A problem of Berry and knotted zeros in the eigenfunctions of the harmonic oscillator

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The quantum harmonic oscillator

It is described by the following spectral problem:

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These curves can be knotted and linked in many complicated ways.

Berry's problem

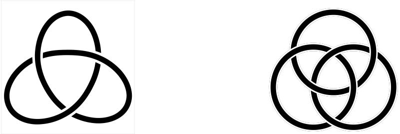

Figure: Trefoil knot and the Borromean rings.

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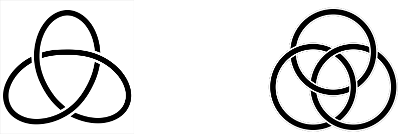

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Berry's problem (2001)

Given a finite link L in $\mathbb{R}^3$, do there exist an eigenfunction ψ of the harmonic oscillator and a diffeomorphism $\Phi : \mathbb{R}^3 \to \mathbb{R}^3$ such that $\Phi(L)$ is a union of connected components of the nodal set $\psi^{-1}(0)$? Is this set structurally stable?

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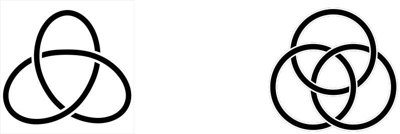

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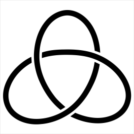

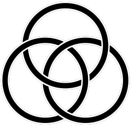

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A link is a union of (pairwise disjoint) smooth closed curves in $\mathbb{R}^3$.

The nodal set is structurally stable if any function φ such that $\|\varphi - \psi\|_{C^1(\mathbb{R}^3)} < \epsilon$ has a nodal set which is a small deformation of the nodal set of ψ.

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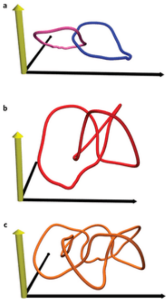

Figure: Numerical reconstruction from measured optical phase fields.

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Remark 3: The eigenfunctions have definite parity. Since the link $\Phi(L)$ is in the positive octant by construction, there is another copy of $\Phi(L)$ in the negative octant.

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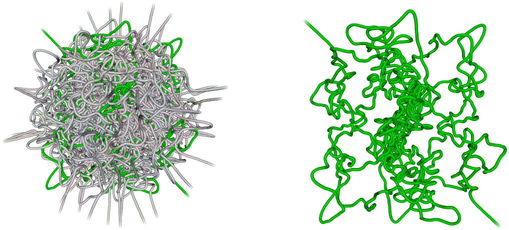

Figure: The nodal set of an eigenfunction of the 3D harmonic oscillator with $N = 21$, and one of its knotted connected components. Figure courtesy of Mark Dennis.

An inverse localization lemma

A first observation: let us rescale the space variables as $\tilde{x} = \sqrt{\lambda} x$. The harmonic oscillator equation then takes the form

$$\Delta_{\tilde{x}} \varphi + \varphi = \frac{|\tilde{x}|^2}{\lambda^2} \varphi \,,$$

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Heuristically: taking $\tilde{x} \in B$ (the unit ball), when $\lambda \to \infty$ the eigenfunction ψ behaves in the ball of radius $1/\sqrt{\lambda}$ as a solution to the Helmholtz equation in the unit ball. The following lemma shows that a converse claim holds:

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Inverse localization lemma for the harmonic oscillator

Let φ be an even (or odd) solution of $\Delta\varphi + \varphi = 0$ in $\mathbb{R}^3$. Fix $\epsilon > 0$ and an integer m. Then for any large enough eigenvalue λ, there is an eigenfunction ψ such that

$$\Big\|\psi\Big(\frac{\cdot}{\sqrt{\lambda}}\Big) - \varphi(\cdot)\Big\|_{C^m(B)} < \epsilon\,.$$

Sketch of the proof of the inverse localization lemma

Using spherical coordinates (r, θ, ϕ), the solution φ of the Helmholtz equation can be approximated in B by a Fourier-Bessel series:

$$\varphi \approx \sum_{l=0}^{l_0} \sum_{m=-l}^{l} c_{lm} j_l(r) Y_{lm}(\theta, \phi)\,,$$

where j_l is the spherical Bessel function, Y_{lm} is the spherical harmonic and c_{lm} are complex constants. Since φ is even we have that $c_{lm} = 0$ for any odd l.

