NUMERICAL LINEAR ALGEBRA AND SOLVABILITY OF PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT. It was observed long ago that the obstruction to the accurate computation of eigenvalues of large non-self-adjoint matrices is inherent in the problem. The basic idea is that the resolvent of a highly non-normal operator can be very large far away from the spectrum. This leads to an easily observable fact that algorithms for locating eigenvalues will typically find some 'false eigenvalues'.

These false eigenvalues also explain one of the most surprising phenomena in linear PDEs, namely the fact (discovered by Hans Lewy in 1957, in Berkeley) that one cannot always locally solve the PDE $Pu = f$. Almost immediately after that discovery, Hörmander provided an explanation of Lewy's example showing that *almost all* operators with non-constanct complex valued coefficients are not locally solvable. In modern language, that was done by considering the essentially dual problem of existence of *non-propagating singularities*.

The purpose of this article is to review this work in the context of "almost eigenvalues" and from the point of view of semi-classical analysis.

The purpose of this article is to describe a connection between the following seemingly unrelated issues:

- Let $A \in M_n(\mathbb{C})$ be an n by n matrix with complex entries. Its eigenvalues, $\lambda_1, \cdots, \lambda_n$, which are the solutions of the characteristic equation $\det(A-\lambda) = 0$, are well defined mathematical objects. Their numerical computation is a delicate problem which in the case when A is not normal ($AA^* \neq A^*A$) may be very unstable. In fact, in many situations it is practically impossible.
- Let V be a non-vanishing vector field in three variables, $V = \sum_{j=1}^3 a_j(x)\partial_{x_j}$. Can the equation $Vu = f$, $f \in \mathcal{C}^\infty(\mathbb{R}^3)$, be locally solved somewhere? That is, does there exist $\Omega \subset \mathbb{R}^3$, open, and $u \in \mathcal{C}^1(\Omega)$ such that $Vu = f$ in Ω? When the coefficients a_j are real valued, that can be done, as by a change of variables V can be locally transformed to ∂_{y_1}. When a_j's are allowed to be complex valued, but both a_j's and f are real analytic then local solvability follows from the classical Cauchy-Kovalevskaya theorem.

  It came as a great surprise to everybody when Hans Lewy [13] discovered a simple vectorfield

  $$V = \partial_{x_1} + i\partial_{x_2} + i(x_1 + ix_2)\partial_{x_3}\,,$$

  for which there exist many functions $f \in \mathcal{C}^\infty(\mathbb{R}^3)$, such that $Vu = f$ cannot be locally solved *anywhere*.

As we will see, some of the difficulties in finding eigenvalues for highly non-selfadjoint problems result from the phenomena which also cause the lack of solvability of most partial differential operators with complex coefficients. I take the point of view of semi-classical analysis, with the "Planck constant" h being small. It should be stressed however that the same methods are applicable in many settings of asymptotic analysis, where h can be replaced by the wave length, step size in discretization of PDEs, the reciprocals of the Péclet number, or the Reynolds number, and even the reciprocal of the size of the matrix.

This article is written from the point of view of a "press-the-button" user of numerical analysis. What I found fascinating was the fact that things which have been standard in microlocal analysis can be easily seen in numerical experiments. I learned this because of the work of Brian Davies and Nick Trefethen.

Spectrum

The simplest operator for which the eigenvalues are interesting and well understood is the quantum harmonic oscillator:

$$P = D_x^2 + x^2\,, \quad D_x = \frac{1}{i}\frac{\partial}{\partial x}\,, \tag{1}$$

where we follow the notational convention which is useful when dealing with Fourier transforms: $\widehat{D_x f}(\xi) = \xi \hat{f}(\xi)$. This is also motivated by quantum mechanics as the operator D_x is the quantization of the classical momentum ξ. The classical object corresponding to the quantum harmonic oscillator is the energy,

$$E = \xi^2 + x^2\,, \tag{2}$$

of the classical harmonic oscillator.

The spectrum, that is the set of eigenvalues of P, can be analyzed using the *creation* and *annihilation* operators

$$A_+ = D_x + ix\,, \quad A_- = A_+^* = D_x - ix\,,$$

which satisfy

$$P = A_+A_- + 1 = A_-A_+ - 1\,.$$

A calculation, which also captures the essence of the uncertainty principle, shows that the lowest eigenvalue is 1:

$$||u||^2 = |\langle [D_x, x]u, u\rangle| = 2|\operatorname{Im}\langle xD_x u, u\rangle| \leq 2||xu||||D_x u|| \leq ||xu||^2 + ||D_x u||^2 = \langle Pu, u\rangle$$

$$Pu_0 = u_0\,, \quad u_0(x) = \exp(-x^2/2)\,.$$

By applying the creation operator A_+ to u_0, we obtain the eigenfunctions corresponding to higher energies:

$$u_n = A_+^n u_0\,, \quad Pu_n = (2n+1)u_n\,.$$

The operator P is self-adjoint on $L^2(\mathbb{R})$ and the time evolution of a state preserves the energy, and can be described using the eigenfunctions:

$$||\exp(-itP)u||_{L^2} = ||u||_{L^2}\,, \quad \exp(-itP)u_n = \exp(-it(2n+1))u_n\,. \tag{3}$$

Here the norm which defines the Hilbert space $L^2(\mathbb{R})$ is given by $||u||_{L^2}^2 = \int_{\mathbb{R}} |u(x)|^2 dx$, and by "evolution" we mean solving the Schrödinger equation,

$$i\frac{\partial}{\partial t}u = Pu\,.$$

Although the operator P is very special, many quantum systems are modeled by ensembles of harmonic oscillators. In general, when the energy of a system is conserved, we have propagation which can be described in terms of oscillations coming from various real modes of the system. These modes are the eigenvalues of a self-adjoint operator

$$P = -\Delta + V(x)\,, \quad \Delta = \sum_{j=1}^n \partial_{x_j}^2\,, \quad V(x) \text{ real valued.} \tag{4}$$

For instance we can be in the situation shown in Fig.1a, where we impose Dirichlet boundary conditions, $u(0) = u(\pi) = 0$.

