Dispersion for the Schrödinger Equation

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Warning: Almost every proof is not mathematically valid!!

1.1. Optics

A simplest wave in d-dimensional space can be written in the form

$$\psi(t, \vec{x}) = A\sin(\vec{k}\cdot\vec{x} - \omega t).$$

There are several terminologies.

- Amplitude A
- Angular frequency $\omega = 2\pi f$
- Wave number $\vec{k}$: ***vector*** with direction of light propagation and size $2\pi/\lambda$

This is a solution of "wave equation"

$$\frac{\partial^2}{\partial t^2}\psi(t, \vec{x}) = v^2\frac{\partial^2}{\partial \vec{x}^2}\psi(t, \vec{x}),$$

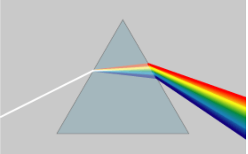
which describes waves of ***constant velocity*** $v = \omega/|\vec{k}|$.

1.1. Optics

The ***index of refraction*** is defined as

$$n := \frac{c}{v_p} = \frac{c}{\omega/|\vec{k}|}.$$

Here ω and $\vec{k}$ are measured in a transparent material.



Dispersion is the phenomenon of optics that

the index of refraction depends on wavelength.

In other words, we have

$$\frac{\omega}{|\vec{k}|} \neq \text{const with respect to } \vec{k},$$

which means the relation between ω and $\vec{k}$ is not like the solutions of the wave equation.

1.2. Dispersion relation

Definition (Dispersion relation)

Dispersion relation is a function $\omega = \omega(\vec{k})$ which describes the relation between angular frequency $\omega \in \mathbb{R}$ and the wave number vector $\vec{k} \in \mathbb{R}^d$.

Many physics can be described by language of waves and dispersion relations.

Example.

Cauchy's formula: dispersion relation of light in transparent materials.

ordinary wave:	$\omega = v\lvert\vec{k}\rvert$
advection:	$\omega = \vec{v} \cdot \vec{k}$
heat distribution:	$\omega = i\alpha\lvert\vec{k}\rvert^2$
quantum mechanics:	$\hbar\omega = \frac{\lvert\hbar\vec{k}\rvert^2}{2m}$

1.2. Dispersion relation

With a dispersion relation, we can think about two different velocities:

$$v_p := \frac{\omega}{|\vec{k}|}, \qquad \vec{v}_g := \nabla_{\vec{k}}\omega.$$

The former is called ***phase velocity*** and the latter is called ***group velocity***.

1.3. Quantization

Then, we will see how each dispersion relation generates a governing equation, by ***quantization***.

Definition (My own definition of "wave")

A ***wave*** is an element of the vector space of functions with basis containing functions of the form:

$$\psi_{\omega,\vec{k}}(t,\vec{x}) = e^{i(\vec{k}\cdot\vec{x}-\omega t)}, \qquad \omega \in \mathbb{R}, \vec{k} \in \mathbb{R}^d.$$

By taking imaginary part, we can see familiar expression for waves: $\sin(\vec{k}\cdot\vec{x}-\omega t)$.

With a specific dispersion relation $\omega = \omega(\vec{k})$, we can restrict the space of "waves" in such a way that the basis only contains

$$\psi_{\omega(\vec{k}),\vec{k}}(t,\vec{x}) = e^{i(\vec{k}\cdot\vec{x}-\omega(\vec{k})t)}, \qquad \vec{k} \in \mathbb{R}^d.$$

1.3. Quantization

Let

$$\psi(t,\vec{x}) = \sum A(\vec{k})e^{i(\vec{k}\cdot\vec{x}-\omega(\vec{k})t)}$$

be a wave satisfying a dispersion relation $\omega = \omega(\vec{k})$. Then,

$$\omega\psi(t,\vec{x}) = i\partial_t\psi(t,\vec{x}), \qquad \vec{k}\psi(t,\vec{x}) = -i\nabla_{\vec{x}}\psi(t,\vec{x}).$$

By changing the classical quantities to differential operators

$$\begin{aligned} \omega &\mapsto i\partial_t, \\ \vec{k} &\mapsto -i\nabla_{\vec{x}}, \\ |\vec{k}|^2 &\mapsto (-i\nabla_{\vec{x}})\cdot(-i\nabla_{\vec{x}}) =: -\Delta_{\vec{x}}, \end{aligned}$$

we get a partial differential equation from the dispersion relation, whose solutions are waves satisfying the dispersion relation. Let me give an example.

