

Publication list with abstracts—Alex Barnett

“Inclusion of Dirichlet eigenvalues in the semiclassical limit via a boundary spectral problem”, Alex H. Barnett, *in preparation*.

The ‘drum problem’— finding the eigenvalues $\{E_j\}$ and eigenmodes of the Laplacian in a domain $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary condition— is numerically challenging and has a wealth of applications. We present a variant of the Method of Particular Solutions (MPS) involving a nonlinear eigenvalue problem, namely a search for parameter values E where a generalized eigenvalue $\lambda_1(E) \rightarrow 0$. By mapping to a spectral problem for a compact operator $A(E) : L^2(\partial\Omega) \rightarrow L^2(\partial\Omega)$, we derive the perturbation of λ_1 as a function of $E - E_j$. This gives, in the limit of small boundary error, eigenvalue inclusion bounds which are $O(E^{1/2})$ tighter than the classical *a priori/a posteriori* bounds of Kuttler-Sigillito. At large eigenvalues (high frequencies), this can lead to higher numerical accuracy, and a route to error analysis of a much accelerated MPS known as the scaling method.

“Quasi-orthogonality on the boundary for Euclidean Laplace eigenfunctions”, Alex. H. Barnett, *submitted, Comm. Pure Appl. Math.*

Consider the Laplacian in a bounded domain in \mathbb{R}^d with general (mixed) homogeneous boundary conditions. We prove that its eigenfunctions are ‘quasi-orthogonal’ on the boundary with respect to a certain norm. Boundary orthogonality is proved asymptotically within a narrow eigenvalue window of width $o(E^{1/2})$ centered about E , as $E \rightarrow \infty$. For the special case of Dirichlet boundary conditions, the normal-derivative functions are quasi-orthogonal on the boundary with respect to the weight function $\mathbf{r} \cdot \mathbf{n}$. The result is independent of any quantum ergodicity assumptions and hence of the nature of the domain’s geodesic flow; however if this is ergodic then known semiclassical results allow an improved asymptotic estimate. Boundary quasi-orthogonality is the key to a highly efficient ‘scaling method’ for numerical solution of the Laplace eigenproblem at large E . One of the main results of this paper is then to place this method on a more rigorous footing.

“Asymptotic rate of quantum ergodicity in chaotic Euclidean billiards”, Alex. H. Barnett, *submitted, Comm. Pure Appl. Math.*

The Quantum Unique Ergodicity (QUE) conjecture of Rudnick-Sarnak is that every quantum (Laplace) eigenfunction ϕ_n of an ergodic, uniformly-hyperbolic classical geodesic flow becomes equidistributed in the semiclassical limit (eigenvalue $E_n \rightarrow \infty$). We report numerical results on the rate of quantum ergodicity, for a uniformly-hyperbolic Euclidean billiard with Dirichlet boundary condition (the ‘drum problem’) at unprecedented high E and statistical accuracy. We calculate matrix elements $\langle \phi_n, \hat{A} \phi_m \rangle$ of a piecewise-constant test observable A , and collect 30000 diagonal matrix elements up to level $n \approx 7 \times 10^5$. Our results support the validity of QUE, that is, there are no ‘strong scars’. We find asymptotic power-law decay $aE^{-\gamma}$ of the diagonal variance with $\gamma \approx 0.48 \pm 0.01$. However convergence to the semiclassical estimate of Feingold-Peres (FP), where $\gamma = 1/2$, appears slow. We also compare off-diagonal variance with the FP sum rule at the highest accuracy (0.7%) known in any chaotic system.

“A fast numerical method for time-resolved photon diffusion in general stratified turbid media”, Alex H. Barnett, *Journal of Computational Physics* 201, 771-797 (2004)

Efficient forward models of photon migration in complex geometries are important for noninvasive imaging of tissue *in vivo* with Diffuse Optical Tomography (DOT). In particular solving the inverse problem requires multiple solutions of the forward model and is therefore computationally intensive. We present a numerical algorithm for the rapid solution of the time-dependent diffusion equation in a semi-infinite inhomogeneous medium whose scattering and absorption coefficients are arbitrary functions of depth, given a point source impulsive excitation. Such stratified media are biomedically important. A transverse modal representation leads to a series of one-dimensional diffusion problems which are solved via finite-difference methods. A novel time-stepping scheme allows effort to scale independently of total time (for fixed system size). Tailoring to the DOT application gives run times of order 0.1 s. We study convergence, computational effort, and

validate against known solutions in the case of 2-layer media. The method will be useful for other forward and inverse diffusion problems, such as heat conduction and conductivity measurement.

