Séminaires & Congrès
15, 2007, p. 181–252

PROPAGATION OF COHERENT STATES IN QUANTUM MECHANICS AND APPLICATIONS

by

Didier Robert

Abstract. — This paper present a synthesis concerning applications of Gaussian coherent states in semi-classical analysis for Schrödinger type equations, time dependent or time independent. We have tried to be self-contained and elementary as far as possible.

In the first half of the paper we present the basic properties of the coherent states and explain in details the construction of asymptotic solutions for Schrödinger equations. We put emphasis on accurate estimates of these asymptotic solutions: large time, analytic or Gevrey estimates. In the second half of the paper we give several applications: propagation of frequency sets, semi-classical asymptotics for bound states and for the scattering operator for the short range scattering.

***Résumé* (Propagation d'états cohérents en mécanique quantique et applications)**

Cet article présente une synthèse concernant les applications des états cohérents gaussiens à l'analyse semi-classique des équations du type de Schrödinger, dépendant du temps ou stationnaires. Nous avons tenté de faire un travail aussi détaillé et élémentaire que possible.

Dans la première partie nous présentons les propriétés fondamentales des états cohérents et nous exposons en détails la construction de solutions asymptotiques de l'équation de Schrödinger. Nous mettons l'accent sur des estimations précises : temps grands, estimations du type analytique ou Gevrey. Dans la dernière partie de ce travail nous donnons plusieurs applications : propagation des ensembles de fréquences, asymptotiques semi-classiques pour les états bornés et leurs énergies ainsi que pour l'opérateur de diffusion dans le cas de la diffusion à courte portée.

Introduction

Coherent states analysis is a very well known tool in physics, in particular in quantum optics and in quantum mechanics. The name "coherent states" was first used by R. Glauber, Nobel prize in physics (2005), for his works in quantum optics

2000 ***Mathematics Subject Classification.*** — 35Q30, 76D05, 34A12.
Key words and phrases. — Semi-classical limit, time dependent Schrödinger equation, Dirac equation, bounded states, scattering operator, analytic estimates, Gevrey estimates.

© Séminaires et Congrès 15, SMF 2007

and electrodynamics. In the book [**27**], the reader can get an idea of the fields of applications of coherent states in physics and in mathematical-physics.

A general mathematical theory of coherent states is detailed in the book [**33**]. Let us recall here the general setting of the theory.

G is a locally compact Lie group, with its Haar left invariant measure dg and R is an irreducible unitary representation of G in the Hilbert space $\mathcal{H}$. Suppose that there exists $\varphi \in \mathcal{H}$, $\|\varphi\| = 1$, such that

$$0 < \int_G |\langle \varphi, R(g)\varphi\rangle|^2 \, dg < +\infty \tag{1}$$

(R is said to be square integrable).

Let us define the coherent state family $\varphi_g = R(g)\varphi$. For $\psi \in \mathcal{H}$, we can define, in the weak sense, the operator $\mathcal{I}\psi = \int_G \langle \psi, \varphi_g\rangle \varphi_g dg$. $\mathcal{I}$ commute with R, so we have $\mathcal{I} = c\mathbb{1}$, with $c \neq 0$, where $\mathbb{1}$ is the identity on $\mathcal{H}$. Then, after renormalisation of the Haar measure, we have a resolution of identity on $\mathcal{H}$ in the following sense:

$$\psi = \int_G \langle \psi, \varphi_g\rangle \varphi_g \, dg, \quad \forall \psi \in \mathcal{H}. \tag{2}$$

(2) is surely one of the main properties of coherent states and is a starting point for a sharp analysis in the Hilbert space $\mathcal{H}$ (see [**33**]).

Our aim in this paper is to use coherent states to analyze solutions of time dependent Schrödinger equations in the semi-classical regime ($\hbar \searrow 0$).

