Nonlinear coherent states and Ehrenfest time for Schrödinger equation

Rémi Carles
(joint work with Clotilde Fermanian-Kammerer)

We consider the semi-classical limit $\varepsilon \to 0$ for the nonlinear Schrödinger equation

$$(1)\quad i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V(x)\psi^\varepsilon + \lambda|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon, \quad (t,x)\in \mathbf{R}_+\times\mathbf{R}^d \quad ; \quad \psi^\varepsilon_{|t=0} = \psi_0^\varepsilon,$$

with $\lambda \in \mathbf{R}$, $d \geqslant 1$. The external potential V is smooth, real-valued, and at most quadratic:

$$V \in C^\infty(\mathbf{R}^d;\mathbf{R}) \quad \text{and} \quad \partial_x^\gamma V \in L^\infty\left(\mathbf{R}^d\right), \quad \forall |\gamma| \geqslant 2.$$

We assume that the initial data ψ_0^ε is a localized wave packet of the form

$$(2)\qquad \psi_0^\varepsilon(x) = \varepsilon^\beta \times \varepsilon^{-d/4} a\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right) e^{i(x-x_0)\cdot\xi_0/\varepsilon}, \quad a\in\mathcal{S}(\mathbf{R}^d), \quad x_0,\xi_0\in\mathbf{R}^d.$$

Such data, which are called *semi-classical wave packets* (or *coherent states*), have been extensively studied in the linear case (see e.g. [2, 4, 5, 10, 11]). In particular, Gaussian wave packets are used in numerical simulation of quantum chemistry like Initial Value Representations methods (see [12, 13, 14] and references therein). These methods rely on the fact that if the data is a wave packet, then the solution of the linear equation ($\lambda = 0$) associated with (1) still is a wave packet at leading order up to times of order $C\log\left(\frac{1}{\varepsilon}\right)$: such a large (as $\varepsilon \to 0$) time is called *Ehrenfest time*, see e.g. [1, 7, 8]. Our aim here is to investigate what remains of these facts in the nonlinear case ($\lambda \neq 0$), since typically (1) appears as a model for Bose–Einstein Condensation, where, for instance, V may be exactly a harmonic potential, or a truncated harmonic potential (hence not exactly quadratic); see e.g. [6, 9].

In the present nonlinear setting, a new parameter has to be considered: the size of the initial data, hence the factor ε^β in (2). There exists a notion of criticality for β: for $\beta > \beta_c := 1/(2\sigma) + d/4$, the initial data are too small to ignite the nonlinearity at leading order, and the leading order behavior of ψ^ε as $\varepsilon \to 0$ is the same as in the linear case $\lambda = 0$, up to Ehrenfest time. On the other hand, if $\beta = \beta_c$, the function ψ^ε is given at leading order by a wave packet whose envelope satisfies a *nonlinear* equation, up to a nonlinear analogue of the Ehrenfest time. We show moreover a nonlinear superposition principle: when the initial data is the sum of two wave packets of the form (2), then ψ^ε is approximated at leading order by the sum of the approximations obtained in the case of a single initial coherent state.

Up to changing ψ^ε to $\varepsilon^{-\beta}\psi^\varepsilon$, we may assume that the initial data are of order $\mathcal{O}(1)$ in $L^2(\mathbf{R}^d)$, and we consider

$$(3)\qquad \begin{cases} i\varepsilon\partial_t\psi^\varepsilon + \dfrac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V(x)\psi^\varepsilon + \lambda\varepsilon^\alpha|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon, \quad (t,x)\in\mathbf{R}_+\times\mathbf{R}^d, \\ \psi^\varepsilon(0,x) = \varepsilon^{-d/4} a\left(\dfrac{x-x_0}{\sqrt{\varepsilon}}\right) e^{i(x-x_0)\cdot\xi_0/\varepsilon}, \end{cases}$$

where $\alpha = 2\beta\sigma$.

Consider the classical trajectories associated with the Hamiltonian $\frac{|\xi|^2}{2} + V(x)$:

$$\dot{x}(t) = \xi(t), \quad \dot{\xi}(t) = -\nabla V(x(t)); \quad x(0) = x_0, \ \xi(0) = \xi_0. \tag{4}$$

We associate with these trajectories the *classical action*

$$S(t) = \int_0^t \left(\frac{1}{2}|\xi(s)|^2 - V(x(s)) \right) ds. \tag{5}$$

We observe that if we change the unknown function ψ^ε to u^ε by

$$\psi^\varepsilon(t,x) = \varepsilon^{-d/4} u^\varepsilon \left(t, \frac{x - x(t)}{\sqrt{\varepsilon}} \right) e^{i(S(t)+\xi(t)\cdot(x-x(t)))/\varepsilon},$$

then, in terms of $u^\varepsilon = u^\varepsilon(t,y)$, (3) is equivalent

$$i\partial_t u^\varepsilon + \frac{1}{2}\Delta u^\varepsilon = V^\varepsilon(t,y)u^\varepsilon + \lambda \varepsilon^{\alpha-\alpha_c}|u^\varepsilon|^{2\sigma}u^\varepsilon \quad ; \quad u^\varepsilon(0,y) = a(y),$$

