  $u$  to

$$i\partial_t u = -\frac{1}{2}\Delta u + U(x)u \quad ; \quad u|_{t=0} = u_0,$$

we see that:

$$\psi^\varepsilon(t, x) = \frac{1}{\varepsilon^{n/2}} u\left(\frac{t}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

By assumption, we have  $u(t, x) \sim e^{i\frac{t}{2}\Delta} \mathcal{F}^{-1}(\psi_\pm)$  as  $t \rightarrow \pm\infty$ , which implies

$$u(t, x) \sim \frac{1}{(it)^{n/2}} \psi_\pm\left(\frac{x}{t}\right) e^{i\frac{|x|^2}{2t}} \quad \text{as } t \rightarrow \pm\infty,$$

where we recall that the Fourier transform is normalized like in (1.6). Back to the initial unknown function  $\psi^\varepsilon$ , this yields:

**PROPOSITION 2.1** (from [61, 62]). *Let  $\psi^\varepsilon$  be the solution to (2.1)–(2.2), where  $U$  is a short range potential and  $u_0 \in \text{Ran } W_- = \text{Ran } W_+$  with  $u_0 = W_- \mathcal{F}^{-1} \psi_- = W_+ \mathcal{F}^{-1} \psi_+$ . Then the Wigner measure of the (pure) family  $\psi^\varepsilon$  is given by*

$$w^0(t, x, \xi) = \begin{cases} \frac{1}{|t|^n} \left| \psi_- \left( \frac{x}{t} \right) \right|^2 dx \otimes \delta_{\xi = \frac{x}{t}} & \text{if } t < 0, \\ \frac{1}{|t|^n} \left| \psi_+ \left( \frac{x}{t} \right) \right|^2 dx \otimes \delta_{\xi = \frac{x}{t}} & \text{if } t > 0. \end{cases}$$

As mentioned in [62], given two functions  $\psi_-$  and  $\psi'_-$  such that  $|\psi_-| \equiv |\psi'_-|$ , one should not expect  $|\psi_+| \equiv |\psi'_+|$ , even in space dimension one. This is a first hint that the propagation of Wigner measures is an ill-posed problem in this context. This argument is made more precise in [61] (this example was not resumed in the complete paper [62]). In space dimension one, assume that the potential  $U$  is even  $U(x) = U(-x)$ , and fix  $T > 0$ . Let  $\psi^\varepsilon$  be a solution to (2.1) such that its Wigner measure satisfies

$$\begin{aligned} w^0(-T, x, \xi) &= \delta_{x=-x_0} \otimes \delta_{\xi=\xi_0}, \\ w^0(T, x, \xi) &= (1 - R^2) \delta_{x=x_0} \otimes \delta_{\xi=\xi_0} + R^2 \delta_{x=-x_0} \otimes \delta_{\xi=-\xi_0}, \end{aligned}$$

where  $R = |R(\xi_0)| = |R(-\xi_0)|$  is the reflection coefficient related to the scattering operator  $S = W_+^* W_-$ . Define  $\check{\psi}^\varepsilon(t, x) = \psi^\varepsilon(-t, -x)$ . Then since  $U$  is even,  $\check{\psi}^\varepsilon$  solves the same equation as  $\psi^\varepsilon$ , and its Wigner measure satisfies

$$\begin{aligned}\check{w}^0(-T, x, \xi) &= (1 - R^2)\delta_{x=-x_0} \otimes \delta_{\xi=\xi_0} + R^2\delta_{x=x_0} \otimes \delta_{\xi=-\xi_0}, \\ \check{w}^0(T, x, \xi) &= \delta_{x=x_0} \otimes \delta_{\xi=\xi_0}.\end{aligned}$$

Define  $\tilde{\psi}^\varepsilon = \psi_1^\varepsilon + \psi_2^\varepsilon$  where the  $\psi_j^\varepsilon$ 's solve (2.1) and whose initial Wigner measures are such that:

$$w_1^0(-T, x, \xi) = (1 - R^2)\delta_{x=-x_0} \otimes \delta_{\xi=\xi_0} \quad ; \quad w_2^0(-T, x, \xi) = R^2\delta_{x=x_0} \otimes \delta_{\xi=-\xi_0}.$$

Then  $\check{w}^0(-T, x, \xi) = \tilde{w}^0(-T, x, \xi)$ , and unless  $R = 0$  or  $1$ ,  $\check{w}^0(T, x, \xi) \neq \tilde{w}^0(T, x, \xi)$ :

$$\tilde{w}^0(T, x, \xi) = ((1 - R^2)^2 + R^4)\delta_{x=x_0} \otimes \delta_{\xi=\xi_0} + 2R^2(1 - R^2)\delta_{x=-x_0} \otimes \delta_{\xi=-\xi_0}.$$

Therefore, the Cauchy problem for the propagation of Wigner measures is ill-posed in this case: knowing the Wigner measure at time  $t = -T$  does not suffice to determine it at time  $t = +T$ .

**2.2. Caustic crossing and ill-posedness in a nonlinear case.** We now give another example on a nonlinear problem, taken from [7], which may be viewed as a nonlinear counterpart of the above example. Consider a Schrödinger equation with power-like nonlinearity:

$$(2.3) \quad i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + \varepsilon^2|\psi^\varepsilon|^{4/d}\psi^\varepsilon \quad ; \quad \psi^\varepsilon|_{t=0} = a_0(x)e^{-i\frac{|x|^2}{2\varepsilon}},$$

where  $x \in \mathbb{R}^d$ ,  $d \geq 1$ . The asymptotic behavior of  $\psi^\varepsilon$  is given in [7] for any time. Note that other powers in the nonlinearity are also considered, provided that the power of  $\varepsilon$  in front of the nonlinearity is well chosen.

**PROPOSITION 2.2** ([7]). *Let  $a_0 \in \mathcal{S}(\mathbb{R}^d)$ , and consider  $\psi^\varepsilon$  solution to (2.3). Then the asymptotic behavior of  $\psi^\varepsilon$  is given by  $\|\psi^\varepsilon(t) - v^\varepsilon(t)\|_{L^2(\mathbb{R}^d)} \rightarrow 0$  as  $\varepsilon \rightarrow 0$ , where:*

$$v^\varepsilon(t, x) = \begin{cases} \frac{1}{(1-t)^{d/2}} a_0\left(\frac{x}{1-t}\right) e^{i\frac{|x|^2}{2\varepsilon(1-t)}} & \text{if } t < 1, \\ \frac{e^{-id\frac{\pi}{2}}}{(t-1)^{d/2}} \mathcal{Z}a_0\left(\frac{x}{t-1}\right) e^{i\frac{|x|^2}{2\varepsilon(t-1)}} & \text{if } t > 1. \end{cases}$$

Here  $\mathcal{Z} = \mathcal{F} \circ S \circ \mathcal{F}^{-1}$ , where  $\mathcal{F}$  stands for the Fourier transform (1.6), and  $S$  denotes the scattering operator associated to  $i\partial_t u + \frac{1}{2}\Delta u = |u|^{4/d}u$  (see e.g. [19]).

Like in Subsection 2.3, we infer the Wigner measure of  $\psi^\varepsilon$ :

$$w^0(t, x, \xi) = \begin{cases} \frac{1}{|t-1|^d} \left| a_0\left(\frac{x}{1-t}\right) \right|^2 dx \otimes \delta_{\xi=\frac{x}{1-t}} & \text{if } t < 1, \\ \frac{1}{|t-1|^d} \left| \mathcal{Z}a_0\left(\frac{x}{t-1}\right) \right|^2 dx \otimes \delta_{\xi=\frac{x}{t-1}} & \text{if } t > 1. \end{cases}$$

Unless  $|a_0|^2 = |\mathcal{Z}a_0|^2$ ,  $w^0$  has a jump at the caustic crossing. The Wigner measure solves the transport equation with a singular source term:

$$\partial_t w^0 + \xi \cdot \nabla_x w^0 = \delta_{x=0} \otimes \left( |\mathcal{Z}a_0(\xi)|^2 - |a_0(\xi)|^2 \right) d\xi \otimes \delta_{t=1}.$$

The pathology is even more serious: the following result was established in [8] in the one-dimensional setting, and its proof extends to any space dimension.

