SCHRÖDINGER OPERATORS

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FOREWORD

In its seven decades of existence, Quantum Mechanics still has many results which are believed not rigorously established, though routinely used in practice by Physicists. The question of unitarity of the S matrix is one such fundamental question, established rigorously only in the last decade, for N particle scattering interacting via a class of pair potentials. The question on transport (or the lack of it) of charge carriers in condensed matter systems, structure of potentials having a given energy spectrum, questions on existence and the number of resonance for a given potential are some other examples of questions in need of a rigorous mathematical framework, not to mention broader questions like existence of Crystals , rigorous foundations for QCD etc.,.

This workshop on "Schrödinger Operators" was aimed to gather a few experts working on such rigorous questions relating to the Schrödinger equation/Operator to introduce the subject to some of the students and teachers in India. I am happy to complement the organisers (Dr Krishna Maddaly in particular) in their effort to bring out the proceedings of the workshop in the Institute of Mathematical Sciences Report series and hope that it will serve as not only a record of the activity that took place here but also serve to enthuse future students to enter this difficult and challenging area of research.

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PREFACE

This is part of the proceedings of a workshop on "Schrödinger Operators" held here at the Institute of Mathematical Sciences during 4-14 December 1995. I hope that this proceedings will give an introduction -to the interested student- to some areas of Mathematical Physics.

I thank the Director. Prof R Ramachandran who supported the workshop whole heartedly and Prof K B Sinha of ISI, New Delhi who was instrumental and supportive for having the workshop. This workshop was funded by a grant from the Department of Science and Technology to defray the expenses for the participants and the cost of production of the proceedings. I thank them for the grant. I also thank my colleagues Prof Rajendra Bhatia, Ghanashyam Date and Sunder of the organizing committee and the office and library staff of the Institute for helping me with the overall administration involved in organizing such a workshop.

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Properties of microlocal smoothing for Schrödinger's equation

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§1. Introduction: I want to talk about a number of recent results on the smoothness of solutions of the Schrödinger equation, which I find striking and quite intuitive to understand, despite the fact that in general the techniques of proof are somewhat technical. In these two lectures I will describe these results, and I will try to give a good picture of the heuristics which govern the smoothness properties of solutions, and as well describe some of the issues that one comes across in studying these questions. Toward the end of the lectures I will give a sketch of the ideas of the proof, and the techniques that are used in it. We will consider the following two equations:

$$\begin{aligned} &i\partial_t\psi = -\tfrac{1}{2}\Delta\psi \\ &x \in R^n \quad \psi_0(x) = \psi(x,0) \in L^2(R^n) \end{aligned} \tag{1}$$

which is the usual free Schrödinger equation, and

$$\begin{aligned} &i\partial_t\psi = -\tfrac{1}{2}\textstyle\sum_{j,\ell=1}^n \partial_{x_j} a^{j\ell}(x)\partial_{x_\ell}\psi + V(x)\psi \\ &x \in R^n \quad \psi_0(x) = \psi(x,0) \in L^2(R^n) \end{aligned} \tag{2}$$

which is a more complicated Schrödinger equation with variable coefficients in a divergence form second order term, as well as lower order potential terms. Equation (1) has a well known explicit fundamental solution the free Schrödinger kernel, so in some sense we know all about its solutions. The equation (2) is more of a challenge, and will require us to work harder. I will start by describing some elementary properties of solutions of equation (1), and then go on to give their analogs for equation (2), to the extent that we know them. These properties of equation (1) are simple, but despite this I still think that they are remarkable,

Typeset by $\mathcal{A}\mathcal{M}\mathcal{S}$-TEX and certain of them are not sufficiently well known. The first theorem concerns solutions of equation (1).

Theorem 1: *Let $\psi_0(x) \in L^2(R^n)$ be initial data for a solution $\psi(x,t)$ of equation (1).*

(i) Then for all $t \in R$, $\psi(x,t) \in L^2(R^n)$, with the same $L^2(R^n)$ norm.

This is the simple and well known fact that evolution by solution of the Schrödinger equation is unitary on $L^2(R^n)$, which is central to the interpretation of quantum mechanics. That is, measurements of a quantum particle are initially made with respect to the probability measure $dP_0(x) = |\psi_0(x)|^2 dx$, and at later time the measurements on the evolution of the particle are made with respect to the probability $dP_t(x) = |\psi(x,t)|^2 dx$. The result (i) is the fact that the evolution conserves probability. It seems then rather natural to impose conditions on the moments of the distribution $dP_0(x)$, as these are information about the location of the quantum paticle at time $t = 0$.

(ii) Suppose that additionally the probility $dP_0(x)$ has finite moments (for reasons of simplicity we will assume that all moments are finite, in order to avoid counting them). That is, we ask that

$$(3) \qquad \forall k \ \textit{multiindices}, \quad \int |x^k \psi_0(x)|^2 dx < +\infty \ .$$

Then for all $t \neq 0$, $\psi(x,t) \in C^\infty$.

The purpose of this talk is to describe the analogous result for the equation (2). In the course of the description, I will give a proof of Theorem 1 as well.

§2. Results (for $V(x) = 0$): In order to start with the analysis of equation (2), I have to give the definition of several things.

Definition 1: (i) The *principal symbol* of the equation is the standard one, from the highest order terms of equation (2);

$$(4) \qquad a(x,\xi) = \tfrac{1}{2} \textstyle\sum_{j,\ell=1}^n a^{j\ell}(x)\xi_j\xi_\ell \ .$$

(ii) The *bicharacteristic flow* is the flow on the cotangent space $(x,\xi) \in T^*(R^n)$ given by solutions of the Hamiltonian system

$$(5) \qquad \begin{aligned} \frac{dx}{ds} &= \partial_\xi a(x,\xi) \\ \frac{d\xi}{ds} &= -\partial_x a(x,\xi) \ , \end{aligned}$$

with the orbit originating at the point (x,ξ) denoted by $\varphi(s; x, \xi)$. Note particularly that the curves that are the orbits of the flow are parametrized by an auxiliary parameter s, which is not the time variable t.

(iii)(a) The classical definition of the *wave front set* of a distribution $f \in D$ is given as follows. One defines the *singular support* $S(f)$ most easily by specifying what is not in it; a point $x_0 \notin S(f)$ if there is a cutoff function $\eta \in C_0^\infty$, with $\eta(x_0) = 1$, such that $(\eta f) \in C_0^\infty$. Using the duality between regularity in space and decay of the Fourier transform, we can alternately ask that

$$|\widehat{(\eta f)}(\xi)| \leq C_N \langle \xi \rangle^{-N}$$

for all $N \geq 0$, where we are using that $\langle x \rangle = (1 + |x|^2)^{1/2}$, notation common to this subject .

(iii)(b) The wave front set $WF(f)$ has a related definition. The point $(x_0, \xi^0) \notin WF(f)$ if there is a cutoff function $\eta \in C_0^\infty$ with $\eta(x_0) = 1$ and an open cone Γ with $\xi^0 \in \Gamma$ such that

$$|\widehat{(\eta f)}(\xi)| \leq C_N \langle \xi \rangle^{-N}$$

for all $\xi \in \Gamma$, for all $N \geq 0$.

The first theorem concerning the microlocal regularity of solutions of equation (2) is the following:

Theorem 2: (L. Boutet de Monvel (1974), R. Lascar (1977)) *For solutions of equation (2), the wave front set is an invariant set under the flow $\varphi(s; x, \xi)$ (with a slightly modified definition of the wave front set in $(x, t, \xi, \tau) \in R^{2(n+1)}$, due to the inequality presented by having two spatial derivatives, compared to only one time derivative). This modification, which I do not give here, was called the quasi-homogeneous wave front set.*

This establishes a relation between the orbits of the flow of (3) and the singularities of the solution of (2), which states essentially that singularities travel with infinite velocity along the bicharacteristics of $a(x, \xi)$. However this statement confines our knowledge to each hyperplane $\{t = \textit{constant}\}$, and it does not tell us how the singularities of the solutions will change in time. Continuing the items in our list,

(iv) Assume that the principal symbol is *nondegenerate*, which usually means elliptic

$$\frac{1}{C}|\xi|^2 \leq a(x, \xi) \leq C|\xi|^2 \tag{6}$$

and *asymptotically flat*,

$$|\partial_x^\alpha (a^{j\ell}(x) - \delta^{j\ell})| \leq C\langle x \rangle^{-\tau(\alpha)}, \qquad \tau(\alpha) > |\alpha| + 1 \; . \tag{7}$$

Speaking of geometrical problems, the operator $-\frac{1}{2}\sum_{j,\ell=1}^n \partial_{x_j} a^{j\ell}(x) \partial_{x_\ell}$ is not quite the Laplace-Beltrami operator in general coordinates on an asymptotically flat manifold, for that requires $\det(a) = 1$. However all the analysis that we have in $L^2(R^n, dx)$ carries over to the case of a Riemannian manifold with metric $ds^2 = \sum_{j\ell} g_{j\ell}(x) dx^j dx^\ell$, with the genuine Laplace-Beltrami operator

$$\Delta_g \psi(x) = \frac{1}{\sqrt{\det(g)}} \sum_{j,\ell=1}^{n} \partial_{x_j}(\sqrt{\det(g)} g^{j\ell}(x) \partial_{x_\ell}) \psi(x)$$

where $g_{j\ell} = (g^{j\ell})^{-1}$, which is also self adjoint using the inner product on $L^2(R^n, \sqrt{\det(g)}dx)$.

(v) One says that the point (x_0, ξ^0) is *not trapped forwards*, (respectively *backwards*) by the bicharacteristic flow φ of the symbol $a(x, \xi)$ if

$$|\varphi(s; x_0, \xi^0)| \to \infty$$

as $s \to +\infty$ (respectively, $s \to -\infty$).

The theorem that we have proved in this subject concerns the time evolution of singularities in the solutions of (2), in contrast to Theorem 2.

Theorem 3 : (W. Craig, T. Kappeler and W. Strauss (1995)) *Suppose that the point (x_0, ξ^0) is not trapped backwards by the bicharacteristic flow φ of $a(x, \xi)$. Suppose that the moment condition (3) holds for the initial data $\psi_0(x)$. Then for any time $t > 0$,*

$$(x_0, \xi^0) \notin WF(\psi(x, t)) . \tag{8}$$

This is an entirely microlocal conclusion about the regularity of the solution of (2), however there is a global element as we must have information about the full backwards bicharacteristic through (x_0, ξ^0). There are also several global corollaries that follow essentially immediately from Theorem 3.

Corollary 4: *If $a(x, \xi)$ has no trapped bicharacteristics, then for initial data $\psi_0(x)$ satisfying (3), for all $t \neq 0$,*

$$WF(\psi(x, t)) = \emptyset ,$$

which is to say that $\psi(x, t) \in C^\infty$.

This latter statement is also a result of L. Kapitanski and Y. Safarov, who study the case of equation (2) when there are no trapped bicharacteristics, with quite different methods for their proof. Their approach is based on a relation between this problem and the classical problem of local time decay for solutions of the wave equation.

It is clear that this result also implies Theorem 1 (you might say it is a proof the hard way). From the Laplacian we have $a(x, \xi) = \frac{1}{2}|\xi|^2$, and therefore Hamilton's canonical equations (5) are

$$\frac{dx}{ds} = \xi , \qquad \frac{d\xi}{ds} = 0 .$$

The solutions are

$$x(s) = x_0 + s\xi^0 , \qquad \xi(s) = \xi^0 ,$$

which are straight line motion at constant velocity, and all bicharacteristics go to infinity in either direction. Thus Corollary 4 holds.

To give a more direct result for equation (1), the fundamental solution for the free problem is

$$S^0(x-y,t) = \frac{1}{\sqrt{2\pi i t}^n} e^{i\frac{|x-y|^2}{2t}} , \tag{9}$$

which is clearly an analytic function for $t \neq 0$. To prove a result related to Theorem 1, consider distributional initial data ψ_0 of compact support. The solution is then $S^0 * \psi_0$, which for any $t \neq 0$ is a compact sum of analytic functions, and is therefore itself analytic.

In general $a(x,\xi)$ may well have trapped bicharacteristics, so we cannot eliminate all singularities from the solution. We can however use Theorem 3 to confine the singularities to a subset of $T^*(R^n)$ characterized by the dynamics. This is the intention of the next result.

Corollary 5: *Consider solutions $\psi(x,t)$ of equation (2), for time $t > 0$. Let R be the recurrent set of the bicharacteristic flow, and $M^u(R)$ the set of orbits which accumulate on R for $s \to -\infty$. Then*

$$WF(\psi(x,t)) \in R \cup M^u(R) . \tag{10}$$

Theorem 3 also allows us to discuss the fundamental solution $S(x,y,t)$ of the equation (2) in these terms. For this we have to consider the four variables $(x,\xi,y,\eta) \in T^*(R^n) \times T^*(R^n)$.

Corollary 6: *The point $(x_0,\xi^0,y_0,\eta^0) \in T^*(R^n) \times T^*(R^n)$ is not in the wave front set $WF(S(x,y,t) \subseteq T^*(R^n) \times T^*(R^n)$ for $t > 0$ if either*

(i) (x_0,ξ^0) is not trapped backwards, or

(ii) (y_0,η^0) is not trapped forwards

by the bicharacteristic flow φ of the principal symbol $a(x,\xi)$.

This result eliminates from the wave front set all points of the cotangent space which have the proper classical scattering behavior, however it is not a full characterization of the set on which the Schrödinger kernal is singular. There is a natural conjecture that one can make as to the full result for the problem, which I will state here. We are however not able with the present methods to prove this, and in fact a characterization of the evolution of $WF(S(x,y,t))$ promises to be a challenging problem. Any singularities must travel at infinite velocity, so points (x,y) at which $S(x,y,t)$ is singular must somehow be associated with noncompact subsets of the orbits of the bicharacteristic. The conjecture goes as follows: for $t > 0$ the point $(x_0,\xi^0,y_0,\eta^0) \in WF(S(x,y,t))$ only if for any conic neighborhoods $(y_0,\eta^0) \in \Omega_1$

and $(x_0, \xi^0) \in \Omega_2$, there is a sequence $\{s_j\}_{j=1}^{\infty}$, with $s_j \to +\infty$, such that $\varphi(s_j; \Omega_1) \cap \Omega_2 \neq \emptyset$.

§3. Idea of the proof of Theorem 3: I want to concentrate on giving a good heuristic picture of the problem, before I talk about the actual analytic techniques that are employed in the proof. Restrict ourselves to the one dimensional case, and study the general (constant coefficient) equation

$$i\partial_t u = \omega(D)u \ , \quad x \in R \tag{11}$$

where we are using the classical notation that $D = (1/i)\partial_x$. There are exponential solutions

$$u_\xi(x,t) = e^{i(\xi x - \omega(\xi)t)} \ ,$$

and for the general solution we can superpose these in a Fourier integral

$$u(x,t) = \int e^{i(\xi x - \omega(\xi)t)} \hat{u}_0 \, d\xi \ . \tag{12}$$

Lets make a solution which looks like a wave packet, by taking u_0 such that $\hat{u}_0 \in C_0^\infty$, in particular $supp(\hat{u}_0) \subset\subset R^n$, centered about some ξ^0. Solve the bicharacteristic equations

$$\frac{d}{dt}x = \partial_\xi \omega \ , \qquad \frac{d}{dt}\xi = -\partial_x \omega = 0 \ . \tag{13}$$

This gives solutions $x(t) = x_0 + t\partial_\xi\omega(\xi^0)$, and $\xi(t) = \xi_0$, which traverses a ray with velocity $\partial_\xi\omega(\xi^0)$ in the (x,t) plane. The following theorem relates this to the solution of (11).

Theorem 7: (the method of stationary phase) *In a cone away from the rays $(x - t\partial_\xi\omega(\xi) = constant$, $\xi \in supp\, \hat{u}_0$; the solution $u(x,t)$ decays faster than any polynomial.*

Proof: Suppose that we consider (x,t) such that for $\xi \in supp\ \hat{u}_0$,

$$\left|\frac{x}{t} - \partial_\xi\omega(\xi)\right| > R \ .$$

Then

$$\begin{aligned}
u(x,t) &= \int e^{i(\xi x - \omega(\xi)t)} \hat{u}_0(\xi) d\xi \\
&= \int \frac{1}{i(x - \partial_\xi\omega(\xi)t)} \partial_\xi (e^{i(\xi x - \omega(\xi)t)}) \hat{u}_0(\xi) d\xi \\
&= \int e^{i(\xi x - \omega(\xi)t)} \Big(-\partial_\xi \frac{1}{i(x - \partial_\xi\omega(\xi)t)}\Big) \hat{u}_0(\xi) d\xi \\
&= \int e^{i(\xi x - \omega(\xi)t)} \Big(-\partial_\xi \frac{1}{i(x - \partial_\xi\omega(\xi)t)}\Big)^N \hat{u}_0(\xi) d\xi \ .
\end{aligned}$$

for regular $\hat{u}_0$, for any integer $N \geq 0$. The denominator grows with magnitude $(Rt)^N$, and the decay result will follow from this. ///

The quantity $\partial_\xi \omega$ is called the *group velocity*, a name given by Kelvin in his work on water waves. Using the picture of the evolution of a wave packet given by Theorem 7, we can give a reason why the moments of the initial data are related to the smoothness of solutions for $t \neq 0$. Consider arbitrary data $u_0(x)$ of rapid decay, and cut its Fourier transform into pieces which each look like a wave packet solution, by using a partition of unity. That is

$$\hat{u}_0(\xi) = \sum_{k \in Z} \hat{u}_k(\xi)$$

with each $\hat{u}_k(\xi) \in C_0^\infty(2Q_k)$, where Q_k is a cube of side one centered at the integer point k. The individual components $u_k(x,t)$ can be tracked (morally speaking) by Theorem 6, and are essentially confined to cones in the (x,t)-plane with slope near to $\partial_\xi \omega(k)$. To discuss the derives of the solution, isolate a bounded region K in x for $t \neq 0$; then the essential contributions of $u(x,t)$ in K are given by those components $u_k(x,t)$ for which the slope $\partial_\xi \omega(k)$ allows propagation from bounded regions of the initial data into our test region K. If the group velocity $\partial_\xi \omega(\xi)$ diverges as $|\xi| \to \infty$, only a finite number of the components are expected to essentially contribute to the solution in K, and therefore we can expect the solution to be smooth there. This is not a proof, but it is a compelling heuristic argument for the smoothing effects described above. Problems (11) for which $\partial_\xi \omega(\xi)$ diverges as $|\xi| \to \infty$ are called *dispersive*, and we expect that their singularities will travel with infinite velocity. The Schrödinger equation has $\omega(\xi) = \frac{1}{2}|\xi|^2$, so that $\partial_\xi \omega(\xi) = \xi$, which is dispersive in the above sense.

I will now give a more precise description of the techniques used in the proof of Theorem 3, which are essentially microlocalized Sobolev estimates of the solution. Rewrite equation (2) as

$$i\partial_t \psi = A\psi \;, \tag{14}$$

where we assume that A is self adjoint. Then for any other operator B, solutions of (14) satisfy an identity

$$\partial_t \, re \, \langle \psi, B\psi \rangle + re \, \langle \psi, \tfrac{1}{i}[A,B]\psi \rangle = re \, \langle \psi, (\partial_t B)\psi \rangle \;. \tag{15}$$

This identity gives us a small proposition, which includes the statement (i) of Theorem 1.

Proposition 8: *Any B which is time independent and commutes with A is preserved by the solutions of (2), that is,*

$$\partial_t \, re \, \langle \psi, B\psi \rangle = 0 \;.$$

In particular, setting $B = I$, the L^2-norm of solutions are preserved.

We will make other choices of operator in the identity (15), in particular we will construct certain pseudodifferential operators for use in the proof. We define $B = b(x, D)$, where

$$(16) \qquad b(x,D)\psi(x) = \int e^{i\xi\cdot(x-y)} b(x,\xi)\psi(y)dy$$

for 'symbol' $b(x,\xi) \in C^\infty(T^*(R^n))$ chosen in a certain class of symbols for which this oscillatory integral is well behaved.

Definition 2: The usual definition of the class of *classical symbols* are those $b(x,\xi) \in C^\infty(T^*(R^n))$ which satisfy

$$(17)(i) \qquad \pi_x supp\ (b) \subseteq K \subset\subset R^n \qquad \textit{compactly supported}$$

$$(17)(ii) \qquad |\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta}\langle\xi\rangle^{m-|\beta|} \ .$$

L. Hörmander noticed that to retain most of the desirable symbol properties, it sufficed to replace (17)(ii) by

$$(17)(iii) \qquad |\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta}\langle\xi\rangle^{m-\delta|\beta|+\rho|\alpha|}$$

for $0 \le \rho < \delta \le 1$. These classes of symbols are denoted $S^m(\delta,\rho)$. When $\rho = \delta < 1$ it is a critical case, which can be addressed to some extent by the theorem of Calderon and Vaillancourt.

The operator A can be written as a pseudodifferential operator, with symbol $a(x,\xi) + a_1(x,\xi)$, where there are both second and first order terms as A is in divergence form. The symbol $a_1(x,\xi) = i\sum_{j\ell}(\partial_{x_j} a^{j\ell}(x))\xi_\ell$. Composition of pseudodifferential operators, whose symbols are in suitable classes such as the above, is well defined in terms of the pseudodifferential calculus, and in fact the commutator in the identity (15) is described by

$$(18) \qquad \frac{1}{i}[A, b(x,D)] = -\{a,b\}(x,D) + e \ ,$$

where the Poisson bracket is

$$(19) \qquad \begin{aligned} \{a,b\}(x,\xi) &= \sum_j (\partial_{\xi_j} a\, \partial_{x_j} b - \partial_{x_j} a\, \partial_{\xi_j} b)(x,\xi) \\ &= \frac{d}{ds}\Big|_{s=0} b(\varphi(s;x,\xi)) \\ &= X_a(b) \ . \end{aligned}$$

The operator e is lower order, and X_a is the Hamiltonian vector field of the symbol a. We will use these operators in the identity (15), and if the relevant symbols are non-negative we can hope to obtain an energy-type estimate. Suppose that $b \in S^m$

of some symbol class, and count the orders of the operators in the identity (15). The error e will be of order m or possibly less, but the operator $\{a,b\}(x,D)$ is of order $m+1$, and is the most important contribution if the expression is to be useful. In fact, take the point of view that, given a symbol $c(x,\xi) \geq 0$ of order $m+1$, we will try to find $b(x,\xi)$ such that

$$b(x,\xi) \geq 0 \,, \qquad \textit{and} \qquad c(x,\xi) = -\{a,b\}(x,\xi) \geq 0 \,. \tag{20}$$

It is a fundamental question then whether pairs of symbols (b,c) exist satisfying the conditions (20).

Proposition 9: *Suppose that $c(x,\xi) \geq 0$, and that the point (x_0,ξ^0) is such that $c(x_0,\xi^0) > 0$ and that it is on a periodic bicharacteristic. Then there is no symbol $b(x,\xi)$ satisfying (20).*

Proof: The equation $\{a,b\} = -c$ is called a cohomological equation, and the regularity of the solution depends highly upon the recurrence properties of the flow φ. In the simple case of periodic orbits, if the symbol $b(x,\xi)$ did exist, then

$$\begin{aligned} 0 &< \int_0^P c(\varphi(s;x_0,\xi^0))ds \\ &= \int_0^P \frac{d}{ds} b(\varphi(s;x_0,\xi^0))ds \\ &= 0 \,, \end{aligned}$$

which proves the result by contradiction. ///

However we can solve the cohomological equation for symbols $c(x,\xi) \geq 0$ by quadrature in the case that $supp(c)$ has support only on bicharacteristics which are not trapped backwards. Indeed take $0 \leq c(x,\xi) \in S^{m+1}$ a classical symbol, with $supp(c)$ in the set of orbits which are not trapped backwards, and set

$$b(x,\xi) = \int_0^{+\infty} c(\varphi(s;x,\xi))ds \,. \tag{21}$$

Then the support of $b(x,\xi)$ cannot be compact and there is a picture of the situation which is somewhat like in figure 1.

Because the support of the symbols relevant to our work will not be compact, we need to keep track of their spatial behavior under differentiation as well as the behavior in the Fourier variables. The following theorem gives the behavior of the symbol $b(x,\xi)$ from (21).

Theorem 10: *Consider a classical symbol $c(x,\xi) \in S^{m+1}$, supported in the set of backwards nontrapping orbits (and suppose that $c(x,\xi) = 0$ for $|\xi| \leq 1$ to avoid troubles for small Fourier variables). Then in general all we can expect of $b(x,\xi)$ is the estimate*

$$|\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \leq C_{\alpha\beta} \langle\xi\rangle^{m-|\beta|} \langle x\rangle^{+|\beta|} \tag{22}$$

That is, all we can expect from quadrature is a result which is in a very bad class of symbols, where no partial derivatives offset a lack of decay in spatial variables. We can call the class of such symbols $S^m(1,0)(0,1)$, where the first pair $(\delta_1,\rho_1)=(1,0)$ quantify the behavior in the Fourier variables, and the second pair $(\delta_2,\rho_2)=(0,1)$ describe their spatial behavior. The class $S^m(1,0)(0,1)$ does not form a symbol calculus, and in general may not even be bounded operators on $L^2(R^n)$. However there is one extra property that is obeyed by symbols $b(x,\xi)$ constructed by the quadrature (21), which is related to their behavior under dilations in the fiber $\xi \in R^n$. The vector field describing infinitessimal dilations is $\xi\cdot\partial_\xi$. Symbols defined by quadrature (21) satisfy the estimate

$$|(\xi\cdot\partial_\xi)^\gamma\partial_x^\alpha\partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta\gamma}\langle\xi\rangle^{m-|\beta|}\langle x\rangle^{+|\beta|} \ . \tag{23}$$

With this estimate with respect to the vector field of dilations, the operators $b(x,D)$ are in fact better behaved than in general.

Theorem 11: *Suppose that $b(x,\xi)$ is a symbol such that*

$$|(\xi\cdot\partial_\xi)^\gamma\partial_x^\alpha b(x,\xi)| \le C_{\alpha\gamma} \ , \tag{24}$$

and suppose that there is a constant $R>0$ such that whenever $|x-y|>R$, and both $(x,\xi),(y,\xi)\in supp\ (b)$, then

$$\tfrac{1}{2}|\xi|\langle x-y\rangle \le |(x-y)\cdot\xi| \ . \tag{25}$$

Then the operator $b(x,D)$ is bounded on $L^2(R^n)$.

The symbols that one gets from quadrature (21) satisfy the estimate (24) and the support property (25) whenever the support of $c(x,\xi)$ is in a non-trapping region and is sufficiently small. From this we can see already an increment of additional regularity for the solutions of Schrödinger's equation (2); this is a microlocal version of what is sometimes called the 'local smoothing' property of dispersive equations. Let $c(x,\xi)$ be a classical symbol of order 1, supported in a sufficiently small conic neighborhood of a point (x_0,ξ^0) in the non-trapping region. Integrating the identity (15) over a time interval $[0,T]$, we obtain

$$\begin{aligned} re\ \langle\psi,b(x,D)\psi\rangle(T) &+ re\int_0^T\langle\psi,c(x,D)\psi\rangle(t)dt \\ &= re\ \langle\psi_0,b(x,D)\psi_0\rangle + re\int_0^T\langle\psi,(e(x,D)-\tfrac{1}{i}[a_1(x,D),b(x,D)])\psi\rangle(t)dt \end{aligned} \tag{26}$$

All terms of this except the second are bounded by $\|\psi(x,t)\|_{L^2}^2$, and therefore, because of Theorem 1 (i), we have

$$re\int_0^T\langle\psi,c(x,D)\psi\rangle(t)dt \le C(T)\|\psi_0\|_{L^2}^2 \ . \tag{27}$$

The symbol of the operator $c(x,D)$ is nonnegative and is of order 1, therefore by Gårding's inequality, for any classical symbol $s(x,\xi)$ such that $0 \le s^2(x,\xi) \le c(x,\xi)$,

$$(28)\qquad \int_0^T \|s(x,D)\psi(t)\|^2 dt \le C(T)\|\psi_0\|_{L^2}^2 .$$

Notice that $s(x,\xi) \in S^{1/2}$, therefore we have control of of a microlocal Sobolev estimate of 1/2-derivative of the solution, averaged in time, for any (x,ξ) in the region of phase space that is not trapped backwards by the bicharacteristic flow.

The full C^∞ result of Theorem 3 is given by an induction, which I will sketch here. Suppose that (x_0,ξ^0) is not trapped backwards, then we construct a conic neighborhood E_-^0 of the backward bicharacteristic $\{\varphi(s;x_0,\xi^0) : s < 0\}$, and a pair of symbols $b(x,\xi) \ge 0, c(x,\xi) \ge 0$, supported in E_-^0 such that

$$(29)(i)\qquad c(x,\xi) = -\{a,b\}(x,\xi)$$

$$(29)(ii)\qquad \begin{aligned} |\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| &\le C_{\alpha\beta}\langle\xi\rangle^{m-|\beta|}\langle x\rangle^{k+\rho|\beta|-\delta|\alpha|} \\ |\partial_x^\alpha \partial_\xi^\beta c(x,\xi)| &\le C_{\alpha\beta}\langle\xi\rangle^{m+1-|\beta|}\langle x\rangle^{k-1+\rho|\beta|-\delta|\alpha|} \end{aligned}$$

These classes of symbols are called $S^{m,k}(1,0)(\delta,\rho)$. We have to manufacture such symbols so that $\rho < \delta$, and this we can do provided that $\delta + \rho > 1$. When $\rho < \delta$ this symbol class gives a calculus of operators, which are used for microlocal bounds in the incoming regions of phase space. Applying the identity (15) to the pair $t^p b(x,D), t^p c(x,D)$, for $b(x,\xi) \in S^{m,k}(1,0)(\delta,\rho)$, and $c(x,\xi) \in S^{m+1,k-1}(1,0)(\delta,\rho)$, the analog of (26) is

$$(30)\qquad \begin{aligned} &re\ \langle\psi, t^p b(x,D)\psi\rangle(T) + re \int_0^T \langle\psi, t^p c(x,D)\psi\rangle(t)dt \\ &= re\ \langle\psi_0, t^p\big|_{t=0} b(x,D)\psi_0\rangle \\ &\quad + re \int_0^T \langle\psi, (pt^{p-1}b(x,D) + t^p(e(x,D) - \tfrac{1}{i}[a_1(x,D), b(x,D)]))\psi\rangle(t)dt \end{aligned}$$

For any $p > 0$, the first term of the RHS vanishes, and the estimate does not depend explicitely upon the initial data. We recognize in the remainder terms symbols in the class $t^{p-1}S^{m,k}(1,0)(\delta,\rho)$, and furthermore they are integrated in time over $[0,T]$. This is used in an induction, in which one starts with $k = K$ bounded orders of growth, and $m = 0$ demands of regularity. At the n-th induction step one takes $m = n, k = K - n$ and $p = n$. This will give the desired regularity result at any point which is not trapped backwards. When in addition the point (x_0,ξ^0) is also not trapped forwards, a similar induction gives the asymptotics of the growth of derivatives as $|x| \to \infty$. The geometry of this situation requires however that we use the worst case symbol class $S^{m,k}(1,0)(0,1)$, with inductive choices $m = n, k = -n - \epsilon$ and again $p = n$. Theorem 11 is used to control the error and to interpret the microlocal regularity of the solution from the resulting estimate.