Non-selfadjoint Operators

There are many ways in which non-selfadjoint operator occur in real life problems. Roughly speaking, any phenomenon in which dissipation or escape are possible (consequently, practically any phenomenon) will be governed by a non-selfadjoint operator. We will consider here an example motivated by quantum chemistry and illustrated in a simplified form in Fig.1b. The situation is still described by a self-adjoint operator of the form (4) but the possible escape to infinity, in the now open system, will cause local decay of states.

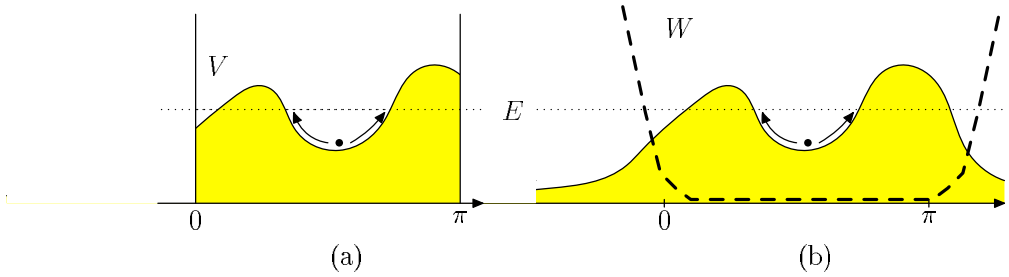

FIGURE 1. (a) A potential well on a finite interval. The spectrum is real and the hard wall causes reflections. (b) A potential on $\mathbb{R}$: same classical picture but a very different quantum picture. The absorbing potential $-iW(x)$ is added to absorb the states escaping from the well (no reflection).

In a concrete example studied in [7], the bottom of the well in the figure corresponds to an unstable molecule of oxirene and the open regions on the left and the right to isomers of ketene. To study the reaction rates in isomerization of ketene it is useful to isolate the unstable system and the simplest way to do so is through the introduction of a *complex absorbing potential* $-iW(x)$. Here, $W(x) \geq 0$ is zero, or nearly zero, in $[0,\pi]$ and becomes very large outside of that interval [7]. The new operator,

$$\widetilde{P} = -\Delta + V(x) - iW(x)\,, \tag{5}$$

is now non-self-adjoint. The difference between a hard barrier in Fig.1a (which could also be modeled by *adding* the real potential $W(x)$), is that the complex absorbing potential produces no reflection and we model an escaping state. The eigenvalues of $\widetilde{P}$ are now complex and lie in the lower half-plane: $z = E - i\Gamma$. The evolution of a pure state is as in (3):

$$\widetilde{P}u = (E - i\Gamma)u\,, \quad \exp(-it\widetilde{P})u = \exp(-itE - t\Gamma)u\,,$$

where we now see decay at the rate given by $-\operatorname{Im} z = \Gamma$. As in [7] the complex absorbing potential method can be used to compute reaction rates and the location of the Breit-Wigner peaks.

Finer description is given in terms of resonances (see [20] for an introduction and pointers to references) and the relation between the two methods is going to be described elsewhere.

A Simple Model

Instead of considering a complicated system such as (5) we follow Davies [1] and study the rotated harmonic oscillator:

$$P_\alpha = D_x^2 + e^{i\alpha}x^2\,, \quad 0 \leq \alpha < \pi\,. \tag{6}$$

The spectrum of this operator is easily computed by making a change of variables $y = e^{i\alpha/4}x$, so that

$$P_\alpha = e^{i\alpha/2}(D_y^2 + y^2) = e^{i\alpha/2}P\,,$$

where P is the harmonic oscillator (1). With a minimal amount of justification, we can see from this that the spectrum of P_α is given by

$$e^{i\alpha/2}(2n+1)\,, \quad n = 0, 1, \cdots,$$

where spectrum is the set of $z \in \mathbb{C}$ for which there exists $u \in L^2(\mathbb{R})$ such that $Pu = zu$.

We can now try to find the same eigenvalues numerically. Although better accounts of this are available in [1] and [19, Chapter 9], out of curiosity, I proceeded directly using *Mathematica*,© and a simple discretization based on taking as a basis of L^2 eigenfunctions, $\{\psi_j\}_{j=0}^{\infty}$, of a different harmonic oscillator ($D_x^2 + 2x^2$). For a truncated basis of 200 elements, and the discretization $(\langle P_\alpha\psi_i, \psi_j\rangle)_{0\leq i,j\leq 200}$, the results of the computation are shown in Fig.2. What we see is a very regular bifurcation, with the correct angle $\alpha/2$ at first, and then