1.3. Quantization

Example. (Schrödinger equation)

The energy conservation can be written in

$$E = \frac{|\vec{p}|^2}{2m} + V.$$

According to de Broglie's relation

$$E = \hbar\omega, \qquad \vec{p} = \hbar\vec{k},$$

we get a dispersion relation

$$\hbar\omega = \frac{|\hbar\vec{k}|^2}{2m} + V$$

If $\psi(t, \vec{x})$ is a wave function satisfying the above dispersion relation, then ψ should be a solution of

$$i\hbar\partial_t\psi(t, \vec{x}) = -\frac{\hbar^2}{2m}\Delta_{\vec{x}}\psi(t, \vec{x}) + V(t, \vec{x})\psi(t, \vec{x}).$$

This is the famous Schrödinger equation.

1.4. Dispersive equation

The term “dispersive” in PDE is little different from optics.

We say a PDE is “dispersive” if the solutions of different wavelengths propagate at different group velocities so that the support of the solution spreads out in space as time flows; the dispersion relation is not linear.

Example.

wave eqn:	$\omega = v\|\vec{k}\|$	$\partial_t^2 - v^2\Delta_{\vec{x}} = 0$	dispersive for $d > 1$
advection eqn:	$\omega = \vec{v} \cdot k$	$\partial_t + \vec{v} \cdot \nabla_{\vec{x}} = 0$	not dispersive
heat eqn:	$\omega = i\alpha\|\vec{k}\|^2$	$\partial_t + \alpha\Delta_{\vec{x}} = 0$	dispersive
Schrödinger's eqn:	$\hbar\omega = \frac{\|\hbar\vec{k}\|^2}{2m}$	$i\hbar\partial_t + \frac{\hbar^2}{2m}\Delta_{\vec{x}} = 0$	dispersive

There are several ways to capture the property, and the most elementary one is to find ***dispersive estimate***.

1.4. Dispersive equation

The objective of this seminar is to prove:

Theorem (Dispersive estimate of Schrödinger operator)

Let $u\colon \mathbb{R}^{1+d} \to \mathbb{C}$ *be the "nice" solution of the initial value problem*

$$\begin{cases} i\partial_t u(t,x) + \Delta u(t,x) = 0, & t > 0,\ x \in \mathbb{R}^d \\ u(0,x) = u_0(x), & t = 0,\ x \in \mathbb{R}^d. \end{cases} \tag{1}$$

Then, there is a constant C_d *depending on* d *such that for* $t > 0$

$$\sup_x |u(t,x)| \le C_d \cdot t^{-\frac{d}{2}} \int |u_0(x)|\, dx.$$

Note that this estimate implies a decay of the solution:

$$\sup_x |u(t,x)| \to 0 \qquad \text{as} \qquad t \to \infty.$$

1.4. Dispersive equation

The following is well-known.

Lemma (Probability conservation)

Let u be "nice" solution of (1). Then, for all $t \in \mathbb{R}$,

$$\int |u(t,x)|^2 \, dx = \int |u_0(x)|^2 \, dx.$$

The following theorem illustrates the mechanism of how the dispersive estimate proves the dispersiveness:

Corollary

Let $S(t) := \mu(\{x \in \mathbb{R}^d : u(t,x) \neq 0\})$ be the area of domain where u does not vanish. Then,

$$S(t) \to \infty \qquad \text{as} \qquad t \to \infty.$$

Proof. Since

$$\int |u_0(x)|^2 \, dx = \int |u(t,x)|^2 \, dx \leq S(t) \times \sup_x |u(t,x)|^2,$$

we get

$$S(t) \geq \frac{\int |u_0(x)|^2 \, dx}{\sup_x |u(t,x)|^2} \to \infty.$$

2.1. Fourier transform

We will say a function is ***nice*** if the function satisfies all conditions needed in the proofs.

Definition (Fourier transform)

Let $f : \mathbb{R}^d \to \mathbb{C}$ be a "nice" function. The ***Fourier transform*** of f is

$$\widehat{f}(\xi) := \frac{1}{\sqrt{2\pi}^d} \int f(x) e^{-ix\cdot\xi}\, dx.$$

We will use another vector variable ξ for the wave number instead of $k = p/\hbar$.

The constant is not important, so do not be pedantic. In Fourier analysis, we can show that $\pi = \frac{1}{2}$.