§4. Results with a potential $V(x)$. The above is a discussion of the Schrödinger equation when no potential terms or other lower order terms are present. Let's now incorporate nonzero potentials in the problem, and see what effect this makes on the question of regularity. Consider potentials $V(x)$ for equation (2) which satisfy the growth conditions

$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x\rangle^{p-|\alpha|} . \tag{31}$$

The power p controls the growth or decay of the potential at infinity. By the same techniques as above, we can prove that if $p < 1$ then the smoothness properties of the solutions with localized initial data ψ_0 are the same as if the potential were not present.

Theorem 12: *If $p < 1$ then then the conclusions of Theorem 3 continue to hold.*

The size of p is important to the problem, and for p sufficiently large the smoothing phenomenon cannot continue to hold. The critical power is $p = 2$, and indeed the quantum harmonic oscillator has explicit solutions which are instructive to discuss;

$$i\partial_t \psi = -\tfrac{1}{2}\Delta\psi + \tfrac{|x|^2}{2}\psi . \tag{32}$$

Theorem 13: *(i) Mehler's formula gives an explicit fundamental solution to (32).*

(33)

$$S^h(x,y,t) = \frac{1}{\sqrt{2\pi i \sin(t)}^{\,n}} e^{i\Phi} , \qquad \Phi(x,y,t) = \tfrac{1}{2}(\cot(t)(|x|^2 + |y|^2) - 2\csc(t) x\cdot y) .$$

The singularities of the quantum harmonic oscillator kernel occur at $x = y$ for $t = 0$, and then recur for every $t = n\pi, n \in Z$. In the intervals between these times, the kernel is analytic, and at $t = 2n\pi$ the singularity is at $x = y$ again, while for $t = (2n+1)\pi$, the singularity is for $x = -y$ on the antipodal point of the potential well.

(ii) (A. Weinstein and S. Zelditch (1981)) For $a(x,\xi) = \frac{1}{2}|\xi|^2$ and $V(x) = \frac{1}{2}|x|^2 + v(x)$, where $v(x)$ is a Schwartz class function, then this same phenomenon of recurring of singularities occurs.

There has been recent work on this problem, with the principal symbol $a(x,\xi) = \frac{1}{2}|\xi|^2$ of the Laplacian, and with various ranges of the growth parameter p.

Theorem 14: (K. Yajima, L. Kapitanski and I. Rodnienski)(1995) *Considering the Schrödinger equation*

$$i\partial_t \psi = -\tfrac{1}{2}\Delta\psi + V(x)\psi ; \tag{34}$$

with the potential satisfying (31) with any $p < 2$. The fundamental solution $S(x,y,t)$ is C^∞ for any $t \neq 0$.

This fills the gap left by Theorem 12 in the allowed values of p for which the smoothness of the fundamental solution is expected. The proofs of this theorem by K. Yajima is through a careful study of the trajectories of the classical Hamiltonian system with Hamiltonian $h(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$, in the case of potentials satisfying (31) with $p < 2$. From this he constructs a parametrix for the problem in the form of those by H. Kitada and H. Kumano-go, which is valid in any finite interval $[-T,T]$. The proof by L. Kapitanski and I. Rodnienski uses completely different techniques, relying on certain specific operators which commute with the Schrödinger equation, modulo error terms which are lower order in derivatives as well as their spatial growth. The latter method depends very much on the fact that the operator A is the Laplacian, but the former construction may not depend so strongly on this, and it would be interesting to construct a proof of Theorem 3 and Theorem 12 for $p < 2$ by use of a parametrix.

Yajima also addresses the case $p > 2$ in his preprint, which gives the result that the fundamental solution lacks regularity.

Theorem 15: (K. Yajima (1995)) *Consider the problem (34) in one space dimension, and take $p > 2$. More precisely, ask that the potential $V(x) \in C^3(R)$, and outside of a bounded set ask that*

(35)(*i*)
$$\partial_x^2 V(x) > 0 \ ,$$

(35)(*ii*)
$$x\partial_x V(x) > pV(x) > 0 \ ,$$

and finally that for $j = 1, 2$ and 3,

(35)(*iii*)
$$\frac{\partial_x^j V(x)}{\partial_x^{j-1} V(x)} = O\left(\frac{1}{\langle x\rangle}\right) .$$

Then the fundamental solution $S(x,y,t)$ is a distribution kernel which is nowhere C^1.

I will finish with a description of the heuristics behind the results on potential terms, which depends upon the description of classical paths, and of course does not constitute a proof. Stay in one dimension for clarity, and consider the classical Hamiltonian systems associated with the problem (34). When $V(x) = 0$, the Hamiltonian is $h(x,\xi) = \frac{1}{2}|\xi|^2$, the system is

(36)
$$\begin{aligned} \frac{d}{dt}x &= \partial_\xi h = \xi \\ \frac{d}{dt}\xi &= -\,\partial_x h = 0 \end{aligned}$$

and the flow $\varphi(t;x,\xi)$ in the phase plane is a shear flow $x(t) = x_0 + t\xi$, $\xi(t) = \xi^0$. The fundamental solution at $t = 0$ is a delta-function at $x = y$, which is schematically represented by marking the line which is its support in the phase plane. The evolution of the partial differential equation (34) can be imagined to be approximated at large Fourier transform variable by a distribution supported on the image of this line under the classical Hamiltonian flow $\varphi(t;x,\xi)$. The support of the delta-function and its evolution under the flow are pictured in figure 2.

When $V(x) = \frac{1}{2}|x|^2$, the classical harmonic oscillator, then $h(x,\xi) = \frac{1}{2}|\xi|^2 + \frac{1}{2}|x|^2$, and the flow in the phase plane is linear and consists of concentric circles about the origin, with every orbit periodic of the same period 2π. These orbits, and the evolution of the support of the initial delta-function are pictured in figure 3.

The feature of recurring singularities at $x = \pm y$ is accurately represented in the fact that the evolution of the line is vertical precisely at $x = \pm y$ at times $t = n\pi$ (see figure 3).

In the case $p < 2$, the interesting situation is for $V(x)$ growing at $|x| \to \infty$, in which case all orbits of classical solutions $\varphi(t;x,\xi)$ are periodic, but with period which becomes infinitely long as the energy $h(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$ is taken to infinity. A rough sketch of the initial delta-function is as below. The feature that no interval of the configuration space $\{x \in R\}$ is covered more than finitely often by the vertical projection of the curve, for $t \neq 0$ reflects accurately the fact that the Schrödinger kernel is smooth (see figure 4).

Finally we can discuss the case of $p > 2$ in this way. For a potential such that $V(x)$ increases to infinity as $|x| \to \infty$ again all the classical orbits are periodic, but this time the period of the orbits decreases to zero as the energy $h(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$ goes to infinity, corresponding to increasingly fast revolutions in phase space around the origin, for increasing radius. The projection of the image under $\varphi(t;x,\xi)$ of the support of the initial delta-function is now wrapped around the origin infinitely often, no matter which small time t is considered, and the projection of the resulting curve onto any interval of configuration space always has infinitely many components, which are unbounded in phase space. This is consistant with the conclusion of Theorem 15, and indeed gives an accurate heuristic argument for the result (see figure 5).

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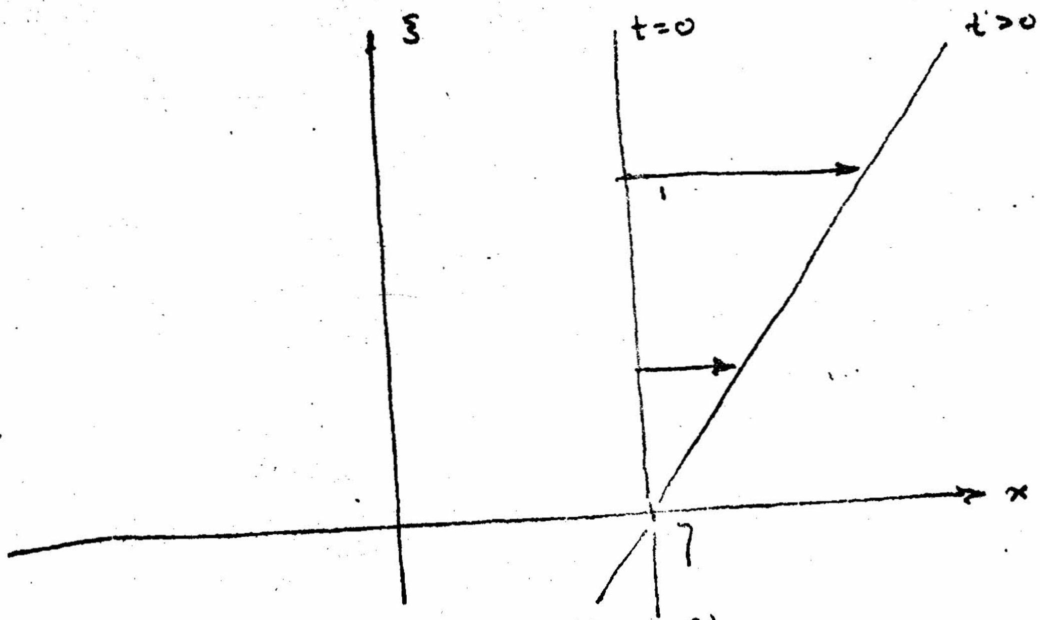
(figure 1)



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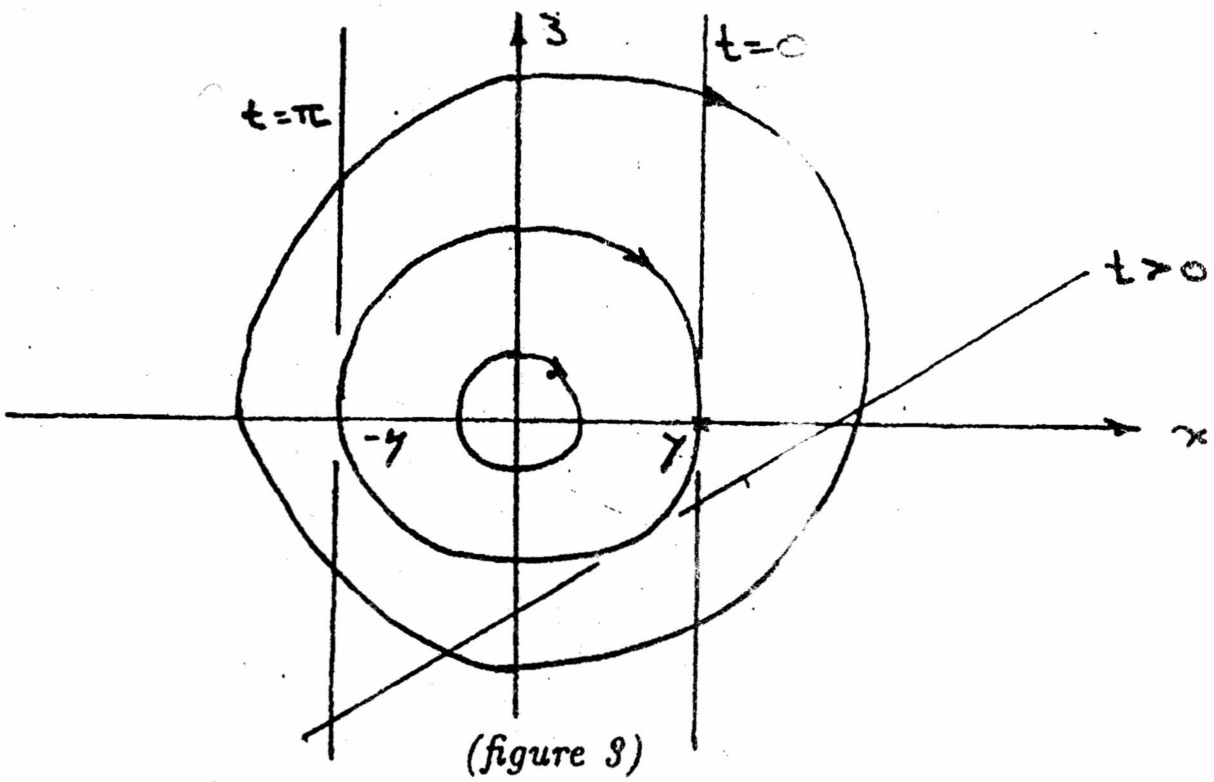

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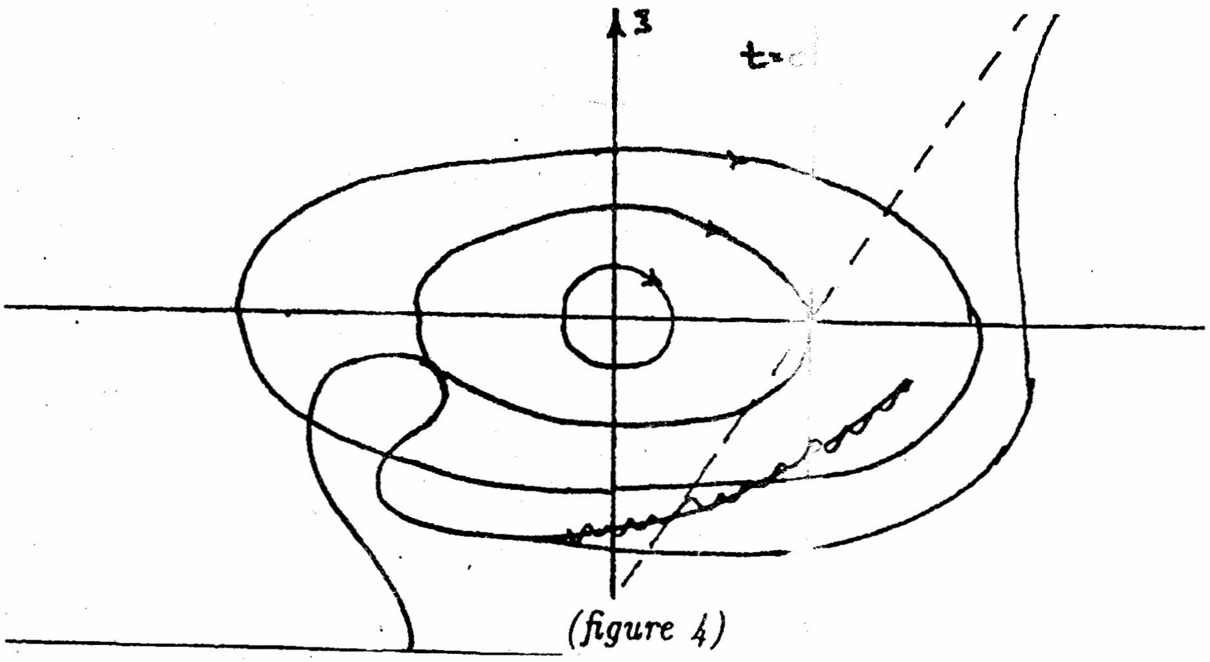

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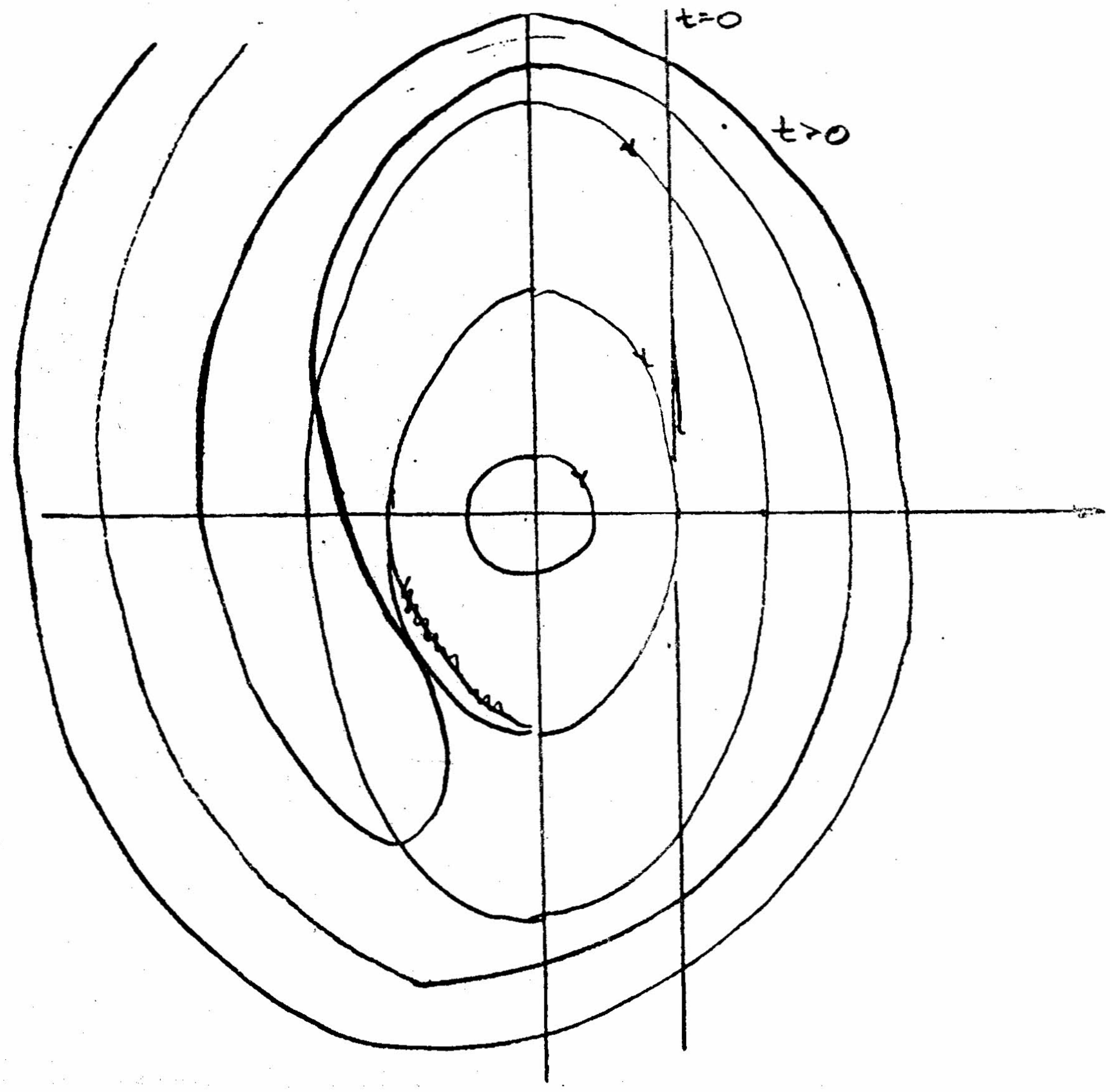

(figure 5)

Counting resonances of Schrödinger operators

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0. Introduction

In the past week we have heard many talks about Schrödinger operators whose spectral measure is singular. In my lectures, I want to examine Schrödinger operators whose spectral measures are analytic. For these operators, the Green's function and the scattering operator have meromorphic continuations into the complex plane. Singularities in these continuations are called resonances, or scattering poles. I will discuss their asymptotic distribution.

In this talk I will consider Schrödinger operators

$$H = -\Delta + V$$

acting in $L^2(\mathbb{R}^n)$, n odd, whose potentials V are super-exponentially decreasing. By definition, this means that for every N there is a constant C such that

$$|V(x)| \leq Ce^{-N|x|}$$

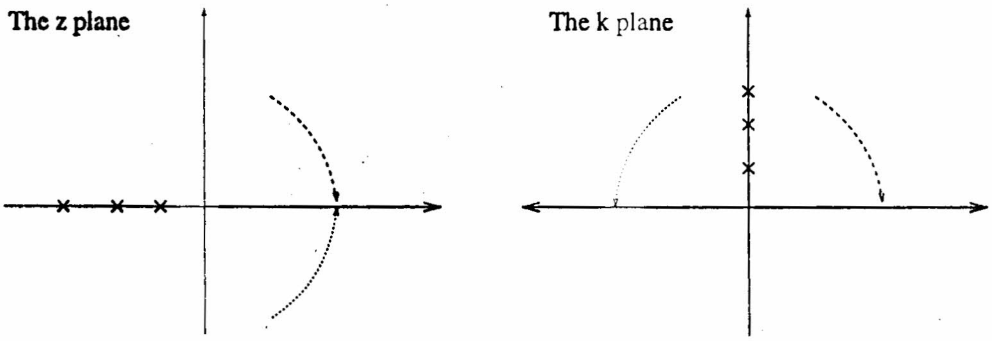
I had originally planned also to talk about some work with Peter Hislop on Laplace operators for a class of infinite volume hyperbolic manifolds. This was my original motivation for thinking about this topic. In that setting it seems more convenient to work with the scattering operator rather than with weighted resolvents. To illustrate this method, I will use the scattering operator in this paper too. I believe that this method might give better constants.

The results for Schrödinger operators that I will talk about are due to Melrose, Zworski, Vodev and others. Two general references that I can recommend are Melrose's book *Geometric Scattering Theory* [Mel] and Zworski's review article [Z1].

1. Definition of resonances

The resolvent $(H-z)^{-1}$ of a selfadjoint operator H blows up in the operator topology as z approaches the spectrum. However, when considered in a different topology, the resolvents of certain operators not only have limits onto a line of continuous spectrum, but have meromorphic continuations across this line. Poles in this continuation are called resonances. Since poles in the resolvent in the original region of definition correspond to eigenvalues, resonances can be thought of as generalized eigenvalues.

The spectrum of a Schrödinger operator with compactly supported potential consists of the positive axis together with finitely many eigenvalues on the negative axis. Thus the resolvent $(H-z)^{-1}$ is a meromorphic function on the complex plane cut along the positive real axis. The poles occur at the eigenvalues. Since the Riemann surface for Schrödinger operators in odd dimensions turns out to be the surface of $\sqrt{z}$, it is convenient to introduce the uniformizing variable $k^2 = z$. We make the convention that the upper half plane $\operatorname{Im} k > 0$ corresponds to the original cut plane (the "physical sheet"). On the k plane, eigenvalues lie on the positive imaginary axis. The two sides of the cut on the z plane become the postive and negative real axes on the k plane.



Define the resolvent $R(k) = (H-k^2)^{-1}$ and the free resolvent $R_0(k) = (-\Delta - k^2)^{-1}$. The Greens functions $G(x,y,k)$ and $G_0(x,y,k)$ are defined to be the integral kernels for the resolvent operators. As a first definition, we will say that a resonance is a pole in the meromorphic continuation of $G(x,y,k)$.

To get a feeling for this, let us compute the free Greens function.

$$G_0(x,y,k) = (2\pi)^{-n} \int_{\mathbf{R}^n} e^{-i\langle\xi,x-y\rangle} \frac{1}{|\xi|^2 - k^2} d^n\xi$$
$$= \frac{i}{4}\left(\frac{k}{2\pi|x-y|}\right)^{(n-2)/2} H^{(1)}_{(n-2)/2}(k|x-y|)$$

Here $H^{(1)}_{(n-2)/2}$ denotes a Hankel function of the first kind. It has a logarithmic singularity if n is even. From now on, we will assume that n is odd. For $n = 1$ and $n = 3$ the expression above simplifies and we obtain

$$G_0(x,y,k) = \begin{cases} \frac{i}{2k} e^{ik|x-y|} & \text{if} \quad n=1 \\ \frac{1}{4\pi|x-y|} e^{ik|x-y|} & \text{if} \quad n=3 \end{cases}$$

This calculation shows that there are no resonances when $V = 0$.

It is convenient to adopt a slightly different definition of resonances. Let χ_1 and χ_2 be functions with compact support. Then the operator $\chi_1 R_0(k)\chi_2$ has integral kernel $\chi_1(x)G_0(x,y,k)\chi_2(y)$. This operator can be analytically continued into the lower half plane, using the continuation of the kernel. Note however that in the lower half plane the middle factor grows exponentially in $|x-y|$, so the continuation cannot be interpreted as an operator product. We can now define resonances as poles in the continuation of $\chi_1 R(k)\chi_2$, whenever this exists. It is convenient to take the potential itself as a weight. Define $V^{\frac{1}{2}} = \operatorname{sgn}(V)|V|^{\frac{1}{2}}$.

Definition: A *resonance* is a pole in the meromorphic continuation of the compact operator valued function

$$R_V(k) = V^{\frac{1}{2}} R(k)|V|^{\frac{1}{2}}$$

As we will see, when V has compact support (or is super-exponentially decreasing) $R_V(k)$ has a continuation to the whole complex plane. If V is decreasing at some fixed exponential rate, the continuation can be made to a strip but (probably) no futher. Given a connected set containing the upper half space, is there a potential V with this set as the domain of meromophicity of $R_V(k)$? It seems like one can use inverse theory to show the existence of such a potential [Ma]. However doesn't seem easy to find out much the potential's properties, such as the decay at infinity.

There are many other definitions of resonances in the literature. The theory of dilation analyticity and translation analyticity gives rise to definitions that do not require the potentials to lie in such a restrictive class. They also correspond to certain exponentially growing solutions of the Schrödinger equation.

Resonances can also be defined as poles in the continuation of the scattering operator. We will show below why this definition co-incides with the one we made above.

2. The counting function

How are properties of V reflected in the locations of the resonances? This is a subject with a huge literature. However, since resonances close to the real axis are the ones that can be measured in experiments, interest has focussed on these. Results on the asymptotic number of resonances for large $|k|$ are comparitively more recent. They were perhaps motivated by analogous results for obstacle scattering, on which there is a large literature, or even by analogous questions for hyperbolic Laplacians, motivated by analytic number theory.

The counting function is defined by

$$n(r) = \#\{\text{resonances } k : |k| < r\}$$

The large r behaviour gives the asymptotic density of resonances. In this lecture I want to survey what is known for $n(r)$ for Schrödinger operators in odd dimensions. Here is an outline.

When $n = 1$ and V has compact support

$$n(r) = \frac{2}{\pi}\text{diam}(\text{supp}(V))r + o(r).$$

This result is due to Zworski [Z2]. For some super-exponentially decaying potentials there is a comparible result [F]

$$n(r) = Cr^{\rho} + o(r^{\rho}),$$

where ρ is the order of growth of the Fourier transform of V. For a class of radially symmetric potentials in dimensions greater than one Zworski [Z3] proves

$$n(r) = C_n \text{radius}(\text{supp}(V))r^n + o(r^n).$$

This exhausts the examples of Schrödinger operators for which the first term in an asymptotic expansion is known.

For a general C_0^∞ potential in dimensions greater than one, only upper bounds are known:

$$n(r) \leq Cr^n.$$

The first polynomial bound (r^{n+1}) was obtained by Melrose [Me2]. The sharp bound (r^n) was first obtained by Zworski [Z4], with additional work by Vodev [V]. A variation on the techniques used for these bounds can also give bounds on super-exponentially decaying potentials in terms of the growth of the Fourier transform of V. We will show that if $\widehat{V}(k)$ grows like $e^{\Phi(|k|)}$, then

$$n(r) \leq C\Phi^n(cr).$$

There are no lower bounds for a general C_0^∞ potential in dimensions greater than one. For $n = 3$ it is known that there are infinitely many resonances [SZ]. This is also known for potentials with some positivity conditions [CPS]. However, for a general C_0^∞ potential in dimensions other than one and three it is not been proved that a single resonance exists!

3. Birman–Schwinger identities

Now we will use some Birman-Schwinger identities to prove that $R_V(k)$ has a meromorphic continuation. For $\operatorname{Im} k > 0$, begin with the resolvent formula

$$R_0(k) - R(k) - R(k)VR_0(k) = 0$$

and multiply on the left with $V^{\frac{1}{2}}$ and on the right with $|V|^{\frac{1}{2}}$. Recall that $R_V(k) = V^{\frac{1}{2}}R(k)|V|^{\frac{1}{2}}$ and define $R_{0V}(k) = V^{\frac{1}{2}}R_0(k)|V|^{\frac{1}{2}}$. Then this equation reads

$$R_{0V}(k) - R_V(k) - R_V(k)R_{0V}(k) = 0.$$

Thus

$$(1 - R_V(k))(1 + R_{0V}(k)) = 1$$

For $\operatorname{Im} k$ large norm of $R_{0V}(k)$ is small, so $(1 + R_{0V}(k))$ is invertible and

$$1 - R_V(k) = (1 + R_{0V}(k))^{-1}$$

The important feature of this equation is that left side only involves the operator $R_{0V}(k)$ which has an explicit integral kernel with an explicit analytic continuation. This analytic continuation defines a compact operator on the whole complex plane (except for a pole at zero in dimension 1). Thus, by analytic Fredholm theory, the left side of this formula defines a meromorphic continuation for $R_V(k)$.

From this formula we can see that the resonances are precisely those values of k for which $R_{0V}(k)$ has an eigenvalue -1. Equivalently, resonances are precisely the zeros of the analytic function $\det(1+R_{0V}(k))$—provided $R_{0V}(k)$ is trace class. Unfortunately, this only happens when $n=1$.

In higher dimensions, it turns out that $R_{0V}^p(k)$ for $p > n/2$ is trace class. If -1 is an eigenvalue for $R_{0V}(k)$, then it is also an eigenvalue for $R_{0V}^p(k)$ for p odd. Thus the set of resonances is contained in the set of zeros of the function $\det(1+R_{0V}^p(k))$ for $p > n/2$ and odd. This function is entire, except for poles arising from eigenvalues. One can therefore estimate the number of resonances by estimating the growth of this function. This is the approach of previous work. Instead of this we will consider the determinant of the scattering operator. I suspect that if one kept track of the constants this method would give a better result, since by taking the pth power one is forced to overcount.

4. Green's function identities

We will need the classical Green's function identity

$$G_0(x,y,k) - G_0(x,y,-k) = \frac{i\pi k^{n-2}}{(2\pi)^n} \int_{S^{n-1}} e^{ik\langle\omega,x-y\rangle} d\omega. \tag{4.1}$$

Here is a formal derivation starting with the expression for G_0 as a Fourier transform, written in polar co-ordinates. For $\operatorname{Im} k > 0$

$$G_0(x,y,k) = (2\pi)^{-n} \int_{S^{n-1}} \int_0^\infty e^{i\rho\langle\omega,x-y\rangle} \frac{1}{\rho^2 - k^2} \rho^{n-1} d\rho d\omega.$$

When k is just above the positive real axis, we deform the ρ contour into the lower half plane close to k. Then we may move k right onto the positive real axis. Similarly, if k is just above the negative real axis, we deform the contour upwards near $-k$ and move k onto the negative real axis. Subtracting this two expressions, we that for k real,

$$G_0(x,y,k) - G_0(x,y,-k) = (2\pi)^{-n} \int_{S^{n-1}} \oint_\Gamma e^{i\rho\langle\omega,x-y\rangle} \frac{1}{\rho^2 - k^2} \rho^{n-1} d\rho d\omega,$$

where Γ is a contour enclosing k. This is easily evaluated by residues to give the desired formula.

The reason why this derivation is formal is that the integral defining G_0 is divergent for large ρ. This can be remedied by thinking of it as a distributional Fourier transform, or by starting with powers of the resolvent (see [Me1]).

