On Fundamental Solution of Schrödinger equations

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We consider **smoothness and boundedness** of FDS of n dim. Schrödinger Eqn.

$$i\frac{\partial u}{\partial t} = H(t)u(t) \tag{1}$$

$$H(t) = \sum_{j=1}^{d} \left(\frac{1}{i}\frac{\partial}{\partial x_j} - A_j(t,x)\right)^2 u + V(t,x)u(t).$$

Electric and magnetic fields are given by

$$F(t,x) = -\partial_t A(t,x) - \partial_x V(t,x),$$
$$B_{jk}(t,x) = (\partial A_k/\partial x_j - \partial A_j/\partial x_k)(t,x).$$

We review some known results and add some new result. $\langle x\rangle = (1+|x|^2)^{1/2}$. We almost always assume the following

Assumption 1. (1) $A,\ \partial_t A,\ V \in C^\infty(x)$ *and* $\partial_x^a A,\ \partial_x^\alpha \partial_t A,\ \partial_x^\alpha V \in C^0(t,x)$ *for all* α.

(2) $\forall \alpha \neq 0$, $\exists \varepsilon_\alpha > 0$ *and* $\exists C_\alpha > 0$ *such that*

$$|\partial_x^\alpha B(t,x)| \le C_\alpha \langle x\rangle^{-1-\varepsilon_\alpha}, \tag{2}$$
$$|\partial_x^\alpha A(t,x)| + |\partial_x^\alpha F(t,x)| \le C_\alpha. \tag{3}$$

Assumption 1 $\Rightarrow \exists_1$ unitary propagator $\{U(t,s)\}$. Solutions with $u(s) = \varphi \in L^2(\mathbf{R}^n)$ are given by

$$u(t) = U(t,s)\varphi.$$

FDS is the distribution kernel of $U(t,s)$:

$$u(t,x) = U(t,s)\varphi(x) = \int E(t,s,x,y)\varphi(y)dy.$$

For the free Schrödinger Eqn

$$E(t,s,x,y) = \frac{e^{\frac{\mp i\pi n}{4}} e^{i(x-y)^2/2(t-s)}}{(2\pi|t-s|)^{n/2}}.$$

Classical Hamiltonian and Lagrangian are

$$\begin{aligned} H(t,x,p) = & \ (p - A(t,x))^2/2 + V(t,x), \\ L(t,q,v) = & \ \ v^2/2 + vA(t,q) - V(t,q). \end{aligned}$$

$(x(t,s,y,k), p(t,s,y,k))$ are solutions of the IVP for Hamilton's equations

$$\begin{aligned} \dot{x}(t) = \partial_p H(t,x,p), \quad & \dot{p}(t) = -\partial_x H(t,x,p); \\ x(s) = y, \quad & p(s) = k \end{aligned} \tag{4}$$

We begin with **short time results** due to D. Fujiwara (1980, $A = 0$) and K. Yajima (1991).

Lemma 2. *Assume* Assumption 1*. Then,* $\exists T > 0$ *such that* $\forall x, y \in \mathbf{R}^d$ *and* $\forall t, s \in \mathbf{R}$ *with* $|t-s| < T$, $\exists_1$ *solutions of Hamilton Eqn's* (4) *such that*

$$x(t) = x, \quad x(s) = y.$$

The action integral of this path

$$S(t,s,x,y) = \int_s^t L(r, x(r), \dot{x}(r))dr$$

is $C^\infty(x,y)$*;* $\partial_x^\alpha \partial_y^b S \in C^1(t,s,x,y)$*; for* $|\alpha+\beta| \geq 2$

$$\left| \partial_x^\alpha \partial_y^\beta \left(S(t,s,x,y) - \frac{(x-y)^2}{2(t-s)} \right) \right| \leq C_{\alpha\beta}.$$

Theorem 3. *Assume* Assumption 1*. Then, FDS is given for* $0 < \pm(t-s) < T$ *by*

$$E(t,s,x,y) = \frac{e^{\frac{\mp i\pi n}{4}} e^{iS(t,s,x,y)} a(t,s,x,y)}{(2\pi|t-s|)^{n/2}},$$

where $a \in C^\infty(x,y)$, $\partial_x^\alpha \partial_y^\beta a \in C^1(t,s,x,y)$ *and*

$$|\partial_x^\alpha \partial_y^\beta a(t,s,x,y)| \leq C_{\alpha\beta}, \quad |\alpha| + |\beta| \geq 0.$$

