The Fundamental Gap

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The second main problem to be focused on at the workshop is what we'll refer to as the **Fundamental Gap Problem**, which is the problem of finding a sharp lower bound to the gap between the first two eigenvalues of a Schrödinger operator on a bounded convex domain with convex potential in terms of the diameter of the domain. We call the lowest eigenvalue gap, i.e., the gap between the first two eigenvalues, the *fundamental gap*. We shall describe two versions of this problem, one for the Laplacian alone and the other for Schrödinger operators. The second problem contains the first as a special case, but the first is of course of substantial interest in its own right, and may possibly be more tractable than the general problem.

In the first problem one just considers the Laplacian $-\Delta$ on a bounded convex domain Ω with Dirichlet boundary conditions. This problem has a purely discrete spectrum, $\{\lambda_i(\Omega)\}_{i=1}^{\infty}$, with ∞ as its only point of accumulation. Listed in increasing order, with multiplicities, we have

$$0 < \lambda_1(\Omega) < \lambda_2(\Omega) \leq \lambda_3(\Omega) \leq \cdots \to \infty. \tag{1}$$

The fundamental gap, $\Gamma(\Omega)$, is given simply as

$$\Gamma(\Omega) = \lambda_2(\Omega) - \lambda_1(\Omega). \tag{2}$$

When the domain Ω is clear we write $\Gamma = \lambda_2 - \lambda_1$ for short.

It was suggesteded by M. van den Berg in 1983 [8] that the fundamental gap $\Gamma = \lambda_2 - \lambda_1$ of a convex domain is bounded below by $3\pi^2/d^2$, i.e., that

$$\Gamma(\Omega) = \lambda_2(\Omega) - \lambda_1(\Omega) \geq 3\pi^2/d^2, \tag{3}$$

where d is the diameter of the domain (we note that van den Berg considered $-\frac{1}{2}\Delta$ and so his lower bound contained an extra factor of $\frac{1}{2}$ compared to (3)). If $3\pi^2/d^2$ is indeed the best lower bound, then that would indicate that the saturating case is when the domain degenerates to a linear strip (a rectangular parallelepiped, with all dimensions but one going to 0). In one dimension the result is clear, since up to scalings there is only one convex domain in $\mathbb{R}$ (and the inequality respects scalings). The problem remains of interest in all dimensions $n \geq 2$, and, indeed, while progress has been made toward obtaining bounds of the "right" general form, no one has as yet established a general bound with the conjectured optimal constant. Further details of the known results on this problem will be given below after we have outlined the more general problem for Schrödinger operators.

In the more general problem one considers the Schrödinger operator

$$H = -\Delta + V(x) \tag{4}$$

where $V(x)$ is the potential, a multiplication operator, and $x \in \Omega \subset \mathbb{R}^n$. We again take Ω a bounded convex set, and now, to avoid double-well examples (see, e.g., Harrell [21, 22], Kirsch and Simon [29, 30], Kirsch [27, 28]), we take V to be a convex function on Ω. We also impose Dirichlet boundary conditions. Just as for $-\Delta$, the spectrum of H is purely discrete and can be described by $\{\lambda_i(\Omega; V)\}_{i=1}^{\infty}$ with ∞ the only point of accumulation. We have included Ω and V as arguments of λ_i to indicate the dependence of the eigenvalues on both the domain and the potential. As above, we choose to arrange the eigenvalues in increasing order, multiplicities included:

$$0 < \lambda_1(\Omega; V) < \lambda_2(\Omega; V) \le \lambda_3(\Omega; V) \le \cdots \to \infty. \tag{5}$$

In this setting, the conjecture now reads exactly as before (modulo including the dependence on V):

$$\Gamma(\Omega; V) = \lambda_2(\Omega; V) - \lambda_1(\Omega; V) \ge 3\pi^2/d^2. \tag{6}$$

The conjecture for this case is that the inequality is saturated when the domain degenerates to a linear strip (a rectangular parallelepiped, with all dimensions but one going to 0) and with the potential going to a constant (the value of which is immaterial, and may be taken to be 0). Due to the inclusion of the potential, this problem is of interest (and nontrivial) in all dimensions $n \ge 1$. We discuss more background to this problem and partial results below.