Let π_k denote the operator that takes a function on $\mathbb{R}^n$ to its Fourier transform restricted to a sphere of radius k. Using this notation, the identity (4.1) for real k can be written as an operator equation

$$R_0(k) = R_0(-k) + c(k)\pi_k^*\pi_k.$$

where

$$c(k) = \frac{i\pi k^{n-2}}{(2\pi)^n}.$$

This has to be interpreted as an equation involving operators between Besov spaces, since none of the operators are bounded on $L^2(\mathbb{R}^n)$ for real k. However, if we multiply on the left by $V^{\frac{1}{2}}$ and on the right by $|V|^{\frac{1}{2}}$ then we do obtain an equation involving operators on $L^2(\mathbb{R}^n)$, namely

$$R_{0V}(k) = R_{0V}(-k) + c(k)F_V^T(k)F_{|V|}(k) \tag{4.2}$$

where the operator $F_{|V|}(k) : L^2(\mathbb{R}^n) \to L^2(S^{n-1})$ is the formal product $\pi_k|V|^{\frac{1}{2}}$ is given by

$$\left(F_{|V|}(k)\psi\right)(\omega) = \int_{\mathbb{R}^n} e^{ik\langle x,\omega\rangle}|V|^{\frac{1}{2}}(x)\psi(x)d^nx,$$

the operator $F_V^T(k) : L^2(S^{n-1}) \to L^2(\mathbb{R}^n)$ is the formal product $V^{\frac{1}{2}}\pi_k^*$ given by

$$\left(F_V^T(k)\phi\right)(x) = V^{\frac{1}{2}}(x)\int_{S^{n-1}} e^{ik\langle x,\omega\rangle}\phi(\omega)d\omega$$

Since all the operators in the equation (4.2) have analytic continuations to complex k, the equation remains valid for all $k \in \mathbb{C}$.

5. Connection with the scattering operator

Recall that resonances are exactly the values of k in the lower half plane for which $1 + R_{0V}(k)$ has a non-trival kernel. However in dimension higher than one we can't take the determinant because $R_{0V}(k)$ is not trace class. One possibility to remedy this is to multiply $1 + R_{0V}(k)$ by a suitable invertible operator and then take the determinant. For k in the lower half plane, $-k$ is in the upper half plane, and so $(1 + R_{0V}(-k))$ is invertible except at the finitely many eigenvalues of the $-\Delta+V$. We will therefore consider

$(1+R_{0V}(-k))^{-1}(1+R_{0V}(k))$. (The disadvantage of this regularization is that we have introduced infinitely many poles in the upper half plane, and will be forced to work in a half plane.) Using (4.2) this can be rewritten

$$
\begin{aligned}
(1+R_{0V}(-k))^{-1}(1+R_{0V}(k)) &= (1+R_{0V}(-k))^{-1}(1+R_{0V}(-k)+c(k)F_V^T(k)F_{|V|}(k)) \\
&= 1+c(k)(1+R_{0V}(-k))^{-1}F_V^T(k)F_{|V|}(k)) \\
&= 1+c(k)(1-R_V(-k))F_V^T(k)F_{|V|}(k)
\end{aligned}
$$

It follows from the estimates on singular values below that the second term on the left side is trace class, so we may take the determinant. Using the identity $\det(1+AB)=\det(1+BA)$ gives

$$\det((1+R_{0V}(-k))^{-1}(1+R_{0V}(k))) = \det(1+c(k)F_{|V|}(k)(1-R_V(-k))F_V^T(k)).$$

The operators on the left are now operators on $L^2(S^{n-1})$. Now

$$c(k)F_{|V|}(k)(1-R_V(-k))F_V^T(k) = c(k)\pi_k(V-VR(-k)V)\pi_k^*,$$

which is exactly the expression from stationary scattering theory for the T matrix defined by $1-S(k)$ where $S(k)$ is the scattering operator. Thus

$$\det(1+R_{0V}(-k))^{-1}(1+R_{0V}(k)) = \det(S(-k)),$$

and we find that resonances correspond to zeros of $S(k)$ in the upper half plane.

We can see from these formulas that zeros of $S(k)$ in the upper half plane correspond to poles in the lower half plane. This also follows from the equation $S(k)S(-k)=1$.

6. Upper bounds

We now need to count the zeros of the determinant of the scattering operator in a half-disk in the upper half plane. Thus we are counting the zeros of a function of the form

$$\phi(k) = \det(S(k)) = \det(1+T(k))$$

where

$$T(k) = c(-k)F_{|V|}(-k)(1-R_V(k))F_V^T(-k)$$

We will show below that $T(k)$ is a trace-class operator valued analytic function in the upper half plane. When s is real, $1+T(s)$ is unitary. Moreover $T(0)=0$.

Lemma 6.1 *Let $\phi(k) = \det(1+T(k))$ where $T(k)$ is a trace-class operator valued analytic function in the closed upper half plane, where $1 + T(s)$ is unitary for $s \in \mathbb{R}$, and where $T(0) = 0$. Let $n(t)$ denote the number of zeros of $\phi(k)$ in a half disk in the upper half plane of radius t. Define*

$$N(r) = \int_0^r \frac{n(t)}{t} dt.$$

Then

$$N(r) \leq \frac{1}{2\pi} \int_0^r t^{-1} \int_{-t}^t \|T'(s)\|_1 ds dt + \frac{1}{2\pi} \int_0^\pi \ln |\phi(re^{i\theta})| d\theta$$

Here $\|\cdot\|_1$ denotes the trace norm.

Proof: Integrating along a contour enclosing the half disk, we have

$$\begin{aligned}
n(t) &= \frac{1}{2\pi i} \oint \frac{\phi'(k)}{\phi(k)} dk \\
&= \frac{1}{2\pi} \operatorname{Im} \int_{-t}^t \frac{\phi'(s)}{\phi(s)} ds + \frac{1}{2\pi} \int_0^\pi t \frac{d}{dt} \ln |\phi(te^{i\theta})| d\theta \\
&\leq \frac{1}{2\pi} \int_{-t}^t |\phi'(s)| ds + \frac{1}{2\pi} \int_0^\pi t \frac{d}{dt} \ln |\phi(te^{i\theta})| d\theta
\end{aligned}$$

We used the fact that $|\phi(s)| = 1$ for real s. We are ignoring the finitely many poles, as these don't affect the counting function. Dividing by t and integrating, we find

$$N(r) \leq \frac{1}{2\pi} \int_0^r t^{-1} \int_{-t}^t |\phi'(s)| ds dt + \frac{1}{2\pi} \int_0^\pi \ln |\phi(re^{i\theta})| d\theta$$

We used $\phi(0) = 1$ to evaluate the second term. Since $\phi'(s) = \phi(s)\operatorname{tr}((1 + T(s))^{-1}T'(s))$, and $|\phi(s)| = \|(1 + T(s))^{-1}\| = 1$ for real s, it follows that for real s

$$\begin{aligned}
|\phi'(s)| &\leq \|((1 + T(s))^{-1}T'(s)\|_1 \\
&\leq \|(1 + T(s))^{-1}\| \|T'(s)\|_1 \\
&= \|T'(s)\|_1.
\end{aligned}$$

This completes the proof. □

This lemma shows that to estimate $N(r)$, we must estimate the trace norm of T' along the real axis, and the growth of ϕ in the upper half plane.

Lemma 6.2 *Let V be a super-exponentially decaying potential. Then for $s \in \mathbb{R}$*

$$\|T'(s)\|_1 \leq C|s|^{n-2}$$

Proof: The operator $T(s)$ is a product $c(s)F_{|V|}(s)(1 - R_V(-s))F_V^T(s)$. We estimate each term and its derivative. To begin, we have

$$|c(s)| \leq C|s|^{n-2}$$
$$|c'(s)| \leq C|s|^{n-3}$$

It follows from the (generalized) limiting absorption principle [JMP] that

$$\|1 - R_V(-s)\| \leq C$$
$$\|R_V'(-s)\| \leq C$$

Using the explicit integral kernels for $F_V^T(s)$ and $F_{|V|}(s)$ it easy to estimate the Hilbert-Schmidt norms

$$\|F_V^T(s)\|_2^2 = \int_{S^{n-1}}\int_{\mathbb{R}^n} |e^{is\langle\omega,x\rangle}V^{\frac{1}{2}}(x)|^2 dx d\omega \leq C$$
$$\|F_V^{T\prime}(s)\|_2^2 = \int_{S^{n-1}}\int_{\mathbb{R}^n} |i\langle\omega,x\rangle e^{is\langle\omega,x\rangle}V^{\frac{1}{2}}(x)|^2 dx d\omega \leq C.$$

The same estimates hold for $\|F_{|V|}(s)\|_2$ and $\|F_{|V|}'(s)\|_2$. The proof is completed by using the Leibnitz rule to write $T'(s)$, and the estimate

$$\|AB\|_1 \leq \|A\|_2^{\frac{1}{2}}\|B\|_2^{\frac{1}{2}}$$

□

It remains to estimate the growth of $\phi(k)$ for complex k.

Lemma 6.3 *Suppose that the Fourier transform of V satisfies the growth estimate*

$$\widehat{V}(z) \leq Ce^{\Phi(|z|)}$$

for some positive, increasing function $\Phi(x)$. Then

$$|\phi(k)| \leq e^{\delta^{-(n-1)}\Phi^n((2+\epsilon)|k|)+O(\Phi^{n-1}((2+\epsilon)|k|))}$$

for any $\epsilon > 0$, and some constant C.

Proof: We will use Weyl's estimate

$$|\phi(k)| = |\det(1+T(k))| \leq \prod_j (1+\mu_j(T(k)))$$

and therefore must estimate the singular values of $T(k)$. Using the estimate

$$\mu_j(AB) \leq \|A\|\mu_j(B)$$

and

$$\mu_j(AB) = \mu_j(BA)$$

(twice) we find

$$\begin{aligned}\mu_j(T(k)) &\leq \|c(-k)(1 - R_V(k)\|\mu_j(F_V^T(-k)F_{|V|}(-k)) \\ &\leq C|k|^{n-2}\mu_j(\mathbf{V}_k).\end{aligned} \tag{6.1}$$

Where the operator $\mathbf{V}_k = F_{|V|}(-k)F_V^T(-k)$ is an integral operator on $L^2(S^{n-1})$ with integral kernel $\widehat{V}(-k(\omega - \omega'))$. To estimate the singular values we will use the following bound without proof. (It follows from the analyticity of $\widehat{V}$.) Let L_ω denote the positive Laplacian on S^{n-1} in the variables ω. Then for any $\epsilon > 0$ there is a constant C such that

$$|L_\omega^{p/2}\widehat{V}(k(\omega - \omega'))| \leq C^p p! e^{\Phi((2+\epsilon)|k|)}$$

Summing the Taylor expansion for the exponential, this gives, for $\delta < C^{-1}$,

$$|e^{\delta L_\omega^{\frac{1}{2}}}\widehat{V}(k(\omega - \omega'))| \leq (1 - \delta C)^{-1}e^{\Phi((2+\epsilon)|k|)}$$

Since the left side is the integral kernel for the operator $e^{\delta L_\omega^{\frac{1}{2}}}\mathbf{V}_k$, this implies that

$$\|e^{\delta L_\omega^{\frac{1}{2}}}\mathbf{V}_k\| \leq Ce^{\Phi((2+\epsilon)|k|)}$$

(The constants C may change from line to line.) Thus

$$\begin{aligned}\mu_j(\mathbf{V}_k) &= \mu_j(e^{-\delta L_\omega^{\frac{1}{2}}}e^{\delta L_\omega^{\frac{1}{2}}}\mathbf{V}_k) \\ &\leq \|e^{\delta L_\omega^{\frac{1}{2}}}\mathbf{V}_k\|\mu_j(e^{-\delta L_\omega^{\frac{1}{2}}}) \\ &\leq Ce^{\Phi - \delta j^{1/(n-1)}}\end{aligned}$$

Using (6.1), we get the same bound for $\mu_j(T(k))$, if we increase ϵ slightly. Thus

$$|\det(1 + T(k))| \leq \prod(1 + Ce^{\Phi - \delta j^{1/(n-1)}}).$$

This product is easily estimated by breaking it into two pieces. For $j \leq (\Phi/\delta)^{n-1}$ we obtain

$$\begin{aligned}\prod_{j \leq (\Phi/\delta)^{n-1}}(1 + Ce^{\Phi - \delta j^{1/(n-1)}}) &\leq \prod_{j \leq (\Phi/\delta)^{n-1}}(C+1)e^{\Phi - \delta j^{1/(n-1)}} \\ &= (C+1)^{(\Phi/\delta)^{n-1}}e^{\Phi^n/\delta^{n-1}}\exp\left(\sum_{j=1}^{(\Phi/\delta)^{n-1}} -\delta j^{1/(n-1)}\right) \\ &= e^{\Phi^n/\delta^{n-1} + O(\Phi^{n-1})}\end{aligned}$$

For $j > (\Phi/\delta)^{n-1}$ we have

$$\prod_{j>(\Phi/\delta)^{n-1}} (1+Ce^{\Phi-\delta j^{1/(n-1)}}) \le \exp\Big(\sum_{j>(\Phi/\delta)^{n-1}} Ce^{\Phi-\delta j^{1/(n-1)}}\Big)$$
$$\le \exp\Big(Ce^{\Phi} \sum_{j>(\Phi/\delta)^{n-1}} e^{-\delta j^{1/(n-1)}}\Big)$$

The sum appearing in this formula can be estimated by an integral.

$$\sum_{j>(\Phi/\delta)^{n-1}} e^{-\delta j^{1/(n-1)}} \le e^{-\delta(\Phi/\delta)} + \int_{(\Phi/\delta)^{n-1}}^{\infty} e^{-\delta x^{1/(n-1)}}\,dx$$
$$\le e^{-\Phi} + Ce^{-\Phi}\Phi^{n-2}$$

Thus the product for large j satisfies the bound

$$\prod_{j>(\Phi/\delta)^{n-1}} (1+Ce^{\Phi-\delta j^{1/(n-1)}}) \le e^{C\Phi^{n-2}}.$$

Combining the estimates for small and large j completes the proof.

□

We can now prove the promised upper bound on the counting function.

Theorem 6.4 *Suppose that V is a super-exponentially decaying potential with*

$$\widehat{V}(z) \le Ce^{\Phi(|z|)}$$

Then

$$n(r) \le C\Phi^n(cr) + O(\Phi^{n-1}(cr))$$

for some constants c and C.

Proof: It follows from the previous lemmas that

$$N(r)$$
$$\le C\int_0^r t^{-1}\int_{-t}^{t} |s|^{n-2}ds dt + (2\pi)^{-1}\int_0^{\pi}\Big(\delta^{-(n-1)}\Phi^n((2+\epsilon)r) + O(\Phi^{n-1}((2+\epsilon)r))\Big)\,d\theta$$
$$\le Cr^{n-1} + 2^{-1}\delta^{-(n-1)}\Phi^n((2+\epsilon)r) + O(\Phi^{n-1}((2+\epsilon)r))$$

By looking at $\widehat{V}$ along the imaginary axis, we see that Φ must grow at least as fast as r. (For compactly supported V's we have $\Phi(r) = Cr$.) Thus we can ignore the first term. This gives

$$N(r) \le 2^{-1}\delta^{-(n-1)}\Phi^n((2+\epsilon)r) + O(\Phi^{n-1}((2+\epsilon)r))$$

To get an estimate on $n(r)$ from this, note that for any $s > 1$, since $n(r)$ is monotone,

$$\begin{aligned} n(r) &= n(r)(\ln s)^{-1} \int_r^{sr} \frac{1}{t} dt \\ &\leq (\ln s)^{-1} \int_r^{sr} \frac{n(t)}{t} dt \\ &= (\ln s)^{-1}(N(sr) - N(r)) \\ &\leq (\ln s)^{-1} N(sr). \end{aligned}$$

This completes the proof. □

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ON THE NORM ESTIMATE OF THE DIFFERENCE BETWEEN THE KAC OPERATOR AND THE SCHRÖDINGER SEMIGROUP

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ABSTRACT. An L^p operator norm estimate of the difference between the Kac operator and the Schrödinger semigroup is proved and used to give a variant of the Trotter product formula for Schrödinger operators in the L^p operator norm. The method of the proof is probabilistic based on the Feynman–Kac formula.
Keywords. Schrödinger operator, Kac operator

1. INTRODUCTION

The aim of this note is to review our recent results in [6] on the estimate in the L^p operator norm of the difference between the Kac operator $e^{-tV/2}e^{-tH_0}e^{-tV/2}$ and the Schrödinger semigroup $e^{-tH} = e^{-t(H_0+V)}$, where $H = H_0 + V \equiv -\frac{1}{2}\Delta + V$ is the nonrelativistic Schrödinger operator with mass 1 and scalar potential $V(x)$, a real-valued continuous function bounded below, in the space $L^p(\mathbf{R}^d)$, $1 \leq p \leq \infty$, and also in the Banach space $C_\infty(\mathbf{R}^d)$ of the continuous functions in $\mathbf{R}^d$ vanishing at infinity. Here as the Kac operator we mention the transfer matrix for a Kac model [10] in statistical mechanics associated with a potential $V(x)$. The operator norm of this difference is estimated by a power of small $t > 0$ with order greater than or equal to 1. As a by-product a variant of the Trotter product formula for the nonrelativistic Schrödinger operator in the L^p operator norm is obtained.

Helffer ([4],[5]) was the first to treat this problem in L^2, when $V(x)$ is a C^∞-function in $\mathbf{R}^d$ bounded below by a constant b and satisfying $|\partial^\alpha V(x)| \leq C_\alpha(1+x^2)^{(2-|\alpha|)_+/2}$ for every multi-index α where $a_+ = \max\{a, 0\}$, in order to relate in some asymptotic limit the spectral properties of the Kac operator to those of the nonrelativistic Schrödinger operator $-\frac{1}{2}\Delta + V$.

In this note we want to give some essential ideas of our result [6] for the nonrelativistic Schrödinger operator with an outline of proof. For a related L^2 result with operator-theoretic methods, we also refer to Doumeki–Ichinose–Tamura [2], where the problem in the trace norm is also treated.

The analogous result for the relativistic Schrödinger operator $H^r = H_0^r + V \equiv \sqrt{-\Delta+1} - 1 + V$ we announce here is new. In this case the operator norm of the difference between the Kac operator and the relativistic Schrödinger semigroup reveals a slightly different behavior for small $t > 0$, compared with the nonrelativistic case.

The results, Theorems 2.1 and 2.2 for the nonrelativistic case and Theorems 2.3 and 2.4 for the relativistic case, are stated in Section 2. Section 3 gives the proof for the nonrelativistic case. The proof for the relativistic case will be given elsewhere.

2. Statement of the Results

To formulate our theorems we want to consider the nonrelativistic Schrödinger operator

$$H = H_0 + V \equiv -\tfrac{1}{2}\Delta + V \tag{2.1}$$

and the relativistic Schrödinger operator

$$H^r = H_0^r + V \equiv \sqrt{-\Delta+1} - 1 + V \tag{2.2}$$

with mass 1 and scalar potential $V(x)$, not only in $L^2 = L^2(\mathbf{R}^d)$ but also in $L^p = L^p(\mathbf{R}^d)$, $1 \le p \le \infty$, and also in the Banach space $C_\infty = C_\infty(\mathbf{R}^d)$ of the continuous functions in $\mathbf{R}^d$ vanishing at infinity, equipped with L^∞ norm.

If $V(x)$ is a real-valued locally square-integrable function in $\mathbf{R}^d$ and bounded below, both H and H^r are essentially selfadjoint on $C_0^\infty = C_0^\infty(\mathbf{R}^d)$, which is shown by use of Kato's inequality (Kato [11], Ichinose–Tsuchida [9]). So their unique selfadjoint extensions are also denoted by the same $H = H_0 + V$ and $H^r = H_0^r + V$.

Then their semigroups e^{-tH} and e^{-tH^r} have the following path integral representations (e.g. Simon [13], Ichinose–Tamura [8]):

$$\left(e^{-tH}f\right)(x) = E_x[\exp\left(-\int_0^t V(X(s))ds\right) f(X(t))], \tag{2.3}$$

$$\left(e^{-tH^r}f\right)(x) = E_x^r[\exp\left(-\int_0^t V(X(s))ds\right) f(X(t))], \tag{2.4}$$

for $f \in L^2$. Here E_x (*resp.* E_x^r) means the expectation or integral with respect to the probability measure μ_x (*resp.* λ_x) on the space of the continuous (*resp.* right-continuous) paths $X : [0,\infty) \to \mathbf{R}^d$ starting at $X(0) = x$ such that

$$E_x[e^{ip(X(t)-x)}] = \exp(-\tfrac{1}{2}tp^2), \tag{2.5}$$

$$E_x^r[e^{ip(X(t)-x)}] = \exp(-t(\sqrt{p^2+1}-1)). \tag{2.6}$$

The measure μ_x is the Wiener measure and (2.3) is called the Feynman–Kac formula, while the measure λ_x is the probability measure associated with a Lévy process with characteristic function (2.6).

We can see via (2.3) and (2.4) that the operators e^{-tH} and e^{-tH^r} defined as bounded operators on L^2 extend from $L^p \cap L^2$ to bounded operators on L^p for $1 \le p < \infty$ (cf. Simon [14]). Both e^{-tH} and e^{-tH^r} are strongly continuous semigroups obeying

$$\|e^{-tH}f\|_p \le e^{-tb}\|f\|_p, \tag{2.7}$$

$$\|e^{-tH^r}f\|_r \le e^{-tb}\|f\|_p, \tag{2.8}$$

for $f \in L^p$, $1 \le p < \infty$. We denote also the generators H_p and H_p^r of these semigroups in L^p by the same $H = H_0 + V$ and $H^r = H_0^r + V$. When $p = \infty$, e^{-tH} and e^{-tH^r} are defined on L^∞ as the duals of the L^1 operators. They are not strongly continuous, but (2.7) and (2.8) hold for the $p = \infty$ operators. The $p = \infty$ operators H_∞ and H_∞^r are the adjoints of the $p = 1$ operators H_1 and H_1^r, respectively.

In addition, if $V(x)$ is continuous, (2.3) and (2.4) define as well the strongly continuous semigroups e^{-tH} and e^{-tH^r} on C_∞ obeying (2.7) and (2.8).

In the following, $\|\cdot\|_{p\to p}$ stands for the operator norm of bounded operators on L^p, $1 \le p \le \infty$, or on C_∞.

THEOREM 2.1. *(The nonrelativistic case) Let $0 < \delta \le 1$. Let m be a nonnegative integer such that $m\delta < 1$ and $(m+1)\delta \ge 1$. Suppose that $V(x)$ is a C^m-function in $\mathbf{R}^d$ bounded below by a constant b which satisfies that*

$$|\partial^\alpha V(x)| \le C(V(x) - b + 1)^{1-|\alpha|\delta}, \quad 0 \le |\alpha| \le m, \tag{2.9}$$

with a constant $C > 0$, and further that $\partial^\alpha V(x), |\alpha| = m$, are Hölder-continuous:

$$|\partial^\alpha V(x) - \partial^\alpha V(y)| \le C|x-y|^\kappa, \quad x, y \in \mathbf{R}^d, \tag{2.10}$$

with constants $C > 0$ and $0 \le \kappa \le 1$ (By $\kappa = 0$ we understand $\partial^\alpha V(x)$, $|\alpha| = m$, bounded). Then it holds that, as $t \downarrow 0$,

$$\|e^{-tV/2}e^{-tH_0}e^{-tV/2} - e^{-t(H_0+V)}\|_{p\to p} = \begin{cases} O(t^{1+(m+\kappa)/2}), & m = 0, 1, \\ O(t^{1+2\delta}), & m \ge 2. \end{cases} \tag{2.11}$$

Note that the condition (2.10) with $\kappa = 1$ is equivalent to that $\partial^\alpha V(x)$, $|\alpha| = m+1$, are essentially bounded.

An immediate consequence of Theorem 2.1 with telescoping is the following variant of the Trotter product formula.

THEOREM 2.2. *(The nonrelativistic case) For the same function $V(x)$ as in Theorem 2.1, it holds that, as $n \to \infty$,*

$$
\begin{aligned}
&\|(e^{-tV/2n}e^{-tH_0/n}e^{-tV/2n})^n - e^{-t(H_0+V)}\|_{p\to p} \\
&\qquad = \begin{cases} n^{-\kappa/2}O(t^{1+\kappa/2}), & m = 0, 0 < \kappa \le 1, \\ n^{-(1+\kappa)/2}O(t^{1+(1+\kappa)/2}), & m = 1, 0 \le \kappa \le 1, \\ n^{-2\delta}O(t^{1+2\delta}), & m \ge 2. \end{cases}
\end{aligned}
\tag{2.12}
$$

The method of our proof is probabilistic based on the Feynman–Kac formula.

Examples. The functions $|x|^2$ (harmonic oscillator potential) satisfies the conditions (2.9) and (2.10) for $V(x)$ in Theorem 2.1 with $(\delta, m, \kappa) = (\frac{1}{2}, 1, 1)$ or $(\frac{1}{2}, 2, 0)$, $|x|^4 - |x|^2$ (double well potential) with $(\delta, m, \kappa) = (\frac{1}{4}, 3, 1)$ or $(\frac{1}{4}, 4, 0)$, and $|x|$ with $(\delta, m, \kappa) = (1, 0, 1)$, while $|x|^{1/2}$, $|x|^{\sqrt{10}}$ satisfy the conditions (2.9) and (2.10) with $(\delta, m, \kappa) = (1, 0, \frac{1}{2}), (1/\sqrt{10}, 3, \sqrt{10} - 3)$, respectively.

Remark 1. It is Helffer [5] (cf. [4], [3]) that first proved (2.11) in the L^2 operator norm ($p = 2$), with $O(t^2)$ on the right-hand side of (2.11), by the pseudo-differential operator calculus, when $V(x)$ is a C^∞–function bounded below by b and satisfying $|\partial^\alpha V(x)| \le C_\alpha(1 + x^2)^{(2-|\alpha|)_+/2}$ for every multi-index α. In fact, as his condition implies that

$$
|\partial^\alpha V(x)| \le C(V(x) - b + 1)^{(1-|\alpha|/2)_+}
\tag{2.13}
$$

for the same α, so his result is included in the case $p = 2, (\delta, m, \kappa) = (1/2, 1, 1)$ or $(\delta, m, \kappa) = (1/2, 2, 0)$ in Theorem 2.1.

With the condition (2.13) Dia–Schatzman [1] also has recently given an operator-theoretical proof of Helffer's result.

Remark 2. Theorems 2.1 and 2.2 are valid with the operator H_0 replaced by the magnetic Schrödinger operator $H_0(A) = \frac{1}{2}(-i\partial - A(x))^2$ with vector potential $A(x)$ including the case of constant magnetic fields (see [6], cf. [2]).

Remark 3. As for the Trotter product formula in operator norm, Rogava [12] proved for nonnegative selfadjoint operators A and B in a Hilbert space that, if the domain $D[A]$ of A is included in the domain $D[B]$ of B and $A + B$ is selfadjoint on $D[A + B] = D[A] \cap D[B] = D[A]$, then, as $n \to \infty$,

$$
\|(e^{-tB/n}e^{-tA/n})^n - e^{-t(A+B)}\| = O(n^{-1/2}\ln n),
$$

$$
\|(e^{-tA/2n}e^{-tB/n}e^{-tA/2n})^n - e^{-t(A+B)}\| = O(n^{-1/2}\ln n).
$$

In this case, B is A–bounded. Notice that in our Theorems 2.1 and 2.2, neither V is H_0–bounded nor H_0 is V–bounded.

For some complementary results to Rogava's we refer to Ichinose–Tamura [7].

THEOREM 2.3. *(The relativistic case) Let $V(x)$ be the same function as in Theorem 2.1. Then it holds that, as $t \downarrow 0$,*

$$\|e^{-tV/2}e^{-tH_0^r}e^{-tV/2} - e^{-t(H_0^r+V)}\|_{p\to p} = \begin{cases} O(t^{1+\kappa}), & m = 0, 0 \le \kappa < 1, \\ O(t^2|\ln t|), & (m,\kappa) = (0,1)\, or\, (1,0), \\ O(t^2), & m = 1, 0 < \kappa \le 1, \\ O(t^{1+2\delta}), & m \ge 2. \end{cases} \tag{2.14}$$

An immediate consequence of Theorem 2.3 is the following variant of the Trotter product formula.

THEOREM 2.4. *(The relativistic case) For the same function $V(x)$ as in Theorem 2.1, it holds that, as $n \to \infty$,*

$$\begin{aligned} &\|(e^{-tV/2n}e^{-tH_0^r/n}e^{-tV/2n})^n - e^{-t(H_0^r+V)}\|_{p\to p} \\ &= \begin{cases} n^{-\kappa}O(t^{1+\kappa}), & m = 0, 0 < \kappa < 1, \\ n^{-1}O(t^2|\ln(t/n)|), & (m,\kappa) = (0,1)\, or\, (1,0), \\ n^{-1}O(t^2), & m = 1, 0 < \kappa \le 1, \\ n^{-2\delta}O(t^{1+2\delta}), & m \ge 2. \end{cases} \end{aligned} \tag{2.15}$$

We need only to prove Theorems 2.1 and 2.3. In the next section we shall give the proof of Theorem 2.1. The proof of Theorem 2.3, which needs a somewhat more elaborated treatment, will be given elsewhere.

3. Proof of Theorem 2.1

Put

$$Q(t) = e^{-tV/2}e^{-tH_0}e^{-tV/2} - e^{-t(H_0+V)}, \quad t > 0. \tag{3.1}$$

Without loss of generality, we may suppose that $V(x) \ge 1$, and the condition (2.9) holds with $b = 1$.

Since $Q(t)$ are uniformly bounded operators on L^p and C_∞ in $t > 0$, and since C_0^∞ is dense in $L^p, 1 \le p < \infty$, and C_∞ , we have only to show that for $f \in C_0^\infty$ with $||f||_p = 1$, $||Q(t)f||_p$ has the order of the power of t as in (2.11). Here note that the L^∞ case follows as the dual of the L^1 case.

By the Feynman–Kac formula (2.3) we have for $f \in C_0^\infty$

$$(Q(t)f)(x) = E_x\Big[\Big(\exp\Big(-\tfrac{t}{2}(V(x) + V(X(t)))\Big) - \exp\Big(-\int_0^t V(X(s))ds\Big)\Big)f(X(t))\Big]. \tag{3.2}$$

Let $p(t,x)$ be the heat kernel, the integral kernel of e^{-tH_0}:

$$p(t,x) = (2\pi t)^{-d/2} e^{-x^2/2t}. \tag{3.3}$$

We have

$$\int |x|^a p(t,x)dx = C(a)t^{a/2}, \tag{3.4}$$

with a constant $C(a)$ depending on $a > 0$ and the dimension d.

To avoid notational complexity, we shall assume $d = 1$; there is no essential change of the following proof in the multi-dimensional case.