2.1. Fourier transform

We will not prove the following:

Theorem (Fourier inversion formula)

Let $f : \mathbb{R}^d \to \mathbb{C}$ be a "nice" function. Then,

$$f(x) = \frac{1}{\sqrt{2\pi}^d} \int \widehat{f}(\xi) e^{ix\cdot\xi} \, d\xi.$$

Fourier transform is a kind of basis change from x to ξ, while the inverse Fourier transform is from ξ to x.

It is a central problem in Fourier analysis to find some conditions allowing the inversion theorem to hold.

In most of applications including our problem, the inversion is always possible.

2.2. Supplementary definitions

Definition (Dirac's delta function)

The Dirac δ fuction is a map from the space of nice functions to a real number defined by

$$\delta[f] = f(0).$$

In other words, δ is the evaluation at 0.

The following notation is frequently used:

$$\delta[f] = \langle \delta, f \rangle = \int \delta(x) f(x)\, dx.$$

In this sense, it is convenient to consider $\delta(x)$ as a "function" of x such that

$$\delta(x) = \begin{cases} \infty & , x = 0 \\ 0 & , x \neq 0 \end{cases}, \qquad \int \delta(x)\, dx = 1$$

since these conditions give

$$\int \delta(x) f(x)\, dx = \int \delta(x) f(0)\, dx = f(0) \int \delta(x)\, dx = f(0)$$

although it is not a function mathematically, but a "generalized" function.

2.2. Supplementary definitions

There is a very good binary operation in studying Fourier analysis, the convolution.

Definition (Convolution)

Let $f, g \colon \mathbb{R}^d \to \mathbb{C}$ be "nice" functions. The ***convolution*** is a binary operation defined by

$$f * g(x) := \int f(x-y)g(y)\,dy.$$

We can show $f * g = g * f$ by change of variable.

The following theorem is not rigorous, but believe me:

Theorem

The δ function is the identity element with respect to convolution.

Pseudo-Proof.

$$\delta * f(x) = \int f(x-y)\delta(y)\,dy = f(x-0) = f(x).$$

□

2.3. Properties

We will give three useful properties of Fourier transform.

Proposition (1)

Let $f : \mathbb{R}^d \to \mathbb{C}$ be a "nice" function. Then,

$$\widehat{xf}(\xi) = i\nabla_\xi \widehat{f}(\xi), \qquad \widehat{\nabla_x f}(\xi) = i\xi \widehat{f}(\xi).$$

Proof.

$$\begin{aligned}\widehat{xf}(\xi) &= \frac{1}{\sqrt{2\pi}^d} \int f(x)[xe^{-ix\cdot\xi}]\,dx \\ &= \frac{1}{\sqrt{2\pi}^d} \int f(x)[i\nabla_\xi e^{-ix\cdot\xi}]\,dx \\ &= \frac{1}{\sqrt{2\pi}^d} i\nabla_\xi \int f(x)e^{-ix\cdot\xi}\,dx \\ &= i\nabla_\xi \widehat{f}(\xi)\end{aligned}$$

The other is same. □

2.3. Properties

Proposition (2)

Let $f, g \colon \mathbb{R}^d \to \mathbb{C}$ be "nice" functions. Then,

$$\frac{1}{\sqrt{2\pi}^d}\widehat{f * g} = \widehat{f}\,\widehat{g}, \qquad \frac{1}{\sqrt{2\pi}^d}\widehat{fg} = \widehat{f} * \widehat{g}.$$

Proof.

$$\begin{aligned}
\widehat{f * g}(\xi) &= \frac{1}{\sqrt{2\pi}^d}\int \left[\int f(x-y)g(y)\,dy\right] e^{-ix\cdot\xi}\,dx \\
&= \frac{1}{\sqrt{2\pi}^d}\int g(y)\left[\int f(x-y)e^{-ix\cdot\xi}\,dx\right] dy \\
&= \frac{1}{\sqrt{2\pi}^d}\int g(y)\left[\int f(x)e^{-i(x+y)\cdot\xi}\,dx\right] dy \\
&= \frac{1}{\sqrt{2\pi}^d}\left[\int f(x)e^{-ix\cdot\xi}\,dx\right]\left[\int g(y)e^{-iy\cdot\xi}\,dy\right] \\
&= \sqrt{2\pi}^d\,\widehat{f}(\xi)\widehat{g}(\xi).
\end{aligned}$$

The other is from the inversion. □

2.3. Properties

Proposition (3)