PROPOSITION 2.3. *Let  $d \geq 1$ .*

(1) *There exists  $a_0 \in \mathcal{S}(\mathbb{R}^d)$  such that the Wigner measure  $w^0$  associated to  $\psi^\varepsilon$  solving (2.3) is discontinuous at  $t = 1$ :*

$$\lim_{t \rightarrow 1^-} w^0(t, dx, d\xi) \neq \lim_{t \rightarrow 1^+} w^0(t, dx, d\xi).$$

(2) *There exist two (pure) families  $(\psi_j^\varepsilon)_{0 < \varepsilon \leq 1}$ ,  $j = 1, 2$ , solutions to (2.3) (with different initial profiles  $a_{0,j}$ ), whose Wigner measures  $w_j^0$  are such that  $w_1^0 = w_2^0$  for  $t < 1$  and  $w_1^0 \neq w_2^0$  for  $t > 1$ .*

SKETCH OF THE PROOF. The point is to show that one can find  $(a_{0,j})_{j=1,2}$  such that  $|a_{0,1}| = |a_{0,2}|$  and  $|\mathcal{Z}(a_{0,1})| \neq |\mathcal{Z}(a_{0,2})|$ . Since very few properties of the scattering operator  $S$  are available, the first two terms of its asymptotic expansion near the origin are computed, following the approach of [40] (the first term is naturally the identity). In the case of  $L^2$ -critical nonlinear Schrödinger equation considered here, we have, for  $\psi_- \in L^2(\mathbb{R}^d)$  and  $0 < \delta \ll 1$ ,

$$S(\delta\psi_-) = \delta\psi_- - i\delta^{1+4/d} \int_{-\infty}^{+\infty} U_0(-t) \left( |U_0(t)\psi_-|^{4/d} U_0(t)\psi_- \right) dt + \mathcal{O}_{L^2(\mathbb{R}^d)}(\delta^{1+8/d}),$$

where  $U_0(t) = e^{i\frac{t}{2}\Delta}$ . The proof of the above identity relies on Strichartz estimates and a bootstrap argument; a complete proof can be found in [16]. The idea is then to consider

$$a_{0,1} = a_0 \in \mathcal{S}(\mathbb{R}^d), \quad a_{0,2} = a_0 e^{ih}, \quad \text{with } h \in C^\infty(\mathbb{R}^d; \mathbb{R}).$$

We proceed as in [8]. Denote

$$P(\psi_-) = -i \int_{-\infty}^{+\infty} U_0(-t) \left( |U_0(t)\psi_-|^{4/d} U_0(t)\psi_- \right) dt.$$

Obviously,

$$|\mathcal{F} \circ S(\delta\psi_-)|^2 = \delta^2 \left| \widehat{\psi_-} \right|^2 + 2\delta^{2+4/d} \operatorname{Re} \left( \widehat{\psi_-} \widehat{P\psi_-} \right) + \mathcal{O}(\delta^{2+8/d}),$$

and we have to prove that we can find  $\psi_- \in \mathcal{S}(\mathbb{R}^d)$ , and  $h \in C^\infty(\mathbb{R}^d; \mathbb{R})$ , such that

$$\operatorname{Re} \left( \overline{\mathcal{F}\psi_-} \mathcal{F}(P\psi_-) \right) \neq \operatorname{Re} \left( \overline{\mathcal{F}(\psi_h)} \mathcal{F}(P(\psi_h)) \right) =: R(\psi_-, h),$$

where  $\psi_h$  is defined by

$$\widehat{\psi_h}(\xi) = e^{ih(\xi)} \widehat{\psi_-}(\xi).$$

If this was not true, then for every  $\psi_- \in \mathcal{S}(\mathbb{R}^d)$ , the differential of the map  $h \mapsto R(\psi_-, h)$  would be zero at every smooth, real-valued function  $h$ . An elementary but tedious computation shows that

$$D_h R(\psi_-, 0)(h) \neq 0,$$

with  $h(x) = |x|^2/2$  and  $\psi_-(x) = e^{-|x|^2/2}$ . The computations uses the fact that the evolution of Gaussian functions under the action of the free Schrödinger group can be computed explicitly. We refer to [13] for more detailed computations.  $\square$

REMARK 2.4. A similar result can be established in the case of the Hartree equation with harmonic potential studied in [15, Sect. 5]. For  $\gamma > 1$  and  $a_0 \in \mathcal{S}(\mathbb{R}^n)$ , consider:

$$(2.4) \quad i\varepsilon \partial_t \psi^\varepsilon + \frac{\varepsilon^2}{2} \Delta \psi^\varepsilon = \frac{|x|^2}{2} \psi^\varepsilon + \varepsilon^\gamma (|x|^{-\gamma} * |\psi^\varepsilon|^2) \psi^\varepsilon \quad ; \quad \psi^\varepsilon|_{t=0} = a_0.$$

Like in [9] in the case of a power-like nonlinearity, the harmonic potential causes focusing at the origin periodically in time; outside the foci, the nonlinearity is negligible, and near the foci, the harmonic potential is negligible while the nonlinearity is not. Like for Proposition 2.2, its influence is described in average by the scattering operator associated to  $i\partial_t u + \frac{1}{2}\Delta u = (|x|^{-\gamma} * |u|^2) u$ , whose existence was proven in [44, 48]. Following the same approach as in [8], one can prove the analogue of Proposition 2.3 in the case of Eq. (2.4).

**2.3. WKB analysis and weak perturbations.** Consider a Schrödinger equation with an  $\mathcal{O}(\varepsilon)$  perturbation and a WKB data:

$$i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V(t, x)\psi^\varepsilon + \varepsilon F^\varepsilon(t, x)\psi^\varepsilon \quad ; \quad \psi^\varepsilon|_{t=0} = a_0(x)e^{i\phi_0(x)/\varepsilon},$$

where  $V$  and  $F^\varepsilon$  are real-valued. If we assume that  $F^\varepsilon$  has an expansion as  $\varepsilon \rightarrow 0$  of the form  $F^\varepsilon = F_0 + \varepsilon F_1 + \dots$ , then a formal WKB analysis yields  $\psi^\varepsilon \approx ae^{i\phi/\varepsilon}$ , where:

$$\begin{cases} \partial_t\phi + \frac{1}{2}|\nabla\phi|^2 + V(t, x) = 0 & ; \quad \phi|_{t=0} = \phi_0. \\ \partial_t a + \nabla\phi \cdot \nabla a + \frac{1}{2}a\Delta\phi = -iF_0 a & ; \quad a|_{t=0} = a_0. \end{cases}$$

The first equation is the eikonal equation. Classically, it is solved locally in space and time, provided that  $V$  and  $\phi_0$  are smooth, by considering the Hamiltonian flow

$$(2.5) \quad \begin{cases} \partial_t x(t, y) = \xi(t, y) & ; \quad x(0, y) = y, \\ \partial_t \xi(t, y) = -\nabla_x V(t, x(t, y)) & ; \quad \xi(0, y) = \nabla\phi_0(y). \end{cases}$$

See e.g. [25, 46]. In addition, if  $\phi_0$  and  $V$  are subquadratic, then one can find a local existence time which is uniform with respect to  $x \in \mathbb{R}^d$ :

**ASSUMPTION 2.5.** *We assume that the potential and the initial phase are smooth and subquadratic:*

- $V \in C^\infty(\mathbb{R}_t \times \mathbb{R}_x^d)$ , and  $\partial_x^\alpha V \in L_{\text{loc}}^\infty(\mathbb{R}_t; L^\infty(\mathbb{R}_x^d))$  as soon as  $|\alpha| \geq 2$ .
- $\phi_0 \in C^\infty(\mathbb{R}^d)$ , and  $\partial_x^\alpha \phi_0 \in L^\infty(\mathbb{R}^d)$  as soon as  $|\alpha| \geq 2$ .