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \widehat{H}(t)\psi(t), \quad \psi(t = t_0) = f, \tag{3}$$

where f is an initial state, $\widehat{H(t)}$ is a quantum Hamiltonian defined as a continuous family of self-adjoint operators in the Hilbert space $L^2(\mathbb{R}^d)$, depending on time t and on the Planck constant $\hbar > 0$, which plays the role of a small parameter in the system of units considered in this paper. $\hat{H}(t)$ is supposed to be the $\hbar$-Weyl-quantization of a classical observable $H(t, x, \xi)$, $x, \xi \in \mathbb{R}^d$ (cf [**37**] for more details concerning Weyl quantization).

The canonical coherent states in $L^2(\mathbb{R}^d)$ are usually built from an irreducible representation of the Heisenberg group $\mathbb{H}_{2d+1}$(see for example [**15**]). After identification of elements in $\mathbb{H}_{2d+1}$ giving the same coherent states, we get a family of states $\{\varphi_z\}_{z\in\mathcal{Z}}$ satisfying (2) where $\mathcal{Z}$ is the phase space $\mathbb{R}^d \times \mathbb{R}^d$. More precisely,

$$\varphi_0(x) = (\pi\hbar)^{-d/4} \exp\left(\frac{x^2}{2\hbar}\right), \tag{4}$$

$$\varphi_z = \mathcal{T}_\hbar(z)\varphi_0 \tag{5}$$

where $\mathcal{T}_\hbar(z)$ is the Weyl operator

$$\mathcal{T}_\hbar(z) = \exp\left(\frac{i}{\hbar}(p \cdot x - q \cdot \hbar D_x)\right) \tag{6}$$

where $D_x = -i\frac{\partial}{\partial x}$ and $z = (q, p) \in \mathbb{R}^d \times \mathbb{R}^d$.

We have $\|\varphi_z\| = 1$, for the L^2 norm. If the initial state f is a coherent state φ_z, a natural ansatz to check asymptotic solutions modulo $O(\hbar^{(N+1)/2})$ for equation (3), for some $N \in \mathbb{N}$, is the following

$$\psi_z^{(N)}(t,x) = \mathrm{e}^{i\frac{\delta_t}{\hbar}} \sum_{0\leq j\leq N} \hbar^{j/2}\pi_j(t, \frac{x-q_t}{\sqrt{\hbar}})\varphi_{z_t}^{\Gamma_t}(x) \tag{7}$$

where $z_t = (q_t, p_t)$ is the classical path in the phase space $\mathbb{R}^{2d}$ such that $z_{t_0} = z$ and satisfying

$$\begin{cases} \dot{q}_t = \dfrac{\partial H}{\partial p}(t, q_t, p_t) \\ \dot{p}_t = -\dfrac{\partial H}{\partial p}(t, q_t, p_t), \quad q_{t_0} = q,\ p_{t_0} = p \end{cases} \tag{8}$$

and

$$\varphi_{z_t}^{\Gamma_t} = \mathcal{T}_\hbar(z_t)\varphi^{\Gamma_t}. \tag{9}$$

φ^{Γ_t} is the Gaussian state:

$$\varphi^{\Gamma_t}(x) = (\pi\hbar)^{-d/4} a(t) \exp\left(\frac{i}{2\hbar}\Gamma_t x.x\right). \tag{10}$$

Γ_t is a family of $d \times d$ symmetric complex matrices with positive non-degenerate imaginary part, δ_t is a real function, $a(t)$ is a complex function, $\pi_j(t,x)$ is a polynomial in x (of degree $\leq 3j$) with time dependent coefficients.