Let $f, g\colon \mathbb{R}^d \to \mathbb{C}$ be "nice" functions.

$$\nabla_x(f * g) = (\nabla_x f) * g = f * (\nabla_x g).$$

Proof.

$$\begin{aligned}\nabla_x(f * g)(x) &= \nabla_x \int f(x-y)g(y)\,dy \\ &= \int [\nabla_x f(x-y)]g(y)\,dy \\ &= (\nabla_x f) * g(x).\end{aligned}$$

The second equality is due to the commutativity. □

3.1. Fundamental solution

Consider our initial value problem:

$$\begin{cases} i\partial_t u(t,x) + \Delta u(t,x) = 0, & t > 0 \\ u(0,x) = u_0(x), & t = 0. \end{cases} \tag{1}$$

We are going to assume the existence and uniquness of solutions.

Definition

The ***fundamental solution*** of this problem is the solution of

$$\begin{cases} i\partial_t K(t,x) + \Delta K(t,x) = 0, & t > 0 \\ K(0,x) = \delta(x), & t = 0, \end{cases} \tag{2}$$

in which the initial data u_0 is changed into δ.

3.1. Fundamental solution

The purpose of finding K is the convolution $K(t,x) *_x u_0(x)$ with respect to x is the desired solution:

Theorem

Let K be the fundamental solution; the solution of (2). Then, the convolution $K(t,x) * u_0(x)$ in x-space is the solution of (1).

Proof.

$$[i\partial_t + \Delta](K * u_0) = ([i\partial_t + \Delta]K) * u_0 = 0 * u_0 = 0,$$
$$(K * u_0)(0,x) = K(0,x) * u_0(x) = \delta(x) * u_0(x) = u_0(x).$$

□

In physics, the kernel K is called ***propagator*** since its convolution with the initial solution is same with the solution at specific time t.

3.2. Computation of fundamental solution (1)

The basic idea is Fourier transform. By taking Fourier transform for (2)

$$\begin{cases} i\partial_t K(t,x) + \Delta K(t,x) = 0, & t > 0 \\ K(0,x) = \delta(x), & t = 0, \end{cases}$$

we have

$$\begin{cases} i\partial_t \widehat{K} - |\xi|^2 \widehat{K} = 0, & t > 0 \\ \widehat{K}(0,\xi) = \widehat{\delta}(\xi), & t = 0. \end{cases}$$

It is an ODE, so we can find the solution

$$\widehat{K}(t,\xi) = C(\xi) e^{-it|\xi|^2},$$

where

$$C(\xi) = \widehat{K}(0,\xi) = \widehat{\delta}(\xi) \equiv \frac{1}{\sqrt{2\pi}^d}.$$

Therefore,

$$\boxed{\widehat{K}(t,\xi) = \frac{1}{\sqrt{2\pi}^d} e^{-it|\xi|^2}.}$$

Note that this is the complex Gaussian, a very special function!

3.2. Computation of fundamental solution (1)

With

$$\widehat{K}(t,\xi) = \frac{1}{\sqrt{2\pi}^d} e^{-it|\xi|^2},$$

differentiating before taking inverse transform,

$$\nabla_\xi \widehat{K} = -2it\xi\widehat{K}.$$

By the inversion formula, we get the ODE

$$xK = -2it\nabla_x K,$$

and its solution

$$\boxed{K(t,x) = C(t)e^{i\frac{|x|^2}{4t}}.}$$

Here,

$$C(t) = K(t,0) = \frac{1}{\sqrt{2\pi}^d}\int \widehat{K}(t,\xi)e^{i\vec{0}\cdot\xi}\,d\xi = \frac{1}{(2\pi)^d}\int e^{-it|\xi|^2}\,d\xi.$$

3.2. Computation of fundamental solution (2)

Since

$$\begin{aligned} C(t) &= \frac{1}{(2\pi)^d} \int e^{-it|\xi|^2}\, d\xi \\ &= \frac{1}{(2\pi)^d} \int \cdots \int e^{-it(\xi_1^2 + \cdots + \xi_d^2)}\, d\xi_1 \cdots d\xi_d \\ &= \left(\frac{1}{2\pi} \int_{\mathbb{R}} e^{-it\xi^2}\, d\xi \right)^d, \end{aligned}$$

we obtain

$$C(t) = \frac{1}{\sqrt{4\pi i t}^{\,d}}$$

by the following theorem:

Theorem

If we let $\sqrt{i} = e^{\frac{1}{4}\pi i}$, then the complex Gaussian is

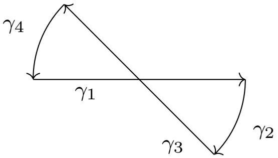
$$\int_{\mathbb{R}} e^{-it\xi^2}\, d\xi = \sqrt{\frac{\pi}{it}}.$$

3.2. Computation of fundamental solution (2)

Proof. By Cauchy's integral theorem,

$$0 = \int_\gamma e^{-itz^2}\,dz = I_1 + I_2 + I_3 + I_4,$$

where $I_i := \int_{\gamma_i} e^{-itz^2}\,dz$ for $i = 1, 2, 3, 4$.



Then, the problem is to show

$$\lim_{R\to\infty} I_1 = \sqrt{\frac{\pi}{it}}.$$

3.2. Computation of fundamental solution (3) - estimate of I_3

Since

$$I_3 = \int_{\gamma_3} e^{-itz^2}\, dz = \int_{\gamma_3} e^{-it(re^{\frac{3}{4}\pi i})^2}\, d(re^{\frac{3}{4}\pi i}) = e^{\frac{3}{4}\pi i} \int_{-R}^{R} e^{-tr^2}\, dr,$$

we have a limit

$$\lim_{R\to\infty} I_3 = e^{\frac{3}{4}\pi i}\sqrt{\frac{\pi}{t}} = -\sqrt{\frac{\pi}{it}}.$$

3.2. Computation of fundamental solution (3) - estimate of I_2 and I_4

By change of variable, we have

$$I_2 = \int_{\gamma_2} e^{-it(Re^{i\theta})^2}\, d(Re^{i\theta}) = \int_0^{-\frac{1}{4}\pi} e^{-itR^2 e^{i2\theta}} Rie^{i\theta}\, d\theta$$

and

$$|I_2| \leq \int_0^{\frac{\pi}{4}} Re^{-tR^2 \sin 2\theta}\, d\theta.$$

We can do for $|I_4|$ similarly, so

$$|I_2| + |I_4| \leq 2\int_0^{\frac{\pi}{4}} Re^{-tR^2 \sin 2\theta}\, d\theta = \int_0^{\frac{\pi}{2}} Re^{-tR^2 \sin \theta}\, d\theta.$$

3.2. Computation of fundamental solution (3) - estimate of I_2 and I_4

If we take $\delta = \frac{2}{\pi} R^{-\frac{3}{2}}$ so that $\sin\delta \geq R^{-\frac{3}{2}}$, then

$$\int_0^{\delta} Re^{-tR^2 \sin\theta}\, d\theta \leq \int_0^{\delta} R\, d\theta = \frac{2}{\pi}\frac{1}{\sqrt{R}} \to 0,$$

$$\int_{\delta}^{\frac{\pi}{2}} Re^{-tR^2 \sin\theta}\, d\theta = \int_{\delta}^{\frac{\pi}{2}} Re^{-tR^2 \sin\delta}\, d\theta \leq \frac{\pi}{2} Re^{-t\sqrt{R}} \to 0$$

as $R \to \infty$; $\lim_{R\to\infty} |I_2| + |I_4| = 0$.

Consequently,

$$\int e^{-it\xi^2}\, d\xi = \lim_{R\to\infty} I_1 = -\lim_{R\to\infty} I_3 = \sqrt{\frac{\pi}{it}},$$

□

3.3. Representation formula

Therefore, we showed

Theorem

The fundamental solution of (1) is

$$K(t,x) = \frac{1}{\sqrt{4\pi i t}^{d}} e^{i\frac{|x|^2}{4t}},$$

where $\sqrt{i} = e^{\frac{1}{4}\pi i}$.

3.3. Representation formula

Theorem

Let u be the solution of (1). Then,

$$u(t,x) = \frac{1}{\sqrt{4\pi i t}^d} \int u_0(y) e^{i\frac{|x-y|^2}{4t}}\, dy.$$

This kind of explicit formula of the solution is called ***representation formula***.

Corollary

$$\sup_x |u(t,x)| \leq (4\pi t)^{-\frac{d}{2}} \int |u_0(x)|\, dx.$$

4.1. Oscillatory integral

This method is applicable for more generalized cases, such as the Airy equation or the fractional Schrödinger equation.