**LEMMA 2.6** (from [12]). *Under Assumption 2.5, there exist  $T > 0$  and a unique solution  $\phi_{\text{eik}} \in C^\infty([0, T] \times \mathbb{R}^d)$  to:*

$$(2.6) \quad \partial_t\phi_{\text{eik}} + \frac{1}{2}|\nabla\phi_{\text{eik}}|^2 + V(t, x) = 0 \quad ; \quad \phi_{\text{eik}}|_{t=0} = \phi_0.$$

*This solution is subquadratic:  $\partial_x^\alpha \phi_{\text{eik}} \in L^\infty([0, T] \times \mathbb{R}^d)$  as soon as  $|\alpha| \geq 2$ .*

Essentially, for  $0 \leq t \leq T$ , the map  $y \mapsto x(t, y)$  given by (2.5) is a diffeomorphism of  $\mathbb{R}^d$ : for  $0 \leq t \leq T$ , the Jacobi determinant

$$J_t(y) = \det\nabla_y x(t, y)$$

is bounded away from zero. For  $0 \leq t \leq T$ , no caustic is formed yet, and the second equation is a transport equation. It is an ordinary differential equation along the rays of geometric optics: introduce  $A$  given by

$$A(t, y) := a(t, x(t, y)) \sqrt{J_t(y)}.$$

The transport equation is then equivalent, for  $0 \leq t \leq T$ , to:

$$(2.7) \quad \partial_t A(t, y) = -iF_0(t, x(t, y)) A(t, y); \quad A(0, y) = a_0(y).$$

We note that since  $F_0$  is real-valued, the modulus of  $A$  is independent of  $t \in [0, T]$ . The influence of  $F_0$  shows up through a phase shift, whose wavelength is  $\mathcal{O}(1)$ :

$$A(t, y) = a_0(y) \exp\left(-i \int_0^t F_0(\tau, x(\tau, y)) d\tau\right).$$

Back to  $a$ , we find

$$a(t, x) = \frac{1}{\sqrt{J_t(y(t, x))}} a(y(t, x)) \exp\left(-i \int_0^t F_0(\tau, x(\tau, y(t, x))) d\tau\right),$$

where  $y(t, x)$  stands for the inverse mapping of  $y \mapsto x(t, y)$ . Wigner measures ignore this integral, since it corresponds to a phase whose wavelength is large compared to  $\varepsilon$ .

The above approach is very general, and includes linear problems. For instance, we may take  $F^\varepsilon(x, t) = f(x) \in \mathcal{S}(\mathbb{R}^d)$ . We could also consider perturbations of order  $\mathcal{O}(\varepsilon^\alpha)$  with  $0 < \alpha \leq 1$  instead of  $\mathcal{O}(\varepsilon)$ , and follow the same line of reasoning. We illustrate this general statement with examples, corresponding to weakly nonlinear phenomena. The term “weakly” means that the nonlinearity does not appear in the eikonal equation (the geometry of propagation is the same as in the linear case), but is present in the leading order transport equation.

Consider the nonlinear Schrödinger equation in  $\mathbb{R}^d$

$$(2.8) \quad i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(t, x) \psi^\varepsilon + \varepsilon f(|\psi^\varepsilon|^2) \psi^\varepsilon \quad ; \quad \psi^\varepsilon|_{t=0} = a_0 e^{i\phi_0/\varepsilon},$$

where  $f \in C^\infty(\mathbb{R}_+; \mathbb{R})$  and Assumption 2.5 is satisfied. Here,

$$F^\varepsilon = f(|\psi^\varepsilon|^2)$$

is a nonlinear function of  $\psi^\varepsilon$ . However, we see from (2.7) that, at leading order, the modulus of  $\psi^\varepsilon$  is independent of time, so that (2.7) turns out to be a linear ordinary differential equation. In [12], the asymptotic behavior of  $\psi^\varepsilon$  is given for  $t \in [0, T]$ , by:

PROPOSITION 2.7 (from [12]). *Let  $f \in C^\infty(\mathbb{R}_+; \mathbb{R})$ ,  $a_0 \in \mathcal{S}(\mathbb{R}^d)$ , and let Assumption 2.5 be satisfied. Then for all  $\varepsilon \in ]0, 1]$ , (2.8) has a unique solution  $\psi^\varepsilon \in C^\infty([0, T] \times \mathbb{R}^d) \cap C([0, T]; H^s)$  for all  $s > d/2$  ( $T$  is given by Lemma 2.6). Moreover,*

$$\left\| \psi^\varepsilon - a e^{iG} e^{i\phi_{\text{eik}}/\varepsilon} \right\|_{L^\infty([0, T]; L^2 \cap L^\infty)} \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0.$$

The functions  $a$  and  $G$  are given by

$$a(t, x) = \frac{1}{\sqrt{J_t(y(t, x))}} a_0(y(t, x)),$$

$$G(t, x) = - \int_0^t f\left(J_s(y(t, x))^{-1} |a_0(y(t, x))|^2\right) ds.$$

In particular, the unique Wigner measure for  $\psi^\varepsilon$  is given by:

$$w^0(t, x, \xi) = \frac{1}{J_t(y(t, x))} |a_0(y(t, x))|^2 dx \otimes \delta_{\xi = \nabla \phi_{\text{eik}}(t, x)}.$$

It is independent of the nonlinearity  $f$ , and therefore, does not take the nonlinear effect, causing the non-trivial presence of  $G$ , into account.

A similar analysis could be carried out by replacing the above local nonlinearity by a non-local Hartree type term. We shall simply exhibit an explicit example in such a framework. In [15], the following Hartree equation with a harmonic potential was considered:

$$(2.9) \quad i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + \frac{|x|^2}{2} \psi^\varepsilon + \varepsilon (|x|^{-\gamma} * |\psi^\varepsilon|^2) \psi^\varepsilon \quad ; \quad \psi^\varepsilon|_{t=0} = a_0,$$

with  $0 < \gamma < 1$  and  $x \in \mathbb{R}^d$  for  $d \geq 2$ . The solution to (2.6) is explicit in this case:

$$\phi_{\text{eik}}(t, x) = -\frac{|x|^2}{2} \tan t, \quad t \notin \frac{\pi}{2} + \pi\mathbb{Z}.$$

PROPOSITION 2.8 ([15, Prop. 4.1]). *Let  $d \geq 2$ ,  $a_0 \in \mathcal{S}(\mathbb{R}^d)$ , and  $0 < \gamma < 1$ . Let  $\psi^\varepsilon$  be the solution to (2.9). Define (for any  $t$ )*

$$g(t, x) = -(|x|^{-\gamma} * |a_0|^2)(x) \int_0^t \frac{d\tau}{|\cos \tau|^\gamma}.$$

- For  $0 \leq t < \pi/2$ , the following asymptotic relation holds:

$$\sup_{0 \leq \tau \leq t} \left\| \psi^\varepsilon(\tau, x) - \frac{1}{(\cos \tau)^{n/2}} a_0 \left( \frac{x}{\cos \tau} \right) e^{-i \frac{|x|^2}{2\varepsilon} \tan \tau + ig(\tau, \frac{x}{\cos \tau})} \right\|_{L_x^2} \xrightarrow{\varepsilon \rightarrow 0} 0.$$

- For  $\pi/2 < t \leq \pi$ ,

$$\sup_{t \leq \tau \leq \pi} \left\| \psi^\varepsilon(\tau, x) - \frac{e^{-in\frac{\pi}{2}}}{(\cos \tau)^{n/2}} a_0 \left( \frac{x}{\cos \tau} \right) e^{-i \frac{|x|^2}{2\varepsilon} \tan \tau + ig(\tau, \frac{x}{\cos \tau})} \right\|_{L_x^2} \xrightarrow{\varepsilon \rightarrow 0} 0.$$

For any time  $t \in [0, \pi] \setminus \{\frac{\pi}{2}\}$ , the Wigner measure  $w^0$  associated to the (pure) family  $(\psi^\varepsilon)_{0 < \varepsilon \leq 1}$  is given by:

$$w^0(t, x, \xi) = \frac{1}{|\cos t|^n} \left| a_0 \left( \frac{x}{\cos t} \right) \right|^2 dx \otimes \delta_{\xi = -x \tan t}.$$

As mentioned in [15], the asymptotic description could be pursued to any time. Like in the first example, the Wigner measure is the same as in the linear case and ignores leading order nonlinear effects measured by  $g$ .

The phenomenon we described in this paragraph is also present in the main result of [14], where a weakly nonlinear perturbation of (1.11) is considered:

$$i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(t, x) \psi^\varepsilon + V_\Gamma \left( \frac{x}{\varepsilon} \right) \psi^\varepsilon + \varepsilon |\psi^\varepsilon|^{2\sigma} \psi^\varepsilon,$$

where  $V$  is as above,  $V_\Gamma$  is lattice-periodic, and  $\sigma \in \mathbb{N}$ . Before the formation of caustics, nonlinear effects show up at leading order through a self-modulation (phase shift), which may be viewed in this case as a nonlinear Berry phase.

We emphasize the fact that the self-modulation described in this paragraph is not bound to the Schrödinger equation. In [17], a nonlinear wave equation is considered in a weakly nonlinear régime. If in [17], we consider a purely imaginary coupling constant, that is, a nonlinear wave equation of the form

$$\partial_t^2 u - \Delta u + i|\partial_t u|^{p-1} \partial_t u = 0,$$

then we meet the same phenomenon as in this paragraph if, following the notations of [17],  $P_- = 0$  or  $P_+ = 0$  (this corresponds to polarized initial data).