Theorem 3 **is sharp and results do not extend beyond a short time under the conditions**. From singularities point of view, this can be seen from Mehler's formula for the harmonic oscillator ($A = 0$ and $V(x) = x^2/2$): If A and V are t independent we write

$$E(t-s, x, y) = E(t, s, x, y).$$

Then, FDS of the harmonic oscillator is given for $m < t/\pi < m+1$, $m \in \mathbf{Z}$, by

$$E(t, x, y) = \frac{e^{-in\pi\mu(t)/2}}{|2\pi \sin t|^{n/2}} e^{(i/\sin t)(\cos t(x^2+y^2)/2 - x\cdot y)}$$

where $\mu(t) = m + \frac{1}{2}$ and

$$E(m\pi, x, y) = e^{-im\pi/2}\delta(x - (-1)^m y).$$

FDS is smooth and bounded for non-resonant times $t \in \mathrm{R} \setminus \pi\mathbf{Z}$ but singularities recur at resonant times $\pi\mathbf{Z}$. We will show toward the end of this talk that **FDS can increase as $|x| \to \infty$ for some fixed t and s** .

Situation is the same for linearly increasing magnetic fields A. Consider non-vanishing constant magnetic force in two dimensions: $V = 0$ and $A = (x_2, -x_1)$ ($\Rightarrow B = 2$). Let

$$T(t) = e^{-iLt}, \quad L = (x_1 p_2 - x_2 p_1) = \frac{1}{i}\frac{\partial}{\partial\theta}$$

and $v(t,x) = T(t)u(t,x) = u(t, R(t)x)$, $R(t)$ being the rotation by angle t. Then

$$i\frac{\partial u}{\partial t} = \frac{1}{2}(p - A)^2 u + V(t,x)u$$
$$\Leftrightarrow i\frac{\partial v}{\partial t} = -\frac{1}{2}\Delta v + \frac{1}{2}x^2 v + V(t, R(t)^{-1})v.$$

It follows for FDSs that

$$E_u(t,s,x,y) = E_v(t,s,R(t)^{-1}x, R(s)^{-1}y).$$

In particular, if $V = 0$, then

$$E(t,x,y) = \frac{-i\pi\mu(t)}{|2\pi\mathrm{sin}t|} e^{(i/\mathrm{sin}t)(\mathrm{cos}t(x^2+y^2)/2 - x\cdot R(t)y)}$$

and

$$E(m\pi, x, y) = e^{-im\pi/2}\delta(x-y).$$

If $A = 0$ and $V(t,x) = o(x^2)$, short time results extend to **any finite time**, $a \to 1$ and $\partial_x^\alpha \partial_y^\beta S$ have limits as $x^2 + y^2 \to \infty$ (Yajima 96, 01):

Definition 4. *V is subquadratic at infinity if*

$$\lim_{|x|\to\infty} \sup_{t\in\mathbf{R}} |\partial_x^2 V(t,x)| = 0.$$
$$|\partial_x^\alpha V(t,x)| \le C_\alpha, \quad |\alpha| \ge 3.$$

Lemma 5. *Let $A = 0$ and V be subquadratic at infinity. Let $T > 0$ be fixed arbitrarily. Then:* (1) $\exists R \ge 0$ *such that*

$$\forall x, y \in \mathbf{R}^d \text{ with } x^2 + y^2 \ge R^2 \text{ and}$$
$$\forall t, s \in \mathbf{R} \text{ with } |t-s| < T,$$

$\exists$ *a unique path of* (4) *such that*

$$x(t) = x \quad \text{and} \quad x(s) = y.$$

For $|\alpha + \beta| \ge 2$, the action of this path satisfies

$$\left| \partial_x^\alpha \partial_y^\beta \left(S(t,s,x,y) - \frac{(x-y)^2}{2(t-s)} \right) \right| \to 0;$$

as $x^2 + y^2 \to \infty$ uniformly for $0 < |t-s| < T$.