“Bayesian estimation of optical properties of the human head via 3D structural MRI”, Alex H. Barnett, Joseph P. Culver, A. Gregory Sorensen, Anders M. Dale, and David A. Boas, *Proc. SPIE* 5138 (2003).

Knowledge of the baseline optical properties of the tissues of the human head is essential for absolute cerebral oximetry, and for quantitative studies of brain activation. In this work we numerically model the utility of signals from a small 6-optode time-resolved diffuse optical tomographic apparatus for inferring baseline scattering and absorption coefficients of the scalp, skull and brain, when complete geometric information is available from magnetic resonance imaging (MRI). We use an optical model where MRI-segmented tissues are assumed homogeneous. We introduce a noise model capturing both photon shot noise and forward model numerical accuracy, and use Bayesian inference to predict errorbars and correlations on the measurements. We also sample from the full posterior distribution using Markov chain Monte Carlo. We conclude that $\sim 10^6$ detected photons are sufficient to measure the brain’s scattering and absorption to a few percent. We present preliminary results using a fast multi-layer slab model, comparing the case when layer thicknesses are known versus unknown.

“Robust inference of baseline optical properties of the human head with 3D segmentation from magnetic resonance imaging”, Alex H. Barnett, Joseph P. Culver, A. Gregory Sorensen, Anders M. Dale, and David A. Boas, *Applied Optics* 42, 3095–3108 (2003).

We model the capability of a small (6-optode) time-resolved diffuse optical tomography (DOT) system to infer baseline absorption and reduced scattering coefficients of the tissues of the human head (scalp, skull and brain). Our heterogeneous three-dimensional diffusion forward model uses tissue geometry from segmented MR data. Handling the inverse problem via Bayesian inference, and introducing a realistic noise model, we predict coefficient errorbars in terms of detected photon number and assumed model error. We demonstrate the large improvement that an MR-segmented model can provide: 2–10% error in brain coefficients (for 2×10^6 photons, 5% model error). We sample from the exact posterior, and show robustness to numerical model error. This opens up the possibility of simultaneous DOT/MR for quantitative cortically-constrained functional neuroimaging.

“Parametric evolution for a deformed cavity”, D. Cohen, A. H. Barnett, and E. J. Heller, *Phys. Rev. E* 63, 46207 (2001), [nlin.CD/0008040](#).

We consider a classically chaotic system that is described by a Hamiltonian $\mathcal{H}(Q, P; x)$, where (Q, P) describes a particle moving inside a cavity, and x controls a deformation of the boundary. The quantum-eigenstates of the system are $|n(x)\rangle$. We describe how the parametric kernel $P(n|m) = |\langle n(x)|m(x_0)\rangle|^2$, also known as the local density of states, evolves as a function of $\delta x = x - x_0$. We illuminate the non-unitary nature of this parametric evolution, the emergence of non-perturbative features, the final non-universal saturation, and the limitations of random-wave considerations. The parametric evolution is demonstrated numerically for two distinct representative deformation processes.

“Mesoscopic scattering in the half-plane: squeezing conductance through a small hole”, A. H. Barnett, M. Blaauuboer, A. Mody, and E. J. Heller, *Phys. Rev. B* 63, 245312/1 (2001), [cond-mat/0008279](#).

We model the 2-probe conductance of a quantum point contact (QPC), in linear response. If the QPC is highly non-adiabatic or near to scatterers in the open reservoir regions, then the usual distinction between leads and reservoirs breaks down and a technique based on scattering theory in the full two-dimensional half-plane is more appropriate. Therefore we relate conductance to the transmission *cross section* for incident plane waves. This is equivalent to Landauer’s formula using a radial partial-wave basis. We derive the result that an arbitrarily small (tunneling) QPC can reach a p-wave channel conductance of $2e^2/h$ when coupled to a suitable reflector. If two or more resonances coincide the total conductance can even exceed this. This relates to recent mesoscopic experiments in open geometries. We also discuss reciprocity of conductance,

and the possibility of its breakdown in a proposed QPC for atom waves.