**2.4. Supercritical WKB régime.** To conclude on the case of scalar equations, consider the case

$$(2.10) \quad i\partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + |\psi^\varepsilon|^2 \psi^\varepsilon \quad ; \quad \psi^\varepsilon(0, x) = a_0^\varepsilon(x) e^{i\phi_0(x)/\varepsilon}.$$

We consider the case of a cubic, defocusing nonlinearity for simplicity; the approach recalled below can be extended to a wider class of nonlinearities, from [2, 67]. Assume that the initial amplitude  $a_0^\varepsilon$  has an asymptotic expansion of the form

$$a_0^\varepsilon = a_0 + \varepsilon a_1 + \mathcal{O}(\varepsilon^2), \quad \text{as } \varepsilon \rightarrow 0,$$

where the functions  $a_0$  and  $a_1$  are independent of  $\varepsilon$ . The case considered in §2.3 was critical as far as WKB analysis is concerned: nonlinear effects are present in the transport equation (which determines the leading order amplitude), and it would not be the case if the power  $\varepsilon$  in front of the nonlinear term was replaced by  $\varepsilon^\kappa$ ,

with  $\kappa > 1$  (see [12]). The above equation is supercritical as far as WKB analysis is concerned. If we seek

$$\psi^\varepsilon(t, x) = (\mathbf{a}_0(t, x) + \varepsilon \mathbf{a}_1(t, x) + \mathcal{O}(\varepsilon^2)) e^{i\phi(t, x)/\varepsilon},$$

then plugging this expression into (2.10) and ordering the powers of  $\varepsilon$  yields:

$$\begin{aligned} \mathcal{O}(\varepsilon^0) : \quad & \partial_t \phi + \frac{1}{2} |\nabla \phi|^2 + |\mathbf{a}_0|^2 = 0, \\ \mathcal{O}(\varepsilon^1) : \quad & \partial_t \mathbf{a}_0 + \nabla \phi \cdot \nabla \mathbf{a}_0 + \frac{1}{2} \mathbf{a}_0 \Delta \phi = 2i \operatorname{Re}(\mathbf{a}_0 \overline{\mathbf{a}_1}) \mathbf{a}_0. \end{aligned}$$

We see that there is a strong coupling between the phase and the main amplitude:  $\mathbf{a}_0$  is present in the equation for  $\phi$ . Moreover, the above system is not closed:  $\phi$  is determined in function of  $\mathbf{a}_0$ , and  $\mathbf{a}_0$  is determined in function of  $\mathbf{a}_1$ . Even if we pursued the cascade of equations, this phenomenon would remain: no matter how many terms are computed, the system is never closed (see [39]). This is a typical feature of supercritical cases in nonlinear geometrical optics (see [20, 21]).

Suppose however that we know  $\phi$ , and that the rays associated to  $\phi$  do not form an envelope for  $t \in [0, T]$  (we prefer not to speak of caustic in that case; see [10]). Then along these rays, and following the same approach as in 2.3, we see that the equation for  $\mathbf{a}_0$  is of the form

$$D_t \mathbf{a}_0 = 2i \operatorname{Re}(\mathbf{a}_0 \overline{\mathbf{a}_1}) \mathbf{a}_0.$$

Therefore, the modulus of  $\mathbf{a}_0$  is constant along rays, and the coupling between  $\mathbf{a}_0$  and  $\mathbf{a}_1$  is present only through a phase modulation for  $\mathbf{a}_0$ . As in 2.3, this phase modulation is not trivial in general: a perturbation of the initial data at order  $\mathcal{O}(\varepsilon)$  in (2.10) leads to a modification of  $\psi^\varepsilon$  at leading order  $\mathcal{O}(1)$  for positive times. This phenomenon was called *ghost effect* in a slightly different context [65]. This discussion is made rigorous in [12], after rewriting the original idea of E. Grenier [45]. Note also that in the above discussion, we have seen that we do not need to know  $\mathbf{a}_1$  to determine  $|\mathbf{a}_0|^2$ : this is strongly related to the following observation. Set  $(\rho, v) = (|\mathbf{a}_0|^2, \nabla \phi)$ . Then the above system for  $\phi$ ,  $\mathbf{a}_0$  and  $\mathbf{a}_1$  implies

$$\begin{cases} \partial_t v + v \cdot \nabla v + \nabla \rho = 0 & ; \quad v|_{t=0} = \nabla \phi_0, \\ \partial_t \rho + \nabla \cdot (\rho v) = 0 & ; \quad \rho|_{t=0} = |\mathbf{a}_0|^2. \end{cases}$$

This system is a polytropic compressible Euler equation. WKB analysis can be justified so long as the solution to this system remains smooth ([45, 12]), and the Wigner measure is given by

$$w^0(t, x, \xi) = \rho(t, x) dx \otimes \delta_{\xi=v(t, x)}.$$

See also [71].

The above remarks can be applied also when  $a_1$  depends on  $\varepsilon$ . Formally, if we replace  $a_1$  by  $\varepsilon^{-\delta} a_1$ ,  $0 < \delta < 1$ , then we should at least replace  $\mathbf{a}_1$  by  $\varepsilon^{-\delta} \mathbf{a}_1$ , and also reconsider the remainder  $\mathcal{O}(\varepsilon^2)$ . Forget this last point. Mimicking the above discussion, the interaction between  $\mathbf{a}_0$  and  $\mathbf{a}_1$  leads to a phase modulation for  $\mathbf{a}_0$ , of order  $\varepsilon^{-\delta}$ : “rapid” oscillations appear. However, such oscillations are not detected at the level of Wigner measures: the  $x$ -component of the Wigner measure ignores this modulation, because it is of modulus one, and the  $\xi$ -component cannot see it, because its wavelength  $\varepsilon^\delta$  is too large compared to  $\varepsilon$ . However, this phenomenon is everything but negligible at the level of the wave functions, since it causes instabilities:



THEOREM 2.9 (from [11]). *Let  $d \geq 1$ ,  $a_0, a_1 \in \mathcal{S}(\mathbb{R}^d)$ ,  $\phi_0 \in C^\infty(\mathbb{R}^d; \mathbb{R})$ , where  $a_0, a_1$  and  $\phi_0$  are independent of  $\varepsilon$ , and  $\nabla \phi_0 \in H^s(\mathbb{R}^d)$  for every  $s \geq 0$ . Let  $u^\varepsilon$  and  $v^\varepsilon$  solve the initial value problems:*

$$\begin{aligned} i\varepsilon \partial_t u^\varepsilon + \frac{\varepsilon^2}{2} \Delta u^\varepsilon &= |u^\varepsilon|^2 u^\varepsilon ; u^\varepsilon|_{t=0} = a_0 e^{i\phi_0/\varepsilon} . \\ i\varepsilon \partial_t v^\varepsilon + \frac{\varepsilon^2}{2} \Delta v^\varepsilon &= |v^\varepsilon|^2 v^\varepsilon ; v^\varepsilon|_{t=0} = (a_0 + \varepsilon^k a_1) e^{i\phi_0/\varepsilon} , \end{aligned}$$

for some  $0 < k < 1$ . Assume that  $\operatorname{Re}(\bar{a}_0 a_1) \neq 0$ . Then we can find  $0 < t^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} 0$  such that

$$\liminf_{\varepsilon \rightarrow 0} \|u^\varepsilon(t^\varepsilon) - v^\varepsilon(t^\varepsilon)\|_{L^2 \cap L^\infty} > 0.$$

More precisely, this mechanism occurs as soon as  $t^\varepsilon \gtrsim \varepsilon^{1-k}$ . In particular,

$$\frac{\|u^\varepsilon - v^\varepsilon\|_{L^\infty([0, t^\varepsilon]; L^2)}}{\|u^\varepsilon|_{t=0} - v^\varepsilon|_{t=0}\|_{L^2}} \rightarrow +\infty \quad \text{as } \varepsilon \rightarrow 0.$$

As pointed out above, the Wigner measures ignore this instability. One could argue that this instability mechanism does not affect the quadratic quantities, and thus may not be physically relevant (the same remark could be made about §2.3). Note however that this phenomenon occurs for very small times, when WKB analysis is still valid. When WKB ceases to be valid (in this case, this corresponds to the appearance of singularities in Euler equations), the approach must be modified. We have seen in §2.2 that even for a weaker nonlinearity, nonlinear effects can alter drastically the Wigner measures when rays of geometric optics form an envelope. The consequence shown in §2.2 was an ill-posedness result for the propagation of Wigner measures. Even if Theorem 2.9 may not seem relevant for Wigner measures, it may very well happen that for larger times, it causes another ill-posedness phenomenon.