Theorem 6. *Let $A = 0$ and V be subquadratic at infinity. Let $T > 0$ be fixed arbitrarily. Then: For $0 < \pm(t-s) < T$,*

$$E(t,s,x,y) = \frac{e^{\frac{\mp i\pi n}{4}} e^{i\tilde{S}(t,s,x,y)} a(t,s,x,y)}{(2\pi|t-s|)^{n/2}},$$

where
(a) $\tilde{S}, a \in C^\infty(x,y), \quad \partial_x^\alpha \partial_y^\beta \tilde{S}, a \in C^\infty(t,s,x,y)$.
(b)$S(t,s,x,y) = \tilde{S}(t,s,x,y)$ *for* $x^2 + y^2 \geq R^2$.
(c) $\forall \alpha, \beta$, *as* $x^2 + y^2 \to \infty$

$$\sup_{0<|t-s|<T} |\partial_x^\alpha \partial_y^\beta (a(t,s,x,y) - 1)| = 0$$

Remark 7. Smoothness *of FDS is known for more general quadratic or subquadratic potentials* **with magnetic fields and for Schrödinger equations on the manifolds** *under the non-trapping condition of backward Hamilton trajectories of $\sum g_{ij}(x)p_ip_j$ starting from y. Results are obtained via* **micro-local propagation of singularities** *theorems. For more information, we refer to recent papers by S. Doi (04) and Martinez, Nakamura and Sordoni (07).*

Results on boundedness of FDS are scarce except when $V(x)$ decays at infinity and $A = 0$. Then, **dispersive estimates**

$$\sup_{x,y} |E_c(t,x,y)| \leq C|t|^{-n/2} \tag{5}$$

are studied for the (spectrally) continuous part of FDS. For more information we refer to W. Schlag's survey article (07). For $A \neq 0$, (5) is not known.

If $V \geq C|x|^{2+\varepsilon}$, then FDS should be non-smooth and unbounded. But, results are only for smoothness in one dimension.

Theorem 8. *Let $n = 1$ and $V \in C^3$. Assume outside a compact set that V is convex;*

$$|V^{(j)}(x)| \leq C_j \langle x \rangle^{-1} |V^{(j-1)}(x)| \text{ for } j = 1, 2, 3;$$

and $xV'(x) \geq 2cV(x)$ ($\Rightarrow V(x) \geq C|x|^{2c}$) for $\exists c > 1$. Then, $E(t,x,y)$ is nowhere $C^1(t,x,y)$.

Because of this sharp transition, it is interesting to study border line cases $V(t,x) = O(x^2)$. We consider **perturbations of harmonic oscillator by subquadratic** W.

$$V(t,x) = \frac{1}{2}x^2 + W(t,x). \tag{6}$$

Non-resonant behavior of FDS is stable under subquadraic perturbations (Kapitanski, Rodnianski and Yajima (97), Yajima(01)):
Lemma 9. *Assume* (6) *and* $A = 0$*. Let* $m \in \mathbf{Z}$ *and* $\varepsilon > 0$*.* $\exists R \geq 0$ *s.t.* $\forall t, s$ *and* $\forall x, y \in \mathbf{R}^d$ *with*

$$m\pi + \varepsilon < t - s < (m+1)\pi - \varepsilon, \quad x^2 + y^2 \geq R^2,$$

$\exists_1$ *path of Hamilton Eqn.* (4) *such that*

$$x(t) = x \text{ and } x(s) = y.$$

The action integral $S(t,s,x,y)$ *of this path satisfies, for* $|\alpha + \beta| \geq 2$ *and as* $x^2 + y^2 \to \infty$

$$\partial_x^\alpha \partial_y^\beta \left(S(t,s,x,y) - \frac{\cos(t-s)(x^2+y^2) - 2x \cdot y}{2\sin(t-s)} \right)$$
$$\to 0 \text{ uniformly wrt } \varepsilon < t - s - m\pi < \pi - \varepsilon.$$

Using this action as phase function, FDS can be written in the same form as for harmonic oscillator:

Theorem 10. *Let $V = (x^2/2) + W(t,x)$ be as above and $A = 0$. Let $m \in \mathbf{Z}$ and $\varepsilon > 0$. Then, $\forall t, s$ as above,*

$$E(t,s,x,y) = \frac{e^{-in\mu(t-s)\pi} e^{i\tilde{S}(t,s,x,y)} a(t,s,x,y)}{(2\pi|\sin(t-s)|)^{n/2}},$$

(a) $\tilde{S}, a \in C^\infty(x,y)$;
$\partial_x^\alpha \partial_y^\beta \tilde{S}, \partial_x^\alpha \partial_y^\beta a \in C^1(t,s,x,y)$, $\forall \alpha,\ \forall \beta$.