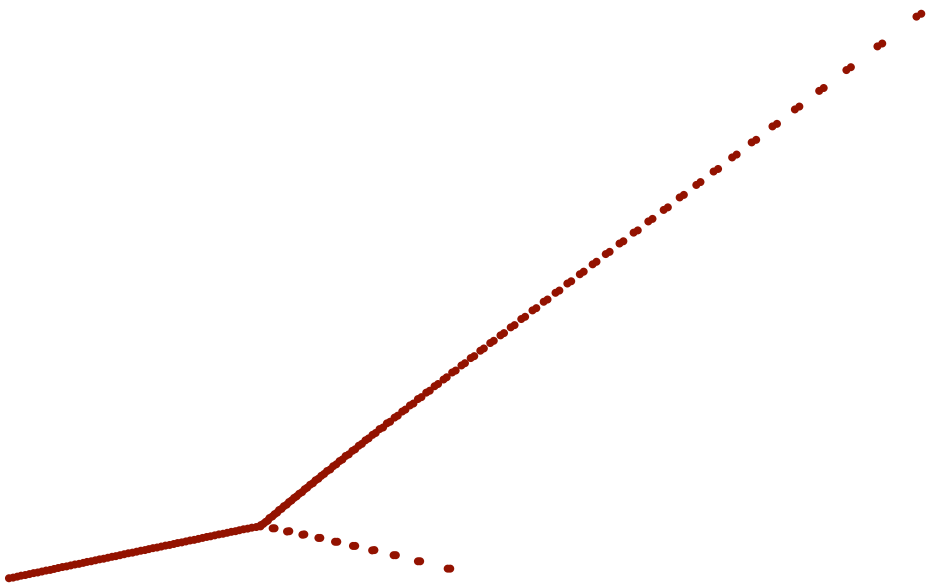

FIGURE 2. Computation of eigenvalues of the discretized rotated harmonic oscillator with $\alpha = \pi/3$.

with one arm of the bifurcation going up at the angle α. The computation is in fact very accurate up to the bifurcation point as seen in the magnified picture shown in Fig.3. The same basis works very well for the normal operator $e^{i\alpha/2}(D_y^2 + y^2)$, which is shown as the "control" result in the same figure.

This example is typical. As emphasized by Trefethen, computations of eigenvalues of highly non-normal operators, will show "pseudo-eigenvalues" and that set will exhibit structure of its own.

Pseudospectrum

We will now follow Trefethen's review article [18], and recall the definition of the *pseudospectrum* for matrices. Thus let $A \in M_{n\times n}(\mathbb{C})$ be a matrix. A well known consequence of the spectral theorem says that

$$A = A^* \implies ||(\lambda - A)^{-1}|| = d(\lambda, \mathrm{spec}(A))^{-1}\,,$$

where $\mathrm{spec}(A)$ is the set of eigenvalues of A, and $d(\bullet,\bullet)$ the usual distance in $\mathbb{C}$.

Nothing of this sort remains valid for non-self-adjoint operators (or strictly speaking, non-normal operators, $AA^* \neq A^*A$). The resolvent $(\lambda - A)^{-1}$ can be *very* large for points very far from the spectrum. This leads to the definition of the ϵ-pseudospectrum:

$$\begin{aligned}\Lambda_\epsilon(A) &= \{\lambda \in \mathbb{C} \,:\, ||(\lambda - A)^{-1}|| \geq \epsilon^{-1}\} \\ &= \{\lambda \in \mathbb{C} \,:\, \lambda \in \mathrm{spec}(A + \delta A) \ \text{ for some } \delta A \text{ with } ||\delta A|| \leq \epsilon\}\,,\end{aligned}$$

where we used the fact that A is a matrix for the second equality.

If the resolvent is large for points away from the spectrum, false eigenvalues will appear. They come from inevitable perturbations originating for instance from the round-off errors, and from the discretization (such as the finite difference, finite element, or spectral method employed in a specific code). That explains, at least roughly, the regularity of the bifurcation in Fig.2. Due to the specifics of the our disretization, and

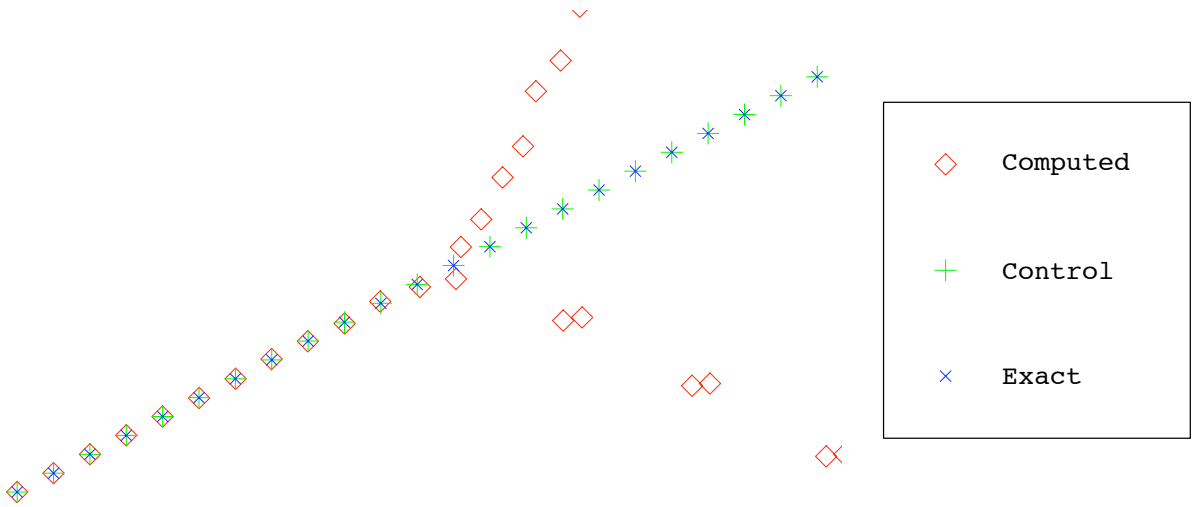

FIGURE 3. Results near the bifurcation point: the eigenvalues of a normal operator with the same spectrum are computed as control data.

computer code[1] used by *Mathematica*©, at some stage of the computation, points on the level sets of the norm of the resolvent, $\Lambda_\epsilon(A)$, with ϵ small, will be chosen over the actual eigenvalues. The computational results presented in Fig.2 and 3 constituted a heuristic experiment, though one that a user of a numerical package is likely to encounter. A proper approach involves the computation of the pseudospectra and for the rotated harmonic oscillator than can be seen in [19, Output 24].