The same discussion remains valid in the case of the Schrödinger–Poisson system (1.14). It was proven in [72] that so long as the solution to a corresponding Euler–Poisson remains smooth, it yields the Wigner measure associated to  $\psi^\varepsilon$ . However, in [1], the approach of Grenier was adapted to the case of (1.14): the above instability mechanism can be inferred in this case as well, and the discussion remains the same.

It turns out that this instability mechanism can be met in the case of a weaker (as far as WKB analysis is concerned) nonlinearity. Using a semi-classical conformal transform, we infer from Theorem 2.9:

COROLLARY 2.10 (from [11]). *Let  $d \geq 2$ ,  $1 < \alpha < d$ , and  $a_0, a_1 \in \mathcal{S}(\mathbb{R}^d)$  independent of  $\varepsilon$ . Let  $u^\varepsilon$  and  $v^\varepsilon$  solve the initial value problems:*

$$\begin{aligned} i\varepsilon \partial_t u^\varepsilon + \frac{\varepsilon^2}{2} \Delta u^\varepsilon &= \varepsilon^\alpha |u^\varepsilon|^2 u^\varepsilon ; u^\varepsilon(0, x) = a_0(x) e^{-i|x|^2/(2\varepsilon)} , \\ i\varepsilon \partial_t v^\varepsilon + \frac{\varepsilon^2}{2} \Delta v^\varepsilon &= \varepsilon^\alpha |v^\varepsilon|^2 v^\varepsilon ; v^\varepsilon(0, x) = \left( a_0(x) + \varepsilon^{1-\alpha/d} a_1(x) \right) e^{-i|x|^2/(2\varepsilon)} . \end{aligned}$$

Assume that  $\operatorname{Re}(\bar{a}_0 a_1) \neq 0$ . There exist  $T^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} 1^-$  and  $0 < \tau^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} 0$  such that:

$$(2.11) \quad \|u^\varepsilon - v^\varepsilon\|_{L^\infty([0, T^\varepsilon]; L^2)} \xrightarrow{\varepsilon \rightarrow 0} 0 \quad ; \quad \liminf_{\varepsilon \rightarrow 0} \|u^\varepsilon - v^\varepsilon\|_{L^\infty([0, T^\varepsilon + \tau^\varepsilon]; L^2)} > 0.$$

Consider the case  $d = 2$ , and compare with the result of §2.2. The assumption  $\alpha < 2$  implies that supercritical nonlinear effects occur near the focusing time  $t = 1$  (see also [6] for a similar result), but not before since  $\alpha > 1$ . This case, along with Proposition 2.3, illustrates the above discussion: Wigner measures do not capture

the above instability mechanism, but for larger times, this instability may affect the Wigner measures.

### 3. Limitation of the Wigner measures in the case of systems

We consider now systems of Schrödinger equations coupled by a matrix-valued potentials. Such systems appear in the framework of Born-Oppenheimer approximation, where the dynamics of molecules can approximately be reduced to matrix-valued Schrödinger equations on the nucleonic configuration space. We consider

$$(3.1) \quad \begin{cases} i\varepsilon\partial_t\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V(x)\psi^\varepsilon, & (t, x) \in \mathbb{R}^+ \times \mathbb{R}^d, \quad \psi^\varepsilon \in \mathbb{C}^j, \\ \psi^\varepsilon|_{t=0} = \psi_0^\varepsilon \in L^2(\mathbb{R}^d, \mathbb{C}^j), \end{cases}$$

where the small parameter  $\varepsilon$  is the square root of the ratio of the electronic mass on the average mass of molecule's nuclear. Of typical interest is the situation where

$$d = 2, \quad j = 2, \quad V(x) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix},$$

which is referred to as a codimension 2 crossing (see [47]). Indeed, the eigenvalues of  $V$  are  $\pm|x|$ , and they cross on a codimension 2 subspace  $S$  of  $\mathbb{R}^d$ ,

$$S = \{x_1 = x_2 = 0\}.$$

The main features of eigenvalue crossings appear on this example which is simple enough so that precise computations can be performed.

According to the analysis of [42] and taking advantage of the fact that the eigenvalues are of multiplicity 1 outside the crossing set  $S$ , any Wigner measure  $w^0$  of the family  $\psi^\varepsilon(t)$  is a 2 by 2 matrix of measures which splits into two parts

$$w^0(t, x, \xi) = w^{0,+}(t, x, \xi)\Pi^+(x) + w^{0,-}(t, x, \xi)\Pi^-(x),$$

where  $\Pi^+(x)$  and  $\Pi^-(x)$  are the spectral projectors associated respectively with the eigenvalues  $+|x|$ ,  $-|x|$  of  $V(x)$  and  $w^{0,+}$ ,  $w^{0,-}$  are scalar non-negative measures. Moreover, outside the crossing set,  $w^{0,\pm}$  propagate along the classical trajectories of  $\frac{|\xi|^2}{2} \pm |x|$  according to

$$\partial_t w^{0,\pm} + \xi \cdot \nabla_x w^{0,\pm} \mp \frac{x}{|x|} \cdot \nabla_\xi w^{0,\pm} = 0.$$

Let us focus on initial data which have only one Wigner measure  $w_I^0$  and which are microlocally localized on two points of the phase space, so that

$$(3.2) \quad w_I^0(x, \xi) = \sum_{j \in \{+, -\}} a_0^j \delta(x - x_0^j) \otimes \delta(\xi - \xi_0^j) \Pi^j(x).$$

By [42], as long as the classical trajectories  $(x^\pm(t), \xi^\pm(t))$ , that is the curves such that

$$\begin{cases} \partial_t x^\pm(t) = \xi^\pm(t) & ; \quad x^\pm(0) = x_0^\pm, \\ \partial_t \xi^\pm(t) = \mp \frac{x^\pm(t)}{|x^\pm(t)|} & ; \quad \xi^\pm(0) = \xi_0^\pm. \end{cases}$$

do not reach the crossing set  $S$ ,  $\psi^\varepsilon(t)$  has only one Wigner measure  $w^0(t, x, \xi)$  which is of the form

$$w^0(t) = a^+(t) \delta(x - x^+(t)) \otimes \delta(\xi - \xi^+(t)) \Pi^+ + a^-(t) \delta(x - x^-(t)) \otimes \delta(\xi - \xi^-(t)) \Pi^-$$

with  $a^\pm(t) = a_0^\pm$  as long as the trajectories have not reached the crossing. Such situations are precisely studied in [34]: it is proved in Proposition 1 of [34] that under the assumptions

$$\begin{aligned} x_0^\pm \wedge \xi_0^\pm &= 0 \quad ; \quad |\xi_0^-|^2 > 2|x_0^-| \quad ; \quad \xi_0^- \cdot x_0^- < 0, \\ \xi_0^+ \cdot \frac{x_0^+}{|x_0^+|} + \sqrt{|\xi_0^+|^2 + 2|x_0^+|} &= -\xi_0^- \cdot \frac{x_0^-}{|x_0^-|} - \sqrt{|\xi_0^-|^2 - 2|x_0^-|} := t^*, \end{aligned}$$

the curves  $(x^\pm(t), \xi^\pm(t))$  reach  $S$  at the same time  $t^*$  with a non-zero speed  $\xi^\pm(t^*)$  and one can choose  $x_0^\pm, \xi_0^\pm$  so that they reach  $S$  at the same point  $(0, \xi^*)$  with  $\xi^* \neq 0$ . One then has

$$x^+(t^*) = x^-(t^*) = 0, \quad \xi^+(t^*) = \xi^-(t^*) = \xi^*.$$

The trajectories are given on  $[0, t^*]$  by

$$\begin{aligned} x^+(t) &= -\frac{t^2}{2} \frac{x_0^+}{|x_0^+|} + t\xi_0^+ + x_0^+ & ; \quad \xi^+(t) &= -t \frac{x_0^+}{|x_0^+|} + \xi_0^+, \\ x^-(t) &= \frac{t^2}{2} \frac{x_0^-}{|x_0^-|} + t\xi_0^- + x_0^- & ; \quad \xi^-(t) &= t \frac{x_0^-}{|x_0^-|} + \xi_0^-. \end{aligned}$$

Then, there exists  $t_1 > t^*$  such that during  $(t^*, t_1)$ , both trajectories do not meet  $S$  again. We will suppose during all this section that we are in this situation and for simplicity, we assume  $|x_0^\pm| = 1$ . We are concerned on the Wigner measure of  $\psi^\varepsilon(t)$  for  $t \in (t^*, t_1)$  which cannot be described by the transport equations above mentioned.