First, though, we give some motivation for why one would want to study the fundamental gap and why bounds for it are important. In the grand scheme of things, beyond studying the first eigenvalue of a differential operator, the most interesting object is the gap between the first two eigenvalues, i.e., the fundamental gap. Note, too, that in cases where the first eigenvalue is trivially 0 one often first focuses on the first **nontrivial** eigenvalue, but this is in reality just the fundamental gap, slightly disguised. The fundamental gap often has interesting physical implications, as well as mathematical ones. For example, in the setting of the heat equation, the gap controls the rate of "collapse" of any initial state toward a state dominated by the first eigenfunction. For similar reasons, the gap is also of central interest in statistical mechanics (cf. van den Berg's work in [8], for example) and quantum field theory. In addition, from a numerical point of view, the gap can be used to control the rate of convergence of numerical methods of computation (for example, discretization or the finite element method leads to matrices as approximations to differential operators, and one's ability to solve for the first eigenvalue and eigenvector of such matrices is controlled by the separation between the first eigenvalue and the rest of the spectrum, i.e., the first eigenvalue gap). There are also a variety of cases in analysis where the gap is important, e.g., in refinements of the Poincaré inequality, a priori estimates, etc.

Beyond the paper of van den Berg, the recent history of the Fundamental Gap Problem primarily stems from the 1985 paper of Singer, Wong, Yau, and Yau [43], who obtained the lower bound $\pi^2/4d^2$ in the case of the general Schrödinger problem (for all dimensions n). Soon after, Yu and Zhong (1986) [48] were able to improve this to π^2/d^2, which provides a better, though presumably not sharp, constant. (We note that a key to the Singer, Wong, Yau, and Yau "breakthrough" for Schrödinger operators with convex potentials was the earlier fundamental work of Brascamp and Lieb [9, 10] proving log-concavity of the groundstate of such Schrödinger operators.) Further work in this vein includes that of F.-Y. Wang [45] (see also a precursor to this paper, [14]) and J. Ling [35].

Related work of Ashbaugh and Benguria [4, 5] suggested that the best bound of this form for the Schrödinger problem was likely $3\pi^2/d^2$ in all dimensions, based on the example of a rectangular parallelepiped, with all dimensions but one very small and with the potential going to a constant. Indeed, even if you fix the domain Ω you can use the potential to get back to this example, by making the potential go to infinity off a rectangular parallelepiped which "parallels a diameter", i.e., you take a parallelepiped having all dimensions but one tiny and with the last dimension being, essentially, the diameter d. This conjecture was made independently of the earlier observations of van den Berg.

The results established by Ashbaugh and Benguria include a one-dimensional result for Schrödinger operators with the sharp constant ($3\pi^2/d^2$) but under the assumption that the potential is symmetric and "single-well" (single-well means that the potential is first decreasing and then increasing), rather than for convex potentials. Of course this class includes the symmetric convex potentials, as well as a variety of nonconvex (but symmetric) potentials. Further work with single-well potentials in one dimension includes that of Horváth [24], who was able to eliminate the symmetry hypothesis of Ashbaugh and Benguria (the only remnant that survives is that the "transition point", i.e., the bottom of the well, must be centered; there are non-convex counterexamples if this condition is not met). A variety of related work on eigenvalue gaps and ratios has been completed by researchers in Taiwan; we cite [26] and [25] as representative works. Several recent papers by Ross Pinsky [41, 40, 39] compare a variety of approaches to an array of one-dimensional gap problems, focusing mainly on probabilistic approaches. The forthcoming book by A. Henrot [23] provides a good survey of much of the work on the one-dimensional gap problem with an emphasis on analytic methods.

Ashbaugh and Benguria also established results in n dimensions with dimension-dependent constants (increasing with n) under the assumption that the domain Ω is a ball and the potential is radially-symmetric and convex (and also under somewhat weaker conditions that imply these). In this case the best constant in the lower bound is determined by the potential which vanishes identically (and the constant is determined in terms of zeros of Bessel functions).

Later Lavine [32] was able to establish the sharp result for a Schrödinger operator with a convex potential in the one-dimensional case. Lavine's approach has been extended to other one-dimensional cases, and, in particular, to the vibrating string; see, for example, [26], [25], [1], [31]. However, all the higher dimensional cases remain open in general.

