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ALBERT BAERNSTEIN II

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Lectures on exponential decay of solutions of second-order elliptic equations: bounds on eigenfunctions of N-body Schrödinger operators, by Shmuel Agmon, Mathematical Notes, Vol. 29, Princeton University Press, Princeton, New Jersey, 1982, 118 pp., $10.50. ISBN 0-6910-8318-5

Square integrable eigenfunctions of the Schrödinger equation decay exponentially. More precisely, let

$$\tilde{H} = -\sum_{i=1}^{N} \frac{1}{2m_i}\Delta_i + \sum_{i<j} V_{ij}(x_i - x_j), \qquad x_i \in \mathbf{R}^\nu,$$

be the Schrödinger Hamiltonian for N particles interacting with real pairwise potentials $V_{ij}(x_i - x_j)$, where $V_{ij}(x_i - x_j) \to 0$ (in some sense) as $x_i - x_j \to \infty$ in $\mathbf{R}^\nu$. Separating out the center of mass ($\tilde{H}$ itself has only continuous spectrum) one obtains the operator

$$H = -\Delta + \sum_{i<j} V_{ij}(x_i - x_j),$$

where Δ denotes the Laplacian on $L^2(X)$, $X = \{x = (x_1,\ldots,x_N)\colon \sum_{i=1}^N m_i x_i = 0\}$. If ϕ is an L^2 solution of $H\phi = E\phi$, and if E lies below the essential spectrum of H, then ϕ decays exponentially in the sense that there exist positive constants A and B for which $|\phi(x)| \leqslant Ae^{-B|x|}$. The phenomenon of exponential decay has long been recognized and was apparent already in Schrödinger's solution of the hydrogen atom, but is is only recently that a satisfactory mathematical theory for the problem has been developed.

There is a considerable chemical, physical, and mathematical literature on the subject, and we refer the reader to **[9, 7]**, and also the notes to Chapter XIII of **[14]**, for extensive historical and bibliographic information. Four general techniques have emerged.

(1) *Comparison methods* (see for example **[4, 5** and **3]**). These methods are based on the maximum principle for second order elliptic operators and are modelled, to a greater or lesser extent, on the standard proofs of such classical theorems of complex analysis as the Hadamard three-line theorem, the Phragmen–Lindelöf theorem, and so on.

(2) *Analytic group methods* (see **[8, 9]**: the work in **[8]** was inspired by earlier work in **[13]**). Here the idea is to combine the invariance properties of the Laplacian under certain analytic group actions with the results of regular perturbation theory. The argument has charm and surprise, and, fortunately, is easy to describe. For example, under the action of translations $p \to p - b$ in Fourier space, the Schrödinger operator $H = -\Delta + V$ is mapped unitarily to

$$H_b = e^{ib\cdot x}(-\Delta + V)e^{-ib\cdot x} = \left(\frac{1}{i}\nabla - b\right)^2 + V(x), \quad \text{where } b \in \mathbf{R}^n.$$

If $\phi \in L^2$ is an eigenfunction for H, $H\phi = E\phi$, then $\phi_b = e^{ib\cdot x}\phi \in L^2$ is an eigenfunction for H_b, $H_b\phi_b = E\phi_b$; but if E is isolated, by regular perturbation theory, H_b has an eigenvalue E_b near E, even if b is (small and) complex. By analytic continuation the associated L^2 eigenfunction must be $\phi_b \equiv e^{ib\cdot x}\phi$. Said differently, this means that if $|b|$ is small enough, $e^{|b||x|}|\phi(x)| \in L^2$!

(3) *Operator positivity methods* **[1, 2]**. In this approach exponential decay follows directly from the positivity of the Schrödinger operator on certain subspaces and an elementary, but nonetheless remarkable, identity for second order elliptic operators. Again the ideas are easy to describe. Suppose $\phi(x)$ is a real, $L^2(\mathbf{R}^n)$ solution of the equation $H\phi = (-\Delta + V)\phi = E\phi$, where $E < 0$ and $V(x) \to 0$ as $|x| \to \infty$. Let f be an arbitrary real, bounded C^1 function with a bounded derivative. Then the interesting, and easily verified, observation is that after multiplying by e^f and integrating by parts, the equation becomes