The work [32] proves that the sole knowledge of the initial Wigner measure is not enough to determine the Wigner measure of the solution after the crossing time  $t^*$ . A second level of observation is required, and the decisive fact is the way the data concentrates on the classical trajectories entering in  $S$  with respect to the scale  $\sqrt{\varepsilon}$ . Since all these trajectories are included in the set

$$J = \{x \wedge \xi := x_1\xi_2 - x_2\xi_1 = 0\},$$

it is enough to study the concentration of  $\psi^\varepsilon(t)$  on  $J$ .

We come up with the first aspect of our purpose, which is that the sole microlocalization consisting in working in the phase space is not enough. The complete analysis of  $\psi^\varepsilon(t)$  after a crossing point requires a second microlocalization: we add to the phase space variables  $(x, \xi)$  a new variable

$$\eta \in \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty, -\infty\}$$

which describes the spread of the wave packet on both sides of  $J$  with respect to the scale  $\sqrt{\varepsilon}$ . Then, one defines two-scale Wigner measures whose projections on the phase space are the Wigner measure. These measures have been first introduced in [60] and developed in [32]; the reader may also find in [30] a survey on the topic.

In the following, we explain the resolution of our problem by means of two-scale Wigner measures (according to [32]). This explains why initial data may have the same Wigner measure and generate solutions of the Schrödinger equation which have different Wigner measures after a crossing time. We give examples of this fact. Then, in a second section, we shall explain and illustrate the limits of the two-scale Wigner measures approach: some situations cannot be studied with the sole knowledge of the two-scale Wigner measures.

**3.1. When one needs a second microlocalization.** One defines a two-scale Wigner measure  $w^{0,(2)}(t, x, \xi, \eta)$  of  $\psi^\varepsilon(t)$  associated with  $J$ , as a weak limit in  $\mathcal{D}'$  of the two-scale Wigner functional defined on  $\mathbb{R}_x^2 \times (\mathbb{R}_\xi^2 \setminus \{0\}) \times \overline{\mathbb{R}}_\eta$  by

$$w^{\varepsilon,(2)}[\psi^\varepsilon(t)](x, \xi, \eta) = w^\varepsilon[\psi^\varepsilon(t)](x, \xi) \otimes \delta\left(\eta - \frac{x \wedge \xi}{\sqrt{\varepsilon}}\right)$$

that we test against smooth functions  $a(x, \xi, \eta)$  which are compactly supported in  $(x, \xi)$ , uniformly with respect to  $\eta$ , and coincide for  $\eta$  big enough with an homogeneous function of degree 0 in  $\eta$ , denoted by  $a_\infty(x, \xi, \eta)$ . The knowledge of  $w^{0,(2)}(t, x, \xi, \eta)$  determines the Wigner measures of  $\psi^\varepsilon(t)$  above  $J$  according to

$$\forall a \in C_0^\infty(\mathbb{R}_x^2 \times (\mathbb{R}_\xi^2 \setminus \{0\})), \quad \langle w^0 \mathbf{1}_J, a \rangle = \int_{\mathbb{R}_x^2 \times (\mathbb{R}_\xi^2 \setminus \{0\}) \times \overline{\mathbb{R}}_\eta} a(x, \xi) dw^{0,(2)}.$$

Let us suppose that the data  $\psi_0^\varepsilon$  has a unique two-scale Wigner measure  $w_I^{0,(2)}$  of the form

$$w_I^{0,(2)}(x, \xi, \eta) = \sum_{j \in \{+, -\}} \delta(x - x_0^j) \otimes \delta(\xi - \xi_0^j) \otimes \nu_{in}^j(\eta) \Pi^j(x),$$

where  $\nu_{in}^\pm(\eta)$  are scalar positive Radon measures on  $\overline{\mathbb{R}}$ , and  $x_0^\pm, \xi_0^\pm$  are as before. Define

$$(3.3) \quad T(\eta) = e^{-\pi|\eta|^2/|\xi^*|^3}.$$

Then, Theorems 2 and 3 in [32] yield

**PROPOSITION 3.1.** *For any  $t \in [0, t^*) \cup (t^*, t_1)$ ,  $\psi^\varepsilon(t)$  has a unique two-scale Wigner measure  $w^{0,(2)}(t)$  which satisfies:*

- For  $t \in [0, t^*)$ ,

$$w^{0,(2)}(t, x, \xi, \eta) = \sum_{j \in \{+, -\}} \delta(x - x^j(t)) \otimes \delta(\xi - \xi^j(t)) \otimes \nu_{in}^j(\eta) \Pi^j(x).$$

- For  $t \in (t^*, t_1)$ ,

$$w^{0,(2)}(t, x, \xi, \eta) = \sum_{j \in \{+, -\}} \delta(x - x^j(t)) \otimes \delta(\xi - \xi^j(t)) \otimes \nu_{out}^j(\eta) \Pi^j(x).$$

Moreover if  $\nu_{in}^+$  and  $\nu_{in}^-$  are singular on  $\{|\eta| < \infty\}$ , the link between the incident measures  $(\nu_{in}^+, \nu_{in}^-)$  and the outgoing ones  $(\nu_{out}^+, \nu_{out}^-)$  is given by

$$\begin{pmatrix} \nu_{out}^+ \\ \nu_{out}^- \end{pmatrix} = \begin{pmatrix} 1 - T(\eta) & T(\eta) \\ T(\eta) & 1 - T(\eta) \end{pmatrix} \begin{pmatrix} \nu_{in}^+ \\ \nu_{in}^- \end{pmatrix}.$$

Let us examine the consequence of this Proposition for initial data of the form

$$\psi_{0,\ell}^\varepsilon = \varepsilon^{-\beta_\ell} \Phi\left(\frac{x - x_0^+}{\varepsilon^{\beta_\ell}}\right) \exp\left(\frac{i}{2\varepsilon} r_0^+ |x|^2\right) E^+(x), \quad \ell \in \{1, 2, 3\},$$

$$\text{with } \beta_1 < \frac{1}{2} = \beta_2 < \beta_3,$$

where  $\xi_0^+ = r_0^+ x_0^+$ ,  $\Phi \in C_0^\infty(\mathbb{R}^2)$ , and  $E^+$  is a smooth bounded function such that  $\Pi^+ E^+ = E^+$  on the support of  $\psi_{0,\ell}^\varepsilon$ , and  $\|E^+\|_{C^2} = 1$ . These three families have the same Wigner measure  $w_I^0$  of the form (3.2) with

$$a_0^+ = \|\Phi\|_{L^2}^2, \quad a_0^- = 0.$$

Simple calculus (see [34, Section 3.2] for details) shows that the two-scale Wigner measures associated with  $J$  for each of these families are different. Let us denote

by  $w_{I,\ell}^{0,(2)}$  the two-scale Wigner measure of  $\psi_{0,\ell}^\varepsilon$ ,  $\ell \in \{1, 2, 3\}$ . If  $v = (v_1, v_2)$ , we denote by  $v^\perp$  the vector  $v^\perp = (-v_2, v_1)$ . Then, we have

$$\begin{aligned} w_{I,1}^{0,(2)}(x, \xi, \eta) &= \|\Phi\|_{L^2}^2 \delta(x - x_0^+) \otimes \delta(\xi - \xi_0^+) \otimes \delta(\eta) \Pi^+(x), \\ w_{I,2}^{0,(2)}(x, \xi, \eta) &= \delta(x - x_0^+) \otimes \delta(\xi - \xi_0^+) \otimes \mathbf{1}_{\eta \in \mathbb{R}} \gamma(\eta) d\eta \Pi^+(x), \\ w_{I,3}^{0,(2)}(x, \xi, \eta) &= \delta(x - x_0^+) \otimes \delta(\xi - \xi_0^+) \otimes (\gamma^- \delta(\eta - \infty) + \gamma^- \delta(\eta + \infty)) \Pi^+(x), \end{aligned}$$

with

$$\xi_0^\pm = r_0^\pm x_0^\pm ; \quad \gamma(\eta) = \frac{1}{(2\pi)^2} \left( \int_{\mathbb{R}} \left| \widehat{\Phi}(rx_0^+ + \eta(x_0^+)^\perp) \right|^2 dr \right) ; \quad \gamma^\pm = \int_{\mathbb{R}^\pm} \gamma(\eta) d\eta.$$

As a consequence of the propagation of two-scale Wigner measures along the classical trajectories (see [34]), we get different behaviors after the crossing time  $t^*$ .