We use the conditional expectation first $E_x[\,\cdot\,|X(t) = y]$ and next $E_0[\,\cdot\,|X(t) = 0]$ to rewrite (3.2) as

$$\begin{aligned}
&(Q(t)f)(x) \\
&= \int f(y)p(t,x-y)E_x[\exp\Big(-\tfrac{t}{2}(V(x)+V(y))\Big) \\
&\qquad\qquad - \exp\Big(-\int_0^t V(X(s))ds\Big)|X(t) = y]dy \\
&= \int f(y)p(t,x-y)E_0[\exp\Big(-\tfrac{t}{2}(V(x)+V(y))\Big) \\
&\qquad\qquad - \exp\Big(-\int_0^t V(x+\tfrac{s}{t}(y-x)+X(s))ds\Big)|X(t) = 0]dy \\
&= \int f(y)p(t,x-y)E_0[\exp\Big(-\tfrac{t}{2}(V(x)+V(y))\Big) \\
&\qquad\qquad - \exp\Big(-\int_0^t V(x+\tfrac{s}{t}(y-x)+X_0^{t,0}(s))ds\Big)]dy \\
&\equiv \int f(y)p(t,x-y)d(t,x,y)dy,
\end{aligned} \tag{3.5a}$$

where

$$d(t,x,y) = E_0[v(t,x,y)] \tag{3.5b}$$

with

$$\begin{aligned}
&v(t,x,y) \\
&= \exp\Big(-\tfrac{t}{2}(V(x)+V(y))\Big) - \exp\Big(-\int_0^t V(x+\tfrac{s}{t}(y-x)+X_0^{t,0}(s))ds\Big).
\end{aligned} \tag{3.5c}$$

Further, $X_0^{t,0}(s)$ in the fourth member of (3.5a) or in (3.5c) is the Brownian bridge:

$$X_0^{t,0}(s) = X(s) - \tfrac{s}{t}X(t), \quad 0 \le s \le t. \tag{3.6}$$

By Taylor's theorem

$$
\begin{aligned}
e^{-a} - e^{-b} &= -(1 - e^{a-b})e^{-a} \\
&= -\sum_{j=1}^{m} \tfrac{1}{j!}(a-b)^j e^{-a} - \tfrac{1}{m!}(a-b)^{m+1} \int_0^1 d\theta (1-\theta)^m e^{-(1-\theta)a - \theta b}.
\end{aligned}
$$

Putting

$$
\begin{aligned}
w(t,x,y) &= \tfrac{t}{2}(V(x) + V(y)) - \int_0^t V(x + \tfrac{s}{t}(y-x) + X_0^{t,0}(s))ds \\
&= -\int_0^{t/2} \left(V(x + \tfrac{s}{t}(y-x) + X_0^{t,0}(s)) - V(x)\right) ds \\
&\qquad - \int_{t/2}^{t} \left(V(y + (1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s)) - V(y)\right) ds,
\end{aligned}
\tag{3.7}
$$

this yields the following expansion of $v(t,x,y)$ in (3.5c).

$$
\begin{aligned}
& v(t,x,y) \\
&= -w(t,x,y)e^{-\frac{t}{2}(V(x)+V(y))} \\
&\quad - \sum_{j=2}^{m} \tfrac{1}{j!} w(t,x,y)^j e^{-\frac{t}{2}(V(x)+V(y))} \\
&\quad - \tfrac{1}{m!} w(t,x,y)^{m+1} \\
&\quad \times \int_0^1 d\theta (1-\theta)^m \exp\left[-(1-\theta)\tfrac{t}{2}(V(x)+V(y)) - \theta \int_0^t V(x + \tfrac{s}{t}(y-x) + X_0^{t,0}(s))ds\right] \\
&\equiv \sum_{i=1}^{3} v_i(t,x,y).
\end{aligned}
\tag{3.8}
$$

Note in (3.8) that if $m = 1$, $v_2(t,x,y)$ is absent, and if $m = 0$, both $v_1(t,x,y)$ and $v_2(t,x,y)$ are absent.

Put

$$
d(t,x,y) = \sum_{i=1}^{3} d_i(t,x,y), \tag{3.9a}
$$

$$
d_i(t,x,y) = E_0[v_i(t,x,y)], \quad i = 1,2,3. \tag{3.9b}
$$

Then the function

$$
q(t,x,y) = p(t,x-y)d(t,x,y) = \sum_{i=1}^{3} q_i(t,x,y) \equiv \sum_{i=1}^{3} p(t,x-y)d_i(t,x,y) \tag{3.10}
$$

is the integral kernel of the operator $Q(t)$ in (3.1). Here, in (3.9ab), if $m=1$, $d_2(t,x,y)$ is absent, and if $m=0$, both $d_1(t,x,y)$ and $d_2(t,x,y)$ are absent, and so are for $q_i(t,x,y)$ in (3.10).

For $m \geq 1$, we have by Taylor's theorem

$$
\begin{aligned}
V(x+z)-V(x) &= \sum_{k=1}^{m-1} \tfrac{1}{k!} z^k V^{(k)}(x) + \tfrac{1}{(m-1)!} z^m \int_0^1 d\tau (1-\tau)^{m-1} V^{(m)}(x+\tau z) \\
&= \sum_{k=1}^{m} \tfrac{1}{k!} z^k V^{(k)}(x) \\
&\qquad + \tfrac{1}{(m-1)!} z^m \int_0^1 d\tau (1-\tau)^{m-1} \big(V^{(m)}(x+\tau z) - V^{(m)}(x)\big).
\end{aligned}
$$

Applying this to the integrands of (3.7) yields

$$
\begin{aligned}
&w(t,x,y) \\
&= -\int_0^{t/2} \big(\tfrac{s}{t}(y-x) + X_0^{t,0}(s)\big) V'(x)\,ds \\
&\quad - \sum_{k=2}^{m} \tfrac{1}{k!} \int_0^{t/2} \big(\tfrac{s}{t}(y-x) + X_0^{t,0}(s)\big)^k V^{(k)}(x)\,ds \\
&\quad - \tfrac{1}{(m-1)!} \int_0^1 d\tau (1-\tau)^{m-1} \\
&\qquad \times \int_0^{t/2} \big(\tfrac{s}{t}(y-x) + X_0^{t,0}(s)\big)^m \Big(V^{(m)}\big(x + \tau(\tfrac{s}{t}(y-x) + X_0^{t,0}(s))\big) - V^{(m)}(x)\Big)\,ds \\
&\quad - \int_{t/2}^{t} \big((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s)\big) V'(y)\,ds \\
&\quad - \sum_{k=2}^{m} \tfrac{1}{k!} \int_{t/2}^{t} \big((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s)\big)^k V^{(k)}(y)\,ds \\
&\quad - \tfrac{1}{(m-1)!} \int_0^1 d\tau (1-\tau)^{m-1} \int_{t/2}^{t} \big((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s)\big)^m \\
&\qquad\qquad \times \Big(V^{(m)}\big(y + \tau((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s))\big) - V^{(m)}(y)\Big)\,ds,
\end{aligned}
\tag{3.11}
$$

where the second and fifth terms $-\sum_{k=2}^{m}$ on the right are absent if $m=1$.

It follows that

$$
w(t,x,y) = \sum_{i=1}^{4} w_i(t,x,y), \tag{3.12a}
$$

where

$$
w_1(t,x,y) = \tfrac{1}{8} t(x-y)(V'(x) - V'(y)), \tag{3.12b}
$$

$$w_2(t,x,y) = -\Big\{V'(x)\int_0^{t/2} X_0^{t,0}(s)ds + V'(y)\int_{t/2}^{t} X_0^{t,0}(s)ds\Big\}, \tag{3.12c}$$

$$\begin{aligned} w_3(t,x,y) = -\sum_{k=2}^{m} \tfrac{1}{k!}\Big\{&V^{(k)}(x)\int_0^{t/2} \big(\tfrac{s}{t}(y-x) + X_0^{t,0}(s)\big)^k ds \\ &+ V^{(k)}(y)\int_{t/2}^{t} \big((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s)\big)^k ds\Big\}, \end{aligned} \tag{3.12d}$$

$$\begin{aligned} w_4(t,x,y) = &-\tfrac{1}{(m-1)!}\int_0^1 d\tau(1-\tau)^{m-1} \\ &\times\Big\{\int_0^{t/2} (\tfrac{s}{t}(y-x) + X_0^{t,0}(s))^m \Big(V^{(m)}(x + \tau(\tfrac{s}{t}(y-x) + X_0^{t,0}(s))) - V^{(m)}(x)\Big) ds \\ &+ \int_{t/2}^{t} ((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s))^m \\ &\qquad\times \Big(V^{(m)}(y + \tau((1-\tfrac{s}{t})(x-y) + X_0^{t,0}(s))) - V^{(m)}(y)\Big) ds\Big\}, \end{aligned} \tag{3.12e}$$

where the first term $w_1(t,x,y)$ and second $w_2(t,x,y)$ come from the first and fourth terms of (3.11), and the third term $w_3(t,x,y) = -\sum_{k=2}^{m} \cdots$ is absent if $m = 1$.

According to the decomposition (3.12a) of $w(t,x,y)$ rewrite $d_1(t,x,y)$ as

$$d_1(t,x,y) = \sum_{i=1}^{4} d_{1i}(t,x,y), \tag{3.13a}$$

$$d_{1i}(t,x,y) = -E_0[w_i(t,x,y)]e^{-\frac{t}{2}(V(x)+V(y))}, \quad 1 \le i \le 4, \tag{3.13b}$$

where $d_{13}(t,x,y)$ is absent if $m = 1$.

We can use (2.9), (2.10) and that for $a > 0$

$$t^a e^{-t/2} \le \left(\tfrac{2a}{e}\right)^a, \quad t \ge 0, \tag{3.14}$$

to show the following lemma.

LEMMA 3.1. *a) If $m = 0$,*

$$|v(t,x,y)| \le |w(t,x,y)| \le C\int_0^t (|x-y| + |X_0^{t,0}(s)|)^\kappa ds. \tag{3.15}$$

b) If $m \ge 1$,

$$v_1(t,x,y) = \sum_{i=1}^{4} v_{1i}(t,x,y) \equiv -\sum_{i=1}^{4} w_i(t,x,y)e^{-\frac{t}{2}(V(x)+V(y))}, \tag{3.16a}$$

and

$$|v_{11}(t,x,y)| \le \sum_{l=2}^{m} |x-y|^l O(t^{l\delta}) + |x-y|^{m+\kappa} O(t), \tag{3.16b}$$

where if $m = 1$, *the first term* $\sum_{l=2}^{m}$ *is absent; if* $m \geq 2$,

$$|v_{13}(t,x,y)| \le \sum_{k=2}^{m} O(t^{-1+k\delta}) \int_0^t (|x-y| + |X_0^{t,0}(s)|)^k ds; \tag{3.16c}$$

if $m \geq 1$,

$$|v_{14}(t,x,y)| \le \frac{C}{m!} \int_0^t (|x-y| + |X_0^{t,0}(s)|)^{m+\kappa} ds. \tag{3.16d}$$

If $m \geq 2$,

$$\begin{aligned} |v_2(t,x,y)| \le \sum_{j=2}^{m} \{ \sum_{k=1}^{m} O(t^{-1+jk\delta}) \int_0^t (|x-y| + |X_0^{t,0}(s)|)^{jk} ds \\ + O(t^{j-1}) \int_0^t (|x-y| + |X_0^{t,0}(s)|)^{j(m+\kappa)} ds \}. \end{aligned} \tag{3.17}$$

If $m \geq 1$,

$$\begin{aligned} |v_3(t,x,y)| \le \sum_{k=1}^{m} O(t^{-1+(m+1)k\delta}) \int_0^t (|x-y| + |X_0^{t,0}(s)|)^{(m+1)k} ds \\ + O(t^m) \int_0^t (|x-y| + |X_0^{t,0}(s)|)^{(m+1)(m+\kappa)} ds. \end{aligned} \tag{3.18}$$

We give here only a few words for the proof of Lemma 3.1. (3.15) follows directly from (3.7). (3.16a), (3.16b), (3.16c) and (3.16d) follow from (3.12b), (3.12c), (3.12d) and (3.12e), respectively, while (3.17) and (3.18) are obtained by using the expression (3.7) of $w(t,x,y)$ to calculate $w(t,x,y)^j$ and $w(t,x,y)^{m+1}$.

Therefore, to prove Theorem 2.1, we need to calculate a basic quantity concerning the Brownian bridge $X_0^{t,0}$ in (3.6) in the following lemma.

LEMMA 3.2. *Let* $t \geq 0$.

$$\int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^a] ds \le \begin{cases} t|x-y|^a + \frac{4}{a+2} C(a) t^{a/2+1}, & 0 < a < 1, \\ 2^{a-1}\left(t|x-y|^a + \frac{2^{a+1}}{a+2} C(a) t^{a/2+1}\right), & a \geq 1. \end{cases} \tag{3.19}$$

Proof. Let $0 \leq s \leq t$.

For $0 < a < 1$,

$$\begin{aligned}
E_0[|X_0^{t,0}(s)|^a] &= E_0[|X(s) - X(t) + \tfrac{t-s}{t}X(t)|^a] \\
&\le E_0[|X(t) - X(s)|^a + (\tfrac{t-s}{t})^a|X(t)|^a] \\
&= \int |x|^a p(t-s,x)dx + (\tfrac{t-s}{t})^a \int |x|^a p(t,x)dx \\
&= C(a)(1 + (\tfrac{t-s}{t})^{a/2})(t-s)^{a/2} \le 2C(a)(t-s)^{a/2}.
\end{aligned}$$

We have

$$\begin{aligned}
E_0[(|x-y| + |X_0^{t,0}(s)|)^a] &\le E_0[|x-y|^a + |X_0^{t,0}(s)|^a] \\
&\le |x-y|^a + 2C(a)(t-s)^{a/2}.
\end{aligned}$$

Integrating this yields (3.19) for $0 < a < 1$.

For $a \ge 1$,

$$\begin{aligned}
E_0[|X_0^{t,0}(s)|^a] &= E_0[|X(s) - X(t) + \tfrac{t-s}{t}X(t)|^a] \\
&\le (E_0[|X(t) - X(s)|^a]^{1/a} + \tfrac{t-s}{t}E_0[|X(t)|^a]^{1/a})^a \\
&= \left[\left(\int |x|^a p(t-s,x)dx\right)^{1/a} + (\tfrac{t-s}{t})\left(\int |x|^a p(t,x)dx\right)^{1/a}\right]^a \\
&= C(a)(1 + (\tfrac{t-s}{t})^{1/2})^a(t-s)^{a/2} \le 2^a C(a)(t-s)^{a/2}.
\end{aligned}$$

We have

$$\begin{aligned}
E_0[(|x-y| + |X_0^{t,0}(s)|)^a] &\le (E_0[|x-y|^a]^{1/a} + E_0[|X_0^{t,0}(s)|^a]^{1/a})^a \\
&= (|x-y| + 2C(a)^{1/a}(t-s)^{1/2})^a \\
&\le 2^{a-1}(|x-y|^a + 2^a C(a)(t-s)^{a/2}).
\end{aligned}$$

Integrating this yields (3.19) for $a \ge 1$. This ends the proof of Lemma 3.2.

Now we complete the proof of Theorem 2.1, using Lemmas 3.1 and 3.2. To do so first we use (3.4) to get that for $a > 0$,

$$\left\| \int p(t, \bullet - y)|\bullet - y|^a |f(y)| dy \right\|_p \le C(a) t^{a/2} \|f\|_p, \qquad f \in L^p, \tag{3.20}$$

for $1 \le p \le \infty$. This is obvious for $p = \infty$ and seen for $1 \le p < \infty$ by the Hölder inequality.

Then for $m = 0$ we have from Lemma 3.1, (3.15), with Lemma 3.2, (3.19)

$$\begin{aligned}
|d(t,x,y)| = |E_0[v(t,x,y)]| &\le C \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^\kappa] ds \\
&= |x-y|^\kappa O(t) + O(t^{1+\kappa/2}).
\end{aligned} \tag{3.21}$$

Hence it follows with (3.20) that

$$\|\int |q(t,\bullet,y)||f(y)|dy\|_p \leq O(t^{1+\kappa/2})\|f\|_p. \tag{3.22}$$

For $m=1$, we have $d(t,x,y)=d_1(t,x,y)+d_3(t,x,y)$ with $d_1(t,x,y)=d_{11}(t,x,y)+d_{12}(t,x,y)+d_{14}(t,x,y)$, so that $q(t,x,y)=q_1(t,x,y)+q_3(t,x,y)$ in (3.10). We have from Lemma 3.1, (3.16b) and (3.12c) with Lemma 3.2, (3.19)

$$|d_{11}(t,x,y)|=|E_0[v_{11}(t,x,y)]|\leq |x-y|^{1+\kappa}O(t), \tag{3.23a}$$

and

$$d_{12}(t,x,y)=E_0[v_{12}(t,x,y)]=0, \tag{3.23b}$$

because $E_0[w_2(t,x,y)]=0$, which is crucial in the present work. We have from Lemma 3.1, (3.16d) and (3.18) with Lemma 3.2, (3.19)

$$\begin{aligned}|d_{14}(t,x,y)|=|E_0[v_{14}(t,x,y)]|&\leq \tfrac{C}{m!}\int_0^t E_0[(|x-y|+|X_0^{t,0}(s)|)^{1+\kappa}]ds\\&=|x-y|^{1+\kappa}O(t)+O(t^{1+(1+\kappa)/2}),\end{aligned} \tag{3.23c}$$

and

$$\begin{aligned}|d_3(t,x,y)|=|E_0[v_3(t,x,y)]|&\leq O(t^{-1+2\delta})\int_0^t E_0[(|x-y|+|X_0^{t,0}(s)|)^2]ds\\&\quad+O(t)\int_0^t E_0[(|x-y|+|X_0^{t,0}(s)|)^{2(1+\kappa)}]ds\\&=|x-y|^2O(t^{2\delta})+O(t^{1+2\delta})+|x-y|^{2(1+\kappa)}O(t^2)+O(t^{3+\kappa}).\end{aligned} \tag{3.24}$$

It follows from (3.23abc) and (3.24) by (3.10) and (3.20) that

$$\|\int |q(t,\bullet,y)||f(y)|dy\|_p \leq O(t^{1+(1+\kappa)/2})\|f\|_p. \tag{3.25}$$

For $m\geq 2$ we have from Lemma 3.1, (3.16b) and (3.12c) with Lemma 3.2, (3.19)

$$|d_{11}(t,x,y)|=|E_0[v_{11}(t,x,y)]|\leq \sum_{l=2}^m |x-y|^l O(t^{l\delta})+|x-y|^{m+\kappa}O(t), \tag{3.26a}$$

and

$$d_{12}(t,x,y)=E_0[v_{12}(t,x,y)]=0, \tag{3.26b}$$

because $E_0[w_2(t,x,y)] = 0$, which is again crucial. We have from Lemma 3.1, (3.16cd), (3.17) and (3.18) with Lemma 3.2, (3.19)

$$
\begin{aligned}
|d_{13}(t,x,y)| = |E_0[v_{13}(t,x,y)]| &\le \sum_{k=2}^{m} O(t^{-1+k\delta}) \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^k] ds \\
&= \sum_{k=2}^{m} (|x-y|^k O(t^{k\delta}) + O(t^{(1+2\delta)k/2})),
\end{aligned}
\tag{3.26c}
$$

and

$$
\begin{aligned}
|d_{14}(t,x,y)| = |E_0[v_{14}(t,x,y)]| &\le \tfrac{C}{m!} \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^{m+\kappa}] ds \\
&= |x-y|^{m+\kappa} O(t) + O(t^{1+(m+\kappa)/2}),
\end{aligned}
\tag{3.26d}
$$

$$
\begin{aligned}
|d_2(t,x,y)| &= |E_0[v_2(t,x,y)]| \\
&\le \sum_{j=2}^{m} \{ \sum_{k=1}^{m} O(t^{-1+jk\delta}) \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^{jk}] ds \\
&\quad + O(t^{j-1}) \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^{j(m+\kappa)}] ds \} \\
&= \sum_{j=2}^{m} \{ \sum_{k=1}^{m} (|x-y|^{jk} O(t^{jk\delta}) + O(t^{(1+2\delta)jk/2})) \\
&\quad + |x-y|^{j(m+\kappa)} O(t^j) + O(t^{(m+2+\kappa)j/2}) \};
\end{aligned}
\tag{3.27}
$$

$$
\begin{aligned}
|d_3(t,x,y)| &= |E_0[v_3(t,x,y)]| \\
&\le \sum_{k=1}^{m} O(t^{-1+(m+1)k\delta}) \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^{(m+1)k}] ds \\
&\quad + O(t^m) \int_0^t E_0[(|x-y| + |X_0^{t,0}(s)|)^{(m+1)(m+\kappa)}] ds \\
&= \sum_{k=1}^{m} (|x-y|^{(m+1)k} O(t^{k\delta}) + O(t^{(1+2\delta)(m+1)k/2})) \\
&\quad + |x-y|^{(m+1)(m+\kappa)} O(t^{m+1}) + O(t^{(m+1)(1+(m+\kappa)/2)}).
\end{aligned}
\tag{3.28}
$$

It follows from (3.26abcd), (3.27) and (3.28) by (3.10) and (3.20) that

$$\begin{aligned}
\| \int |q(t,\bullet,y)||f(y)|dy\|_p \le & \{\sum_{l=2}^{m} O(t^{(1+2\delta)l/2}) + O(t^{1+(m+\kappa)/2}) \\
& + \sum_{k=2}^{m} O(t^{(1+2\delta)k/2}) + O(t^{1+(m+\kappa)/2}) \\
& + \sum_{j=2}^{m+1}(\sum_{k=1}^{m} O(t^{(1+2\delta)jk/2}) + O(t^{(m+2+\kappa)j/2}))\}\|f\|_p \\
& = O(t^{1+2\delta})\|f\|_p.
\end{aligned} \tag{3.29}$$

This ends the proof of Theorem 2.1.

Remark. In view of (3.10) we have obtained, with (3.21), (3.23abc)–(3.24) and (3.26abcd)–(3.27)–(3.28) above, the estimate of the integral kernel $q(t,x,y)$ in terms of $p(t,x-y)$ times a finite positive linear combination of powers of $|x-y|$ and t.

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THE DENSITY OF STATES FOR MULTIDIMENSIONAL CONTINUOUS RANDOM SCHRÖDINGER OPERATORS WITH SINGULAR RANDOMNESS

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0. Introduction

The present paper is the text of a set of two lectures given at the Institute of Mathematical Sciences (Madras) during the conference "Spectral Theory of Schrödinger Operators". These lectures deal with the density of states for random Schrödinger operators especially in the case of singular randomness.

The motivation for the study of random Schrödinger operators comes mainly from solid state physics. These operators are the hamiltonians modeling cristals with impurities (see e.g [16] and the lectures by W. Kirsch in this volume).

This paper will deal with the d-dimensional continuous Anderson model with singular randomness. The random potentials we consider will be of Bernoulli type.

1. The continuous Anderson model - The density of states

1.1. The continuous Anderson model. Let W be a $\mathbb{Z}^d$-periodic, bounded, real-valued function on $\mathbb{R}^d$. Let us define the following periodic Schrödinger operator: $H_0 = -\Delta + W$. H_0 is essentially self-adjoint on C_0^∞, lower semi-bounded and its self-adjoint extension on $L^2(\mathbb{R}^d)$ has $H^2(\mathbb{R}^d)$ as domain. Let $\sigma(H_0)$ be the spectrum of H_0. We know that the spectrum of H is made of bands of purely absolutely continuous spectrum (cf [18] or [21]).

Let V be a function that is not identically 0 and that satisfies

$$\exists \eta > 0,\ C > 0 \text{ such that } \forall x \in \mathbb{R}^d,\ |V(x)| \leq Ce^{-\eta|x|}.$$

Let $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ be independently identically distributed (i.i.d) bounded random variables. We then consider the following random Schrödinger operator

$$H_\omega = H_0 + \sum_{\gamma\in\mathbb{Z}^d} \omega_\gamma V_\gamma \text{ where } V_\gamma(x) = V(x-\gamma). \tag{1}$$

H_ω is *the continuous Anderson model.* As the $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ are supposed to be bounded, all the possible H_ω (i.e the realizations of the Anderson model) are bounded perturbation of H_0; hence they are self-adjoint $L^2(\mathbb{R}^d)$ with domain $H^2(\mathbb{R}^d)$.

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Rather than a single operator, a random operator is a family of operators endowed with a probability structure; in the case of the Anderson model, the probability structure is the one induced by the random variables $\omega = (\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$.

Under the assumptions made above, one proves that the Anderson model is stationnary and ergodic (for a proof of these and all the following general facts, the reader may turn to the lectures by W. Kirsch in the same volume or to [17]). Ergodicity ensures the existence of a closed subset of $\mathbb{R}$ denoted by Σ such that, for almost every ω, Σ is the spectrum of H_ω. Σ is the *(almost sure) spectrum* of H_ω. The same way the spectral type of this family of operators is almost surely the same. The aim is then to understand what is the almost sure behaviour of this family.

In the sequel, we will be interested in the special case when the common law of the random variables $\omega = (\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ is a Bernoulli law. More precisely, we will assume that their common distribution law is defined by $P(\omega_0 = 1) = \mu$ and $P(\omega_0 = 0) = 1-\mu$, where μ is chosen in $(0,1)$. In this case, we will speak of the *continuous Bernoulli Anderson model.* μ is the *concentration*; it is easily seen that μ is the expectation of the number of impurities per units of volume in the Bernoulli Anderson model.

1.2. The density of states. Let $l > 0$ and Λ_l be a cube in $\mathbb{R}^d$ centered at 0 and of sidelength l. Define $H^D_{\omega,l} = H_{\omega|\Lambda_l}$ that is H_ω restricted to Λ_l with Dirichlet boundary conditions. For $\lambda \in \mathbb{R}$, define

$$(2) \qquad \mathcal{N}_l(\lambda) = \frac{1}{\mathrm{Vol}(\Lambda_l)}\#\{\lambda_n;\ \lambda_n \text{ is an eigenvalue of } H^D_l(t) \text{ and } \lambda_n \leq \lambda\}$$

and $N_l(d\lambda) = \partial_\lambda \mathcal{N}_l$, its derivative; it is a positive discrete measure on $\mathbb{R}$. Then one shows that there exists a non-random measure $N(d\lambda)$ such that, with probability 1,

$$\lim_{l\to+\infty} N_l(d\lambda) = N(d\lambda) \text{ (in the vague topology),}$$

and, one has the following formula

$$(3) \qquad N(d\lambda) = \mathbb{E}_\omega\{\mathrm{Tr}(\chi_0 E_\omega(d\lambda)\chi_0)\}$$

where $E_\omega(d\lambda)$ is the spectral resolution of H_ω, χ_0 is the characteristic function of the cube centered in 0 with sidelength 1, $\mathbb{E}_\omega$ is the average with respect to the probability measure defined by the $(t_\gamma)_{\gamma\in\mathbb{Z}^d}$ and $\mathrm{Tr}(A)$ is the trace of A. For a proof of these facts, we refer to the lectures by W. Kirsch in this volume and to [17].

$N(d\lambda)$ is the *density of states* of H_ω. It is a positive measure supported in Σ. Moreover it is a tempered distribution, that is an element of the Schwartz space S'. When dealing with the continuous Bernoulli Anderson model, we will denote the density of states by $N_\mu(d\lambda)$.

The main questions concerning this measure are

1. What is its support?
2. How regular is it?

The first question we answered already, even if only in an implicit way, as we do not know in general how to compute Σ (nevertheless see, e.g W. Kirsch's lectures, [10] or [17]). We will not dwell any longer on this question.

As for the regularity, it is the main motivation for the rest of this lecture.

2. Some known results about the regularity of N

The regularity of the density of states depends crucially on the regularity of the distribution of the random variables $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$. To underline this aspect, we will first give a heuristic proof of the Wegner estimate in the case of continuous probability distributions for the $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$, then recall some known results in the case of singular distributions.

2.1. **The Wegner estimate: a heuristic.**

A so called Wegner estimate is an estimate on

(4)
$$N_l((\lambda_0-\varepsilon,\lambda_0+\varepsilon]) = \mathbb{E}_\omega(\#\{\lambda;\ \lambda \text{ is an eigenvalue of } H^D_{\omega,l} \text{ and } \lambda\in(\lambda_0-\varepsilon,\lambda_0+\varepsilon]\})$$

for l large and ε small, when λ_0 is some fixed energy. As we already saw, when renormalized by the volume of Λ_l, this quantity converges to the integrated density of states at $\lambda_0+\varepsilon$ minus the integrated density of states at $\lambda_0-\varepsilon$. So one expects it to grow with Λ_l and decrease with ϵ (if the density of states is to be regular).

For the sake of simplicity, let us assume that the potential V has compact support in some cube centered at 0 of side length less than 1. So

$$H^D_{\omega,l} = (-\Delta)^D_l + \sum_{\gamma\in\mathbb{Z}^d\cap\Lambda_l} \omega_\gamma V_\gamma$$

where $(-\Delta)^D_l$ is the Dirichlet Laplacian in Λ_l.

So we are only left with a finite dimensional space of random parameters. Let us call these finitely many parameters $\omega=(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$. Let $(\lambda_j(\omega))_{j=1}^N$ be the eigenvalues of $H^D_{\omega,l}$ that lie in $[\lambda_0-\varepsilon_0,\lambda_0+\varepsilon_0]$ for some possible choice of ω that is for some ω in the support of the probability measure defined by the initial random variables (here $\varepsilon_0>0$ is fixed). The existence of the density of states guarantees that their number N is of order the volume of Λ_l.

We can write

$$\begin{aligned} N_l((\lambda_0-\varepsilon,\lambda_0+\varepsilon]) &= \mathbb{E}_\omega\left(\sum_{1\le j\le N}\chi_{(\lambda_0-\varepsilon,\lambda_0+\varepsilon]}(\lambda_j(\omega))\right)\\ &\le \sum_{1\le j\le N}\mathbb{P}\{\lambda_j(\omega)\in(\lambda_0-\varepsilon,\lambda_0+\varepsilon]\}. \end{aligned}$$

(here χ_A is the characteristic function of the set A and $\mathbb{P}\{E\}$ is the probability of the event E).

So we need to estimate $\mathbb{P}\{\lambda_j(\omega) \in (\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]\}$. The mapping $\omega \mapsto \lambda_j(\omega)$ realizes a projection from the parameter space onto the real axis; and we want to measure the size (with respect to the probability measure on the parameter space) of the preimage of some interval. The idea is then to find $\mathcal{V}$ a vector field in the parameters ω such that the eigenvalue $\lambda_j(\omega)$ moves when ω moves along the flow of the vector field. The flow of $\mathcal{V}$ foliates the parameter space nicely and the volume we want to measure is just the volume contained in a layer between two leaves (see figure 1). This volume will then be of size the width of this layer at least when the probability measure has a nice density. So if one is able to do this for all the eigenvalues, one gets an estimate of the form

$$N_l((\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]) \leq C\varepsilon \mathrm{Vol}(\Lambda_l).$$

To be able to do this for all eigenvalues at a time, one may choose $\mathcal{V}$ so that $H^D_{\omega,l}$ derivated along $\mathcal{V}$ has nice properties (e.g positivity).

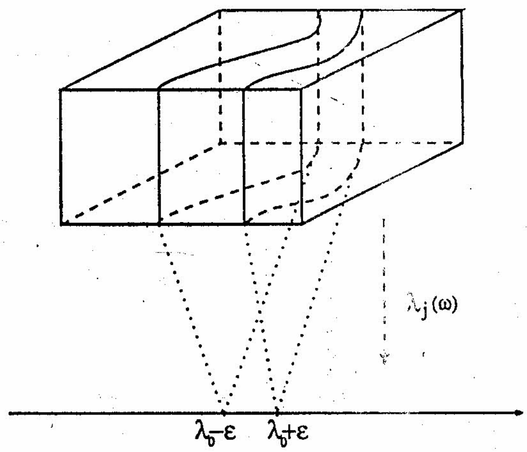


FIGURE 1. Foliation and projection of the probability space

In singular cases like the Bernoulli case, the probability measure is supported by discrete points in the parameter space; so to be able to conclude we would need to compute the number of points in the given layer; this is a much harder problem, as it comes up to knowing more or less exactly the nature of the mappings $(\omega \mapsto \lambda_j(\omega))_{1\leq j\leq N}$.