The importance of the size of the resolvent in computational problems was stressed early on by Kreiss [12]. Many systems in science and engineering are described using some form of linearized propagation

$$\exp(tA)\,,$$

not unlike the quantum mechanical propagation (3). The following intuitive statement is quite standard:

$$\textbf{Stability} \iff \max_{\lambda\in\mathrm{spec}(A)} \mathrm{Re}\,\lambda < 0\,. \tag{7}$$

This is correct in the asymptotic sense as for a matrix A, we always have

$$||\exp(tA)|| \leq \exp\left(\max_{\lambda\in\mathrm{spec}(A)} \mathrm{Re}\,\lambda + \delta\right) t\,,\quad t \geq t(\delta) \gg 0\,.$$

If however $\sup\{|z| \;:\; z \in \Lambda_\epsilon(A)\} > 0$, the linearized propagator, $\exp tA$, can be very large for very long times – see [18, Theorem 5], and references there. What matters in specific problems is far from clear and, in some cases, somewhat controversial.

[1]The choice of this particular code was motivated only by easy availability.

Semi-classical Explanation

The problem of finding eigenvalues for the operator P_α defined by (6), is the same as that of solving the equation $(P_\alpha - \lambda)u = 0$. We will rephrase it semi-classically by putting $y = h^{\frac{1}{2}}x$, so that

$$\begin{aligned} P_\alpha - \lambda &= D_x^2 + e^{i\alpha}x^2 - \lambda \\ &= h^{-1}\left((hD_y)^2 + e^{i\alpha}y^2 - h\lambda\right) \\ &= h^{-1}(P(h) - z)\,, \quad z = h\lambda\,. \end{aligned}$$

Since we are interested in the behaviour of the resolvent as λ gets larger, we can work with z in a fixed region, and let $h \to 0$.

As was observed by Davies [1], [2], and discussed further in [21], the resolvent becomes very large inside of the open set given by the values of the *symbol* of the operator $P(h)$: $\xi^2 + e^{i\alpha}x^2$:

$$\forall\, N \quad \|(P(h) - z)^{-1}\| \geq C_N(\Omega)h^{-N}\,, \quad z \in \overline{\Omega} \Subset \{w \,:\, 0 < \arg w < \alpha\}\,, \quad h < h_0(\Omega)\,. \tag{8}$$

In fact, as will be discussed later, the 'super-polynomial' lower bound could be replaced by an exponential bound $\exp(1/C(\Omega)h)$. Rescaling back to λ shows that the level sets of the resolvent are close to lines homothetic to the boundary of the range of the symbol (a more precise description will be given later). The two arms of the bifurcation in Fig.2 are getting close to these level sets.

In general, the symbol is defined by substituting ξ for hD_x in a differential operator, and we think of the differential operator as the quantization of its classical symbol, just as (1) was the quantization of (2). The principal symbol comes from neglecting the terms which depend on h (none in this case). Conversely, if we think of (x, ξ) as an element of the classical configuration space, $T^*\mathbb{R}$ (or more generally T^*X where X is our physical space), then any function $p(x, \xi)$ satisfying

$$|\partial_x^\alpha \partial_\xi^\beta p(x,\xi)| \leq C_{\alpha\beta}(1 + |\xi|)^m\,, \quad \text{for some } m \tag{9}$$

can be quantized to give an operator $P(h) = p(x, hD)$. Differential operators are obtained from polynomials in ξ – see [3] for a comprehensive introduction to semi-classical analysis.

The estimate (8) follows from the existence of 'almost eigenvalues' or what in mathematical physics would be called *quasi-modes*:

$$\|(P(h) - z)u(h)\|_{L^2} = \mathcal{O}(h^\infty)\,, \quad \|u(h)\|_{L^2} = 1\,. \tag{10}$$

In addition, the states $u(h)$ are highly localized, which in the semi-classical/microlocal language means that they are non-propagating. Normally, we expect states to propagate according to the rules of classical mechanics, just as light, governed by the Helmholtz equation, $(-h^2\Delta - 1)u = 0$, propagates[2]. Consequently, to construct approximate solutions, global properties of the classical flow, such as existence of invariant sets, need to be considered, leading to Bohr-Sommerfeld quantization conditions (see [14] and references given there). Different mechanisms take over in the case of complex coefficients.

To describe them we need some elementary symplectic geometry. The configuration space T^*X is a symplectic manifold, that is, a manifold equipped with non-degenerate closed differential two-form ω. By the classical theorem of Darboux (which will be essential below), any symplectic form can be locally transformed to the standard one: $\omega_0 = \sum_{i=1}^n d\xi_i \wedge dx_i$. Classical evolution is described by flows which preserve the symplectic form, and a natural object which arises is the *Poisson bracket*:

$$\{f, g\} = \sum_{i=1}^n \frac{\partial f}{\partial \xi_i}\frac{\partial g}{\partial x_i} - \frac{\partial g}{\partial \xi_i}\frac{\partial f}{\partial x_i}\,.$$