(b) $S(t,s,x,y) = \tilde{S}(t,s,x,y)$ *for* $x^2 + y^2 \geq R^2$;

(c) *For all α and β, uniformly with respect to $m\pi + \varepsilon < t - s < (m+1)\pi - \varepsilon$.*

$$\lim_{x^2+y^2 \to \infty} |\partial_x^\alpha \partial_y^\beta (a(t,s,x,y) - 1)| = 0.$$

What happens at resonant times? We set $s = 0$ and write $E(t,x,y)$ for $E(t,0,x,y)$.

Recurrence of singularities at resonant times $\pi\mathbf{Z}$ persists under sub-linear perturbations (Zelditch(83), Kapitanski, Rodnianski and Yajima (97), Doi(04)). $R^n_* = \mathbf{R}^n \setminus \{0\}$.

Theorem 11. *Let $A = 0$, $V = (1/2)x^2 + W(t,x)$. Suppose*

$$|\partial_x^\alpha W(t,x)| \le C_\alpha \langle x\rangle^{\delta-|\alpha|}, \quad \delta < 1.$$

Then, for $N = 0, 1, \ldots,$

$$\langle x-y\rangle^N |E(m\pi,x,y)| \le C_N \text{ for } |x-y| > 1,$$
$$WF_x E(m\pi,x,y) = \{(-1)^m(y,\xi)\colon \xi \in \mathbf{R}^n_*\}.$$

For linearly increasing perturbations, **singularities can propagate but $E(m\pi,x,y)$ falls off as** $|x| \to \infty$. For example, if $V = (1/2)x^2 + a\langle x\rangle$, then, with $\hat{\xi} = \xi/|\xi|$,

$$WF_x E(m\pi,x,y) = \{(-1)^m(y + 2a\hat{\xi},\xi)\colon \xi \in \mathbf{R}^n_*\},$$
$$\lim_{|x-y|\to\infty} \langle x-y\rangle^N |E(m\pi,x,y)| = 0.$$

However, **superlinear perturbations satisfying a certain sign condition can sweep away singularities and creat growth of FDS at infinity**. Let $\chi \in C_0^\infty(1/4 < |x| < 4)$ be such that

$$\chi(x) = 1 \quad \text{for} \quad 1/2 < |x| < 2.$$

Theorem 12. *Let $A = 0$, $V = (1/2)x^2 + W(t,x)$. Suppose W is subquadratic and*

$$C_1\langle x\rangle^{-\delta} \le \partial_x^2 W(t,x) \le C_2\langle x\rangle^{-\delta}, \qquad 0 < \delta < 1.$$

Then, $E(m\pi, 0, x, y) \in C^\infty(x,y)$. Moreover, for a fixd y, $E(m\pi, 0, x, y) \sim |x|^{n\delta/(1-\delta)}$ in the sense

$$\left(\int_{\mathbf{R}^n} |E(m\pi, 0, x, y)|^2 \chi\left(\frac{x}{R}\right)^2 \frac{dx}{R^n}\right)^{1/2} \sim R^{n\delta/(2-2\delta)}$$

for sufficiently large $R > 0$.

Note that growth rate of $E(m\pi, x, y)$ as $|x| \to \infty$ increases (dereases) when $W(x) = O(|x|^{2-\delta})$ becomes weaker(stronger):

$$\lim_{\delta \uparrow 1} \frac{n\delta}{2(1-\delta)} = \infty \quad \text{and} \quad \lim_{\delta \downarrow 0} \frac{n\delta}{2(1-\delta)} = 0.$$