The right choice of vector field is model dependent; for the Anderson model, discrete or continuous, in many cases, one may use the divergence vector field (for exemple, see [22], [9], [2], [13] or W. Kirsch's lectures in this volume). For the continuous Anderson model, another, more elegant, way of proving Wegner estimates has been developed in [3] (see also P. Hislop's lectutes in this volume); it is nevertheless based on the same picture.

Different types of randomness may require different vector fields (cf [11], [14]).

2.2. **Some results in the singular case.** We will recall some of the mathematically proven results about the density of states for random Schrödinger operators with singular randomness. These results are mostly one dimensional or they deal only with the discrete case. The problem is open for continuous models in dimension larger than one.

In one dimension or for the discrete Anderson model in higher dimension, it has been proved (se [5], [4]) that the integrated density of states in Log-Hölder continuous that is, it satisfies locally an estimate of the form

$$|N(\lambda) - N(\lambda')| \leq \frac{C}{\log|\lambda - \lambda'|} \text{ for some } C > 0.$$

This result was proved for general ergodic models. To the author's knowledge, such general results do not yet exist for continuous random Schrödinger operators in dimension greater than 1.

For the one dimensional discrete Bernoulli Anderson model, it was proved in [1], that for large enough disorder, the density of states has a singular continuous component. A heuristics given in [7] and made rigourous in [20] shows that the maximal possible regularity of the density of states for the one dimensional Bernoulli Anderson hamiltonian is decreasing as μ tends to 0. Let us notice here that the limit $\mu \to 0$ and $\mu \to 1$ are equivalent as one can pass from one to the other by a change in H_0 (i.e a change in the periodic potential).

A rigorous study of the density of states has also been done near certain critical energies. At these thresholds, the density of states tends very quickly to 0; when the threshold is an edge of the spectrum, the density of states exhibits a Lifshitz tail behaviour (see [6]). There exists also a lot of enlightening numerical and physical studies on the regularity of the density of states; we will not review this material here; for these one may look up [16] or [17].

3. An asymptotic expansion in the concentration

The asymptotic expansion we want to give now is not directly related to the regularity of the density of states; nevertheless in the limit of the concentration tending to 0, it gives a picture of why the density could be singular. Such expansions for the density of states and the related picture have been used by physicists (e.g [15], [16]).

3.1. Krein's spectral shift. Let A be a finite subset of $\mathbb{R}^d$. Let us define $H_A = H_0 + \sum_{\gamma \in A} V_\gamma$. H_A is H_0-relatively compact. Moreover, for φ, a function in $\mathcal{S}(\mathbb{R})$, the Schwartz space of rapidly decreasing functions, the operator $\varphi(H_A) - \varphi(H_0)$ is trace class. One defines the temperate distribution $\zeta'(A)$ by

$$\forall \varphi \in \mathcal{S}'(\mathbb{R}),\ \langle \zeta'(A), \varphi \rangle = \mathrm{Tr}(\varphi(H_0) - \varphi(H_A)). \tag{5}$$

$\zeta'(A)$ is supported in the spectrum of H_A; outside of the spectrum of H_0, it is positive linear combination of Dirac deltas located at the discrete eigenvalues of H_A (see [23]).

3.2. **The expansion theorem.** One has

Theorem 3.1. *N_μ admits an asymptotic expansion in $S'(\mathbb{R})$ in powers of μ when μ tends to 0. More precisely, there exists a sequence of distributions $(n_k)_{k\in\mathbb{N}}$ such that*

- *for $k \geq 0$, $n_k \in S'(\mathbb{R})$,*
- *for $N > 0$, there exists $|\cdot|_N$, a semi-norm in $S(\mathbb{R})$ such that, for φ in $S(\mathbb{R})$, one has*

$$|\langle N_\mu, \varphi\rangle - \sum_{k=0}^{N} \mu^k \langle n_k, \varphi\rangle| \leq \mu^{N+1} | \varphi |_N \tag{6}$$

for μ in $]0,1[$.

Moreover the $(n_k)_{k\in\mathbb{N}}$ are given by the following

- *n_0 is the density of states of H_0,*
- *for $k \geq 1$, n_k is given by the following convergent (in $S'(\mathbb{R})$) series*

$$n_k = -\sum_{\substack{\Lambda\subset\mathbb{Z}^d \\ \#\Lambda=k \text{ and } 0\in\Lambda}} \sum_{A\subset\Lambda} (-1)^{\#\Lambda-\#A} \zeta'(A), \tag{7}$$

We will not give a complete proof of this result; it may be found in [13]. Let us first explain the convergence of (7) in the simplest non trivial case that is $k = 2$ (in the case $k = 1$, there is only 1 term). For $k = 2$, (7) becomes

$$n_2 = -\sum_{\gamma\in\mathbb{Z}^d} \sum_{A\subset\{0,\gamma\}} (-1)^{\#A} \zeta'(A). \tag{8}$$

We will just consider the convergence problem outside of the spectrum of H_0. So let us compute n_2 on φ, a C^∞ function compactly supported outside of the spectrum of H_0. Then either of two cases occurs: either the support of φ does not intersect the spectrum of $H_{\{0\}}$ or it contains finitely many discrete eigenvalues of $H_{\{0\}}$. Let us assume we are in the first case. Then the sum $\sum_{\gamma\in\mathbb{Z}^d}\sum_{A\subset\{0,\gamma\}}(-1)^{\#A}\mathrm{Tr}(\varphi(H_A) - \varphi(H_0))$ has only a finite number of terms as the eigenvalues of H_A tend to those of $H_{\{0\}}$ when γ tends to infinity.

If we are in the second case, then we may assume that the support of φ contains a single eigenvalue of $H_{\{0\}}$ that we will denote by λ. For the sake of simplicity let us assume that λ is of multiplicity 1. For $\gamma \in \mathbb{Z}^d$, let $(\lambda_j(\gamma))_{1\leq j\leq J}$ be the eigenvalues of $H_{\{0,\gamma\}}$ in the support of φ. The eigenfunctions associated to the $(\lambda_j(\gamma))_{1\leq j\leq J}$ are exponentially localized either near 0 or near γ. By standard perturbation theory, we know that for some $\gamma_0 > 0$, if $|\gamma| > \gamma_0$, there will be at most two eigenvalues of $(\lambda_j(\gamma))_{1\leq j\leq J}$ contained in the support of φ. Let us denote these eigenvalues by $\lambda_\pm(\gamma)$. One has the following estimate

$$|\lambda_\pm(\gamma) - \lambda| \leq Ce^{-c|\gamma|} \text{ for some } c, C > 0. \tag{9}$$

Hence,

$$(10)\quad \langle n_2,\varphi\rangle = -\sum_{\substack{\gamma\in\mathbb{Z}^d\\|\gamma|\le\gamma_0}} \sideset{}{'}\sum_{A\subset\{0,\gamma\}} (-1)^{\#A}\operatorname{Tr}(\varphi(H_A)-\varphi(H_0))$$

$$-\sum_{\substack{\gamma\in\mathbb{Z}^d\\|\gamma|>\gamma_0}} (\varphi(\lambda_+(\gamma))+\varphi(\lambda_-(\gamma))-2\varphi(\lambda)).$$

By (9), the second term in the right hand side of (10) converges absolutely. Moreover we see that to estimate it we will need one derivative of φ so n_2 is distribution of order 1 and not a measure anymore.

For $k\ge 2$, the alternate series in (7) are convergent in $\mathcal{S}'(\mathbb{R})$ but its sum is not a measure: it is a distribution the order of which is increasing in k. So the asymptotic expansion (6) is a diverging series. Nevertheless, in the sequel, we will see that for a certain restricted class of test functions it converges.

4. The behavior of N_μ in the spectral gaps of H_0

The asymptotic expansion (6) permits us to study the behavior of the integrated density of states in the gaps of the spectrum of H_0 when μ tends to 0. In this limit, it is clear that the integrated density of states goes to 0 in the spectral gaps of H_0. One also knows that, it concentrates at the possible discrete eigenvalues of H_0+V (see [8]). We will see that it actually concentrates near the eigenvalues created by any finite number of perturbations of H_0.

Let Λ be a finite subset of $\mathbb{Z}^d$; let $\sigma(\Lambda)$ be the spectrum of H_Λ. Our assumptions on V guarantee that H_Λ is a relatively compact perturbation of H_0. By Weyl's Theorem H_Λ has only discrete eigenvalues outside of the spectrum of H_0. These eigenvalues can only accumulate at the edges of the essential spectrum of H_Λ. Let us define $\Sigma_{\text{disc}}(\Lambda)$ as the closure of the discrete spectrum of H_Λ; so $\Sigma_{\text{disc}}(\Lambda)$ contains the discrete eigenvalues of H_Λ and possibly some endpoints of the spectrum of H_0.

Definition 4.1. For $k\ge 1$, we define the set of the k-eigenvalues of (H_0,V) by $\mathcal{E}_k = \bigcup_{\#\Lambda=k} \Sigma_{\text{disc}}(H_\Lambda)$.

Remark 4.1. For $A\subset\mathbb{Z}^d$, A finite, $\zeta'(A)$ is supported in $\sigma(A)$. Hence $\operatorname{supp}(n_k)\subset \sigma(H_0)\bigcup\left(\bigcup_{1\le j\le k}\mathcal{E}_k\right)$.

One shows

Proposition 4.1. *$\overline{\mathcal{E}_1} = \mathcal{E}_1$, and for $k \geq 2$, $\overline{\mathcal{E}_k} = \mathcal{E}_k \bigcup \overline{\mathcal{E}_{k-1}} = \bigcup_{j=1}^{k} \mathcal{E}_j$. Moreover, for I, a closed interval in $\mathbb{R} \setminus \sigma(H)$, the points in $\overline{\mathcal{E}_k \cap I} \setminus \overline{\mathcal{E}_{k-1} \cap I}$ are isolated in $\overline{\mathcal{E}_k \cap I}$ ($\overline{I}$ denotes the closure of I).*

The proof of this proposition is given in [13]. Let us just recall its main ideas. It relies on the exponential localization for eigenfunctions associated to eigenvalues of H_Λ located in gaps of H_0. From this localization property, one deduces that a converging sequence of k-eigenvalues can only have two different types of limits either a j-eigenvalue for j less than k or a k-eigenvalue (that is not a j-eigenvalue for j less than k); in the latter case, the sequence has to be almost constant (i.e constant for large enough indices).

For $I \subset \mathbb{R} \setminus \sigma(H_0)$, we define $\mathfrak{n}_k(I)$ to be the number of k-eigenvalues of (H_0, V) in I counted with multiplicity; more precisely, if we denote the spectral projector of H_Λ associated to the eigenvalue λ by $\Pi_\Lambda(\lambda)$, then

$$\mathfrak{n}_k(I) = \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k \text{ et } 0 \in \Lambda}} \; \sum_{\lambda \in I \cap \sigma(H_\Lambda)} \operatorname{rank}(\Pi_\Lambda(\lambda)).$$

Obviously, $\mathfrak{n}_k(I)$ takes its values in $[0, +\infty]$. The behaviour of the integrated density of states inside the gaps of $\sigma(H_0)$ is then given by the

Theorem 4.1. *Let I be an open interval such that its closure is contained in a gap of $\sigma(H_0)$. Then*

- *if $I \cap \mathcal{E}_k \neq \emptyset$ and if for $1 \leq j \leq k-1$, $\overline{I} \cap \mathcal{E}_j = \emptyset$ then $0 < \mathfrak{n}_k(I) < +\infty$ and*

$$N_\mu(I) = \int_I N_\mu(dE) = \mathfrak{n}_k(I)\mu^k(1 + O(\mu)) \quad \text{when } \mu \to 0, \ \mu > 0,$$

- *if for $1 \leq j \leq k$, $\overline{I} \cap \mathcal{E}_j = \emptyset$ then,*

$$N_\mu(I) = \int_I N_\mu(d\lambda) = O(\mu^{k+1}) \quad \text{when } \mu \to 0, \ \mu > 0.$$

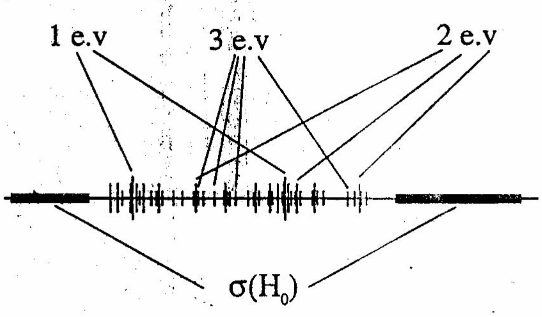


FIGURE 2. The "fractal" structure

In figure 2, some 1, 2 and 3-eigenvalues are shown. A k-eigenvalue is represented by a dash. The dash is of size logarithmically proportional to the inverse of the asymptotic (when $\mu \to 0$) size of N_μ at the k-eigenvalue. In the limit μ tends to 0, the density of states exhibits a fractals structure. This explains the possible existence of singularities for the density of states. Physical heuristics and numerical experiments suggest that such singularities should only exist in dimension 1 but should be smoothed out in higher dimensions (see [16] for physical arguments, and [1] for 1 dimensional mathematical results).

5. Convergence of the asymptotic expansion

As we already underlined, the expansion (6) is only asymptotic. We will now prove that, for a restricted set of test functions (that we will characterize) this asymptotic expansion is absolutely convergent, and that its sum is the density of states computed against the test function. More precisely, one has

Theorem 5.1. *Let φ be an entire function in $\mathbb{C}$ such that, for some $\varepsilon > 0$, φ is rapidly decreasing in a domain of the form $\{z \in \mathbb{C};\ |\Im z| < \varepsilon\, |\Re z|\}$. Then,*

1. *the power series $\sum_{k\in\mathbb{N}} \langle n_k, \varphi\rangle \mu^k$ is absolutely convergent for $\mu \in \mathbb{C}$,*
2. *for $\mu \in [0,1]$,*

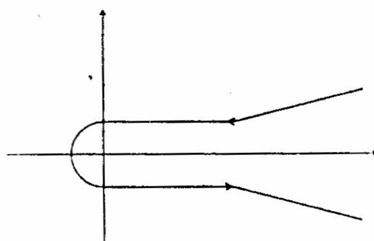
$$\langle N_\mu(d\lambda), \varphi\rangle = \sum_{k=0}^{+\infty} \mu^k \langle n_k, \varphi\rangle.$$

Remark 5.1. In Theorem 5.1, we did not try to obtain the largest class of functions φ for which this result holds. From the proof, one sees that one can certainly restrict the domain where φ needs to be analytic and relax the decay conditions at infinity. Nevertheless, analyticity and decay will be required in some neighborhood of Σ, the almost sure spectrum.

5.1. The proof of Theorem 5.1.

The proof of Theorem 5.1 will more or less follow the lines of the proof of the asymptotic expansion.

As Σ is lower semi-bounded, we may assume that Σ is contained in the positive half-axis (one just needs to shift H_0 by some constant). Then, by [10], for any realization of ω, $\sigma(H_\omega)$ is contained in the positive half-axis. Let $T > 0$. Define Γ_T to be the following path in the complex plane $\Gamma_T = \Gamma_1 \cup \Gamma_2^{\pm} \cup \Gamma_3^{\pm}$ where $\Gamma_1 = \{z = Te^{i\theta};\ \theta \in (\pi/2, 3\pi/2)\}$, $\Gamma_2^{\pm} = \{\Im z = \pm T,\ 0 \le \Re z \le 2T/\varepsilon\}$ and $\Gamma_3^{\pm} = \{\Im z = \pm\varepsilon \Re z/2,\ \Re z \ge 2T/\varepsilon\}$.



Γ_T

Notice that for any $T > 0$

$$\forall z \in \Gamma_T,\ 1 \le \frac{|z|}{\mathrm{dist}(z, (0, +\infty))} \le \sqrt{1 + \varepsilon^{-2}}. \tag{11}$$

Then, using the Cauchy Formula, the Spectral Theorem and Fubini's Theorem, one gets, for $\omega \in \Omega$,

$$\varphi(H_\omega) = \frac{1}{2i\pi} \int_\Gamma \varphi(z) \cdot (z - H\omega)^{-1} dz.$$

Using (3) and Fubini's Theorem, we know that

$$\langle N_\mu, \varphi \rangle = \mathbb{E}_\omega\{\mathrm{Tr}(\chi_0 \varphi(H_\omega)\chi_0)\} = \mathrm{Tr}(\mathbb{E}_\omega\{\chi_0\varphi(H_\omega)\chi_0\}), \tag{12}$$

(by [12], $\sup\limits_\omega \|\chi_0\varphi(H_\omega)\chi_0\|_1 < +\infty$, here $\|\cdot\|_1$ is the trace-class norm).
Fubini's Theorem yields

$$\mathbb{E}_\omega\{\chi_0\varphi(H_\omega)\chi_0\} = \frac{1}{2i\pi} \int_\Gamma \varphi(z) \cdot \mathbb{E}_\omega\{\chi_0(z - H_\omega)^{-1}\chi_0\} dz.$$

Then we get,

Lemma 5.1. *There exists $C > 0$ such that, for $T > (C\mu)^2$, one has the following uniformly norm-convergent expansion for $z \in \Gamma_T$*

$$\mathbb{E}_\omega\{\chi_0(z - H_\omega)^{-1}\chi_0\} = \sum_{k \in \mathbb{N}} \mu^k M_k(z), \tag{13}$$

where M_k is defined by the following uniformly norm-convergent expansion for z in Γ_T,

$$M_k(z) = \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k}} \sum_{A \subset \Lambda} (-1)^{k - \#A} \chi_0 (z - H_A)^{-1} \chi_0. \tag{14}$$

Moreover, for $k \geq 2d$, $M_k(z)$ is a trace-class operator and one has

$$\sup_{z \in \Gamma_T} \|M_k(z)\|_1 \leq \left(\frac{C}{\sqrt{T}}\right)^k. \tag{15}$$

Let us now compute, for $k \geq 1$,

$$\begin{aligned}
\int_\Gamma \varphi(z) \cdot M_k(z) dz &= \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k}} \sum_{A \subset \Lambda} (-1)^{k-\#A} \int_\Gamma \varphi(z) \chi_0 (z - H_A)^{-1} \chi_0 dz \\
&= \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k}} \sum_{A \subset \Lambda} (-1)^{k-\#A} \int_\Gamma \varphi(z) \chi_0 \left((z - H_A)^{-1} - (z - H_0)^{-1} \right) \chi_0 dz \qquad (16) \\
&= 2i\pi \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k}} \sum_{A \subset \Lambda} (-1)^{k-\#A} \chi_0 \left(\varphi(H_A) - \varphi(H_0) \right) \chi_0.
\end{aligned}$$

By equations (2.9) and (2.3) in [12], we know that the last term of this equality converges absolutely in trace-class norm, so $\int_\Gamma \varphi(z) \cdot M_k(z) dz$ is trace class for any k. Moreover for

$k > 2d$ and some $C > 0$ (depending on T), as φ is rapidly decreasing at infinity, one has

$$\| \int_\Gamma \varphi(z) \cdot M_k(z) dz \|_1 \leq C' \left(\frac{C}{\sqrt{T}} \right)^k . \tag{17}$$

So, for $T > (C\mu)^2$, one has

$$\mathbb{E}_\omega \{ \chi_0 \varphi(H_\omega) \chi_0 \} = \sum_{k \in \mathbb{N}} \mu^k \frac{1}{2i\pi} \int_\Gamma \varphi(z) \cdot M_k(z) dz, \tag{18}$$

and the series on the right hand side converges absolutely in trace class norm. Plugging (16) and (18) into (12) gives

$$\langle N_\mu, \varphi \rangle = \sum_{k \in \mathbb{N}} \mu^k \mathrm{Tr} \left(\frac{1}{2i\pi} \int_\Gamma \varphi(z) \cdot M_k(z) dz \right) \tag{19}$$

and

$$\begin{aligned}
&\mathrm{Tr} \left(\frac{1}{2i\pi} \int_\Gamma \varphi(z) \cdot M_k(z) dz \right) \\
&= \mathrm{Tr} \left(\sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k}} \sum_{A \subset \Lambda} (-1)^{k - \#A} \chi_0 \left(\varphi(H_A) - \varphi(H_0) \right) \chi_0 \right) \\
&= \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k \text{ and } 0 \in \Lambda}} \sum_{\gamma \in \mathbb{Z}^d} \sum_{A \subset \Lambda} (-1)^{k - \#A} \mathrm{Tr} \left(\left(\varphi(H_{A+\gamma}) - \varphi(H_0) \right) \chi_0 \right) \\
&= \sum_{\substack{\Lambda \subset \mathbb{Z}^d \\ \#\Lambda = k \text{ and } 0 \in \Lambda}} \sum_{A \subset \Lambda} (-1)^{k - \#A} \sum_{\gamma \in \mathbb{Z}^d} \mathrm{Tr} \left(\left(\varphi(H_A) - \varphi(H_0) \right) \chi_\gamma \right) \\
&= \langle n_k, \varphi \rangle .
\end{aligned}$$

This ends the proof of Theorem 5.1.

5.2. **Proof of Lemma 5.1.** We are now just left with proving Lemma 5.1. To do this we will follow the same strategy as in [12]. Therefore we will use the following estimates. For $\alpha \in \mathbb{Z}^d$, let χ_α be the characteristic function of the cube of sidelength 1 centered in α. There exists $\eta > 0$ and $C > 0$ such that for $\omega \in \Omega$, for $T > 1$, for $z \in \Gamma_T$, for $(\alpha, \beta) \in \mathbb{Z}^d \times \mathbb{Z}^d$,

$$\| \chi_\alpha (z - H_\omega)^{-1} \chi_\beta \| \leq \frac{C}{\mathrm{dist}(z, [0, +\infty))} e^{-\eta |\alpha - \beta|}, \tag{20}$$

and, for $p > d/2$,

$$\| \chi_\alpha (z - H_\omega)^{-1} \chi_\beta \|_p \leq C_p e^{-\eta |\alpha - \beta|}, \tag{21}$$

(where $\| \cdot \|_p$ is the p-th Schatten class norm).

These estimates are obtained using a Combes-Thomas argument (see [19] and [12]). The uniformity of these results with respect to T and z is an immediate consequence from (11).

For $l > 0$ and $\omega \in \Omega$, we define $H_{\omega,l} = H + \sum_{\gamma\in\Lambda_l} \omega_\gamma V_\gamma$ (here Λ_l is cube in $\mathbb{Z}^d$ of center 0 and sidelength l). Using (20), one proves

$$\mathbb{E}_\omega\{\chi_0(z-H_\omega)^{-1}\chi_0\} = \lim_{l\to+\infty} \mathbb{E}_\omega\{\chi_0(z-H_{\omega,l})^{-1}\chi_0\} \text{ (in norm sense)}. \tag{22}$$

By definition $H_{\omega,l}$ depends only on finitely many random variables (i.e. the one indexed by $\gamma \in \Lambda_l$). Hence, if we define

$$\begin{aligned} P_l(z,\mu) &:= \mathbb{E}_\omega\{(\chi_0(z-H_{\omega,l})^{-1}\chi_0)\} \\ &= \int_{[0,1]^{\Lambda_l}} (\chi_0(z-H_l(t))^{-1}\chi_0) \bigotimes_{\Lambda_l} (\mu\delta_1 + (1-\mu)\delta_0). \end{aligned} \tag{23}$$

then $P_l(z,\mu)$ is a bounded operator-valued polynomial in μ of degree $\#\Lambda_l$. Hence we may expand it using Taylor's formula to an arbitrary order N and get

$$P_l(z,\mu) = \sum_{k=0}^{N} \frac{P_l^{(k)}(z,0)}{k!}\mu^k + \frac{\mu^{N+1}}{N!}\int_0^1 P_l^{(N+1)}(z,u\mu)(1-u)^N du. \tag{24}$$

To compute the coefficients in this expansion, we notice that in (23), we are integrating a function with respect to a measure on a finite set; this measure depends analytically in the parameter μ; so we just have to write the Taylor expansion in μ for this measure and integrate the function against it; we compute

$$\begin{aligned} &\frac{d^k}{d\mu^k}\left(\bigotimes_{\Lambda_l}(\mu\delta_1 + (1-\mu)\delta_0)\right) \\ &= \sum_{\substack{\gamma_1\in\Lambda_l,\dots,\gamma_k\in\Lambda_l \\ \gamma_i\neq\gamma_j \text{ for } i\neq j}} \sum_{\substack{A\cup B=\{\gamma_1,\dots,\gamma_k\} \\ A\cap B=\emptyset}} (-1)^{\#B} \bigotimes_A \delta_1 \bigotimes_B \delta_0 \bigotimes_{\Lambda_l\setminus\{\gamma_1,\dots,\gamma_k\}} (p\delta_1 + (1-p)\delta_0). \end{aligned} \tag{25}$$

Hence, for $k \geq 1$, we get

$$\begin{aligned} P_l^k(z,\mu) &= \frac{P_l^{(k)}(z,\mu)}{k!} \\ &= \frac{1}{k!}\sum_{\substack{\gamma_1\in\Lambda_l,\dots,\gamma_k\in\Lambda_l \\ \gamma_i\neq\gamma_j \text{ for } i\neq j}} \sum_{A\subset\{\gamma_1,\dots,\gamma_k\}} (-1)^{\#(\Lambda\setminus A)}\mathbb{E}_\omega\{\chi_0(z-H_{\gamma_1,\dots,\gamma_k,A,\omega})^{-1}\chi_0\}, \end{aligned} \tag{26}$$

where

$$H_{\gamma_1,\dots,\gamma_k,A,\omega} = H + \sum_{\gamma\in A} V_\gamma + \sum_{\gamma\in(\Lambda_l\setminus\{\gamma_1,\dots,\gamma_k\})} \omega_\gamma V_\gamma.$$

One easily checks that this equality may be rewritten in the following form

$$(27)\qquad P_l^k(z,\mu)=\frac{1}{k!}\sum_{\substack{\gamma_1\in\Lambda_l,\dots,\gamma_k\in\Lambda_l\\ \gamma_i\neq\gamma_j \text{ for } i\neq j}}\int_{[0,1]^k}\mathbb{E}_\omega\left\{\chi_0\partial_t\left[(z-H_{\gamma_1,\dots,\gamma_k,\omega,t})^{-1}\right]\chi_0\right\}dt,$$

where

- $H_{\gamma_1,\dots,\gamma_k,\omega,t}=H+\sum_{1\leq j\leq k}t_jV_{\gamma_j}+\sum_{\gamma\in(\Lambda_l\setminus\{\gamma_1,\dots,\gamma_k\})}\omega_\gamma V_\gamma$,
- $(t_j)_{1\leq j\leq k}$ are i.i.d. random variables taking value in $[0,1]$,
- $\partial_t=\bigotimes_{1\leq j\leq k}\partial_{t_j}$ and $dt=\bigotimes_{1\leq j\leq k}dt_j$.

We define

$$\begin{aligned}a_{\gamma_1,\dots,\gamma_k,l}(z,\mu)&=\int_{[0,1]^\Lambda}\mathbb{E}_\omega\left\{\chi_0\partial_t\left[(z-H_{\gamma_1,\dots,\gamma_k,\omega,t})^{-1}\right]\chi_0\right\}dt\\&=\sum_{\sigma\in\mathfrak{S}_k}\int_{[0,1]^\Lambda}\mathbb{E}_\omega\left\{b_{\sigma,\gamma_1,\dots,\gamma_k,l}(z,\mu)\right\}dt.\end{aligned}$$

where $\mathfrak{S}_k$ is the group of permutation of $\{1,\dots,k\}$ and

$$(28)\quad \begin{aligned}b_{\sigma,\gamma_1,\dots,\gamma_k,l}(z,\mu)=\chi_0(z-H_{\gamma_1,\dots,\gamma_k,\omega,t})^{-1}V_{\gamma_{\sigma(1)}}(z-H_{\gamma_1,\dots,\gamma_k,\omega,t})^{-1}V_{\gamma_{\sigma(2)}}\cdots\\ \cdots V_{\gamma_{\sigma(k)}}(z-H_{\gamma_1,\dots,\gamma_k,\omega,t})^{-1}\chi_0.\end{aligned}$$

Using (20), one gets, for some $\eta>0$, $C>0$ and for any $z\in\Gamma_T$,

$$(29)\quad \begin{aligned}&\sup_{\mu\in[0,1]}\int_{[0,1]^\Lambda}\mathbb{E}_\omega\left\{\|b_{\sigma,\gamma_1,\dots,\gamma_k,l}(z,\mu)\|\right\}dt\\ &\leq\left(\frac{C}{\text{dist}(z,[0,+\infty))}\right)^{k+1}e^{-\eta|\gamma_{\sigma(1)}|}e^{-\eta|\gamma_{\sigma(1)}-\gamma_{\sigma(2)}|}\dots\\ &\qquad\dots e^{-\eta|\gamma_{\sigma(k-1)}-\gamma_{\sigma(k)}|}e^{-\eta|\gamma_{\sigma(k)}|}.\end{aligned}$$

Hence, for $l \geq 1$,

$$\sup_{\mu\in[0,1]} \|P_l^k(z,\mu)\| \leq \frac{1}{k!} \sum_{\substack{\gamma_1\in\Lambda_l,\dots,\gamma_k\in\Lambda_l \\ \gamma_i\neq\gamma_j \text{ for } i\neq j}} \sup_{\mu\in[0,1]} \|a_{\gamma_1,\dots,\gamma_k,l}(z,\mu)\|$$

$$(30)\qquad \leq \frac{1}{k!}\left(\frac{C}{\mathrm{dist}(z,[0,+\infty))}\right)^{k+1} \sum_{\sigma\in\mathfrak{S}_k} \left(\sum_{\substack{\gamma_1\in\Lambda_l,\dots,\gamma_k\in\Lambda_l \\ \gamma_i\neq\gamma_j \text{ for } i\neq j}} e^{-\eta|\gamma_{\sigma(1)}|} e^{-\eta|\gamma_{\sigma(1)}-\gamma_{\sigma(2)}|} \dots e^{-\eta|\gamma_{\sigma(k-1)}-\gamma_{\sigma(k)}|} e^{-\eta|\gamma_{\sigma(k)}|} \right)$$

$$\leq \left(\frac{C}{\eta\,\mathrm{dist}(z,[0,+\infty))}\right)^{k+1}.$$

Using the same arguments, one gets, for $l \geq l' \geq 1$ for $z \in \Gamma_T$,

$$\sup_{\mu\in[0,1]} \|P_l^k(z,0) - P_{l'}^k(z,0)\| \leq \frac{1}{k!}\left(\frac{C}{\mathrm{dist}(z,[0,+\infty))}\right)^{k+1} \sum_{\sigma\in\mathfrak{S}_k}\sum_{n=1}^{k}$$

$$(31)\qquad \left(\sum_{\substack{\gamma_1\in\Lambda_l,\dots,\gamma_k\in\Lambda_l \\ \gamma_i\neq\gamma_j \text{ for } i\neq j \\ |\gamma_n|>l'}} e^{-\eta|\gamma_{\sigma(1)}|} e^{-\eta|\gamma_{\sigma(1)}-\gamma_{\sigma(2)}|} \dots e^{-\eta|\gamma_{\sigma(k-1)}-\gamma_{\sigma(k)}|} e^{-\eta|\gamma_{\sigma(k)}|} \right)$$

$$\leq \left(\frac{C}{\eta\,\mathrm{dist}(z,[0,+\infty))}\right)^{k+1} e^{-\eta l'}.$$

So one has that $(P_l^k(z,0))_{k\in\mathbb{N}}$ is a norm Cauchy sequence, hence it converges in norm, so $\lim_{l\to+\infty} P_l^k(z,0) = M_k(z)$. Then using (30), (22) and (24), taking the limit $l \to +\infty$, we get that, for $z \in \Gamma_T$,

$$(32)\qquad \mathbb{E}_\omega\{\chi_0(z-H_\omega)^{-1}\chi_0\} = \sum_{k\in\mathbb{N}} \mu^k M^k(z),$$

where the convergence is uniform for $z \in \Gamma_T$. This gives (13) of Lemma 5.1. To get (14) for $k > 2d$, in the estimate (28), one replaces half of the norm estimates used in (28) to get (29) by the Schatten class estimate (21). So one gets that the terms $b_{\sigma,\gamma_1,\dots,\gamma_k,l}(z,\mu)$ are trace-class and satisfy estimates of the type (29) but for the trace class norm (with $k/2$ inverse powers of $\mathrm{dist}(z,[0,+\infty))$). (14) follows from this by the summation performed in (30).