The Poisson bracket is essential in quantization theories, through the following fundamental relation:

$$[f(x, hD), g(x, hD)] = \frac{h}{i}\{f, g\}(x, hD) + \mathcal{O}(h^2)\,,$$

[2]see the remark after the proof of the main theorem for an explanation

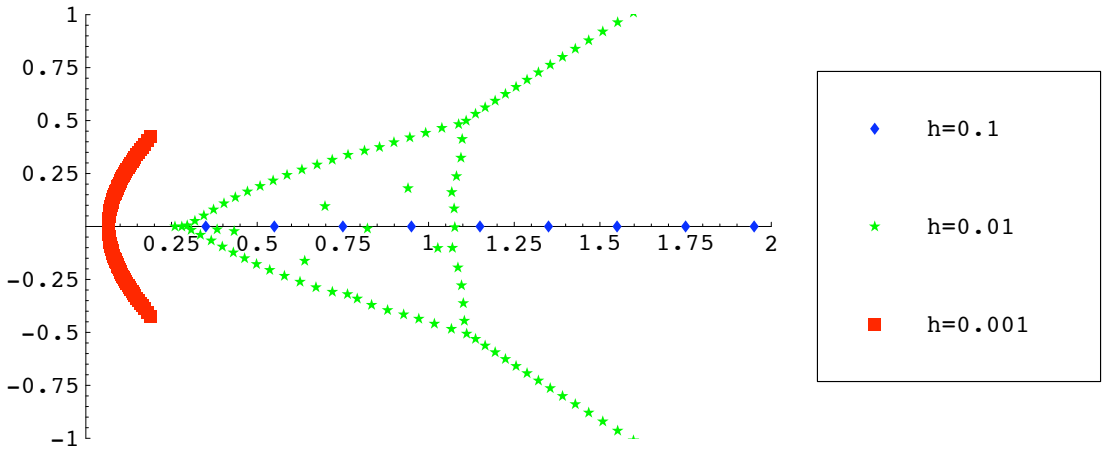

FIGURE 4. Computation of the eigenvalues of a convection-diffusion operator with a quadratic potential

where in the roughest form $\mathcal{O}(h^2)$ may mean an operator bound in L^2, provided that f and g satisfy (9) with $m = 0$.

With this definition, we can state a semi-classical generalization of Hörmander's theorem [8], which is an immediate adaptation of the results of Duistermaat and Sjöstrand [4]:

Theorem. *Suppose that $p(x,\xi)$ satisfies (9) and that*

$$p(x_0,\xi_0) = 0\,, \quad \{\mathrm{Re}\, p, \mathrm{Im}\, p\}(x_0,\xi_0) < 0\,.$$

Then for any $P(h) = p(x,hD) + hp_1(x,hD,h)$, there exist $u(h)$ such that

$$\begin{aligned} &||P(h)u(h)||_{L^2} = \mathcal{O}(h^\infty)\,, \quad ||u(h)||_{L^2} = 1\,, \\ &||q(x,hD)u(h)||_{L^2} = \mathcal{O}(h^\infty) \quad \textit{for any } q(x,\xi) \textit{ which vanishes in a neighbourhood of } (x_0,\xi_0). \end{aligned} \tag{11}$$

The last statement in (11) says that $u(h)$ is localized in space (x) and momentum (ξ). A moment's reflection also shows that the $\mathcal{O}(h^\infty)$ smallness of the L^2 norms implies smallness of norms including derivatives. When $p(x,\xi)$ is real analytic (for instance, when we are dealing with differential operator with real analytic coefficients), then using the work of Kashiwara-Kawai [11] (which provided partial motivation for [4]), the estimates can be improved to exponential ones, that is, $\mathcal{O}(h^\infty)$ can be replaced by $\exp(-1/Ch)$. The level sets of the norm of the resolvent are also related to the level sets of $\{\mathrm{Re}\, p, \mathrm{Im}\, p\}$.

In the simple example discussed above we take

$$P(h) = (hD_x)^2 + e^{i\alpha}x^2 - z\,,$$

so that $p(x,\xi) = \xi^2 + e^{i\alpha}x^2 - z$, and

$$\{\mathrm{Re}\, p, \mathrm{Im}\, p\}(x,\xi) = 2x\xi \sin\alpha\,.$$

For any z in the interior of $\{w : 0 < \arg w < \alpha\}$ we can find (x_0,ξ_0) such that the assumptions of the theorem are satisfied. That produces the complex quasi-modes, and results in the blow-up of the resolvent as $h \to 0$. The estimates are uniform on compact sets in which the Poisson bracket is uniformly bounded away from 0.

We conclude this section with another numerical experiment motivated by [18, Example 5]. Let us put

$$P(h) = (hD_x)^2 + ihD_x + V(x)\,, \quad V(x) \geq 0\,,$$

where $V(x)$ grows very fast outside of a finite interval (faster than x^2, we can take $V(x) = x^2$ for simplicity). This is a form of a *convection-diffusion operator* where the small constant h can be interpreted as the inverse of the Péclet number, rather than as the Planck constant.

If we conjugate the operator by the exponential $\exp(-x/2h)$ we see that the spectrum is real and bounded from below by $1/4$:

$$e^{-x/2h}\left((hD_x)^2 + ihD_x\right)e^{x/2h} = (hD_x)^2 + \frac{1}{4}\,.$$

On the other hand, if $p(x,\xi) = \xi^2 + i\xi + V(x)$, then

$$\{\mathrm{Re}\, p, \mathrm{Im}\, p\}(x,\xi) = -V_x'(x)\,,$$

and that is negative for sufficiently large x (the potential is supposed to grow). This will produce complex quasi-modes concentrated where $V'(x) > 0$ (for $V(x) = x^2$, at points x_0, with $x_0 > 0$).

A naïve numerical experiment confirms that the resolvent gets large inside the set of values of $p(x,\xi)$:

$$\{z\,:\,\mathrm{Re}\, z > (\mathrm{Im}\, z)^2\}\,.$$

This is shown in Fig.4, where the computations are done for $V(x) = x^2$ with 100 basis vectors used in the previous computation. We take $h = 10^{-k}$, $k = 1, 2, 3$. What is strange is the fact that in principle the number of basis vectors for $h = 10^{-3}$ should be too small: in one dimension we ordinarily need $\sim h^{-1}$ basis vectors. Yet, we already see the semi-classically determined pattern of a parabola.

Finally, let us point out that if we put $A = 1/8 - P(h)$, we obtain a simple example in which the criterion for stability (7) is not accurate for a very long time: the eigenvalues lie left of $-1/8$ but the resolvent is very large (for small h) for $\mathrm{Re}\, z \sim 1/8$.