This is somewhat against intuition and surprizing. But, **this can be understood semi-classically.** Consider the ensemble Γ of classical particles sitting at time 0 at the position $y \in \mathbf{R}^n$ with uniform momentum distribution. This is described by the wave function $\delta(x-y) = E(0,x,y)$ semiclassically. After time $m\pi$, Γ will be mapped by the Hamilton flow to Lagrangian manifold $\{(x(m\pi,y,k), p(m\pi,y,k)) \colon k \in \mathbf{R}\}$. Here we have $p(m\pi,y,k) \sim k$ and $|x(m\pi,y,k)| \sim |k|^{1-\delta}$ as $|k| \to \infty$. It follows semi-classically

$$|E(m\pi,x,y)| \sim \left|\det\left(\frac{\partial x}{\partial p}\right)\right|^{-1/2} \sim |k|^{n\delta/2} \sim |x|^{n\delta/(2-2\delta)}$$

as $|x| \to \infty$.

Notice also that when $\delta \to 0$, then

$$V(x) = \frac{1}{2}x^2 + c\langle x\rangle^{2-\delta} \to x^2/2 + c\langle x\rangle^2$$

and $m\pi$ is non-resonant for the latter and FDS at $t = m\pi$ is smooth and bounded. On the other hand as $\delta \to 1$

$$V(x) = \frac{1}{2}x^2 + c\langle x\rangle^{2-\delta} \to \frac{1}{2}x^2 + c\langle x\rangle.$$

For the latter potential, singularities fill the sphere $|x-y| = 2cm$ and we may naively consider $E(m\pi, x, y) = \infty$ there.

We remark **smoothness properties of FDS both at non-resonant and resonant times have been generalized by S. Doi (04 in CMP)** to more general situations including perturbations of non-isotropic harmonic oscillators by using Egorov type argument.

We emphasize that there still are a lot of things to be understood. In particular:

(1) What happens **for finite time FDS when magnetic fields are present?**

(2) **Is FDS spatially unbounded when V is superquadratic at infinity?** If so, how is it unbounded, locally in space or at infinity? Note that for the free particle in an interval $[0, \pi]$ with Dirichlet condition, the FDS

$$E(t, x, y) = (\pi/2) \sum_{n=1}^{\infty} e^{in^2 t} \sin nx \sin ny$$

is not integrable wrt x for almost all t, y.

(3) **What happens in multi-dimensions when V is superquadratic?**

Proof of the last statement of Theorem 12.

Proof of theorems and their generalizations may be found in the literature mentioned above except the last statement of Theorem 12, viz. the growth of $E(m\pi, 0, x, y)$ as $|x| \to \infty$, which we prove for $m = 1$. We write

$$(x(\pi, 0, y, k), p(\pi, 0, y, k)) = (x(y, k), p(y, k))$$

for solutions of Hamilton Eqn. (4).

Lemma 13. $\exists R > 0$ *such that canonical map*

$$(y,k) \mapsto (x(y,k), p(t,y))$$

has a generating function $\varphi(\xi, y)$ *defined for* $\xi^2 + y^2 \geq R^2$ *such that*

$$(\partial_\xi \varphi)(p(y,k), y) = x(y,k), \;\; (\partial_y \varphi)(p(y,k), k) = k$$

For fixed y, φ *satisfies:*

$$C_1 |\xi|^{1-\delta} \leq |\nabla_\xi \varphi(\xi, y)| \leq C_2 |\xi|^{1-\delta}.$$
$$|\partial_\xi^\alpha \varphi(\xi, y)| \leq C_\alpha, \quad |\alpha| \geq 2.$$

Theorem 14. *By using* $\tilde{\varphi} \in C^\infty(\xi, y)$ *such that* $\tilde{\varphi}(\xi, y) = \varphi(\xi, y)$ *for* $\xi^2 + y^2 \geq R^2$ *and* $a \in C^\infty(\xi, y)$ *such that*

$$\lim_{\xi^2 + y^2 \to \infty} |\partial_\xi^\alpha \partial_y^\beta (a(\xi, y) - 1)| = 0,$$

the FDS $E(x,y) = E(\pi, x, y)$ *may be written*

$$E(x,y) = \frac{-i}{(2\pi)^n} \int e^{ix\xi - i\tilde{\varphi}(\xi, y)} a(\xi, y) d\xi$$