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KREIN'S SPECTRAL SHIFT FUNCTION AND TRACE FORMULA

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This article is purely mathematical in nature and for some of the applications the reader is referred to [SM], [S] and [K]. In the first section we briefly discuss the existence of the spectral shift function for a pair of unitary operators whose difference is trace class and as an application of it we obtain the same for two self adjoint operators whose resolvent difference is trace class. In the second section we discuss the function classes for which the trace formula is valid.

Notations. $\mathcal{H}$ stands for infinite dimensional separable Hilbert space, H and H_0 stand for a pair of self adjoint operators in $\mathcal{H}$ with $D(H)$ and $D(H_0)$ the respective domains, $\rho(H)$ and $\rho(H_0)$ the respective resolvent sets, $R_z = (H - zI)^{-1}$ and $R_z^0 = (H_0 - zI)^{-1}$ the corresponding resolvent operators, and U and U_0 a pair of unitary operators. The symbols $||.||$, $||.||_1$, represent the operator or vector norm and the trace norm respectively. $\mathcal{B}_1$ stands for the class of all trace class operators in $\mathcal{H}$.

1 THE XI FUNCTION

In a finite dimensional Hilbert space $\mathcal{H}$, if H and H_0 are two self adjoint operators, then setting $\xi(\lambda) = E_\lambda^0 - E_\lambda$, E_λ and E_λ^0 being the spectral families of H and H_0 respectively, one can easily check that

$$(i) \quad \int_{I\!R} \xi(\lambda)d\lambda = \mathrm{Tr}[H - H_0], \tag{1.1}$$

$$(ii) \quad \mathrm{Tr}[\phi(H) - \phi(H_0)] = \int_{I\!R} \xi(\lambda)\phi'(\lambda)d\lambda \tag{1.2}$$

for any $\phi \in C^1(I\!R)$.

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The function ξ is called the Krein's spectral shift function and the second eqaulity is called the trace formula. In finite dimension the operators as well as their spectral families are trace class. But if dimension of $\mathcal{H}$ is not finite, then the difference of the operators may be trace class but the difference of their spectral families may not be (see [SM] for an example). However, in this case there exists $\xi \in L^1(\mathbb{R})$, unique almost every where with respect to Lebesgue measure such that (1.1) holds and that the trace formula (1.2) is true for the class $\mathcal{K}$ of functions $\phi : \mathbb{R} \to \mathbb{C}$ satisfying

$$\phi(\lambda) = \int_{\mathbb{R}} \frac{e^{it\lambda} - 1}{it} \nu(dt) + C_1 \tag{1.3}$$

for some constant C_1 and complex measure ν on $\mathbb{R}$. M. G. Krein, in 1963, proved that the shift function is the boundary value of certain Herglotz function (see [Kr]). In 1987, Dan Voiculescu [V] gave a function theoritic proof for a pair of bounded self adjoint operators and in [SM] it was further generalised to the unbounded case. Voiculescu's trick is to prove the result in finite dimension and then get the final result by a limiting argument.

So one would be interested to know whether the function theoritic method of Voiculescu can be applied for a pair of self adjoint operators whose resolvent difference is trace class. Note that if the difference of two self adjoint operators is trace class then so is their resolvent difference, but the converse is not true (for example if $\mathcal{H} = L^2(\mathbb{R}^3)$, $H_0 = -\Delta$ and $H = H_0 + V$ where V is the multiplication operator by $V \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, then $R_z - R_z^0 \in \mathcal{B}_1$ for $\text{Im} z \neq 0$ but V is not).

Since unitaries are related to the resolvents via Cayley transform, we will show the existance of the spectral shift function for a pair of unitaries whose difference is trace class and then obtain the same for the resolvent difference case from it. First notice that given an unitary operator U_0 there exists $\phi \in (-\pi, \pi]$ and a self adjoint operator (not necesserily bounded) such that $U_0' \equiv e^{-i\phi}U_0 = \frac{i-H_0}{i+H_0}$. This follows from the fact that the eigen values of U_0 are at most countable, lying on the unit circle.

Given two unitaries U and U_0, set $T = U_0^*(U - U_0)$. Note that T is normal and $I + T$ is unitary. Assume that $T = \tau|g >< g|$ with $||g|| = 1$. Then since $I + T$ is unitary one has $1 + \tau = e^{i\theta}$ for some $\theta \in (-\pi, \pi]$. Hence $I + T = e^{i\theta Q}$, where $Q = |g >< g|$. If $\mathcal{H}$ is of finite dimension, then for given two unitaries U and U_0, we can find a $\phi \in \rho(U) \cap \rho(U_0)$ such that both $U + e^{i\phi}$ and $U_0 + e^{i\phi}$ are invertible. Then setting $U' = e^{-i\phi}U$ and $U_0' = e^{-i\phi}U_0$ observe that T remains invariant under this transformation. So for simplicity we may assume that $-1 \in \rho(U) \cap \rho(U_0)$. With these two assumption one can prove the following:

THEOREM 1.1 *Let* $\dim\mathcal{H} = n$ *and* U, U_0, T *be as above with* $T = (e^{i\theta} - 1)|g >< g|$, $||g|| = 1$ *and* $\theta \in (-\pi, \pi]$. *Then there exists a bounded function* η *such that*

$$(i) \quad \int_{-\pi}^{\pi} \eta(t)dt = \theta, \quad 0 \leq \eta(t)\ (\text{sgn}\ \theta) \leq 1$$

(ii) *for every integer* m,

$$\text{Tr}(U^m - U_0^m) = im \int_{-\pi}^{\pi} e^{imt}\eta(t)dt.$$

SKETCH OF THE PROOF: By the above discussion assume that $-1 \in \rho(U) \cap \rho(U_0)$ and define two self adjoint operators

$$H = i\frac{I - U}{U + I} \quad \text{and} \quad H_0 = i\frac{I - U_0}{U_0 + I}$$

so that

$$U = \frac{i-H}{H+i} = -I + 2i(H+i)^{-1} \text{ and } U_0 = \frac{i-H_0}{H_0+i} = -I + 2i(H_0+i)^{-1}.$$

An easy computation shows that $H - H_0$ is rank one and is $+ve$ or $-ve$ accordingly as θ is $+ve$ or $-ve$. Let $0 \le \theta \le \pi$. Then by the minimax principle (see [HJ]) the eigen values $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ of H_0 and the eigen values $\mu_1 \le \mu_2 \le \cdots \le \mu_n$ of H are interlaced, i.e. $\lambda_k \le \mu_k \le \lambda_{k+1} \le \mu_n$ for $1 \le k \le n-1$. Define ξ by

$$\xi(\lambda) = \sum_{k=1}^{n} \chi_{[\lambda_k,\mu_k]}(\lambda) = \mathrm{Tr}[E^0_\lambda - E_\lambda],$$

where $\chi_{[\lambda,\mu]}$ is the characterstic function of the interval $[\lambda,\mu]$. Then setting $\phi(\lambda) = \ln \frac{i-\lambda}{\lambda+i}$ (ln stands for the principal branch of the logarithm function), making substitution $\frac{i-\lambda}{\lambda+i} = e^{it}$ and setting $\eta(t) \equiv \xi(\tan\frac{t}{2}) = \xi(\lambda)$ in (1.2), one gets

$$\begin{aligned} i\theta = & \ \ln \det(U_0^* U) \\ = & \ \ln \det\{(i-H)(H+i)^{-1}\} - \ln \det\{(i-H_0)(H_0+i)^{-1}\} \\ = & \ \mathrm{Tr}\ln\{(i-H)(H+i)^{-1}\} - \mathrm{Tr}\ln\{(i-H_0)(H_0+i)^{-1}\} \\ = & \ 2i\int_{-\infty}^{\infty} \xi(\lambda)/(1+\lambda^2)d\lambda \\ = & \ i\int_{-\pi}^{\pi} \eta(t)dt. \end{aligned}$$

Similarly assertion (ii) follows from (1.2) by putting $\phi(\lambda) = (\frac{i-\lambda}{\lambda+i})^m = e^{imt}$. If $-\pi \le \theta \le 0$, then we just interchange U and U_0, and write $\eta(t)$ for $-\eta(t)$ to get the same expression.

■

If we emphasize on the ϕ dependence of η, then one can check that $\eta_\phi(t+\phi) = \eta_0(t)$.

Our next aim is to construct two sequences of finite dimensional unitary operators $\{U_n\}$ and $\{U_{0,n}\}$ such that as $n \to \infty$, $\mathrm{Tr}[U_n^m - U_{0,n}^m]$ converges to $\mathrm{Tr}[U^m - U_0^m]$ for every integer m. We discuss it breifly omitting the details (for details see [MS]). Let $U_0 = e^{i\phi}(i-H_0)(i+H_0)^{-1}$, normalised g and $1 > \epsilon > 0$ be given. If $F(.)$ is the spectral measure associated with H_0, choose $a > 0$ such that $||(I - F(-a,a])g|| < \epsilon$. For each positive integer l and $1 \le k \le l$, set $F_k = (\frac{2k-2-l}{l}a, \frac{2k-l}{l}a]$ and note that $\{F_k\}_1^l$ are pairwise disjoint and $\sum_1^l F_k = F(-a,a]$. Set $g_k = \frac{F_k g}{||F_k g||}$ if $F_k g \ne 0$, and $= 0$ otherwise. The sequence $\{g_k\}_1^l$ are pairwise orthogonal and $g_k \in F_k\mathcal{H} \subset D(H_0)$. Let P be the projection onto the subspace spanned by $\{g_k\}_1^l$. Then one can show that $||(I-P)g|| < \epsilon$. Next set $U_{0,P} = e^{i\phi}(i - PH_0P)(i + PH_0P)^{-1}$ and $U_P = U_{0,P}e^{i\theta PQP}$, where Q is the one dimensional projection onto the subspace generated by g. Observe that P commutes with $(i \pm PH_0P)$ and $(i \pm PH_0P)^{-1}$, so it commutes with $U_{0,P}$ as well as U_P. Hence in $P\mathcal{H}$, PU_PP and $PU_{0,P}P$ are unitaries. Furthermore one can show that for every integer m,

$$|\mathrm{Tr}P(U_P^m - U_{0,P}^m)P - \mathrm{Tr}(U^m - U_0^m)| < K(|m|,|\theta|)\epsilon, \tag{1.4}$$

where $K(|m|,|\theta|)$ is a positive constant depending on $|m|$ and $|\theta|$ only. Next is our main result:

THEOREM 1.2 *Let U and U_0 be two unitary operators in $\mathcal{H}$ such that $U-U_0$ is trace class. Then there exists a real valued function $\eta \in L^1(-\pi,\pi]$ such that*

$$(i) \quad \int_{-\pi}^{\pi} |\eta(t)|dt \leq \frac{\pi}{2}||U_0^*(U-U_0)||_1,$$

$$(ii) \quad \textit{for every integer } m, \ \operatorname{Tr}(U^m - U_0^m) = im \int_{-\pi}^{\pi} e^{imt}\eta(t)dt,$$

$$(iii) \quad \textit{for any } \omega \textit{ with } |\omega| \neq 1, \ (U-\omega)^{-1} - (U_0-\omega)^{-1} \in \mathcal{B}_1 \textit{ and}$$
$$\operatorname{Tr}[(U-\omega)^{-1} - (U_0-\omega)^{-1}] = -\int_{-\pi}^{\pi} (e^{it}-\omega)^{-2}\eta(t)d_t(e^{it}).$$

PROOF: The sketch is in two steps. In the first step we assume that $U-U_0$ is rank one and show the existence of the shift f function. In the second step $U-U_0$ is considered to be trace class and the existence of shift function is shown by sucessive rank one perturbation.

Step (1). Assume that $U-U_0 = (e^{i\theta}-1)|U_0g >< g|$ with $||g|| = 1$. Then rephrasing the above discussion and (1.4) there exists a sequence of finite dimensional projections $\{P_n\}$ such that $P_ng \to g$ and two sequences $\{U_n\} = \{P_nU_{P_n}P_n\}$ and $\{U_{0,n}\} = \{P_nU_{0,P_n}P_n\}$ of unitary operators in the finite dimensional Hilbert space $P_n\mathcal{H}$ such that

$$\lim_{n\to\infty}\operatorname{Tr}(U_n^m - U_{0,n}^m) = \operatorname{Tr}(U^m - U_0^m). \tag{1.5}$$

If $\theta > 0$, then by the finite dimensional result there exists real valued function η_n on $(-\pi,\pi]$ such that $0 \leq \eta_n \leq 1$ and

$$\operatorname{Tr}(U_n^m - U_{0,n}^m) = im \lim_{n\to\infty}\theta||P_ng||^2 \int_{-\pi}^{\pi} e^{imt}\, d\mu_n(t),$$

where $\mu_n(t) = (\theta||P_ng||^2)^{-1}\int_{-\pi}^{t}\eta_n(s)\,ds$. Since

$$\begin{aligned}\int_{-\pi}^{\pi} \eta_n(t)dt &= -i \ln \det(U_{0,n}^*U_n) \\ &= -i \ln \det e^{i\theta P_nQP_n} = \theta||P_ng||^2,\end{aligned}$$

$0 = \mu_n(-\pi) \leq \cdots \leq \mu_n(\pi) = 1$ for each n. So by Helley's selection principle there exists a subsequence $\{\mu_{n_k}\}$ of $\{\mu_n\}$ and a probability measure μ such that μ_{n_k} converges weakly to μ. By an application of bounded convergence theorem, μ is absolutely continuous with respect to the Lebesgue measure. So there exists a real valued function $\eta \in L^1(-\pi,\pi]$ (setting $\eta(t) = \theta\frac{d\mu(t)}{dt}$) one gets $\int_{-\pi}^{\pi}\eta(t)dt = \theta$. For $\theta < 0$ one can also apply the above procedure. Thus (1.5) yields

$$\operatorname{Tr}[U^m - U_0^m] = im \int_{-\pi}^{\pi} e^{imt}\,\eta(t)\,dt.$$

Step (2). Let $T = U_0^*(U-U_0) = \sum \tau_jF_j$, where $F_j = |g_j >< g_j|$ for some orthonormal set $\{g_j\}$ and $\sum|\tau_j| < \infty$. Since U_0^*U is unitary, $1+\tau_j = e^{i\theta_j}$ for some $\theta_j \in (-\pi,\pi]$. By virtue of the identity $i\,\theta_j = e^{-i\theta_j/2}(\frac{\theta_j/2}{\sin(\theta_j/2)})\tau_j$, we get $\sum|\theta_j| \leq \frac{\pi}{2}\sum|\tau_j| < \infty$ since $|\frac{\theta_j/2}{\sin(\theta_j/2)}| \leq \pi/2$ for $|\theta_j/2| \leq \pi/2$. For $j = 1,2,\cdots$, set $U_j = U_{j-1}(I+\tau_jF_j)$ and observe that

$$||U-U_j||_1 \leq \sum_{k=j+1}^{\infty} |\tau_j| \to 0 \tag{1.6}$$

as $j \to \infty$. By step (1) there exists a real valued function $\eta_j \in L^1(-\pi, \pi]$ associated with each pair U_j and U_{j-1} such that $\int_{-\pi}^{\pi} \eta_j(t)\, dt = \theta_j$ and $\int_{-\pi}^{\pi} |\eta_j(t)|\, dt = |\theta_j|$. Set $\eta(t) = \sum_{j=1}^{\infty} \eta_j(t)$ and note that the series converges in L^1 since $\sum |\theta_j| < \infty$. Thus we have $\int |\eta(t)| dt \leq \pi/2\|T\|_1$ which proves (i). By the identity

$$U^m - U_0^m = \begin{cases} \sum_{j=1}^{m} U^{m-j}(U - U_0)U_0^{j-1} & \text{if } m \geq 1 \\ -\sum_{j=0}^{|m|-1} U^{m+j}(U - U_0)U_0^{-j-1} & \text{if } m \leq -1, \end{cases} \tag{1.7}$$

and (1.6), $U_j^m - U_0^m \to U^m - U_0^m$ in $\mathcal{B}_1$ as $j \to \infty$. So

$$\begin{aligned} \mathrm{Tr}(U^m - U_0^m) &= \lim_{j\to\infty} \mathrm{Tr}(U_j^m - U_0^m) \\ &= \lim_{j\to\infty} \sum_{k=1}^{j} \mathrm{Tr}(U_k^m - U_{k-1}^m) \\ &= im \lim_{j\to\infty} \int_{-\pi}^{\pi} \sum_{k=1}^{j} \eta_k(t) e^{imt} dt \\ &= im \int_{-\pi}^{\pi} \eta(t) dt, \end{aligned}$$

which proves (ii). For part (iii), one can expand $(U-\omega)^{-1} - (U_0 - \omega)^{-1}$ in terms of Neumann series and apply part (ii) and Fubini.

■

As a Corollary we obtain

COROLLARY 1.3 *Let H and H_0 be two self adjoint operators in $\mathcal{H}$ such that $R_z - R_z^0$ is trace class for some* $\mathrm{Im}\, z \neq 0$. *Then there exists a real valued function ξ defined uniquely upto an additive constant such that*

$$(i) \quad \int_{-\infty}^{\infty} \xi(\lambda)/(1+\lambda^2) d\lambda < \infty$$

$$(ii) \quad \mathrm{Tr}\left[R_z - R_z^0\right] = -\int_{-\infty}^{\infty} \xi(\lambda)/(\lambda - z)^2 d\lambda.$$

PROOF: By virtue of the identity

$$R_{-i} - R_{-i}^0 = (H - z)R_{-i}[R_z - R_z^0](H_0 - z)R_{-i}^0,$$

we may assume that $R_{-i} - R_{-i}^0 \in \mathcal{B}_1$. Set $U = (i - H)(i + H)^{-1}$ and $U_0 = (i - H_0)(i + H_0)^{-1}$ and note that $U - U_0 = 2i\,[R_{-i} - R_{-i}^0] \in \mathcal{B}_1$. So there exists $\eta \in L^1(-\pi, \pi]$ such that parts (i)-(iii) of Theorem 1.2 are satisfied.

By the map $e^{it} = (i - \lambda)(\lambda + i)^{-1}$ or conversely $t = 2\tan^{-1}\lambda$, t moves from $-\pi$ to π as λ moves from $-\infty$ to ∞. Setting $\xi(\lambda) = \eta(t) \equiv \eta(2\tan^{-1}\lambda)$ and using $dt/d\lambda = 2/(1+\lambda^2)$, we obtain from Theorem 1.2(i)

$$\begin{aligned} \int_{-\infty}^{\infty} |\xi(\lambda)|/(1+\lambda^2) d\lambda &= \frac{1}{2}\int_{-\pi}^{\pi} |\eta(t)| dt \\ &\leq \frac{\pi}{4}\|U_0^*(U - U_0)\|_1 < \infty \end{aligned}$$

The map $z \to \omega = (i-z)(z+i)^{-1}$ maps the open upper half plane onto the open unit disc and open lower half plane onto the exterior of the unit disc. By virtue of the identities

$$(U-\omega)^{-1} = \frac{i}{2}(z+i)[I-(z+i)(z-H)^{-1}]$$

and

$$(U_0-\omega)^{-1} = \frac{i}{2}(z+i)[I-(z+i)(z-H_0)^{-1}],$$

and Theorem 1.2(iii) we get

$$\begin{aligned}
\frac{i}{2}(z+i)^2\mathrm{Tr}(R_z-R_z^0) &= \mathrm{Tr}[(U-\omega)^{-1}-(U_0-\omega)^{-1}] \\
&:= -i\int_{-\pi}^{\pi}\frac{e^{it}}{(e^{it}-\omega)^2}\eta(t)dt \\
&= -i\{\int_{-\infty}^{\infty}\xi(\lambda)\frac{dt}{d\lambda}\cdot d\lambda\{\frac{(i-\lambda)}{(\lambda+i)}[2i\frac{z-\lambda}{(\lambda+i)(z+i)}]^{-2}\}\} \\
&= -i\frac{(z+i)^2}{2}\int_{-\infty}^{\infty}\frac{\xi(\lambda)}{(\lambda-z)^2}d\lambda,
\end{aligned}$$

which proves to (ii).

Lastly, to show the uniqueness of ξ upto an additive constant, let ξ_1 and ξ_2 be two shift functions satisfying (i) and (ii). Then setting $\zeta = \xi_1 - \xi_2$, we have for $z = \mu + i\epsilon, \epsilon > 0$, $\int_{-\infty}^{\infty}\frac{\zeta(\lambda)}{(\lambda-z)^2}d\lambda = 0$. Thus

$$0 = \mathrm{Im}\int_{-\infty}^{\infty}\frac{\zeta(\lambda)d\lambda}{(\lambda-\mu)^2-\epsilon^2-2i\epsilon(\lambda-\mu)} = \frac{d}{d\mu}\epsilon\int_{-\infty}^{\infty}\frac{\zeta(\lambda)\,d\lambda}{(\lambda-\mu)^2+\epsilon^2}$$

or

$$\epsilon\int_{-\infty}^{\infty}\frac{\zeta(\lambda)\,d\lambda}{(\lambda-\mu)^2+\epsilon^2} = C(\epsilon)$$

independent of $\mu \in \mathbb{R}$. By taking limit $\epsilon \to 0$ and using Theorem 13 of [T], $\zeta(\mu) = \mathit{constant}$ for almost all μ, which proves the assertion.

■

2 THE TRACE FORMULA

In this section we will discuss briefly the function classes for the unitaries and for the resolvent difference case for which trace formula holds. Since the resolvents are related to the unitaries, it would be interesting to compare these two classes.

A function $\psi : \boldsymbol{T}^1 \to \mathbb{C}$ is said to be in $\mathcal{U}$ if it is given by

$$\psi(e^{it}) = \sum_{m=-\infty}^{\infty} a_m e^{imt}, \tag{2.1}$$

where a_m are complex numbers satisfying

$$\sum |ma_m| < \infty. \tag{2.2}$$

THEOREM 2.1 *Let U and U_0 be unitary operators such that $U - U_0$ is trace class and $\psi \in \mathcal{U}$. Then $\psi(U) - \psi(U_0)$ is trace class. Furthermore,*

$$\operatorname{Tr}[\psi(U) - \psi(U_0)] = \int_{-\pi}^{\pi} \eta(t) \frac{d}{dt}[\psi(e^{it})]dt \tag{2.3}$$

PROOF: First observe that, by (2.2), ψ is differentiable and has a bounded derivative. By functional calculus, define $\psi(U)$ and $\psi(U_0)$ and note that again by (2.2) and (1.7) the right hand side of

$$\psi(U) - \psi(U_0) = \sum_{m=-\infty}^{\infty} a_m (U^m - U_0^m)$$

converges in trace norm. Now the desired trace formula (2.3) follows from Theorem 1.2(ii) and Fubini's theorem.

■

A function ϕ belongs to class $\tilde{\mathcal{K}}$ if there exists a complex measure ν such that

$$\phi(\lambda) = \frac{1}{1+\lambda^2} \int_{-\infty}^{\infty} \frac{e^{it\lambda} - 1}{it} d\nu(t) + \frac{C_1}{1+\lambda^2} + C_2 \tag{2.4}$$

for some constants C_1, C_2 and complex measure ν. In terms of $\mathcal{K}$ (see (1.3)), the function class $\tilde{\mathcal{K}}$ can also be viewed as (setting $C_2 = 0$)

$$\tilde{\mathcal{K}} = \{\phi : \mathbb{R} \to \mathbb{C} \text{ such that } (1+\lambda^2)\phi(\lambda) \in \mathcal{K}\}. \tag{2.5}$$

For the resolvent difference case the trace formula for the class $\tilde{\mathcal{K}}$ can be shown to hold by virtue of an abstract result which we state without proof.

For any bounded continuous function ϕ on $\mathbb{R}$ and $\epsilon > 0$, define

$$\phi_\epsilon(\lambda) = \frac{\epsilon}{\pi} \int_{-\infty}^{\infty} \frac{\phi(\mu)}{(\lambda - \mu)^2 + \epsilon^2} d\mu.$$

Then the abstract theorem says

THEOREM 2.2 *Let $R_{-i} - R_{-i}^0 \in \mathcal{B}_1$ and ϕ be a bounded continuous function on $\mathbb{R}$ such that both $(1+\lambda^2)\phi(\lambda)$ and $(1+\lambda^2)\phi'(\lambda)$ are bounded on $\mathbb{R}$. Suppose that ϕ_ϵ be as above. Then*

(i) $\phi_\epsilon(H) - \phi_\epsilon(H_0) \in \mathcal{B}_1$ *for every* $\epsilon > 0$,

(ii) *If* $\phi_\epsilon(H) - \phi_\epsilon(H_0)$ *converges to* $\phi(H) - \phi(H_0)$, *then*

$$\operatorname{Tr}[\phi(H) - \phi(H_0)] = \int_{-\infty}^{\infty} \phi'(\lambda)\, \xi(\lambda)\, d\lambda.$$

The proof of this can be found in Theorem 4.2 of [SM]. As a consequence of this we have

LEMMA 2.3 *Let $D(H) = D(H_0)$ and $R_{-i} - R_{-i}^0 \in \mathcal{B}_1$. For $t \neq 0$ and $\lambda \in \mathbb{R}$, set $\phi^{(t)}(\lambda) = \frac{e^{it\lambda} - 1}{\lambda^2 + 1}$. Then*

(i) $\phi^{(t)} \in C(\mathbb{R})$, *both* $\phi^{(t)}(\lambda)(1+\lambda^2)$ *and* $\phi^{(t)\prime}(\lambda)(1+\lambda^2)$ *are bounded in* $\mathbb{R}$, *and* $|\phi^{(t)'}(\lambda)(1+\lambda^2)| \leq 3|t|$,

(*ii*) $\psi_\epsilon^{(t)}(\lambda) = \mp\chi_\pm(t)\left[\frac{1-e^{it\lambda}e^{-\epsilon|t|}}{1+(\lambda\pm i\epsilon)^2} + \frac{1-e^{-|t|}}{(\lambda\mp i)^2+\epsilon^2}\right]$

for $t > 0$ *and* $t < 0$ *respectively,*

(*iii*) $\phi^{(t)}(H) - \phi^{(t)}(H_0) \in \mathcal{B}_1$ *and*

$||\phi^{(t)}(H) - \phi^{(t)}(H_0)||_1 \leq (2||R_i - R_i^0||_1 + ||R_{-i} - R_{-i}^0||_1)|t|$,

(*iv*) $\phi_\epsilon^{(t)}(H) - \phi_\epsilon^{(t)}(H_0) \in \mathcal{B}_1$ *for every* $\epsilon > 0$ *and converges to* $\phi^{(t)}(H) - \phi^{(t)}(H_0)$ *in* $\mathcal{B}_1 -$ *norm as* $\epsilon \to 0^+$,

(*v*) $\mathrm{Tr}[\phi^{(t)}(H) - \phi^{(t)}(H_0)] = \phi^{(t)'}(\lambda)\,\xi(\lambda)\,d\lambda$.

SKETCH OF THE PROOF: Part (i) is straight forword and part (ii) follows from direct computation using contour integration.

Next

$$\begin{aligned}\phi^{(t)}(H) - \phi^{(t)}(H_0) = &\quad R_i(e^{itH} - I)R_{-i} - R_i^0(e^{itH_0} - 1)R_{-i}^0 \\ = &\quad (R_i - R_i^0)(e^{itH} - I)R_{-i} + R_i^0(e^{itH_0} - I)(R_{-i} - R_{-i}^0) \\ &\quad + R_i^0(e^{itH} - e^{itH_0})R_i\{(H-i)R_{-i}\}.\end{aligned}$$

Since $(e^{itH} - I)R_{-i} = \int_0^t i\ e^{isH}HR_{-i}\ ds$ and $R_i^0(e^{itH_0} - I) = R_i^0\int_0^t i\ e^{isH_0}H_0\ ds$ are bounded operators, upon premultiplying the first by $R_i - R_i^0$ and postmultiplying the second by $R_{-i} - R^0_{-i}$, the trace norm these terms are dominated by $|t|\ ||R_i - R_i^0||_1$ and $|t|\ ||R_{-i} - R_{-i}^0||_1$ respectively. Since $D(H) = D(H_0)$, the third term in the above can be rewritten as

$$i\int_0^t e^{i(t-s)H_0}R_i^0(H - H_0)R_ie^{isH}\{(H-i)R_{-i}\}\ ds,$$

which is trace class by virtue of the resolvent identity $R_i - R_i^0 = R_i(H_0 - H)R_i^0$. So the trace norm of the integral is dominated by $|t|\ ||R_i - R_i^0||_1$. This proves (iii). The proof of (iv) is not difficult but long which uses the assumption $D(H) = D(H_0)$. We omit its proof here. Now part (v) follows from (i)-(iv) and Theorem 2.2.

■

Finally we have

THEOREM 2.4 *Let* $R_{-i} - R_{-i}^0 \in \mathcal{B}_1$ *and* $D(H) = D(H_0)$. *Then for any* $\phi \in \tilde{\mathcal{K}}$, $\phi(H) - \phi(H_0) \in \mathcal{B}_1$ *and the trace formula (1.2) holds.*

PROOF: Let $\phi^{(t)}$ be as defined in Lemma 2.3. By Lemma 2.3(iii) $||\int \frac{\phi^{(t)}(H)-\phi^{(t)}(H_0)}{it}\ \nu(dt)||_1 \leq |\nu|(I\!R)(2||R_i - R_i^0||_1 + ||R_{-i} - R_{-i}^0||_1)$. So $\phi(H) - \phi(H_0) \in \mathcal{B}_1$. Now the trace formula follows from Corollary 1.3(ii), Lemma 2.3(v) and a change of order of integration.