Lack of Solvability

Hörmander's theorem quoted in the previous section was motivated by a very different problem. It was a tool to explain Lewy's example mentioned in the very beginning, and to provide a general condition for the lack of solvability. The idea used in [8] can be roughly described as follows. Suppose we want to solve

$$Pu = f\,. \tag{12}$$

If one succeeds in constructing a family of $u(h)$ such that

$$P^*u(h) = \mathcal{O}(h^\infty)\,, \quad \lim_{h\to 0}\langle u(h), f\rangle = \infty\,,$$

then (12) is clearly impossible:

$$\mathcal{O}(h^\infty) = \langle P^*u(h), u\rangle = \langle u(h), Pu\rangle = \langle u(h), f\rangle \longrightarrow \infty\,,$$

a contradiction.

The implementation of this idea for $f \in \mathcal{C}^\infty$ and $u \in \mathcal{D}'$ (the space of distributions) involves an elegant use of functional analysis (Banach's applications of Baire's Category Theorem). The main point is the construction of approximate solutions for the adjoint P^*, and that is in essence the theorem of the previous section. Its translation to the classical differential operator gives the celebrated *commutator condition*. Suppose that $P(x,D) = \sum_{|\alpha|\leq m} a_\alpha(x)D_x^\alpha$, $p(x,\xi) = \sum_{|\alpha|=m} a_\alpha(x)\xi^\alpha$, and that

$$p(x_0,\xi_0) = 0\,, \quad \{\mathrm{Re}\, p, \mathrm{Im}\, p\}(x_0,\xi_0) \neq 0\,, \quad \xi_0 \neq 0\,,$$

Then for a large class (generic) of $f \in \mathcal{C}^\infty$, the equation (12) cannot be solved in *any* neighbourhood of x_0. For differential operators, the sign of the Poisson bracket is irrelevant as the sign can be changed by changing the sign of ξ (it is a polynomial of degree $2m-1$). Hence the vanishing of the symbol of the commutator of P and P^* is a necessary condition for solvability (the commutator condition). The commutator condition

appeared already in Hörmander's thesis *before* Lewy's example. In a stronger form it was used to guarantee solvability for some operators with complex coefficients (see [9] and references given there).

In Lewy's example we have $p(x,\xi) = \xi_1 + i\xi_2 + i(x_1 + ix_2)\xi_3$, so that at any $x \in \mathbb{R}^3$ we can find $\xi(x) = (-x_1\xi_3, -x_2\xi_3, \xi_3) \neq 0$ such that

$$p(x,\xi(x)) = 0\,, \quad \{\mathrm{Re}\, p, \mathrm{Im}\, p\}(x,\xi(x)) = 2\xi_3 \neq 0\,,$$

which shows lack of solvability anywhere.

Let us also use this example to indicate the relation to the semi-classical discussion before. If we take the Fourier transform in x_3, put $h = 1/\xi_3$, $\xi_3 \to +\infty$, and multiply P by h, then we obtain a semi-classical operator,

$$P(h) = hD_{x_1} + ihD_{x_2} + ix_1 - x_2\,.$$

The smoothness properties are now translated to decay properties as $h \to 0$. The adjoint of $P(h)$ has the symbol $\xi_1 - i\xi_2 - ix_1 - x_2$ which satisfies the assumptions needed for (11) (with $P(h)$ replaced by $P(h)^*$). The approximate solutions used to prove lack of solvability can be obtained from the quasi-modes constructed there.

Since the early papers [8],[13], the question of solvability of differential and pseudodifferential equations was studied by the leading analysts – see [10], and also [9] for an excellent survey.

Proof of Theorem

Replacing technical arguments by heuristics, we can present an outline of the modern proof of the main theorem. It essentially follows [10, Sect.26.2] with simplifications in the semi-classical setting.

Let $P(h)$ be a semi-classical operator with a principal symbol $p(x,\xi)$:

$$P(h) = p(x, hD_x) + hp_1(x, hD_x, h)\,.$$

Suppose that the commutator condition holds in a stronger form,

$$\{\mathrm{Re}\, p, \mathrm{Im}\, p\}(x,\xi) = -1\,,$$

in a neighbourhood of a point (x_0,ξ_0), such that $p(x_0,\xi_0) = 0$[3]. The classical theorem of Darboux shows that there exists a symplectic change of variables (that is, a change of variables preserving the symplectic form, or in other words, classical mechanics)

$$\kappa(y,\eta) = (x,\xi)\,,$$

defined near $(0,0)$, and such that

$$\kappa(0,0) = (x_0,\xi_0)\,, \quad \mathrm{Re}\, p(\kappa(y,\eta)) = \eta_1\,, \quad \mathrm{Im}\, p(\kappa(y,\eta) = -y_1\,.$$

In other words,

$$\kappa^* p(y,\eta) = \eta_1 - iy_1\,,$$

which is the symbol of the annihilation operator $A_- = hD_{y_1} - iy_1$ which appeared in the discussion of the quantum harmonic oscillator. This operator has a highly localized solution given by the ground state of the harmonic oscillator, and we can localize it trivially to $(0,0)$ in all variables:

$$u_0(h,y) = \exp(-|y|^2/2h)\,, \quad (hD_{y_1} - iy_1)u_0(h,y) = 0\,.$$

The question now lies in transplanting u_0 to the (x,ξ) coordinates so that we obtain an approximate solution of $P(h)u = 0$.