$$(1) \qquad \int |\nabla\psi|^2 + \left(V - |\nabla f|^2 - E\right)\psi^2 = 0,$$

where $\psi \equiv e^f\phi \in L^2$. On the other hand, as $V(x) \to 0$ as $|x| \to \infty$, for any $\varepsilon > 0$, we may choose R such that $V(x) - E \geqslant (1 - \varepsilon)(-E)$ for $|x| \geqslant R$. Thus the Schrödinger operator satisfies the *positivity* condition

$$(2) \qquad \int_{|x|\geqslant R} |\nabla\chi|^2 + (V - E)\chi^2 \geqslant (1 - \varepsilon)(-E)\int_{|x|\geqslant R} \chi^2$$

for all real χ. Splitting equation (1) into $\{|x| < R\}$ and $\{|x| \geqslant R\}$, one obtains

$$(3) \qquad \int_{|x|\geqslant R} \left((1 - \varepsilon)(-E) - |\nabla f|^2\right)\psi^2 \leqslant \int_{|x|<R} \left|\left(v - |\nabla f|^2 - E\right)\right|\psi^2.$$

Now let $b \in \mathbf{R}^n$ satisfy $|b|^2 < (1 - \varepsilon)(-E)$ and choose a sequence of real bounded C^1 functions f_n satisfying $|\nabla f_n|^2 < (1 - \varepsilon)(-E)$ and which converge to $f \equiv b \cdot x$ ($\notin L^\infty$). The point is that as $n \to \infty$, the right side of (2) remains bounded, by C say, and this in turn implies the a priori exponential bound

$$\int_{|x|\geqslant R} \left(e^{b\cdot x}\phi\right)^2 \leqslant \frac{C}{\left((1 - \varepsilon)(-E) - |b|^2\right)}!$$

In particular, ϕ decays (in the L^2 sense) like $e^{-|b||x|}$, as long as $|b| < \sqrt{(-E)} = \sqrt{0 - E} = \sqrt{\inf(\operatorname{ess\,spec} H) - E}$.

(4) *Probabilistic methods* **[6, 7]**. Here the eigenfunction ϕ is expressed in terms of the semigroup $\phi = e^{(\Delta - V + E)t}\phi$, which is in turn reexpressed as a

Feynman–Kac integral. Exponential decay then follows by carefully singling out and estimating the important contributions to the integral.

The first result for general N-body systems ($N > 3$) was obtained by O'Connor [**13**], who proved the L^2 exponential bound for ϕ, $H\phi = E\phi$,

$$(4) \qquad \int_X dx\, |\phi(x)|^2 e^{2B\|x\|} < \infty,$$

as long as

$$(5) \qquad B < \sqrt{\Sigma - E},$$

where $\Sigma = \inf(\text{ess spec}\, H)$ and $\|x\|^2 = 2\sum_{i=1}^N m_i x_i \cdot x_i$ is the natural norm on X. Using analytic group methods as in (2), Combes and Thomas substantially simplified O'Connor's proof and also proved an extension of the result to eigenvalues embedded in the continuum. In [**15**] Simon showed that the L^2 bound (4) implies the pointwise bound

$$(6) \qquad |\phi(x)| \leqslant Ae^{-B\|x\|}$$

for the same range of B. Bounds such as (4) and (6), which depend only on $\|x\|$, are called *isotropic*. However, as first remarked by Morgan [**12**], in regions of configuration space where all the particles are separated, the eigenfunction ϕ automatically satisfies $-\Delta\phi = E\phi$, so that one expects falloff like $\exp(\Sigma_{i=1}^N b_i x_i)$, with $\Sigma b_i^2/2m_i = -E$, which may be considerably more rapid than (6). This observation then led the authors in [**9**] to discover nonisotropic bounds of the form $|\phi(x)| \leqslant Ae^{b\cdot x}$, which were sensitive to the decay of the potentials $V_{ij}(x_i - x_j)$ in different directions of configuration space. The authors obtained their bounds through an extension of the analytic group method and stated their results in the form of a series of inequalities, similar to (5), but now containing directional information that b should satisfy in order that $e^{b\cdot x}$ be a bound for $\phi(x)$. Simultaneously and independently, Alrichs and M. and T. Hoffmann-Ostenhof [**4, 5**] used comparison methods to study the atomic case (with fixed nucleus) and obtained similar results.