■

Note that $\lambda \to (\lambda - z)^{-m} \in \mathcal{K}$ for $m \geq -1$. So for $m \geq 1$

$$(\lambda^2 + 1)(\lambda - z)^{-m} = (\lambda - z)^{-m+2} + 2z(\lambda - z)^{-m+1} + (z^2 + 1)(\lambda - z)^{-m} \in \mathcal{K}.$$

Hence by (2.5) $\lambda \to (\lambda - z)^{-m} \in \tilde{\mathcal{K}}$ for $m \geq 1$. Also setting $\nu(dt) = \frac{it}{2\pi}\hat{\zeta}(t)\,dt$ and $C_1 = 0$, where $\zeta \in \mathcal{S}(I\!R)$ and $\hat{\zeta}$ its Fourier transform, one has $\mathcal{S}(I\!R) \subset \tilde{\mathcal{K}}$

For $|\omega| \neq 1$, sucessive differentiation of $(e^{it} - \omega)^{-1}$ with respect to e^{it} yields $t \to (e^{it} - \omega)^{-k} \in \mathcal{U}$ for all $k \geq 1$. By the identification $e^{it} = \frac{i-\lambda}{i+\lambda}$ and $\omega = \frac{i-z}{i+z}$ (so that the upper half plane and lower half plane are mapped onto the interior and exterior of the unit disc) it is easy to check that for $\mathrm{Im} z \neq 0$, $t \to (\lambda - z)^{-k} \in \mathcal{U}$ for $k \geq 1$. Let $\phi \in \mathcal{S}(I\!R)$. Then if we look ϕ as a function of t (say ψ) one has $\psi(\pm\pi) = \lim_{\lambda \to \pm\infty} \phi(\lambda) = 0$; more over $\psi^{(k)}(\pm\pi) = \lim_{\lambda \pm\infty} \left[\frac{1+\lambda^2}{2}\frac{d}{d\lambda}\right]^k \phi(\lambda) = 0$. So ψ is periodic and is in $L^1(-\pi, \pi]$, hence has a power series expansion $\psi(e^{it}) = \sum a_m e^{imt}$ with

$$a_m = \frac{1}{2\pi}\int_{-\pi}^{\pi} \psi(t) e^{imt}\,dt = \frac{1}{2\pi}\int_{-\infty}^{\infty} \phi(\lambda)\left(\frac{i-\lambda}{i+\lambda}\right)^m \frac{2}{1+\lambda^2}\,d\lambda$$

from which sucessive integration by part yields $\sup_k |m|^k |a_m| < \infty$. So $\mathcal{S}(I\!R) \subset \mathcal{U}$.

Consider $\phi(\lambda) = \frac{e^{i\lambda\alpha}-1}{i\alpha(1+\lambda^2)}$ for some nonzero real α. Then $\phi \in \tilde{\mathcal{K}}$ ($C_1 = C_2 = 0$, $d\nu(t) = \delta(t-\alpha)dt$). If ϕ also belongs to $\mathcal{U}$, then $\phi(\lambda) = \sum a_m e^{imt}$ with $\sum |ma_m| < \infty$. Applying $(1+\lambda^2)\frac{d}{d\lambda}$ on both sides (note that ψ is differentiable, and the interchange of summation and differentiation on the right hand side is possible since $\sum |ma_m| < \infty$) we get

$$e^{i\lambda\alpha} = \frac{2\lambda(e^{i\lambda\alpha} - 1)}{1+\lambda^2} + 2i\sum m a_m e^{imt}.$$

Now letting $\lambda \to \pm\infty$ or equivalently $t \to \pm\pi$, the limit on the left hand side does not exist, but the right hand side converges to $2i\sum(-1)^m m a_m$, which shows that $\phi \notin \mathcal{U}$. However we do not know whether $\mathcal{U} \subset \tilde{\mathcal{K}}$ or not.

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Multipliers for the Weyl Transform

by

R.RADHA[1]

Abstract

The purpose of this paper is to discuss the multipliers for the Weyl transform, which is related to the Schrödinger representation of the Heisenberg group, and its connection with the special Hermite operator.

1 Introduction

The Hermite functions $\tilde{h}_k$ on the real line are defined by

$$\tilde{h}_k(x) = H_k(x)e^{-\frac{1}{2}x^2}, k = 0, 1, 2, \ldots .$$

where $H_k(x)$ denotes the Hermite polynomial. These are eigen functions of the Hermite operator (harmonic oscillator) $-\Delta + x^2$ with the eigen values $2k + 1$. The normalised Hermite functions $h_k(x)$ are defined by

$$h_k(x) = (2^k k! \sqrt{\pi})^{-\frac{1}{2}} \tilde{h}_k(x)$$

which form a complete orthonormal family in $L^2(\mathbb{R}, dx)$. These Hermite functions are also eigen functions of the Fourier transform:

$$\hat{h_k}(\xi) = (-i)^k h_k(\xi).$$

Let μ be a multiindex and $x \in \mathbb{R}^n$. Then the n-dimensional Hermite functions $\Phi_\mu(x)$ are defined by

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taking the product of the one dimensional Hermite functions $h_{\mu_j}(x_j)$:

$$\Phi_\mu(x) = \prod_{j=1}^{n} h_{\mu_j}(x_j).$$

Then they form a complete orthonormal system for $L^2(\mathbb{R}^n, dx)$ and $H = -\Delta + |x|^2$ is the Hermite operator on $\mathbb{R}^n$.

The Laguerre polynomials may be regarded as generalizations of the Hermite polynomials in the sense that Laguerre polynomials of order $-\frac{1}{2}$ give the Hermite polynomials of even degree and those of order $\frac{1}{2}$ give the Hermite polynomials of odd degree.

The special Hermite functions, which occupy a central place in the study of Hermite and Laguerre expansions, are defined by

$$\Phi_{\mu\nu}(x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{ix\xi} \phi_\mu(\xi + \frac{1}{2}y)\phi_\nu(\xi - \frac{1}{2}y)d\xi.$$

These are called special Hermite functions by Strichartz for the following reason: These are actually Hermite functions on $\mathbb{C}^n$ viewed as $\mathbb{R}^{2n}$ because

$$(-\Delta + \frac{1}{4}|z|^2)\Phi_{\mu\nu} = (|\mu| + |\nu| + n)\Phi_{\mu\nu}$$

but they do not give all Hermite functions on $\mathbb{C}^n$. These functions appear as the entry functions of the Schrödinger representation of the Heisenberg group (see Strichartz [9]). They form a complete orthonormal system in $L^2(\mathbb{C}^n)$. Let

$$L = -\Delta_z + \frac{1}{4}|z|^2 - iN$$

where

$$N = \sum_{j=1}^{n} \left(x_j \frac{\partial}{\partial y_j} - y_j \frac{\partial}{\partial x_j} \right).$$

Then $\phi_{\mu\nu}$ are eigen functions of L, with eigenvalue $(2|\nu| + n)$ and hence L is called the special Hermite operator.

Analysis on the Heisenberg group and expansions in terms of Hermite and Laguerre functions are interrelated. Infact, the first summability theorem for multiple Hermite expansions was deduced from the corresponding result on the Heisenberg group. A multiplier theorem for Laguerre expansions was likewise proved using a multiplier theorem on the Heisenberg group. The first multiplier theorem for Hermite expansions followed from considerations of the Weyl transform which is related to the Schrödinger representation of the Heisenberg group.

The Weyl transform W takes functions on $\mathbb{C}^n$ into bounded operators on $L^2(\mathbb{R}^n)$. As W enjoys many properties of the Fourier transform and is closely related to expansions in terms of Laguerre, Hermite and special Hermite expansions, it will be interesting to study multipliers for the Weyl transform analogous to Fourier multipliers.

We organise this paper as follows. In section 2, we give the basic concept of Fourier multipliers for L^p spaces. In section 3, we define Weyl transform and twisted convolution using the schrödinger representation of the Heisenberg group. In section 4, we discuss the Weyl multipliers for $L^p(\mathbb{C}^n)$. In section 5, we state two types of Weyl multiplier problems (without proofs) using special Hermite Operator.

2 Multipliers for the Fourier transform

Let m be a bounded measurable functions on $\mathbb{R}^n$. Define a linear transformation T_m on $L^2 \cap L^p(\mathbb{R}^n)$ by $\widehat{T_m f} = m\hat{f}$ for $f \in L^2 \cap L^p(\mathbb{R}^n)$. We say that m is a multiplier for L^p $(1 \leq p < \infty)$ if whenever $f \in L^2 \cap L^p$, then $T_m f$ is also in L^p and T_m is bounded i.e.

$$\|T_m f\|_p \leq C\|f\|_p \quad \forall\, f \in L^2 \cap L^p. \tag{1}$$

The smallest constant C for which (1) holds is called the norm of the multiplier. Clearly, the above equation shows that T_m has a unique bounded extension to L^p, which again satisfies the same inequality. We denote this extension also by T_m. Observe that the operator T_m commutes with translations. And for translation invariant operators, we have the following results.

Proposition 2.1 *Let T be a bounded linear transformation mapping $L^1(\mathbb{R}^n)$ to itself. Then a necessary and sufficient condition that T commutes with translations is that there exists a finite Borel measure μ on $\mathbb{R}^n$ such that $Tf = \mu * f$ for every $f \in L^1(\mathbb{R}^n)$ and $\|T\| = \|\mu\|$.*

Proposition 2.2 *Let T be a bounded linear transformation mapping $L^2(\mathbb{R}^n)$ to itself. Then a necessary and sufficient condition that T commutes with translations is that there exists a bounded measurable function ϕ such that $\widehat{Tf} = \phi\hat{f}$ for every $f \in L^2(\mathbb{R}^n)$ and $\|T\| = \|\phi\|$.*

Let $m(L^p)$ denote the class of L^p multipliers with the multiplier norm.Then $m(L^1)$ is the class of Fourier transforms of finite Borel measures on $\mathbb{R}^n$ ($M(\mathbb{R}^n)$) and the norm of $m(L^1)$ is identical with that of $M(\mathbb{R}^n)$. $m(L^2)$ is the class of all bounded measurable functions and multiplier norm is identical with the $L^\infty(\mathbb{R}^n)$ - norm.

Suppose that T is a bounded linear transformation on $L^p(\mathbb{R}^n), 1 \leq p < \infty$, which commutes with translations. Then, it is easy to see that

$$T(f * g) = Tf * g = f * Tg \quad \forall\, f \in C_c(\mathbb{R}^n).$$

Hence

$$\int_{\mathbb{R}^n} Tf(x)\tilde{g}(x)dx = \int_{\mathbb{R}^n} f(x)(\tilde{Tg})(x)$$

where $\tilde{g}(x) = g(-x)$.

Then, by usual duality argument, one can show that T is bounded on $L^{p'}, \frac{1}{p} + \frac{1}{p'} = 1$. It then follows from Marcinkewicz interpolation theorem that T is bounded on L^2 . Hence there exists a bounded measurable function m such that $\widehat{Tf} = m\hat{f} = \widehat{T_m f}$. By uniqueness of Fourier transform, we get $T = T_m$. Thus, on $L^p(\mathbb{R}^n)$, the concept of multipliers coincide with the study of bounded linear translation invariant operators.

Initially, no simple characterisation was known for $m(L^p)$ except for $p = 1$ and $p = 2$. However, there is an important sufficient conditions for L^p multipliers, $1 < p < \infty$:

Theorem 2.1 *Suppose that $m(x)$ is of class C^k in the complement of the origin of $\mathbb{R}^n$, where k is an integer greater than $\frac{n}{2}$. Suppose $m(x)$ satisfies*

$$|\frac{\partial^\alpha}{\partial x^\alpha}m(x)| \leq B|x|^{-\alpha} \text{ whenever } |\alpha| \leq k$$

where $\alpha = (\alpha_1, \ldots \alpha_n)$ with $|\alpha| = \alpha_1 + \alpha_2 + \ldots + \alpha_n$. Then $m \in m(L^p)$ for $1 < p < \infty$.

The proof is based on Littlewood-Paley theory. For a detailed study on Fourier multipliers on $L^p(\mathbb{R}^n)$, we refer to Hormander [4] or Stein [8].

Later, a necessary condition, namely, if m is a multiplier for $L^p(\mathbb{R}^n)$, then there exists a pseudomeasure σ such that $T_m f = \sigma * f$, was also obtained. Infact, this result was proved for a general locally compact abelian group G in place of $\mathbb{R}^n$. This is based on the works of Hormander [4] and Gaudry [3]. Infact, Gaudry in [3] obtained a representation theorem through quasi measures for an (L^p, L^q) multiplier. This idea motivates to obtain such type of representation theorems for various types of multipliers. To cite a few, Unni in [12] obtained the result for the multipliers between any two Segal algebras, Chan in [1] for the Banach valued multipliers $m(L^1(G, A))$, Radha in [6] for $m(L^1(G, A), L^p(G, A)), 1 < p < \infty$.

3 Weyl transform and twisted convolution

Consider the Heisenberg group H^n, which is a nilpotent Lie group, whose underlying manifold is $\mathbb{C}^n \times \mathbb{R}$ where the group operation is defined by

$$(z, t)(w, s) = (z + w, t + s + \frac{1}{2}\text{Im}z\overline{w})$$

and the Haar measure is the Lebesgue measure $dzdt$ on $\mathbb{C}^n \times \mathbb{R}$. The corresponding Lie algebra is generated by the $(2n+1)$ left invariant vector fields

$$X_j = \frac{\partial}{\partial x_j} - \frac{1}{2} y_j \frac{\partial}{\partial t}$$

$$Y_j = \frac{\partial}{\partial y_j} + \frac{1}{2} x_j \frac{\partial}{\partial t}$$

$$T = i \frac{\partial}{\partial T}$$

$j = 1, 2, ... n$.

By stone-Von Neumann theorem, every infinite dimensional irreducible unitary representation on the Heisenberg group is unitairly equivalent to the representation $\pi_\lambda, \lambda \in \mathbb{R} - \{0\}$, where π_λ is defined by

$$\pi_\lambda(z,t)\phi(\xi) = e^{i\lambda t} e^{i\lambda(x\xi + \frac{1}{2}xy)} \phi(\xi + y) \quad (z = x + iy)$$

for each $\phi \in L^2(\mathbb{R}^n)$. This is called Schrödinger representation of H^n with parameter λ. (Infact, there are only two types of representations on H^n, infinite dimensional and one dimensional. The one dimensional representations are not important to us in our discussions).

To define the Weyl transform and twisted convolution, we consider the representation π_1 of H^n. Notice that π_1 is not a faithful representation. The kernel of π_1 is the subgroup

$$K = \{(0,t) / \ t \in \mathbb{Z}\}$$

For some purposes, it is better to throw away this kernel, so we define the reduced Heisenberg group H^n_{red} to be $H^n_{red} = H^n/K$. We still denote the elements of H^n_{red} by (z,t) with the understanding that $0 \leq t < 2\pi$. Then π_1 is a representation of H^n_{red}, which is now faithful. Since the central variable t always acts in a simple minded way, as multiplication by the scalar e^{it}, it is convenient to disregard it entirely. Therefore we define $W(z) = \pi_1(z,0)$.

The unitary representation π_1 of H^n_{red} determines a representation of the convolution algebra $L^1(H^n_{red})$, still denoted by π_1 in the usual way: if $f \in L^1(H^n_{red})$, then

$$\begin{aligned}\pi_1(f) &= \int_{H^n_{red}} f(z,t)\pi_1(z,t)dzdt \\ &= \int_{\mathbb{C}^n}\int_o^{2\pi} f(z,t)e^{it}W(z)dzdt \\ &= \sqrt{2\pi}\int_{\mathbb{C}^n} f_1(z)W(z)dz,\end{aligned}$$

where $f_1(z) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} f(z,t)e^{it}dt.$

For details regarding representation theory of Heisenberg group, we refer to Folland [2].

Given a function f in $L^1(\mathbb{C}^n)$, the function $f^{\#}(z,t) = (2\pi)^{-1}e^{-it}f(z)$ belongs to $L^1(H^n_{red})$ and

$$\pi_1(f^{\#}) = \int_{\mathbb{C}^n} f(z)W(z)dz.$$

This transform which takes f into the operator $W(f) = \pi_1(f^{\#})$ is called the Weyl transform.

The group convolution on H^n_{red} can be transferred to $\mathbb{C}^n$ as a non standard convolution. Given two function f, g in $L^1(\mathbb{C}^n)$, consider

$$\begin{aligned}f^{\#} * g^{\#}(z,t) &= \int_{H^n_{red}} f^{\#}(z-w, t-s-\frac{1}{2}\mathrm{Im} z\overline{w})g^{\#}(w,s)dwds \\ &= (2\pi)^{-1}\left(\int_{\mathbb{C}^n} f(z-w)g(w)e^{\frac{i}{2}\mathrm{Im} z\overline{w}}dw\right)e^{-it}.\end{aligned}$$

If we now define $f \times g$ by

$$f \times g(z) = \int_{\mathbb{C}^n} f(z-w)g(w)e^{\frac{i}{2}\mathrm{Im} z\overline{w}}dw,$$

then we have the relation $f^{\#} * g^{\#} = (f * g)^{\#}$. This convolution is called the twisted convolution and $L^1(\mathbb{C}^n)$ becomes a non commutative algebra under this.

The Weyl transform $W(f)$ enjoys many properties of the Fourier transform. For example, we have an analogue of the Fourier inversion formula

$$f(z) = (2\pi)^{-n}\mathrm{tr}(W(z)^*W(f))$$

and a Plancheral formula

$$\|f\|_2^2 = (2\pi)^{-n}\|W(f)\|_{HS}^2$$

for $f \in L^2(\mathbb{C}^n)$, where $W(z)^*$ denotes the adjoint of $W(z)$ and $W(f \times g) = W(f)W(g)$. Like ordinary convolution, twisted convolution extends from $L^1(\mathbb{C}^n)$ to other $L^p(\mathbb{C}^n)$ and satisfies the Young's inequality

$$\|f \times g\|_r \leq \|f\|_p\|g\|_q, \frac{1}{r} = \frac{1}{p} + \frac{1}{q} - 1.$$

We state here that twisted convolution has better behaviour in some contexts. For example, for $f, g \in L^2(\mathbb{C}^n), f \times g$ will also be in $L^2(\mathbb{C}^n)$ and

$$\|f \times g\|_2 \leq (2\pi)^{\frac{n}{2}}\|f\|_2\|g\|_2,$$

and the equations $f \times g = 0$ and $f \times f = f$ do have non trivial solution, given by special Hermite functions. For details of the above, we refer to Thangavelu [11].

4 Weyl multipliers for $L^p(\mathbb{C}^n)$

A bounded operator $M \in B(L^2(\mathbb{R}^n))$ is called a (left) Weyl multiplier for $L^p(\mathbb{C}^n)$ if the operator T_M defined on $f \in L^1 \cap L^p(\mathbb{C}^n)$ by $W(T_M f) = MW(f)$ extends to a bounded operator on $L^p(\mathbb{C}^n)$. We denote the Weyl multiplier class by m_W. As in the case of Fourier multipliers, $m_W(L^1(\mathbb{C}^n))$ is identified with $M(\mathbb{C}^n)$, the Banach algebra of finite Borel measures on $\mathbb{C}^n$. And $m_W(L^2(\mathbb{C}^n))$ is identified with $B(L^2(\mathbb{R}^n))$ of all bounded operators on $L^2(\mathbb{R}^n)$.

A Hormander type multiplier theorem, which gives sufficient conditions for L^p - multipliers for the Weyl transform, was proved by Mauceri in [5]. Let $A_j = \frac{-\partial}{\partial x_j} + x_j, A_j^* = \frac{\partial}{\partial x_j} + x_j$ be the "creation" and "annihilation" operators considered as unbounded operators on $L^2(\mathbb{R}^n)$ defined on their natural domains.

Let

$$\delta_j S = [A_j^*, S], \quad \overline{\delta}_j S = [S, A_j]$$

for every operator $S \in B(L^2(\mathbb{R}^n))$ whose range is contained in the domain of $A_j, A_j^*, j = 1, 2, \ldots n$. Given an operator $S \in B(L^2(\mathbb{R}^n))$, we say that S is of class C^m if $\delta^\alpha \delta^\beta S$ is in $B(L^2(\mathbb{R}^n))$ for all $\alpha, \beta \in N^n$ such that $|\alpha| + |\beta| \leq m$. Let φ_α be the n-dimensional normalised Hermite functions. Let P_N denote the orthogonal projection on the subspace of $L^2(\mathbb{R}^n)$ generated by $\{\varphi_\alpha / |\alpha| = N\}$. For every $k \in N$, let ψ_k be the dyadic projection defined by $\psi_0 = P_0$ and $\psi_k = \sum_N P_N$ for $2^{k-1} \leq N < 2^k, k > 0$. Then we have

Theorem 4.1 [5] *Suppose that $M \in m_W(L^2(\mathbb{C}^n))$ is of class C^{n+1}. Assume also that*

$$\mathrm{Sup}_{k \in \mathbb{N}} 2^{k(|\alpha|+|\beta|-n)} \| \ (\delta^\alpha \overline{\delta}^\beta M) \psi_k \|_{HS}^2 \leq C \tag{1}$$

whenever $|\alpha| + |\beta| \leq n + 1$. Then $M \in m_W(L^p(\mathbb{C}^n)), 1 < p < 2$.
If assumption (1) is replaced by

$$\mathrm{Sup}_{k \in \mathbb{N}} 2^{k(|\alpha|+|\beta|-n)} \| \psi_k (\delta^\alpha \overline{\delta}^\beta M) \|_{HS}^2 \leq C$$

then $M \in m_W(L^p(\mathbb{C}^n)), 2 \leq p < \infty$.

However, for necessary condition for L^p - multipliers, (for $p \neq 1, p \neq 2$), only the following was known.

Proposition 4.1 *Let $M \in m_W(L^p(\mathbb{C}^n)), 1 \leq p < \infty$. Then there exists a tempered distribution $\rho \in S'(\mathbb{C}^n)$ such that $T_M f = \rho \times f$ for every $f \in S(\mathbb{C}^n)$.*

Recently, Radha and Thangavelu in [7] obtained a concrete characterisation for $m \in m_W(L^p(\mathbb{C}^n)), 1 < p < \infty$. Let $A(\mathbb{C}^n)$ denote the space of functions f on $\mathbb{C}^n$ whose Weyl transforms $W(f)$ are in $B_1(L^2(\mathbb{R}^n))$. Then $A(\mathbb{C}^n)$ is a Banach algebra under $\|\cdot\|_A$ given by

$$\|f\|_A = \|W(f)\|_1 \quad \forall f \in A(\mathbb{C}^n)$$

and a multiplication as twisted convolution. Let $P(\mathbb{C}^n)$ denote the dual space of $A(\mathbb{C}^n)$. Then we have

Theorem 4.2 [7] *Let $M \in m_W(L^p(\mathbb{C}^n))$, $1 < p < \infty$. Then there exists a pseudomeasure σ such that $T_M f = \sigma \times f$ for every $f \in L^1 \cap L^p(\mathbb{C}^n)$.*

5 Connection with Special Hermite Operator

Let $\phi_{\mu\nu}$ be the special Hermite functions and L be the special Hermite operator. Given a function f in $L^p(\mathbb{C}^n), 1 \leq p \leq \infty$, we can formally expand f in terms of the special Hermite functions as

$$f(z) = \sum_{\mu}\sum_{\nu} < f, \overline{\Phi}_{\mu\nu} > \Phi_{\mu\nu}(z) \tag{1}$$

As $\Phi_{\mu\nu}$ are Schwarz class functions, the coefficients

$$< f, \Phi_{\mu\nu} >= \int_{\mathbb{C}^n} f(z)\overline{\Phi}_{\mu\nu}(z)dz$$

are well defined. As $\Phi_{\mu\nu}$ satisfies

$$\Phi_{\mu\nu} \times \Phi_{\alpha\beta} = 0 \quad \text{if } \nu \neq \alpha$$

$$\Phi_{\mu\nu} \times \Phi_{\nu\beta} = (2\pi)^{\frac{n}{2}} \Phi_{\mu\beta},$$

we get

$$\begin{aligned} f \times \Phi_{\alpha\alpha} &= \sum_{\mu}\sum_{\nu} < f, \Phi_{\mu\nu} > \Phi_{\mu\nu} \times \Phi_{\alpha\alpha} \\ &= (2\pi)^{\frac{n}{2}} \sum_{\mu} < f, \Phi_{\mu\alpha} > \Phi_{\mu\alpha}, \end{aligned}$$

the series (1) can be put in the form

$$f(z) = (2\pi)^{-\frac{n}{2}} \sum_{\nu} f \times \phi_{\nu\nu}(z) \tag{2}$$

the special Hermite expansion of f. For various results concerning special Hermite expansions, we refer to [11].

Now, we can state a multiplier problem for special Hermite expansions, proof of which can be found in [11]. Let

$$T_m f(z) = (2\pi)^{-\frac{n}{2}} \sum_{\nu} m(\nu) f \times \phi_{\nu\nu}(z)$$

where m is a bounded function defined on the set of all multiindices. This operator is clearly bounded on $L^2(\mathbb{C}^n)$ but not on $L^p(\mathbb{C}^n), p \neq 2$. So we need to impose further conditions on m to ensure that T_m is bounded on $L^p(\mathbb{C}^n), 1 < p < \infty$, which is achieved by finite difference operators. Let

$$\Delta_j m(\mu) = m(\mu + \epsilon_j) - m(\mu)$$

and define Δ_j^k inductively. If β is a multiindex, we define

$$\Delta^\beta m(\mu) = \Delta_1^{\beta_1}, \ldots \Delta_n^{\beta_n} m(\mu).$$

Then we have

Theorem 5.1 [11] *Assume that $k = n + 1$ if n is odd and $k = n + 2$ if n is even. Let m be a function defined on $\mathbb{N}^n$ which satisfies*

$$|\Delta^\beta m(\mu)| \leq C_\beta(1+|\mu|)^{-|\beta|}$$

for all β with $|\beta| \leq k$. Then T_m is bounded on $L^p(\mathbb{C}^n), 1 < p < \infty$. The proof is based on Littlewood-Paley-Stein theory of g functions defined by the special Hermite semigroup e^{-tL} generated by the operator L.

To state another multiplier problem, let

$$\varphi_k(z) = L_k^{n-1}(\frac{1}{2}|z|^2)e^{-\frac{1}{4}|z|^2},$$

where L_k^{n-1} denotes the Laguerre polynomial of type $(n-1)$. As

$$\sum_{|\mu|=k} \Phi_{\mu\mu}(z) = (2\pi)^{-n/2}\varphi_k(z),$$

the special Hermite expansion can be written as

$$f(z) = (2\pi)^{-n}\sum_{k=0}^{\infty} f \times \varphi_k(z).$$

The Laguerre Sobolev space $W_L^{s,2}(\mathbb{C}^n)$ was introduced by Thangavelu in [10] in connection with spherical means on the Heisenberg group H^n.

For $m \in Z^+$ and $1 < p < \infty$, we define $W_L^{m,p}(\mathbb{C}^n)$ to be image of $L^p(\mathbb{C}^n)$ under L^{-m} where L^m is defined by

$$L^m f = (2\pi)^{-n}\sum_{k=0}^{\infty}(2k+n)^m f \times \varphi_k.$$

In otherwords, $f \in W_L^{m,p}(\mathbb{C}^n)$ if and only if

$$\|f\|_{m,p}^p = \|(2\pi)^{-n}\sum_{k=0}^{\infty}(2k+n)^m f \times \varphi_k\|_p^p$$

is finite. Then the problem is to characterise the multipliers for $W_L^{m,p}(\mathbb{C}^n)$. It turns out that

Theorem 5.2 [7] *The space of Weyl multipliers for $W_L^{m,p}(\mathbb{C}^n)$ coincides with the space of Weyl multiplier for $L^p(\mathbb{C}^n)$ for $1 < p < \infty$.*

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Asymptotic Solutions to Hyperbolic Equations - a brief overview

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The purpose of this write-up is to discuss certain aspects of linear and nonlinear wave propagation in homogeneous and nonhomogeneous media. It is going to be a brief over-view of problems, methods and ideas rather than technicalities. This presentation contains both classical material and moden developments. Bibliographic material is by no means meant to be complete. The goal is merely to understand the significance of some recent developments viewed in the light of classical problems of wave propagation. Most of the arguments are heuristic and so hopefully accessible also to non-specialists in the field.

Talking of wave propagation in non-homogeneous media, two essential parameters come to our mind : wavelength of the waves (denoted as ε) and wavelength of the medium (denoted by λ). We can distinguish qualitatively three different cases.

(a) $\lambda << \varepsilon$: An instructive example of this case would be homogenization of elliptic problems with periodically oscillating coefficients. There is a huge literature on this topic presenting a wide variety of methods : method of asymptotic expansion [1], Tartar's method [1], two-scale convergence method [2], [3], Γ-convergence method [4]. Bloch-wave method [3],[5]. We are not concerned with this important development in this write-up.

(b) $\lambda \approx \varepsilon$: In this case, there is resonant interaction between the medium and the propagating waves and as a consequence new waves are produced (e-g : Bloch waves). Since such waves and their perturbation were widely discussed in this meeting, we do not intend to pursue further these lines.

(c) $\varepsilon << \lambda$: in this case, oscillation of the waves is much more compared with the variations of the medium. Heuristically for such short waves, the medium looks almost homogeneous and so a perturbation theory from the homogeneous case is possible. This is the basic idea behind the method of Geometrical Optics and we will be concerned with this aspect in the sequel. Laws governing the propagation of waves are quite often described by Partial Differential Equations (PDE) which may be linear or nonlinear and are usually complicated. The task at hand is to get a simplified picture of propagation under the above asymptotic limit. A classical example is Newton's theory of light which predicted straight line motion of light waves.

In carrying out the above task, our discussions centre around Maxwell type classical waves rather than Schrodinger type Quantum Mechanical waves. The essential characteristics of the first type of waves (referred to as hyperbolic) are finiteness of the speed of propagation, boundedness of group velocity w.r.t the wave numbers etc. In contrast, the second family of waves has infinite propagation speed and their behaviour was the main point of discussion in the contribution of W. Craig to this volume. Some of the recent advances which we will be discussing below have taken place only in the hyperbolic set-up ; similar developments in the understanding of other types of waves should be hotly pursued in future.

Linear waves - Homogeneous case

By this we mean a situation where the PDE involved is linear and with constant coefficients. Moreover, the initial profile of the wave is a plane wave. More precisely, we have the problem

$$(1) \qquad \begin{cases} P(\partial_t, \partial_x)u = & 0 \ , \ x \in \mathbb{R}^d, \ t > 0 \ , \\ u(x,0) = & e^{i\xi x}, x \in \mathbb{R}^d \ . \end{cases}$$

Here $\xi \in \mathbb{R}^d \backslash (0)$ is given and P is a partial differential operator in (x,t) variables. Assuming that $\{t = 0\}$ is non-characteristic w.r.t P, we demand that there are m ($=$ order of P) real and distinct roots $w = w(\xi)$ for the polynomial equation $P(-iw, i\xi) = 0 \quad \forall \quad \xi \in \mathbb{R}^d$. This is called hyperbolicity condition. For each such root, we can generate a plane wave $u(x,t) = \exp\left[i(x \cdot \xi - wt)\right]$ which solves the above problem. Thus we get a very satisfying picture : each initial plane wave bifurcates into m-families of plane waves, each one is identified by its phase speed $\frac{w(\xi)}{|\xi|}$. General wave patterns may be obtained via super position.