More precisely Γ_t is given by the Jacobi stability matrix of the Hamiltonian flow $z \mapsto z_t$. If we denote

$$A_t = \frac{\partial q_t}{\partial q}, \quad B_t = \frac{\partial p_t}{\partial q}, \quad C_t = \frac{\partial q_t}{\partial p}, \quad D_t = \frac{\partial p_t}{\partial p} \tag{11}$$

then we have

$$\Gamma_t = (C_t + iD_t)(A_t + iB_t)^{-1}, \ \ \Gamma_{t_0} = \mathbb{1}, \tag{12}$$

$$\delta_t = \int_{t_0}^{t} (p_s \cdot \dot{q}_s - H(s, z_s))\, ds - \frac{q_t p_t - q_{t_0} p_{t_0}}{2}, \tag{13}$$

$$a(t) = [\det(A_t + iB_t)]^{-1/2}, \tag{14}$$

where the complex square root is computed by continuity from $t = t_0$.

In this paper we want to discuss conditions on the Hamiltonian $H(t, X)$ ($X = (x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d$) so that $\psi_z^{(N)}(t,x)$ is an approximate solution with an accurate control of the remainder term in $\hbar$, t and N, which is defined by

$$R_z^{(N)}(t,x) = i\hbar\frac{\partial}{\partial t}\psi_z^{(N)}(t,x) - \widehat{H}(t)\psi_z^{(N)}(t,x). \tag{15}$$

The first following result is rather crude and holds for finite times t and N fixed. We shall improve later this result.

Theorem 0.1. — *Assume that $H(t,X)$ is continuous in time for t in the interval $I_T = [t_0 - T, t_0 + T]$, C^∞ in $X \in \mathbb{R}^{2d}$ and real.*

Assume that the solution z_t of the Hamilton system (8) exists for $t \in I_T$.

Assume that $H(t,X)$ satisfies one of the following global estimate in X

1. $H(t,x,\xi) = \frac{\xi^2}{2} + V(t,x)$ *and there exists $\mu \in \mathbb{R}$ and, for every multiindex α there exists C_α, such that*

$$|\partial_x{}^\alpha V(t,x)| \leq C_\alpha \mathrm{e}^{\mu x^2}; \tag{16}$$

2. *for every multiindex α there exist $C_\alpha > 0$ and $M_{|\alpha|} \in \mathbb{R}$ such that*

$$|\partial_X^\alpha H(t,X)| \leq C_\alpha (1 + |X|)^{M_{|\alpha|}}, \quad \text{for } t \in I_T \text{ and } X \in \mathbb{R}^{2d}.$$

Then for every $N \in \mathbb{N}$, there exists $C(I_T, z, N) < +\infty$ such that we have, for the L^2-norm in $\mathbb{R}^d_x$,

$$\sup_{t \in I_T} \|R_Z^{(N)}(t, \bullet)\| \leq C(I_T, z, N)\hbar^{\frac{N+3}{2}}, \quad \forall \hbar \in]0, \hbar_0],\ \hbar_0 > 0. \tag{17}$$

Moreover, if for every $t_0 \in \mathbb{R}$, the equation (3) has a unique solution $\psi(t) = U(t,t_0)f$ where $U(t,s)$ is family of unitary operators in $L^2\mathbb{R}^d)$ such that $U(t,s) = U(s,t)$, then we have, for every $t \in I_T$,

$$\|U(t,t_0)\varphi_z - \psi_z^{(N)}(t)\| \leq |t - t_0| C(I_T, z, N)\hbar^{\frac{N+1}{2}}. \tag{18}$$

In particular this condition is satisfied if H is time independent.

The first mathematical proof of results like this, for the Schrödinger Hamiltonian $\xi^2 + V(x)$, is due to G. Hagedorn [**18**].

There exist many results about constructions of asymptotic solutions for partial differential equations, in particular in the high frequency regime. In [**35**] J. Ralston constructs Gaussian beams for hyperbolic systems which is very close to construction of coherent states. This kind of construction is an alternative to the very well known WKB method and its modern version: the Fourier integral operator theory. It seems that coherent states approach is more elementary and easier to use to control estimates. In [**8**] the authors have extended Hagedorn's results [**18**] to more general Hamiltonians proving in particular that the remainder term can be estimated by $\rho(I_T, z, N) \leq K(z,N)\mathrm{e}^{\gamma T}$ with some $K(z,N) > 0$ and $\gamma > 0$ is related with Lyapounov exponents of the classical system.