Progress has occurred, however, for cases with symmetry. Thus, Burgess Davis [19] obtained the sharp constant $3\pi^2/d^2$ for the case of the Laplacian on a bounded domain in $\mathbb{R}^2$ under the condition that the domain be symmetric with respect to both the x and y axes and that it be convex in both x and y ("convex in x" means that the intersection of the domain with any line parallel to the x-axis is an interval; "convex in y" is defined analogously). Also, at about the same time, Bañuelos and Méndez-Hernández [7] obtained comparison results for integrated heat kernels of a Schrödinger operator acting on L^2 functions on a bounded domain in $\mathbb{R}^2$ with the domain symmetric with respect to the y-axis and convex in x, and where the potential is assumed to be symmetric single-well in x for each y. This result gives, as corollaries, the Davis result given above and also the one-dimensional symmetric single-well result of Ashbaugh and Benguria. Further work in this area includes the papers of D. You [47] and C. Draghici [20].

If one gives up the convexity of the potential and also (possibly) of the domain, one can still obtain lower bounds to the fundamental gap, but the bounds must involve something about the potential, or more about the geometry of the domain, and not just its diameter. In particular, for double-well potentials the gap can be made arbitrarily small, and similarly for "dumbbell-shaped domains". Various references on these matters include [21], [22], [16], [17], [29], [36], [30], [27], [28], [42], [18], [2], and [11] (but note that this list makes no claim to completeness, nor to identifying the earliest references; in fact, it is likely far from complete in either sense).

Generalizations (building on the work of Singer, Wong, Yau, and Yau and, most directly, on that of Yu and Zhong) have been made to domains in spheres in the work of Y. I. Lee and A. N. Wang [33], with later refinements by J. Ling [34] (see also his recent preprint [35]). Work for domains in general manifolds (and involving more than convexity hypotheses and a lower bound in terms of a "diameter") includes that of K. Oden and coauthors (see, for example, [15], [37]), and F.-Y. Wang and coauthors [14], [45].

Although our focus has been on problems with Dirichlet boundary conditions, we also mention that for the Laplacian there are generally close analogies between results for the fundamental gap for Dirichlet problems and for the first nonzero Neumann eigenvalue (which, as mentioned above, can also be viewed as the fundamental gap of the Neumann problem). Thus, the early result of Payne and Weinberger [38] (also treated in Bandle [6], pp. 155–158) that the first nonzero Neumann eigenvalue of the Laplacian on a bounded convex domain is bounded below by π^2/d^2 is relevant to the present discussion. Further developments of this theme occur in the work of R. Smits [44]. Beyond that, R. Chen [12, 13] has considered the case of Neumann problems on general Riemannian manifolds.

Beginner's Guide

For more background on this subject we suggest the following articles as being particularly useful:

- I. M. Singer, B. Wong, S.-T. Yau, and S. S.-T. Yau, *An estimate of the gap of the first two eigenvalues in the Schrödinger operator*, Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4) **12** (1985), 319–333.

- S.-T. Yau, **Nonlinear Analysis in Geometry**, Enseignement Math., Geneva, 1986. [This also appeared as an article: *Nonlinear analysis in geometry*, Enseign. Math. **33** (1987), 109–158.]

- Q. H. Yu and J.-Q. Zhong, *Lower bounds of the gap between the first and second eigenvalues of the Schrödinger operator*, Trans. Amer. Math. Soc. **294** (1986), 341–349.

- M. S. Ashbaugh and R. D. Benguria, *Optimal lower bound for the gap between the first two eigenvalues of one-dimensional Schrödinger operators with symmetric single-well potentials*, Proc. Amer. Math. Soc. **105** (1989), 419–424.
- R. Lavine, *The eigenvalue gap for one-dimensional convex potentials*, Proc. Amer. Math. Soc. **121** (1994), 815–821.
- R. Bañuelos and P. J. Méndez-Hernández, *Sharp inequalities for heat kernels of Schrödinger operators and applications to spectral gaps*, J. Funct. Anal. **176** (2000), 368–399.
- R. G. Smits, *Spectral gaps and rates to equilibrium for diffusions in convex domains*, Mich. Math. J. **43** (1996), 141–157.
- A. Henrot, **Extremum Problems for Eigenvalues of Elliptic Operators**, 2006 (to appear).

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