Here and in what follows various integrals should be understood as an oscillatory integrals. Omit y and write φ for $\tilde{\varphi}$. We need estimate

$$\frac{1}{(2\pi R)^n}\int\left|\chi\left(\frac{x}{R}\right)\int e^{i(x\xi-\varphi(\xi))}a(\xi)d\xi\right|^2 dx$$
$$=\iint\widehat{\chi_2}(R(\eta-\xi))e^{i(\varphi(\eta)-\varphi(\xi))}a(\xi)\overline{a(\eta)}d\xi d\eta.$$

Here $\chi_2=\chi^2$. Change variables:

$$\eta=\xi+R^{-1}\zeta$$

and expand $a(\xi+R^{-1}\zeta)$ by Taylor's formula. This produces with $a^{(a)}=\partial^\alpha a$ and etc.

$$=\sum_{|\alpha|\le N}\frac{1}{\alpha!}\frac{(-i)^{|\alpha|}}{R^{n+|\alpha|}}\iint\mathcal{F}(\chi_2^{(\alpha)})(\zeta)$$
$$\times e^{i(\varphi(\xi+R^{-1}\zeta)-\varphi(\xi))}a(\xi)\overline{a^{(\alpha)}(\xi)}d\xi d\zeta \quad (7)$$

plus the remainder which is shown to be $O(R^{-N})$ by integration by parts with respect to the ζ variables.

Writing

$$\varphi(\xi + R^{-1}\zeta) - \varphi(\xi, y) = \frac{\zeta}{R}\nabla\varphi(\xi) + \Psi(\xi, \zeta/R),$$

$$\Psi(\xi, \zeta/R) = \frac{\zeta}{R}\left(\int_0^1 (1-\theta)\frac{\partial^2\varphi}{\partial\xi^2}(\xi + (\theta/R)\zeta)d\theta\right)\frac{\zeta}{R}$$

we then expand the exponential:

$$e^{i(\varphi(\xi+R^{-1}\zeta)-\varphi(\xi))}$$
$$= e^{i(\zeta/R)\nabla\varphi(\xi)}\sum_{m=0}^{N}\frac{(i\Psi)^m}{m!} + R_N(\xi, R^{-1}\zeta)$$

Integartion by parts wrt ζ shows that $R_N(\xi, R^{-1}\zeta)$ produces $O(R^{-N})$ in (7). Thus, we need study

$$\sum_{m,\alpha}\frac{(-i)^{|\alpha|}}{\alpha! R^{n+|\alpha|}}\iint e^{i(\zeta/R)\nabla\varphi(\xi)}\mathcal{F}(\chi_2^{(\alpha)})(\zeta)$$
$$\times\frac{(i\Psi(\xi,\zeta/R))^m}{m!}a(\xi)\overline{a^{(\alpha)}(\xi)}d\zeta d\xi. \quad (8)$$

We further expand $\Psi(\xi, \zeta/R)$ by Taylor's formula

$$\Psi(\xi, \zeta/R) = \sum_{2\le|\alpha|\le N}\frac{(\zeta/R)^\alpha}{\alpha!}\varphi^{(\alpha)}(\xi) + L_N(\xi, \zeta/R)$$

and expand $(i\Psi(\xi,\zeta/R))^m$ in (8) accordingly. Integaration by parts shows terms which contain L_N produce $O(R^{-N})$. When $(i\Psi(\xi,\zeta/R))^m$ is replaced by terms which do not contain L_N, (8) can be explicitly computed and produces

$$\frac{C_{\alpha\beta m}}{R^{n+|\alpha+\beta|}}\int \chi_2^{(\alpha+\beta)}(\nabla\varphi(\xi)/R) \\ \times \varphi^{(\beta_1)}(\xi)\dots\varphi^{(\beta_m)}(\xi)a(\xi)\overline{a^{(\alpha)}(\xi)}d\xi.$$

Thus, as $R\to\infty$, main term in (8) is given by the term with $\alpha=0$ and $m=0$:

$$M(R)=\frac{1}{R^n}\int \chi^2(\nabla\varphi(\xi)/R)|a(\xi)|^2d\xi.$$

Since $a(\xi)\to 1$ as $|\xi|\to\infty$ and $|\nabla\varphi(\xi)|\sim|\xi|^{1-\delta}$ for large $|\xi|$, we have

$$C_R^{n\delta/(1-\delta)}\le M(R)\le C_2R^{n\delta/(1-\delta)},$$

which yields the theorem. $\square$