The point of semi-classical analysis, and of its reflection in the theory of partial differential equations, microlocal analysis, is that the symplectic transformation κ can also be quantized (just as we quantized functions to obtain generalized differential operators, or pseudo-differential operators). That gives the theory

[3]As shown by Duistermaat and Sjöstrand [4],[10, Lemma 21.3.4], this can always be arranged by multiplying p by a non-vanishing function.

of Fourier Integral Operators (see [10, Chapter XXV], and also [17] for a self-contained discussion of local theory in the semi-classical setting). More precisely, we can associate to κ a family of operators

$$U_\kappa(h) \,:\, L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n)\,,$$

uniformly bounded, invertible for small h, such that for any function $q(x,\xi)$ satisfying (9) we have

$$U_h(\kappa)^{-1} q(x,hD_x) U_h(\kappa) = \kappa^* q(y,hD_y) + \mathcal{O}_{L^2\to L^2}(h)\,. \tag{13}$$

This relations is called the *Egorov Theorem* and for simplicity we assumed here that κ is globally defined. There are many operators which satisfy (13) and with care, one can choose $U_h(\kappa)$, and $q(x,\xi,h)$, so that

$$\begin{gathered} U_h(\kappa)^{-1} P(h) U_h(\kappa) = q(y,hD_y,h)(hD_{y_1} - iy_1) + \mathcal{O}_{L^2\to L^2}(h^\infty)\,,\\ q(y,hD_y;h) = q_0(y,hD_y) + hq_1(y,hD_y;h)\,,\quad q_0(0,0)\neq 0\,, \end{gathered}$$

is valid for functions localized near $(0,0)$ (in the sense given in (11)). This concludes the proof of the theorem as by putting $u(h) = U_h(\kappa)u_0(h)$ we obtain a family of quasi-modes satisfying (11).

In the case when we have analyticity, similar results can be obtained, but now, with exponentially small errors. That involves the geometric result from [11] (existence of an analytic symplectic transformation) and the theory of the theory of Fourier Integral Operators in complex domains [15].

Remark. We should briefly mention what happens for operators, $P(h)$, with real symbols satisfying the *principal type* condition:

$$p(m) = 0 \implies dp(m) \neq 0\,.$$

In that case, we can proceed as before, obtaining $\kappa^* p(y,\eta) = \eta_1$, and then

$$U_h(\kappa)^{-1} P(h) U_h(\kappa) = hD_{y_1} + \mathcal{O}_{L^2\to L^2}(h^\infty)\,.$$

If we consider solutions of $hD_{y_1}u = 0$, we see that in solving (11) the condition on q has to be modified: the support of q has to be invariant under the flow of the Hamilton vector field of p (∂_{y_1} in the (y,η) coordinates; the Hamilton vectorfield is defined by $H_p f = \{p,f\}$). In the actual construction of approximate solutions (quasi-modes) global properties of the flow are important and "matching conditions" will allow only for a discrete set of z's. An easy way to see it is to consider the problem $(hD_x - z)u(h) = \mathcal{O}(h^\infty)$, $x\in \mathbb{S}^1 = \mathbb{R}/2\pi\mathbb{Z}$. A complex analogue is obtained when we consider the case where $\{\operatorname{Re} p, \operatorname{Im} p\} = 0$ but $d\operatorname{Re} p$ and $d\operatorname{Im} p$ are independent – see [10, Sect.26.2] and [14].

Annihilation Operator in Linear Algebra

The annihilation operator $A_- = hD_{y_1} - iy_1$ has spectrum equal to $\mathbb{C}$ and it satisfies the commutator condition globally:

$$[A_-, A_-^*] = 2Id\,,$$

a property which we already used in in deriving the lower bound for the quantum harmonic oscillator. As discussed in the previous section this is also the microlocal model for an operator with a non-propagating semi-classical singularity (quasi-mode). From the point of view of linear algebra the simplest model exhibiting "almost eigenvalues", or more precisely pseudospectrum away from the actual eigenvalues, is the *Jordan block* matrix:

$$J_n = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots \\ 0 & \dots & \dots & \ddots & 1 \\ 0 & \dots & \dots & \dots & 0 \end{pmatrix}$$

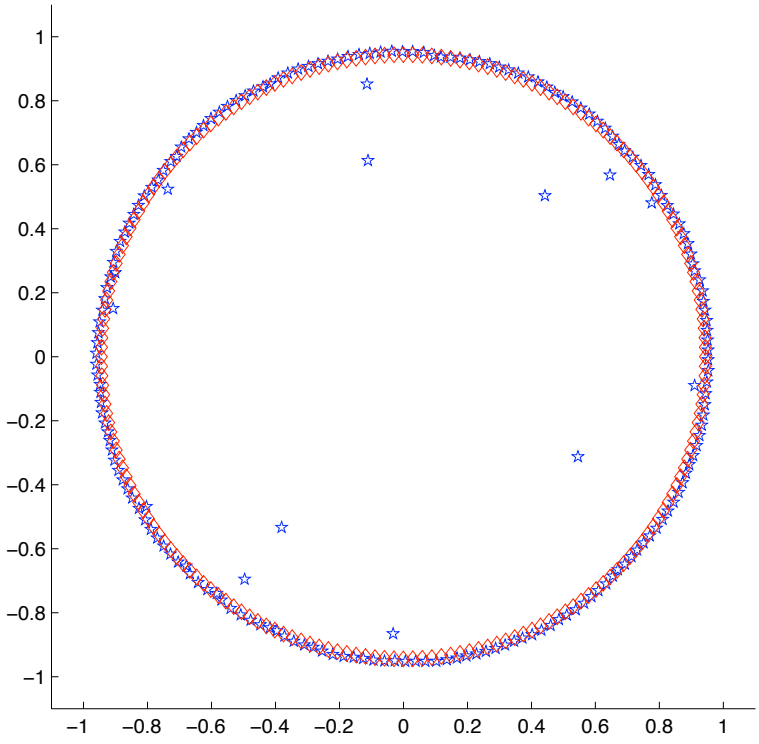

FIGURE 5. Eigenvalues of perturbations of 200×200 Jordan matrices: 10^{-5} put in the lower left hand corner, and a random perturbation with entries bounded by 10^{-5}.