The methods (1)–(4) described above specifically for the eigenvalue problem, can in fact be used in a wide variety of analytical situations. We mention two. For $E <$ spec$(-\Delta + V)$ and for fixed y, the Green's function $G(x, y)$, $(-\Delta_x + V(x) - E)\, G(x, y) = \delta(x - y)$, is an $L^2(dx)$ solution of the Schrödinger equation away from $x = y$, and so the methods (1)–(4) immediately provide exponential decay rates for G as $|x| \to \infty$. In a less obvious development, for the parametric Hamiltonian $-\Delta + \lambda^2 V$, not only do the methods provide information about the decay of eigenfunctions of $-\Delta + \lambda^2 V$ for fixed λ as $|x| \to \infty$, but also for fixed x as $\lambda \to \infty$. This then can be used to study eigenvalue splittings in tunnelling situations, where one learns that the gap between the first and second eigenvalues of $-\Delta + \lambda^2 V$ decays exponentially in λ at a rate given by the distance between two wells in the potential V, as measured in the Agmon metric (see [**16, 17** and **18**]).

The authors in [**9**] obtained improvements on the isotropic bounds (6) by constructing partial solutions of the above inequalities in a rather hit and miss fashion. It was Agmon [**1, 2**], however, who realized that the inequalities could be regarded as inducing a metric on X and that the best bound of the form $|\phi(x)| \leqslant Ae^{-(1-\varepsilon)\rho(x)}$, $\varepsilon > 0$, could be obtained by choosing $\rho(x)$ to be geodesic distance in this metric. Agmon's beautiful and, at this stage, definitive result for L^2 eigenfunctions ϕ of N-body Hamiltonians H, $H\phi = E\phi$, is as follows. For each partition D of N particles into disjoint clusters, set

$$H_D = -\Delta + \sum_{i,j}^{(D)} V_{ij}(x_i - x_j),$$

where $V_{ij}(x_i - x_j)$ is set to zero in the sum $\Sigma_{i,j}^{(D)}$ unless i and j belong to the *same* cluster. Define the threshold energy by $\Sigma_D = \inf(\mathrm{spec}(H_D))$. By a well-known result (see e.g. **[14]**), $\Sigma \equiv \min_D \Sigma_D$ is the infimum of the essential spectrum of H. For each $x = (x_1, \ldots, x_n) \in X$, let $D(x)$ be the partition obtained by lumping together those i and j with $x_i = x_j$. Mostly, $D(x)$ is the N cluster partition, but along directions where $x_i - x_j = 0$, $D(x)$ has fewer clusters, etc. The result is that if $\rho(x)$ is the geodesic distance (from the origin, say) to x in the metric

$$ds^2 = \left(\Sigma_{D(x)} - E\right) \sum_{i=1}^{N} 2m_i |dx_i|^2,$$

then for all $\varepsilon > 0$,

$$|\phi(x)| \leqslant A_\varepsilon e^{-(1-\varepsilon)\rho(x)}, \tag{7}$$

provided that $E < \Sigma$. Agmon proved his results using operator positivity methods as in (3). Precursors of the method can be found, for example, in (a subsection) of **[11]**.

In the case of the ground state, where E lies at the bottom of the spectrum of H and the eigenfunction ϕ is strictly positive, it is possible to show that the bound (7) is the best possible by proving a lower bound of the same form:

$$|\phi(x)| \geqslant A'_\varepsilon e^{-(1+\varepsilon)\rho(x)}. \tag{8}$$

Taking limits one obtains

$$\lim_{\|x\| \to \infty} \frac{\log \phi(x)}{\rho(x)} = -1.$$

The lower bound (7) for the general N-body problem is due to Carmona and Simon [7] (a special case was obtained by T. Hoffman–Ostenhof in **[10]**), who used probabilistic techniques as in method (4). It turns out that probabilistic methods are particularly well suited to describing lower bounds for the ground state. This is because ϕ is positive, and one can simply neglect the contribution to the Feynman–Kac integral from all except those paths in a neighborhood of a certain distinguished path. This distinguished path is chosen to minimize the classical Lagrangian action, and in an elegant circle of ideas connected with Jacobi's geometrization of mechanics, the minimum value of the action turns out to be precisely the geodesic length in Agmon's metric.