Linear waves - Nonhomogeneous case

Inhomogenities may be introduced into (1) by making the coefficients of the operator in (1) to depend on x or by considering initial condition which is not a plane wave. In such situations, there is a new phenomenon which was not present in homogeneous case and the purpose of this section is to highlight it in an example. It is quite clear that plane wave solutions will not work anymore and the idea is to get a propagation picture which is a perturbation from the homogeneous case when inhomogenities vary slowly. How to quantify this statement ? By introducing a small parameter $\varepsilon > 0$, it is reasonable to propose the following Ansatz for the approximate solution $u^\varepsilon = a(\varepsilon x, \varepsilon t)e^{i\varepsilon^{-1}\phi(\varepsilon x, \varepsilon t)}$ where the amplitude a is no more a constant and a slowly varying complex-valued function of (x,t) and the phase function ϕ is no more linear but slowly varying and real-valued. This is the fundamental idea in Linear Geometrical Optics (LGO) and in mathematics literature, it has been pioneered by LAX [6]. Theory of Pseudo Differential Operators and Fourier Integral Operators formalizes his ideas.

Below, we shall see how this Ansatz works in the example of the wave equation which governs propagation of waves in an isotropic medium with speed unity :

(2) $$u_{tt} - \Delta u = 0\,, \qquad x \in \mathbb{R}^d,\ t > 0\,.$$

Even though this has constant coefficients, we will consider an initial wave front $\sum_0$ which is not necessarily planar. Since the equation is homogeneous, our previous Ansatz reduces to

(3) $$u^\varepsilon = a(x,t)e^{i\varepsilon^{-1}\theta(x,t)}\,.$$

What are then the equations governing the evolution of a and θ ? They are obtained by simply inserting (3) into (2) and equating the coefficient of ε^{-2} and ε^{-1} to zero. This procedure yields

(4) $$\theta_t^2 = |\nabla\theta|^2\,,$$

(5) $$2\theta_t a_t - 2\nabla\theta\cdot\nabla a + (\theta_{tt} - \Delta\theta)\,a = 0\,.$$

Discussion of (4)

In fact (4) consists of two equations $\theta_t + |\nabla\theta| = 0$ and $\theta_t - |\nabla\theta| = 0$. This simply signifies that there are two families of waves generated by (2). We will deal with one of them in the sequel :

(6) $$\theta_t + w(\nabla\theta\,) = 0 \quad \text{with} \quad w(\xi) = -|\xi|\,.$$

This is a scalar, first order equation for the phase θ called Eikonal equation. Even though, the original equation (2) is linear, the equation (6) obtained from it is nonlinear. Hamilton-Jacobi theory reduces the resolution of (6) to a system of ordinary differential equations (ODE) by the method of characteristics. They are defined by

(7) $$\frac{dx}{dt} = \frac{\partial w}{\partial\xi}(x(t),\xi(t))\ , \quad \frac{d\xi}{dt} = -\frac{\partial w}{\partial x}(x(t),\xi(t))\,.$$

Since the equation (2) has constant coefficients, we have $\frac{\partial w}{\partial x} \equiv 0$ and so we obtain

(8) $$\xi(t) \equiv \xi(0), \quad x(t) = \frac{\xi(0)}{|\xi(0)|}t + x(0)\,.$$

Further we have $\xi(t) = \nabla\theta(x(t),t)$ and (6) reduces to $\frac{d}{dt}\theta(x(t),t) \equiv 0$. These informations enable us to construct the wave-front at time t :

$$\Sigma_t = \{x/\theta(x,t) = \text{ constant }\}\,.$$

Indeed $x(t)$ lies on Σ_t and $\xi(t)$ is normal to Σ_t at $x(t)$ and hence defines an infinitesimal piece of Σ_t at $x(t)$. From this picture, it is clear that we are not only able to follow the evolution of Σ_t as a whole but also that of individual points on it. It is also worth to note that even though (6) is an equation in x-space, it is necessary to work in (x,ξ) space to solve it. We refer to $x(t)$ as rays and $(x(t),\xi(t))$ as bicharacteristic strip.

Discussion of (5)

Given θ, (5) is a linear, first order equation for a (called transport equation) which can easily be solved once again by method of characteristics. We note that the characteristics of (5) are precisely the rays of (4) given by (7). (5) is reduced to a linear ODE along the rays $x(t)$ which can be integrated.

Caustics

The classical picture of propagation described above is, in general, valid only locally. In this paragraph, we are going to see what the obstacles are for a global theory. First of all, given initial condition $(x(0),\xi(0))$, unique solution to the Hamiltonian system (7) exists in general only locally in time. Secondly, even if global solution exists as in (8), we have the formation of caustics ($\equiv$ envelope of rays) due to the focussing effect of rays. To illustrate the point, let us consider a spherical wave front $\theta(x,t) = t+|x|$ which solves (4). As time evolves, one can easily see the associated rays $x(t)$ tend to focus at the origin. What happens to the amplitude at the origin ? In fact, the transport equation (5) is reduced to $a_s + \frac{d-1}{2s}a = 0$ along rays. Explicit solution is $a = s^{-\frac{1}{2}(d-1)}$ which shows blow-up of the amplitude at the focus. Thus our Ansatz breaks down in such cases and we need to modify it to overcome the difficulties arising out of caustics. Without going into details, let us remark that this can be overcome by the introduction of multi-phases and by assuming some apriori knowledge on the nature of caustics. One example which is intuitive has been worked out in LUDWIG [7].

Justification

In this paragraph, we will give some indications as to why the solution constructed above is an approximate solution. To this end, we need to talk about initial conditions. We have already seen that there are two families of waves generated. Let us denote their phases by $\theta^\pm$ and the corresponding amplitudes by $a^\pm$. Since the equation is linear, it is reasonable to propose a general Ansatz by super position : $u^\varepsilon = a^+e^{i\varepsilon^{-1}\theta^+} + a^-e^{i\varepsilon^{-1}\theta^-}$. It is then reasonable to take initial conditions for the exact solutions of (2) of the following form

$$(9)\qquad \begin{cases} u(x,0) = & f(x)e^{i\varepsilon^{-1}\tilde\theta(x)}, \\ u_t(x,0) = & i\varepsilon^{-1}g(x)e^{i\varepsilon^{-1}\tilde\theta(x)}, \end{cases}$$

where $f, g, \tilde\theta$ are all given functions. To see what are the initial conditions for $\theta^\pm$ and $a^\pm$, let us calculate u_t^ε :

$$u_t^\varepsilon = \left(a_t^+ + i\varepsilon^{-1}\theta_t^+a^+\right)e^{i\varepsilon^{-1}\theta+} + \left(a_t^- + i\varepsilon^{-1}\theta_t^-a^-\right)e^{i\varepsilon^{-1}\theta-}.$$

Comparing u^ε with u and u_t^ε with u_t, we are led to the following conditions :

$$\begin{cases} \theta^\pm(x,0) = \tilde{\theta}(x) , \\ a^+(x,0) + a^-(x,0) = f(x), \quad \left(\theta_t^+ a^+ + \theta_t^- a^-\right)(x,0) = g(x) . \end{cases}$$

Thanks to (4), these determine $a^\pm(x,0)$ uniquely.

Thus, in a formal manner, it follows from the very construction of u^ε, that $u - u^\varepsilon$ satisfies

$$(10) \qquad \begin{cases} (u-u^\varepsilon)_{tt} - \Delta(u-u^\varepsilon) = O(1) , \\ (u-u^\varepsilon)(x,0) = 0 , \\ (u-u^\varepsilon)_t(x,0) = O(1) . \end{cases}$$

It is therefore natural to measure the error $(u - u^\varepsilon)$ in the energy norm. For a function $u = u(x,t)$, the energy at time t is defined by

$$E(u;t) = \frac{1}{2}\int_{\mathbf{R}^d} \left(|u_t|^2 + |\nabla u|^2\right) dx .$$

If u satisfies (2), it is well-known that $E(u;t)$ is independent of t. However $u - u^\varepsilon$ satisfies (10) where there is a non-zero right hand side denoted by F. In such situations, it is common to use the energy inequality which can be written as follows :

$$E(u-u^\varepsilon;t) \le c\left[E(u-u^\varepsilon;0) + \int_0^t \|F(\cdot,s)\|^2_{L^2(\mathbf{R}^d)} ds\right]$$

Because of (10), we get

$$(11) \qquad E(u-u^\varepsilon;t) \le ct .$$

Certain remarks are in order regarding the above estimate. Recall that $E(u,;t) = E(u;0) = 0(\varepsilon^{-2})$. Thus (11) is indeed a non-trivial estimate. We can refine (11) by calculating approximate solution of the form $v^\varepsilon = u^\varepsilon + \varepsilon u_1^\varepsilon + \varepsilon^2 u_2^\varepsilon + \ldots + \varepsilon^N u_N^\varepsilon$ in which case, we can derive $E(u - v^\varepsilon;t) \le c\varepsilon^{2N}t$. It is also to be noted that these estimates are not uniform as $t \to \infty$. Another inference one can make from the estimate (11) is that the two families of waves with phases $\theta^\pm$ decouple and they do not interact to the highest order.

Energy Propogation in LGO limit

Having addressed the problem of the validity of LGO approximation of the entire wave field u, let us now pay attention to a particular functional namely energy functional of the field. In this paragraph, we are going to derive a law of propagation for the limiting energy density as $\varepsilon \to 0$. Since the two families of waves decouple, it is enough to consider only the family described by (6). Energy density of u is defined by

$$E^\varepsilon(x,t) = \frac{1}{2}\left(|\partial_t u|^2 + |\nabla u|^2\right)$$

The corresponding energy flux density is defined by

$$F^\varepsilon(x,t) = \frac{1}{2}\left(\partial_t u \nabla \overline{u} + \partial_t \overline{u} \nabla u\right)$$

Since u satisfies the wave equation (2), we have the following conservation law :

$$\partial_t E^\varepsilon + \text{ div } F^\varepsilon = 0 \ .$$

If, as shown in the previous paragraph, there is an approximation in the energy norm then we have

$$u = a e^{i\varepsilon^{-1}\theta} + O(\varepsilon)$$

and this gives

$$\begin{aligned} E^\varepsilon &= \varepsilon^{-2}|\theta_t|^2|a|^2 + O(\varepsilon^{-1}) + R \\ F^\varepsilon &= \varepsilon^{-2}\theta_t|a|^2\nabla\theta + O(\varepsilon^{-1}) + R \end{aligned}$$

where R is a remainder consisting of ε^0 terms and $e^{i\varepsilon^{-1}\theta}$ terms. Thus, to the highest order in ε, we must have the following conservation law :

$$\partial_t(|\theta_t|^2|a|^2) + \text{ div}_x \left(\theta_t|a|^2\nabla\theta\right) = 0 \ .$$

which can be rewritten as (using (6))

$$\partial_t\left(|\theta_t|^2|a|^2\right) + \text{ div}_x \left(\frac{\nabla\theta}{|\nabla\theta|}|\theta_t|^2|a|^2\right) = 0 \ . \tag{12}$$

This is a first order equation whose characteristics is again the rays $x(t)$ defined by (7). When this equation is restricted to the rays, it becomes an ODE which shows that the energy at LGO limit propagates with velocity $\frac{\xi(0)}{|\xi(0)|}$ along rays.

Microlocal Energy measures

We have already seen the difficulties involved in the justification of the full wave field under LGO approximation. Can we justify at least the energy field ? Of course, caustics is the main problem. To see the difficulties more closely, let us consider general sequences of solutions of the wave equation :

$$\begin{cases} \partial_t^2 u_n - \Delta u_n = 0 \ , \ x \in \mathbb{R}^d, \ t > 0 \ , \\ u_n(x,0) = u_n^0(x), \ \partial_t u_n(x,0) = u_n^1(x), \ x \in \mathbb{R}^d \ . \end{cases} \tag{13}$$

For simplicity, assume that u_n^0, u_n^1 have compact support. Because of finite speed of propagation, $u_n(\cdot,t)$ will have compact support $\forall\, t$. We assume further that

$$u_n^0 \rightharpoonup 0 \text{ in } H^1(\mathbb{R}^d) \text{ weak} \ , \ u_n^1 \rightharpoonup 0 \text{ in } L^2(\mathbb{R}^d) \text{ weak} \ . \tag{14}$$

Energy considerations yield very easily that $\forall\, T > 0$

$$u_n \rightharpoonup 0 \text{ in } L^\infty\left(0,T;H^1(\mathrm{IR}^d)\right) \quad \text{weak} * ,$$
$$\partial_t u_n \rightharpoonup 0 \text{ in } L^\infty\left(0,T;L^2(\mathrm{IR}^d)\right) \quad \text{weak} * .$$

The question on the energy field in LGO approximation is related to the behaviour of the energy $E(u_n;t)$ as $n \to \infty$. (Indeed a simple comparison between (13) and (9) shows that $u = \varepsilon^{-1}u_n$ and so $E(u;t) = \varepsilon^{-2}E(u_n;t)$. Using non-stationary phase method, one can easily verify that the conditions (14) are satisfied by G.O. data (9) if we assume that $\tilde{\theta}$ has no stationary point). Since $E(u_n;t)$ is a quadratic, weak convergence of u_n will not suffice to pass to the limit. It is well-known that oscillations and concentrations are the sources of non-compactness. In this particular case, it is already seen that too much of energy is concentrated at caustics. One idea which was fruitful in elliptic problems (see LIONS [8]), is the consideration of the weak limit of the energy density $E_n(x,t) = \frac{1}{2}\left(|\partial_t u_n(x,t)|^2 + |\nabla u_n(x,t)|^2\right)$ in the sense of measures. However, we have here a hyperbolic problem where there is the effect of propagation ; in particular, we have seen the need to work in the phase space instead of physical space.

The introduction of micro-local energy measures formalizes the above ideas. These measures are in some sense weak limits of energy densities against test functions which depend on (x,ξ). With this at the background, let us introduce a micro-localized version of the energy

$$E(u_n;t,A) = \frac{1}{2}\int_{\mathbf{R}^d} Au_n(x,t)\overline{u}_n(x,t)dx + \frac{1}{2}\int_{\mathbf{R}^d} A\nabla u_n(x,t)\nabla\overline{u}_n(x,t)dx$$

whose A is a pseudo differential operator of order zero. The introduction of the above object is due to GERARD [9] and TARTAR [10] who prove the following compactness result :

Theorem *Fix $t > 0$. Then there is a subsequence of u_n (denoted again by n) and a positive Radon measure $\mu^t(x,\xi)$ on $\mathrm{IR}^d \times \mathrm{S}^{d-1}$ such that*

$$E(u_n;t;A) \longrightarrow \int_{\mathbf{R}^d\times \mathrm{S}^{d-1}} \sigma_0(A)(x,\xi)d\mu^t(x,\xi)$$

for all pseudo differential operators A of order 0. (Its principal symbol is denoted by $\sigma_0(A)$).

■

This is the basic compactness Theorem giving the existence of micro-local energy measure μ^t at time t. μ^t describes the energy field of $u_n(\cdot,t)$ as $n \to \infty$ in a weak sense with all its concentrations and oscillations. Our question therefore is to know the law of propagation of μ^t as t varies. That this is the same as the one found (via heuristics) at the end of the previous paragraph is the content of the following result due to FRANCFORT & MURAT [11] and GERARD [12] :

Theorem *Fix $T > 0$. Assume that $\mu_\pm^0$ are the micro-local measures associated to $u_n^1 \pm i|D|u_n^0$. Then one can choose a subsequence of u_n independent of $t \in [0,T]$ and A such that*

$$E(u_n; t; A) \longrightarrow \int_{\mathbb{R}^d \times S^{d-1}} \sigma_0(A)(x,\xi) d\mu^t(x,\xi)$$

uniformly on $[0,T]$. Further we have

$$\mu^t(x,\xi) = \frac{1}{2}\left[\mu_+^0(x+t\xi,\xi) + \mu_-^0(x-t\xi,\xi)\right]$$

on $\mathbb{R}^d \times S^{d-1}$. ∎

Above result gives a very satisfying picture of energy propagation overcoming the caustics problem. It shows that total energy is the sum of the energies of two families of moves propagating with velocities $\pm\xi$ along bicharacteristics strips.

We end this paragraph by giving references to other "weak" theories which ought to be pointed out in the present context. On one hand, there is a basic work of CRANDALL & LIONS [13] on viscosity solutions to (4) and on the other hand DIPERNA & LIONS [14] establish the existence of a global flow associated with (7). The possible interconnection between these view-points are to be investigated.

Nonlinear waves-Ansatz

From now on, we will be concerned with the task of generalizing the topics discussed so far to nonlinear equations. Since this is a growing field, many problems are open or under development. So we have decided to highlight mainly some basic issues connected with the works of the author [15], [16] in this field.

We consider quasi-linear equations. A simple but instructive example is the Hopf equation :

$$u_t + \left(\frac{u^2}{2}\right)_x = 0 \qquad x \in \mathbb{R},\ t > 0\ . \tag{15}$$

The first task we face is to find a suitable Ansatz. For this purpose, it will be helpful to have a knowledge of the waves generated by (15). It is well-known that discontinuities develop in the solution at a finite time even if the initial condition is smooth. This is because of the focussing of characteristic curves associated with (15). (This is, in some sense, worse than focussing of rays described in LGO). In terms of Fourier analysis, this signifies the generation of higher harmonics in the solution starting from a single harmonic in the initial condition. Hence exponential dependence on the phase will not be a good idea here ; we must allow arbitrary dependence apriori if we want a self-consistent Ansatz. Secondly, since the system depends on u, we cannot, in general, hope to deve'op a big amplitude theory. Since ours is a perturbation theory from homogeneous medium to cover slowly varying medium, the hope is that an Ansatz containing a small amplitude perturbation from a known smooth function u^0 will work.

Accordingly, we set out with a constant $u^0 \in \mathbb{R}$ and propose an Ansatz of the form

$$u^\varepsilon = u^0 + \varepsilon u_1(\varepsilon^{-1}\phi, x, t) + O(\varepsilon^2) \tag{16}$$

where $\phi = \phi(x,t)$ is the phase function to be determined. The dependence of $u_1 = u_1(\theta, x, t)$ on θ cannot obviously be arbitrary and it will be decided by the equation satisfied by u^ε. The point we would like to stress is that it is not going to be exponential.

Let us consider the equation

$$u_t + f(u)_x = 0 \ , \ x \in \mathbb{R}, \ t > 0 \ , \tag{17}$$

where $f : \mathbb{R} \to \mathbb{R}$ is a smooth function. The solution $u = u(x,t)$ is a scalar function. Assuming $u^0 = 0$ without loss of any generality, we develop by Taylor expansion

$$f(u) = f(u^0) + \lambda^0 u + bu^2 + cu^3 + .$$

where $\lambda^0 = f'(u^0), b = \frac{1}{2}f''(u^0), c = \frac{1}{6}f^{(3)}(u^0)$. Several simplifications occur because (17) is an equation in one-space dimension. First of all, substituting (16) into (17) and equating the coefficient of ε^0 to zero, we find

$$\left(\phi_t + \lambda^0\phi_x\right)\frac{\partial u_1}{\partial \theta} = 0 \ .$$

By the very principle of nonlinear geometrical optics (NGO), u_1 depends on θ and so $\phi_t + \lambda^0\phi_x = 0$ which means that the phase is linear $\phi = x - \lambda^0 t$.

Secondly, the equation (17) remains invariant by dilations $(x,t) \mapsto (\alpha x, \alpha t) \quad \forall\, \alpha > 0$. Thus (16) can be rewritten as

$$u^\varepsilon = u^0 + \varepsilon u_1(x - \lambda^0 t, \ \varepsilon x, \varepsilon t) + O(\varepsilon^2)$$

where $u_1 = u_1(\theta, y, \tau)$ is a function to be determined.

Next, we impose initial conditions for (17) which are of the form

$$u^\varepsilon(x,0) = u^0 + \varepsilon v(x) \ . \tag{18}$$

This choice eliminates the dependence of u_1 on the variable $y = \varepsilon x$. Thus, we arrive at

$$u^\varepsilon = u^0 + \varepsilon u_1(x - \lambda^0 t, \varepsilon t) + O(\varepsilon^2) \ . \tag{19}$$

Our next step is to substitute this expansion into (17) which yields the following equation for u_1 :

(20)
$$\begin{cases} \frac{\partial u_1}{\partial \tau} + b\frac{\partial}{\partial \theta}(u_1^2) = 0, \quad \theta \in \mathbb{R}\ , \ \tau > 0\ , \\ u_1(\theta, 0) = v(\theta\ )\ . \end{cases}$$

This system is OK provided $b \neq 0$. If $b = 0$ then this shows that $\frac{\partial u_1}{\partial \tau} = 0$ and so u_1 does not depend on τ. This indicates that (19) is not a good Ansatz in case $b = 0$, i.e., when $f''(u^0) = 0$.

It is well-known from the theory of equations of type (17), (18) that the cases $f''(u^0) \neq 0$ and $f''(u^0) = 0$ are qualitatively different which means that the structure of corresponding solutions are not the same. Thus it is no surprise that the same is reflected in our asymptotic analysis.

Assuming $f''(u^0) = 0$ but $f^{(3)}(u^0) \neq 0$, we modify (19) as follows :

(21)
$$u^\epsilon = u^0 + \varepsilon u_2(x - \lambda^0 t,\ \varepsilon^2 t) + O(\varepsilon^2)\ .$$

In the above expansion, we have introduced a slower time variable, viz $\varepsilon^2 t$, which can be heuristically justified as follows : Due to the fact that $f''(u^0) = 0$, the characteristic speed $f'(u)$ gets lowered when u is near u^0. If we do not introduce a slower time variable as in (21), it is clear that there will be important phase differences which will make the approximation bad. Once we accept (21), it remains to use it in (17), (18) and deduce the following equation for u_2 :

(22)
$$\begin{cases} \frac{\partial u_1}{\partial \tau} + c\frac{\partial}{\partial \theta}(u_2^3) = 0, \quad \theta \in \mathbb{R}\ , \ \tau > 0\ , \\ u_2(\theta, 0) = v(\theta\ )\ . \end{cases}$$

Justification

The purpose of this paragraph is to give elements of proof of validity of the Ansatz suggested above and make a comparison with the linear case.

First of all, the right space for solutions of the equations we have been considering is $L^\infty \cap BV$ on $[0, T] \times \mathbb{R}$ for any $T < \infty$. Recall that BV is defined as the space functions whose distributional derivatives are measures. Such a space is required to incorporate solutions which exhibit discontinuities. Secondly, solutions in this space are not uniquely determined by the equation and the initial condition. This is because the focusing of characteristics makes the solution overdetermined at the points of discontinuity. We must stipulate other conditions to make a suitable selection. They are called entropy inequalities in the literature. We discuss them briefly here. An entropy is convex function $\eta(u)$. We associate to η, the corresponding flux function $q(u)$ specified by $q'(u) = \eta'(u)f'(u)$. If u is a solution of (17), we demand that

(23)
$$\eta(u)_t + q(u)_x \leq 0 \qquad \forall \text{ convex } \eta\ .$$

If $u \in L^\infty \cap BV$ then the left side of (23) is a measure and (23) is required to hold in the sense of measures. It is also clear that the support of this measure is contained in the set where u exhibits discontinuities. Thus (23) offers a selection criterion among possible discontinuities. The maximal entropy measure $m(u)$ is defined to be

$$m(u) = \sup_{\eta \text{ convex}} \{\eta(u)_t + q(u)_x\} .$$

The important result which we will not discuss further here is that entropy solutions u (i.e., solutions for which $m(u) \leq 0$) are unique.

Apart from uniqueness questions, these measures play important role in stability analysis also. Let $u_1, u_2 \in L^\infty \cap BV$ satisfy

$$\frac{\partial u_1}{\partial t} + \frac{\partial}{\partial x} F(u_i) = \mu_i \quad , \quad i = 1, 2,$$

where μ_i are (signed) measures. Then one has

$$(24) \quad \int_{\mathbb{R}} |u_1(x,t) - u_2(x,t)| dx \leq \int_{\mathbb{R}} |u_1(x,0) - u_2(x,0)| dx + \Sigma_{i=1}^2 m_i(S_t) + \Sigma_{i=1}^2 |\mu_i|(S_t)$$

where m_1, m_2 are maximal entropy measures associated with u_1, u_2 respectively and $S_t = \{(x,s); 0 \leq s \leq t\}$. Above estimate has to be compared with the energy inequality written down earlier in the linear case. The only new phenomenon is the appearance of the measures m_i which we have discussed just above.

With this preparatory material out of our way, we can now proceed with the justification of the Ansatz introduced in the earlier paragraph. We introduce

$$\begin{aligned} U_1(x,t) &= u^0 + \varepsilon u_1(x - \lambda^0 t, \varepsilon t) \quad \text{if } b \neq 0 , \\ U_2(x,t) &= u^0 + \varepsilon u_2(x - \lambda^0 t, \varepsilon^2 t) \quad \text{if } b = 0, c \neq 0 . \end{aligned}$$

They satisfy

$$(25) \quad \begin{cases} \frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x} f(U_i) = \frac{\partial}{\partial x}(f(U_i) - Pf(U_i)) \\ U_i(x,0) = u^0 + \varepsilon v(x) , \end{cases}$$

where

$$\begin{aligned} Pf(v) &= u^0 + f'(u^0)v + \frac{1}{2} f''(u^0)v^2 \quad \text{if } b \neq 0 , \\ Pf(v) &= u^0 + f'(u^0)v + \frac{1}{3!} f^{(3)}(u^0)v^3 \quad \text{if } b = 0, c \neq 0 . \end{aligned}$$

It remains to compare each of the solution of (25) with the solution of (17) an the stability estimate (24). We get

Theorem *Assume $v \in L^\infty(\mathbb{R}) \cap \mathrm{BV}(\mathbb{R})$ has compact support. Then*

(a) *if $b \neq 0$ we have*

$$\sup_{0<t<\infty} \|u(\cdot,t) - U_1(\cdot,t)\|_{L^1(\mathbf{R})} = O(\varepsilon^2) .$$

(b) *if $b = 0, c \neq 0$, we have*

$$\sup_{0<t<\infty} \|u(\cdot,t) - U_2(\cdot,t)\|_{L^1(\mathbf{R})} = O(\varepsilon^2) . \blacksquare$$

The proof of the above result is essentially reduced to estimating the maximal entropy measures and the measures occuring in the right hand side of (25). The details of these estimates can be found in VANNINATHAN [16]. We finish this paragraph by pointing out one important difference from the linear case. In LGO, error estimate was not uniform as $t \to \infty$ contrary to the above result which assets that the error estimate is uniform as $t \to \infty$. This is because nonlinear equations under our discussion define dissipative systems and the waves decay as $t \to \infty$. These decay estimates, essential ingredient in the proof of above Theorem, are also discussed in VANNINATHAN [16].

Further discussion on NGO

In this final paragraph, we attempt to define very briefly the problems in the analysis of Nonlinear Geometrical Optics (NGO). We also give references to works where some progress is achieved. The nonlinear propagation laws can be in the form of semi-linear system or quasi-linear system which are strictly hyperbolic :

$$u_t + \sum_{j=1}^{d} A_j(x,t)\frac{\partial u}{\partial x_j} = F(x,t,u) , \ x \in \mathbb{R}^d, \ t > 0 , \tag{26}$$

$$u_t + \sum_{j=1}^{d} A_j(x,t,u)\frac{\partial u}{\partial x_j} = F(x,t,u) , \ x \in \mathbb{R}^d, \ t > 0 . \tag{27}$$

Here $u = u(x,t)$ is a N-vector, A_j is a $N \times N$ matrix depending smoothly on its arguments. F is also a N-vector depending smoothly on its arguments. Appropriate initial conditions in NGO are respectively

$$u(x,0) = H(x, \varepsilon^{-1}\phi^0(x)), \quad x \in \mathbb{R}^d , \tag{28}$$

$$u(x,0) = H_0(x) + \varepsilon H(x, \varepsilon^{-1}\phi^0(x)), \quad x \in \mathbb{R}^d \tag{29}$$

where H, H_0 are given functions. The corresponding Ansatz are respectively of the form

$$u^\varepsilon = \sum_j U_j(x,t,\varepsilon^{-1}\phi_j(x,t)) + o(1) , \tag{30}$$

$$u^\varepsilon = v(x,t) + \varepsilon \sum_j U_j(x,t,\varepsilon^{-} \ \phi_j(x,t)) + o(\varepsilon) . \tag{31}$$

Unlike linear equations, even the existence of solution u cannot be taken for granted. Even if it exists locally, the domain of existence may shrink as $\varepsilon \to 0$. Thus a modest formulation of the task in NGO can be put down along the following lines :

(T1) Prove the existence of solutions u satisfying the initial condition in a domain independent of ε.

(T2) Find equations satisfied by phases ϕ_j, profiles U_j and the mean flow V for the Ansatz (30), (31). Solve these equations.

(T3) Prove that the Ansatz (30), (31) indeed provide approximation to the exact solution as $\varepsilon \to 0$ in a suitable norm.

In the previous paragraph, we have carried out these tasks in a global way in one example where the existence and the stability of solutions are known. The general case is difficult as it can involve several instabilities.

Each phase ϕ_j usually satisfies the Eikonal equation of LGO. The resulting caustics, well-understood in linear regime, pose grave difficulties in the nonlinear case. Above programme with single phase expansion is carried out in [17], [18]. Multi-phase expansions are more difficult because typically there is a resonant interaction between the waves respresented by these phases and new phases may be created. The resulting wave pattern may be very complicated as demonstrated by [19]. Hence in order to have a reasonable picture, one is forced to impose hypotheses on the nature of the phases that can be generated by the system. By means of such assumptions, it is shown in [20] that the profiles U_j satisfy a coupled system of integro-differential equations. These equations were earlier obtained via heuristic arguments by [21] who also showed that they are greatly simplified in some physical models of compressible fluid flows. If there is no resonant interaction, then these equations become simple and decoupled.

The next task is to analyze the behaviour of the NGO waves after the formation of caustics. Depending on the nature of the nonlinearities, amplitude may blow-up, decay or can be continued. For examples, let us refer to [22], [23].

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PROGRAMME

LECTURES

W Craig	Micro-local dispersive smoothness properties for Schrödinger equation
R Froese	The counting function for resonances
P Hislop	Localization of Random operators
W Kirsch	Random Schrödinger operators
F Klopp	The density of states for singular randomness

TALKS

R Bhatia	Perturbation of discrete spectra
T Bhattacharya	A new spectral radius formula
G Date	Quantization of a pseudo integrable system
T Ichinose	On the estimate of the difference between the Kac operator and the Schrödinger semigroup
M Krishna	Inverse theory
A Mohapatra	Krein shift function and the trace formula
S Padhi	Third order differential equations
Radha Balakrishnan	C-Integrability of the Belavin-Polyakov equation using classical differential geometry
R Radha	Multipliers for the Weyl transform
S Sastry	Upper bounds on the counting function
T Sengadir	Stability of a functional differential equation
K B Sinha	Dynamical semigroup and its representation
V S Sunder	Inverse theory and singular spectra
M Vanninathan	Asymptotic solutions to hyperbolic equations
N Wildberger	Hypergroups and random walks on symmetric spaces

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