Note that

$$u(t,x) = K(t,x) * u_0(x).$$

By Hölder's inequality,

$$\|u\|_{L^\infty_x} \le \|K(t,-)\|_{L^\infty_x} \|u_0\|_{L^1}.$$

We have seen that

$$\widehat{K}(t,\xi) = \frac{1}{\sqrt{2\pi}^d} e^{-it|\xi|^2}.$$

Fourier transforming,

$$K(t,x) = \frac{1}{(2\pi)^d} \int e^{i(x\cdot\xi - t|\xi|^2)}\, d\xi.$$

We can find this by Fourier transform of complex Gaussian, but we will use another approach.

4.1. Oscillatory integral

Define ***phase*** and ***amplitude*** by

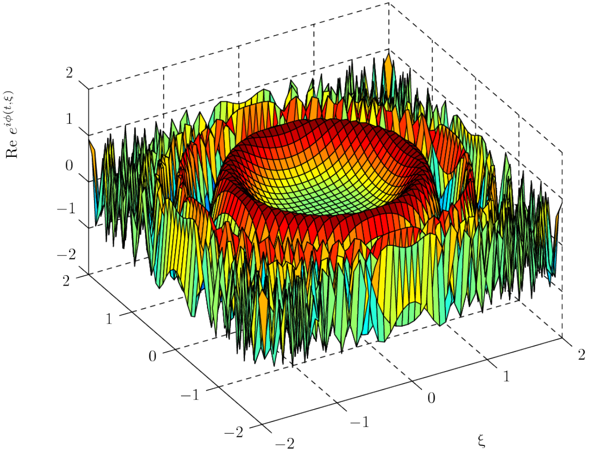
$$\phi(t,x,\xi) := x\cdot\xi - t|\xi|^2, \qquad a(\xi) := \frac{1}{(2\pi)^d}\chi(\xi),$$

so that the limit $(\chi \to 1)$ of the following integral is the fundamental solution:

$$I(t,x) := \int a(\xi)e^{i\phi}\,d\xi.$$

An integral of this form is called ***oscillatory integral***.
We are going to obtain a pointwise estimate of this! $\Rightarrow$ Fix x.

4.2. Principle of non-stationary phase



Where $\nabla_\xi \phi$ is big, the integral $\int a(\xi) e^{i\phi}\, d\xi$ will be cancelled by oscillation.

4.2. Principle of non-stationary phase

Definition

Let ϕ be the phase function defined previously. A ***stationary point*** is a point $\xi^o(t,x)$ at which $\nabla_\xi \phi$ vanishes.

For the Schrödinger equation, we have $\xi^o = \frac{x}{2t}$. The strategy is to divide the integral I as

$$\boxed{I = I_{stat} + I_{nonstat}}$$

We can control each integral by

- I_{stat} : base $\times$ height.
- $I_{nonstat}$: cancellation by fast oscillation.

The wider the region of stationary phase, the bigger I_{stat} is.
The smaller the region of stationary phase, the bigger $I_{nonstat}$ is.

We should find the balance: in fact $t^{-\frac{1}{2}}$ is the boundary of the regions:

$$I_{stat} \simeq (t^{-\frac{1}{2}})^d \times 1 = t^{-\frac{d}{2}}.$$

4.3. Heuristic method: Linearization of the phase

There is a nice heuristic method for finding the boundary (, which we already know it is $t^{-\frac{1}{2}}$).

Let $\xi' = \xi - \xi^o$ be a new variable in the Fourier space. Intuitively, the region of stationary phase is determined as

$$\{\xi' : |\phi(\xi) - \phi(\xi^o)| \lesssim 2\pi\}.$$

Since

$$\begin{aligned} 2\pi &\gtrsim |\phi(\xi) - \phi(\xi^o)| \\ &\simeq |\,\mathrm{Hess}_{\xi^o}(\xi', \xi')| \\ &\simeq t|\xi'|^2, \end{aligned}$$

the region of stationary phase is $|\xi'| \lesssim t^{-\frac{1}{2}}$.

4.4. Repeated integration by parts

So, the rest is to show $|I_{nonstat}| \lesssim t^{-\frac{d}{2}}$, where

$$I_{nonstat} = \int \chi_{|\xi|>t^{-\frac{1}{2}}}(\xi)a(\xi)e^{i\phi}\,d\xi.$$

By the Taylor expansion

$$\nabla_\xi \phi = \frac{1}{2}\,\mathrm{Hess}_{\xi^o}(\xi') + O(|\xi|^2) = t\xi' + O(|\xi|^2),$$