**COROLLARY 3.2.** *For  $\ell \in \{1, 2, 3\}$ , the family  $\psi_\ell^\varepsilon(t)$  solution to (3.1) with the initial data  $\psi_{0,\ell}^\varepsilon$  has a unique Wigner measure  $w_\ell^0(t)$  such that*

$$\begin{aligned} w_\ell^0(t, x, \xi, \eta) &= a_\ell^+(t) \delta(x - x^+(t)) \otimes \delta(\xi - \xi^+(t)) \Pi^+(x) \\ &\quad + a_\ell^-(t) \delta(x - x^-(t)) \otimes \delta(\xi - \xi^-(t)) \Pi^-(x). \end{aligned}$$

Moreover, for all  $t \in [0, t^*)$

$$a_1^+(t) = a_2^+(t) = a_3^+(t) = \|\Phi\|_{L^2}^2, \quad a_1^-(t) = a_2^-(t) = a_3^-(t) = 0,$$

and for all  $t \in (t^*, t_1)$ ,

$$\begin{aligned} a_1^+(t) &= \|\Phi\|_{L^2}^2, \quad a_1^-(t) = 0, \\ a_2^+(t) &= (1 - T(\eta)) \gamma(\eta), \quad a_2^-(t) = T(\eta) \gamma(\eta), \\ a_3^+(t) &= 0, \quad a_3^-(t) = \|\Phi\|_{L^2}^2. \end{aligned}$$

In the first case, the mass propagates along the classical trajectory associated with the mode  $+$ , while in the third case the mass switches from the mode  $+$  to the mode  $-$ . In the second case, the mass parts between both modes  $+$  and  $-$ .

**3.2. When the quadratic approach fails.** The assumption of singularity on the incident measures is crucial in Proposition 3.1. Indeed, if it fails, the two-scale Wigner measures after the crossing point cannot be calculated in terms of the incident ones. Our aim is now to explain and to illustrate that similar Wigner measures (and even similar two-scale Wigner measures) can generate different measures after the crossing point. The example given here is precisely discussed in [31].

We consider

$$\begin{aligned} \psi_0^\varepsilon &= \varepsilon^{-\beta d/2} \Phi \left( \frac{x - x_0^+}{\varepsilon^\beta} \right) \exp \left( \frac{i}{2\varepsilon} r_0^+ \left| x - \varepsilon^{\alpha^+} \omega_0^+ \right|^2 \right) E^+(x) \\ &\quad + \varepsilon^{-\beta d/2} \Psi \left( \frac{x - x_0^-}{\varepsilon^\beta} \right) \exp \left( \frac{i}{2\varepsilon} r_0^- \left| x - \varepsilon^{\alpha^-} \omega_0^- \right|^2 \right) E^-(x), \end{aligned}$$

where

$$0 < \alpha^\pm \leq 1/2 \quad ; \quad 0 < \beta < 1/2 \quad ; \quad \omega_0^+, \omega_0^- \in \mathbb{R}^d \quad ; \quad \xi_0^\pm = r_0^\pm x_0^\pm,$$

and  $\Phi$  and  $\Psi$  are smooth, compactly supported, functions on  $\mathbb{R}^d$ ,  $E^+(x)$  (resp.  $E^-(x)$ ) is a smooth bounded function such that on the support of  $\Phi \left( \frac{x - x_0^+}{\varepsilon^\beta} \right)$  (resp. of  $\Psi \left( \frac{x - x_0^-}{\varepsilon^\beta} \right)$ ) one has  $\Pi^\pm(x) E^\pm(x) = E^\pm(x)$  and  $\|E^\pm(x)\|_{\mathbb{C}^2} = 1$ . We shall focus on both situations  $\omega_0^+ \neq \omega_0^-$  and  $\omega_0^+ = \omega_0^-$ . We set

$$c^{+,in} = \|\Phi\|_{L^2}, \quad c^{-,in} = \|\Psi\|_{L^2}$$

and we suppose

$$\eta_0^\pm := -r_0^\pm(x_0^\pm \wedge \omega_0^\pm) \neq 0.$$

PROPOSITION 3.3. *The family  $\psi^\varepsilon(t)$  solution to (3.1) with the initial data  $\psi_0^\varepsilon$  has a unique Wigner measure  $w^0(t, x, \xi)$  such that*

- For  $t \in [0, t^*)$ ,

$$w^0(t, x, \xi) = \sum_{j \in \{+, -\}} c^{j, in} \delta(x - x^j(t)) \otimes \delta(\xi - \xi^j(t)) \Pi^j(x).$$

- For  $t \in (t^*, t_1)$ ,

$$w^0(t, x, \xi) = \sum_{j \in \{+, -\}} c^{j, out} \delta(x - x^j(t)) \otimes \delta(\xi - \xi^j(t)) \Pi^j(x),$$

where the coefficients  $c^{j, out}$  depend on the position of  $\alpha^+$  and  $\alpha^-$  with respect to  $1/2$ :

	$c^{+, out}$	$c^{-, out}$
$\alpha^-, \alpha^+ < 1/2$	$c^{+, in}$	$c^{-, in}$
$\alpha^+ < \alpha^- = 1/2$	$c^{+, in} + T(\eta_0^-)c^{-, in}$	$c^{-, in} (1 - T(\eta_0^-))$
$\alpha^- < \alpha^+ = 1/2$	$c^{+, in} (1 - T(\eta_0^+))$	$c^{-, in} + T(\eta_0^+)c^{+, in}$
$\begin{cases} \alpha^+ = \alpha^- = 1/2 \\ \eta_0^+ \neq \eta_0^- \end{cases}$	$c^{+, in} (1 - T(\eta_0^+))$ $+ T(\eta_0^-)c^{-, in}$	$c^{-, in} (1 - T(\eta_0^-))$ $+ T(\eta_0^+)c^{+, in}$

If  $\alpha^+ = \alpha^- = 1/2$  and  $\eta_0^+ = \eta_0^- := \eta_0$ , there exists  $\rho_0 \in \mathbb{R}^+$  and  $\phi_0 \in \mathbb{R}$  such that

$$\begin{cases} c^{+, out} = c^{+, in} (1 - T(\eta_0)) + T(\eta_0)c^{-, in} + \rho_0 \cos(\phi_0), \\ c^{-, out} = c^{-, in} (1 - T(\eta_0)) + T(\eta_0)c^{+, in} - \rho_0 \cos(\phi_0). \end{cases}$$

Besides, for any  $\phi \in \mathbb{R}$ , if one turns  $\Psi$  into  $e^{i\phi}\Psi$ , then one has

$$(3.4) \quad \begin{cases} c^{+, out} = c^{+, in} (1 - T(\eta_0)) + T(\eta_0)c^{-, in} + \rho_0 \cos(\phi_0 - \phi), \\ c^{-, out} = c^{-, in} (1 - T(\eta_0)) + T(\eta_0)c^{+, in} - \rho_0 \cos(\phi_0 - \phi). \end{cases}$$

Here again, we see that the interaction between both incident modes cannot be described only by the knowledge of the Wigner measure: one needs to know the two-scale Wigner measure. Indeed, for each case described in the above array, the two-scale Wigner measure is different:

$$w^{0, (2)}(t, x, \xi, \eta) = \sum_{j \in \{+, -\}} c^{j, out} \delta(x - x^j(t)) \otimes \delta(\xi - \xi^j(t)) \otimes \nu^j(\eta) \Pi^j(x),$$

with  $\nu^j(\eta)$  supported on  $\infty$  for  $\alpha^j < 1/2$  and  $\nu^j(\eta)$  supported on  $\eta_0^j$  if  $\alpha^j = 1/2$ . Therefore, the situations of the array enters in the range of validity of Proposition 3.1. In the last situation where  $\alpha^+ = \alpha^- = 1/2$  and  $\eta_0^+ = \eta_0^-$ , the two incident wave functions interact and some coupling term appears. By modifying the initial data, turning  $\Psi$  into  $e^{i\lambda}\Psi$ , one does not modify the two-scale Wigner measure but one can transform the coupling (and even suppress it) so that the outgoing Wigner measures change. The same thing happens for any initial data provided it has the same two-scale Wigner measure as our example.