It is a truncation of the shift operator $\widetilde{A}_-$, which can also be interpreted as an annihilation operator ($\widetilde{A}_- u_{n+1} = u_n$, $n \geq 0$). The spectrum of $\widetilde{A}_-$ is the unit disc and $[\widetilde{A}_-, \widetilde{A}_-^*] \geq 0$. We have $J_n = \Pi_n \widetilde{A}_- \Pi_n$, where Π_n is the truncation to the first n basis vectors. The resolvent is given by

$$(\lambda - J_n)^{-1} = \frac{I}{\lambda} + \frac{J_n}{\lambda} + \cdots + \frac{J_n^{n-1}}{\lambda^n},$$

and although the spectrum of J_n is equal to $\{0\}$ (with multiplicity n), the norm of the resolvent grows exponentially with n for $|\lambda| < 1 - \delta$, $\delta > 0$. Hence for any $\epsilon > 0$, the ϵ-pseudospectrum will approach the the disc of radius $1 + \epsilon$ as the size of the matrix goes to infinity.

¿From the spectral point of view, the most dramatic perturbation of J_n comes from adding to it the matrix

$$\begin{pmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ x & \dots & 0 \end{pmatrix},$$

with the resulting matrix denoted by $\widetilde{J}_n(x)$. Its characteristic polynomial is given by $\lambda^n - x$. Hence, for an arbitrarily small x, the spectrum will be very close to the *boundary* of the pseudospectrum, $|x|^{1/n} \to 1$, as $n \to \infty$. This is the phenomenon which we have seen in our numerical experiments: in Figures 2 and 4 the "false eigenvalues" were computed near the boundary of the semi-classically determined pseudospectrum.

In fact, this can be used to explain the effect of the pseudospectra on some numerical computations. The proximity to Jordan block-like matrices will cause small perturbations (caused in turn by the properties

of the discretization used, and by round-off errors) to push the computed eigenvalues, which are the actual eigenvalues of $A+\delta A$, for δA small, to the boundary of the pseudospectrum.

We refer to [5] for a discussion of related issues and content ourselves with another naïve experiment. Fig.5 shows the eigenvalues of $\widetilde{J}_{200}(10^{-5})$ and the eigenvalues of a matrix obtained by adding to J_{200} a random matrix with entries of size bounded by 10^{-5}. The eigenvalues of the random perturbation are certainly closer to the unit circle than to zero.

Other Directions

There are at least two natural directions for further investigation of the connection described here:

- The commutator condition and the rôle of the annihilation operator can be understood in a more abstract framework. Classes of large matrices can be understood in terms of quantization of compact symplectic manifolds with the Planck constant corresponding to the inverse of the size of the matrix. In other words, the phenomena described here can be seen directly on the level of large matrices, and not only in discretization of differential operators.
- Better estimates are expected to hold in the regions where $\{\mathrm{Re}\, p, \mathrm{Im}\, p\} = 0$, and those regions are often most interesting physically. The estimates on the resolvent are expected to be better there, and consequently numerical computations should be more stable.

We motivate the second item above by the example from chemistry, schematically illustrated by Fig.1. The complex eigenvalues which are of interest (that is, the ones which model the unstable states) are expected to have imaginary parts, Γ, of size much smaller than h (since the factor Γ/h will appear as the decay rate). Also, the artificial potential $-iW(x)$, will produce its own irrelevant eigenvalues in a region with $\mathrm{Im}\, z \ll -h$. Hence, any eigenvalues there are "false" – either due to $-iW(x)$ or to numerical problems, and in any case of no interest. Consequently all interest lies in an h-dependent neighbourhood of the boundary "semi-classical pseudospectrum". The Poisson bracket vanishes there and consequently the general results do not apply.

For more subtle objects, namely resonances (see [20] and references given there), a similar statement is true. Of various recently studied cases, the furthest that one ever gets from the real axis is in the case of scattering by convex obstacles [16][4], and a similar distance is $Ch^{2/3}$. In computing resonances one also has a lot of freedom in choosing the non-selfadjoint operator of which they are eigenvalues. Deforming so that $\{\mathrm{Re}\, p, \mathrm{Im}\, p\} = 0$ holds in a relevant region was recently exploited by Melin and Sjöstrand [14]. To get an heuristic understanding of such deformations, we refer to the example shown in Fig. 4: the operator became normal after a conjugation by $\exp(-x/2h)$, and that could be considered as a deformation of our operator. In the case shown in 3, the conjugation involves a differential operator in the exponential weight, and has a geometric interpretation as *a deformation* into the complex domain, which is in fact what we used.

Consequently one arrives again at an issue similar to the one which arises in the study of solvability: $\{\mathrm{Re}\, p, \mathrm{Im}\, p\} = 0$ is necessary for solvability, but what other condition would make it sufficient as well? We refer to Hörmander's review [9] for a discussion of that. The relation of solvability to quantum mechanics and semi-classics was emphasized by Fefferman [6] but the relation to practical problems described here remains unclear.

ACKNOWLEDGMENTS. I would like to thank Mike Christ, Peter Greiner, and Lars Hörmander for helpful discussions of the issues of solvability, Alan Edelman, William Kahan, and Beresford Parlett for advice on numerical linear algebra, Bill Miller for the explanation of the CAP method in a concrete situation, and Carl Wunsch and Jared Wunsch for comments on the first version of this paper. I am also grateful to Nick Trefethen and Mark Embree for their detailed and instructive comments, and to Tom Wright for providing the correct version of Fig.5

[4]That is in fact also the oldest case, as the resonances for the sphere appear in the Watson transform used to study the behaviour of a diffracted wave in the deep shadow, a real but subtle thing.

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