where the external time-dependent potential V^ε is given by

$$V^\varepsilon(t,y) = \frac{1}{\varepsilon}\left(V(x(t) + \sqrt{\varepsilon}y) - V(x(t)) - \sqrt{\varepsilon}\left\langle \nabla V(x(t)), y \right\rangle \right), \tag{6}$$

and $\alpha_c = 1 + \dfrac{d\sigma}{2}$. The real number α_c appears as a critical exponent. The expression (6) reveals the first terms of the Taylor expansion of V about the point $x(t)$. Passing formally to the limit, V^ε converges to the Hessian of V at $x(t)$ evaluated at (y,y). One does not even need to pass to the limit if V is a polynomial of degree at most two: in that case, we see that the solution ψ^ε remains exactly a coherent state for all time. Let us denote by $Q(t)$ the symmetric matrix

$$Q(t) = \operatorname{Hess} V(x(t)).$$

If $\lambda = 0$ or $\alpha > \alpha_c$, then ψ^ε is approximated by $\varphi^\varepsilon_{\text{lin}}$, up to time of order $C \log \frac{1}{\varepsilon}$, where

$$\varphi^\varepsilon_{\text{lin}}(t,x) = \varepsilon^{-d/4} v \left(t, \frac{x - x(t)}{\sqrt{\varepsilon}} \right) e^{i(S(t)+\xi(t)\cdot(x-x(t)))/\varepsilon},$$

and v is given by

$$i\partial_t v + \frac{1}{2}\Delta v = \frac{1}{2}\left\langle Q(t)y, y \right\rangle v \quad ; \quad v(0,y) = a(y).$$

In the critical nonlinear case $\lambda \neq 0$ and $\alpha = \alpha_c$, we have typically the following result. Consider the solution to

$$i\partial_t u + \frac{1}{2}\Delta u = \frac{1}{2}\langle Q(t)y, y\rangle u + \lambda |u|^{2\sigma} u \quad ; \quad u(0,y) = a(y), \tag{7}$$

and let

$$\varphi^\varepsilon(t,x) = \varepsilon^{-d/4} u \left(t, \frac{x - x(t)}{\sqrt{\varepsilon}} \right) e^{i(S(t)+\xi(t)\cdot(x-x(t)))/\varepsilon}. \tag{8}$$

Theorem 1. *Assume $d = \sigma = 1$, and let $a \in \mathcal{S}(\mathbf{R})$. There exist $C, C_0 > 0$ independent of ε, and $\varepsilon_0 > 0$ such that for all $\varepsilon \in]0, \varepsilon_0]$,*

$$\|\psi^\varepsilon(t) - \varphi^\varepsilon(t)\|_{L^2(\mathbf{R})} \lesssim \sqrt{\varepsilon}\exp(C_0 t), \quad 0 \leqslant t \leqslant C \log \frac{1}{\varepsilon}.$$

Consider now initial data corresponding to the superposition of two wave packets:

$$\psi^\varepsilon(0,x) = \varepsilon^{-d/4} a_1 \left(\frac{x - x_1}{\sqrt{\varepsilon}}\right) e^{i(x-x_1)\cdot\xi_1/\varepsilon} + \varepsilon^{-d/4} a_2 \left(\frac{x - x_2}{\sqrt{\varepsilon}}\right) e^{i(x-x_2)\cdot\xi_2/\varepsilon},$$

with $a_1, a_2 \in \mathcal{S}(\mathbf{R})$, $(x_1, \xi_1), (x_2, \xi_2) \in \mathbf{R}^2$, and $(x_1, \xi_1) \neq (x_2, \xi_2)$. For $j \in \{1, 2\}$, $(x_j(t), \xi_j(t))$ are the classical trajectories solutions to (4) with initial data (x_j, ξ_j). We denote by S_j the action associated with $(x_j(t), \xi_j(t))$ by (5) and by u_j the solution of (7) for the curve $x_j(t)$ and with initial data a_j. We consider φ_j^ε associated by (8) with u_j, x_j, ξ_j, S_j, and ψ^ε solution to (3) with $\alpha = \alpha_c$ and the above data.

Theorem 2. *Assume $d = \sigma = 1$, and let $a_1, a_2 \in \mathcal{S}(\mathbf{R})$. Suppose $E_1 \neq E_2$, where*

$$E_j = \frac{\xi_j^2}{2} + V(x_j).$$

There exist $C, C_1 > 0$ independent of ε, and $\varepsilon_0 > 0$ such that for all $\varepsilon \in]0, \varepsilon_0]$,

$$\|\psi^\varepsilon(t) - \varphi_1(t)^\varepsilon - \varphi_2^\varepsilon(t)\|_{L^2(\mathbf{R})} \lesssim \varepsilon^\gamma e^{C_1 t}, \quad 0 \leqslant t \leqslant C \log \frac{1}{\varepsilon}, \quad \textit{with } \gamma = \frac{k-2}{2k-2}.$$

Even though the profiles are nonlinear, the superposition principle, which is a property of linear equations, still holds. The assumption $E_1 \neq E_2$ is probably only technical, but we cannot conclude without it, unless we consider time intervals which do not depend upon ε. Detailed proofs can be found in [3].

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