For proving Proposition 3.3, we use the normal form one can obtain for (3.1), and which is crucial for proving Proposition 3.1. The reader can refer to [23] for the more elaborate result for general systems presenting codimension 2 crossings (see also [24] for the case of hermitian matrix-valued symbol). One can find in [32] a weaker result which covers the case of Schrödinger equation (3.1), and is enough for calculating Wigner measures. Through a change of symplectic coordinates in

space-time phase space, and a change of unknown by use of a Fourier Integral operator, one reduces to the system:

$$(3.5) \quad \frac{\varepsilon}{i} \partial_s u^\varepsilon = \begin{pmatrix} s & z_1 \\ z_1 & -s \end{pmatrix} u^\varepsilon, \quad (s, z = (z_1, z_2)) \in \mathbb{R}^3.$$

We outline two important features of this normal form. On the one hand, this normal form is microlocal, near the crossing point  $(t^*, 0, \tau^*, \xi^*)$  where  $\tau^*$  is the energy variable  $\tau^* = \frac{|\xi^*|^2}{2}$ . On the other hand, space time coordinates are involved by the canonical transform (i.e. by the change of symplectic coordinates)

$$\kappa : (t, x, \tau, \xi) \mapsto (s, z, \sigma, \zeta).$$

Through  $\kappa$ , the crossing set  $S$  becomes  $S = \{s = z_1 = 0\}$  and the set  $J = \{x \wedge \xi = 0\}$  becomes  $J = \{z_1 = 0\}$ . Moreover, the classical trajectories in space time coordinates  $(r, x^\pm(r), \tau, \xi^\pm(r))_{r>0}$  (where  $\tau = -\frac{1}{2}|\xi^\pm(r)|^2 \pm |x^\pm(r)| = \text{Const.}$ ) which enters in  $S$  maps on the curves  $(r, 0, z_2, \pm|r|, \zeta_1, \zeta_2)_{r>0}$  and the link between  $z_1$  and  $x \wedge \xi$  is given by  $z_1 = e(t, x, \tau, \xi) x \wedge \xi$ , where  $e$  is a smooth function such that  $e(t^*, 0, \tau^*, \xi^*) = |\xi^*|^{-3/2}$ . Finally, the Wigner measure is invariant by this change of coordinates, and if we denote by  $\lambda$  the additional variable of the two-scale Wigner measure in the variables  $(s, z)$ , and by  $\eta$  the corresponding variables in  $(x, \xi)$ , we have  $\lambda = e(t, x, \tau, \xi) \eta$  because of the link between  $z_1$  and  $(t, x, \tau, \xi)$ .

We focus now on system (3.5). This system of o.d.e. is simple enough so that direct calculations are possible. This has been done by Landau and Zener in the 30's (see [52] and [70]). We use the description of  $u^\varepsilon$  near  $z_1 = 0$  as stated in [32, Proposition 9], which is obtained by means of stationary phase method. One can also find a resolution of this system in [47], where special functions are used.

**PROPOSITION 3.4.** *There exist families of vectors of  $\mathbb{C}^2$ ,  $\alpha^\varepsilon = (\alpha_1^\varepsilon, \alpha_2^\varepsilon)$ ,  $\omega^\varepsilon = (\omega_1^\varepsilon, \omega_2^\varepsilon)$ , such that, as  $\varepsilon$  goes to 0 and for  $\frac{z_1}{\sqrt{\varepsilon}}$  bounded,*

- For  $s < 0$ ,

$$u_1^\varepsilon(s, z) = e^{i\frac{s^2}{2\varepsilon}} \left| \frac{s}{\sqrt{\varepsilon}} \right|^{i\frac{z_1^2}{2\varepsilon}} \alpha_1^\varepsilon + o(1), \quad u_2^\varepsilon(s, z) = e^{-i\frac{s^2}{2\varepsilon}} \left| \frac{s}{\sqrt{\varepsilon}} \right|^{-i\frac{z_1^2}{2\varepsilon}} \alpha_2^\varepsilon + o(1).$$

- For  $s > 0$ ,

$$u_1^\varepsilon(s, z) = e^{i\frac{s^2}{2\varepsilon}} \left| \frac{s}{\sqrt{\varepsilon}} \right|^{i\frac{z_1^2}{2\varepsilon}} \omega_1^\varepsilon + o(1), \quad u_2^\varepsilon(s, z) = e^{-i\frac{s^2}{2\varepsilon}} \left| \frac{s}{\sqrt{\varepsilon}} \right|^{-i\frac{z_1^2}{2\varepsilon}} \omega_2^\varepsilon + o(1).$$

Moreover  $\begin{pmatrix} \omega_1^\varepsilon \\ \omega_2^\varepsilon \end{pmatrix} = S \left( \frac{z_1}{\sqrt{\varepsilon}} \right) \begin{pmatrix} \alpha_1^\varepsilon \\ \alpha_2^\varepsilon \end{pmatrix}$  with

$$(3.6) \quad S(\lambda) = \begin{pmatrix} a(\lambda) & -\bar{b}(\lambda) \\ b(\lambda) & a(\lambda) \end{pmatrix}; \quad a(\lambda) = e^{-\pi\frac{|\lambda|^2}{2}} \quad ; \quad a(\lambda)^2 + |b(\lambda)|^2 = 1.$$

**PROOF OF PROPOSITION 3.3.** Let us use the relation between the classical trajectories to identify  $\nu^{+,in}$  (resp.  $\nu^{-,in}$ ) as the two-scale Wigner measure of  $\alpha_1^\varepsilon$  (resp.  $\alpha_2^\varepsilon$ ) for  $\{z_1 = 0\}$ , and  $\nu^{+,out}$  (resp.  $\nu^{-,out}$ ) as the one of  $\omega_2^\varepsilon$  (resp.  $\omega_1^\varepsilon$ ).

- If  $(\alpha^\pm < \alpha^\mp = 1/2)$  or  $(\alpha^\pm = 1/2$  and  $\eta_0^+ \neq \eta_0^-)$ , the two incoming measures are mutually singular. Therefore, the measure of

$$\omega_1^\varepsilon(z) = a \left( \frac{z_1}{\sqrt{\varepsilon}} \right) \alpha_1^\varepsilon(z) - \bar{b} \left( \frac{z_1}{\sqrt{\varepsilon}} \right) \alpha_2^\varepsilon(z)$$

is the sum of the measures of each term. We obtain

$$\nu^{-,out}(z, \zeta, \lambda) = a(\lambda)^2 \nu^{+,in}(z, \zeta, \lambda) + |b(\lambda)|^2 \nu^{-,in}(z, \zeta, \lambda),$$

which gives in the variables  $(x, \xi, \eta)$

$$\nu^{-,out}(x, \xi, \eta) = T(\eta)\nu^{+,in}(x, \xi, \eta) + (1 - T(\eta))\nu^{-,in}(x, \xi, \eta),$$

where we have used

$$a\left(\eta|\xi^*|^{-3/2}\right)^2 = T(\eta), \quad \left|b\left(\eta|\xi^*|^{-3/2}\right)\right|^2 = 1 - T(\eta).$$

Similarly, we get

$$\nu^{+,out}(x, \xi, \eta) = (1 - T(\eta))\nu^{+,in}(x, \xi, \eta) + T(\eta)\nu^{-,in}(x, \xi, \eta).$$

We see here how the singularity relation plays a role for finite  $\eta$  in Proposition 3.1.

• If  $\alpha^\pm < 1/2$ , both incident measures are localized in  $\eta = \infty$ , Prop. 3.1 yields

$$\nu^{\pm,out}(x, \xi, \eta) = \nu^{\pm,in}(x, \xi, \eta).$$

• If  $\alpha^\pm = 1/2$  and  $\eta_0^+ = \eta_0^-$ . Observing that  $\nu^{\pm,out}$  is localized above  $\eta_0^+ = \eta_0^- := \eta_0$  and taking into account the two-scale joint measure  $\theta$  between  $\alpha_1^\varepsilon$  and  $\alpha_2^\varepsilon$  which is also supported above  $\eta_0$ , we obtain

$$\begin{aligned} \nu^{+,out} &= (1 - T(\eta_0))\nu^{+,in} + T(\eta_0)\nu^{-,in} + 2\operatorname{Re}\left(a\left(\eta_0|\xi^*|^{-3/2}\right)b\left(\eta_0|\xi^*|^{-3/2}\right)\theta\right), \\ \nu^{-,out} &= T(\eta_0)\nu^{+,in} + (1 - T(\eta_0))\nu^{-,in} - 2\operatorname{Re}\left(a\left(\eta_0|\xi^*|^{-3/2}\right)b\left(\eta_0|\xi^*|^{-3/2}\right)\theta\right). \end{aligned}$$

There exists  $(\rho_0, \phi_0) \in \mathbb{R}^+ \times [0, 2\pi]$  such that

$$a\left(\eta_0|\xi^*|^{-3/2}\right)b\left(\eta_0|\xi^*|^{-3/2}\right) = \rho_0 e^{i\phi_0}.$$

One then observes that if one multiplies the minus component of the initial data by  $e^{i\phi}$ , one turns  $\alpha_2^\varepsilon$  into  $e^{i\phi}\alpha_2^\varepsilon$  and  $\theta$  into  $e^{-i\phi}\theta$ , whence the result.  $\square$

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