It is well known that the main difficulty of real WKB methods comes from the occurring of caustics (the WKB approximation blows up at finite times). To get rid of the caustics we can replace the real phases of the WKB method by complex valued phases. This point of view is worked out for example in [**41**] (FBI transform theory, see also [**29**]). The coherent state approach is not far from FBI transform and can be seen as a particular case of it, but it seems more explicit, and more closely related with the physical intuition.

One of our main goal in this paper is to give alternative proofs of Hagedorn-Joye results [**20**] concerning large N and large time behaviour of the remainder term $R_N(t,x)$. Moreover our proofs are valid for large classes of smooth classical Hamiltonians. Our method was sketched in [**38**]. Here we shall give detailed proofs of the estimates announced in [**38**]. We shall also consider the short range scattering case, giving uniform estimates in time for $U_t\varphi_z$, with short range potential $V(x) = \mathcal{O}(|x|^{-\rho)}$ with $\rho > 1$. We shall show, through several applications, efficiency of coherent states: propagation of analytic frequency set, construction of quasi-modes, spectral asymptotics for bounded states and semi-classical estimates for the scattering operator.

1. Coherent states and quadratic Hamiltonians

1.1. Gaussians Coherent States. — We shall see in the next section that the core of our method to build asymptotic solutions of the Schrödinger equation, (3) for $f = \varphi_z$, it to rescale the problem by putting $\hbar$ at the scale 1 such that we get a regular perturbation problem, for a time dependent quadratic Hamiltonian.

For quadratic Hamiltonians, using the dilation operator $\Lambda_\hbar f(x) = \hbar^{-d/4} f(\hbar^{-1/2}x)$, it is enough to consider the case $\hbar = 1$. We shall denote g_z the coherent state φ_z for $\hbar = 1$ ($\varphi_z = \Lambda_\hbar g_{\hbar^{-1/2}z}$).

For every $u \in L^2(\mathbb{R}^n)$ we have the following consequence of the Plancherel formula for the Fourier transform.

$$\int_{\mathbb{R}^d} |u(x)|^2\, dx = (2\pi)^{-d} \int_{\mathbb{R}^{2d}} |\langle u, g_z\rangle|^2\, dz. \tag{19}$$

Let $\hat{L}$ be some continuous linear operator from $\mathcal{S}(\mathbb{R}^d)$ into $\mathcal{S}'(\mathbb{R}^d)$ and K_L its Schwartz distribution kernel. By an easy computation, we get the following representation formula for K_L:

$$K_L(x,y) = (2\pi)^{-d} \int_{\mathbb{R}^{2d}} (\hat{L} g_z)(x)\overline{g_z(y)}\, dz. \tag{20}$$

In other words we have the following continuous resolution of the identity

$$\delta(x-y) = (2\pi)^{-n} \int_{\mathbb{R}^{2d}} g_z(x)\overline{g_z(y)}\, dz.$$

Let us denote by $\mathcal{O}^m$, $m \in \mathbb{R}$, the space of smooth (classical) obervables L (usually called symbols) such that for every $\gamma \in \mathbb{N}^{2d}$, there exists C_γ such that,

$$|\partial_X^\gamma L(X)| \le C_\gamma < X >^m, \quad \forall X \in \mathcal{Z}.$$

So if $L \in \mathcal{O}^m$, we can define the Weyl quantization of L, $\hat{L}u(x) = Op_\hbar^w[L]u(x)$ where

$$Op_\hbar^w[L]u(x) = (2\pi\hbar)^{-d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \exp\{i\hbar^{-1}(x-y)\cdot\xi\} L\left(\frac{x+y}{2}, \xi\right) u(y)\, dy\, d\xi \tag{21}$$