“Rate of energy absorption for a driven chaotic cavity”, A. H. Barnett, D. Cohen, and E. J. Heller, J. Phys. A 34, 413–437 (2001), nlin.CD/0006041

We consider the response of a chaotic cavity in d dimensions to periodic driving. We are motivated by older studies of one-body dissipation in nuclei, and also by anticipated mesoscopic applications. For calculating the rate of energy absorption due to time-dependent deformation of the confining potential, we introduce an improved version of the wall formula. Our formulation takes into account that a special class of deformations causes no heating in the zero-frequency limit. We also derive a mesoscopic version of the Drude formula, and explain that it can be regarded as a special example of our calculations. Specifically we consider a quantum dot driven by electro-motive force which is induced by a time-dependent homogeneous magnetic field.

“Deformations and dilations of chaotic billiards: dissipation rate, and quasi-orthogonality of the boundary wavefunctions”, A. H. Barnett, D. Cohen, and E. J. Heller, Phys. Rev. Lett. 85, 1412 (2000), nlin.CD/0003018

We consider chaotic billiards in d dimensions, and study the matrix elements M_{nm} corresponding to general deformations of the boundary. We analyze the dependence of $|M_{nm}|^2$ on $\omega = (E_n - E_m)/\hbar$ using semiclassical considerations. This relates to an estimate of the energy dissipation rate when the deformation is periodic at frequency ω . We show that for dilations and translations of the boundary, $|M_{nm}|^2$ vanishes like ω^4 as $\omega \rightarrow 0$, for rotations like ω^2 , whereas for generic deformations it goes to a constant. Such special cases lead to quasi-orthogonality of the eigenstates on the boundary.

“Substrate-based atom waveguide using guided two-color evanescent light fields”, A. H. Barnett, S. P. Smith, M. Olshanii, K. S. Johnson, A. W. Adams, M. Prentiss, Phys. Rev. A 61, 023608 (2000), physics/9907014.

We propose a dipole-force linear waveguide which confines neutral atoms up to $\lambda/2$ above a microfabricated single-mode dielectric optical guide. The optical guide carries far blue-detuned light in the horizontally-polarized TE mode and far red-detuned light in the vertically-polarized TM mode, with both modes close to optical cut-off. A trapping minimum in the transverse plane is formed above the optical guide due to the differing evanescent decay lengths of the two modes. This design allows manufacture of mechanically stable atom-optical elements on a substrate. We calculate the full vector bound modes for an arbitrary guide shape using two-dimensional non-uniform finite elements in the frequency-domain, allowing us to optimize atom waveguide properties. We find that a rectangular optical guide of $0.8\,\mu\text{m}$ by $0.2\,\mu\text{m}$ carrying 6 mW of total laser power (detuning $\pm 15\,\text{nm}$ about the D2 line) gives a trap depth of $200\,\mu\text{K}$ for cesium atoms ($m_F = 0$), transverse oscillation frequencies of $f_x = 40\,\text{kHz}$ and $f_y = 160\,\text{kHz}$, collection area $\sim 1\,\mu\text{m}^2$ and coherence time of 9 ms. We discuss the effects of non-zero m_F , the D1 line, surface interactions, heating rate, the substrate refractive index, and the limits on waveguide bending radius.

“Bayesian Comparison of Models for Images”, A. H. Barnett and D. J. C. MacKay, in *Maximum Entropy and Bayesian Methods* (Kluwer, 1996), p. 239–248.

Probabilistic models for images are analysed quantitatively using Bayesian hypothesis comparison on a set of image data sets. One motivation for this study is to produce models which can be used as better *priors* in image reconstruction problems.

The types of model vary from the simplest, where spatial correlations in the image are irrelevant, to more complicated ones based on a radial power law for the standard deviations of the coefficients produced by Fourier or Wavelet Transforms. In our experiments the Fourier model is the most successful, as its *evidence* is conclusively the highest. It is shown how the radial power law ties in with the statistical scaling self-similarity (fractal property) of many images. Discussion of the invariances of the models, and a theoretical analysis of their performance leads to suggestions for further investigations.