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On the other hand, an orthogonal basis of harmonic oscillator eigenfunctions is given by:

$$\psi_{klm} = \exp(-r^2/2) r^l L_k^{l+1/2}(r^2) Y_{lm}(\theta, \phi) \,,$$

where L denotes the Laguerre polynomial. The eigenvalues have the expression

$$\lambda_{kl} = 2(2k + l) + 3 \,.$$

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We have the following asymptotic expansion uniformly for $r \leqslant 1$, as $k \to \infty$:

Lemma

$$\psi_{klm}(x) = A_{kl}\left[j_l(\sqrt{\lambda_{kl}}r) + O(\tfrac{1}{k})\right] Y_{lm}$$

$$\nabla\psi_{klm}(x) = \sqrt{\lambda_{kl}}A_{kl}\left[j_l'(\sqrt{\lambda_{kl}}r) + O(\tfrac{1}{k})\right] Y_{lm}e_r + A_{kl}\left[j_l(\sqrt{\lambda_{kl}}r) + O(\tfrac{1}{k})\right]\frac{\nabla_{\mathbb{S}^2}Y_{lm}}{r}$$

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In this lemma, e_r is the unit vector in the radial direction and A_{kl} is an explicit constant whose asymptotics is:

$$A_{kl} = \frac{2}{\sqrt{\pi}} k^{\frac{l+1}{2}} + O(k^{\frac{l-1}{2}})$$

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Now, to prove the localization lemma we proceed as follows. Fix a large constant $\hat{k} \gg l_0/2$, and define for any $l \leqslant l_0$ the number

$$\hat{k}_l := \hat{k} - \frac{l}{2}\,.$$

Sketch of the proof of the inverse localization lemma (III)

With these choices we have that $\lambda_{\hat{k}_l l} = 4\hat{k} + 3 =: \lambda$, so it is a fixed number. We can construct an eigenfunction of the harmonic oscillator for this eigenvalue as

$$\psi := \sum_{l=0}^{l_0} \sum_{m=-l}^{l} \frac{c_{lm}}{A_{\hat{k}_l l}} \psi_{\hat{k}_l lm} \,.$$

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Using the lemma for the asymptotic expansion of the eigenfunctions, we can derive the following estimate:

$$\left\| \psi\left(\frac{\cdot}{\sqrt{\lambda}}\right) - \varphi(\cdot) \right\|_{C^1(B)} \leqslant \sum_{l=0}^{l_0} \sum_{m=-l}^{l} |c_{lm}| O\left(\frac{1}{\hat{k}_l}\right) \leqslant \frac{C}{\hat{k} - \frac{l_0}{2}} < \epsilon$$

for any $\hat{k}$ that is large enough. The localization lemma is then proved.

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Remark 2: the techniques to prove this result are based on previous ideas developed by Enciso and the speaker to study the level sets of harmonic functions and the vortex structures in fluid mechanics. To this end, we need to develop a Runge-type global approximation theorem.

Knotted zeros for the Helmholtz equation (II)

A global approximation theorem for the Helmholtz equation

Let $\tilde{\varphi}$ be a function that satisfies the equation $\Delta\tilde{\varphi} + \tilde{\varphi} = 0$ in a (possibly disconnected) compact set $K \subset \mathbb{R}^3$. Assume that $\mathbb{R}^3 \backslash K$ has no bounded connected components. Then, there exists a function φ satisfying $\Delta\varphi + \varphi = 0$ in $\mathbb{R}^3$ such that $\|\tilde{\varphi} - \varphi\|_{C^m(K)} < \delta$, for any integer m and positive δ that are fixed a priori. Moreover, φ falls off at infinity as $|D^j\varphi(x)| < C_j|x|^{-1}$.

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Assuming that this result holds true, the proof of the theorem on the nodal set reduces to show that there exists a complex-valued solution $\tilde{\varphi} =: \tilde{\varphi}_1 + i\tilde{\varphi}_2$ of the equation $\Delta\tilde{\varphi} + \tilde{\varphi} = 0$ in a neighborhood N_L of the link L such that $\tilde{\varphi}^{-1}(0) = L$ and is structurally stable. The structural stability follows if we assume that $\tilde{\varphi}$ satisfies the condition:

$$\operatorname{rank}(\nabla\tilde{\varphi}_1(x), \nabla\tilde{\varphi}_2(x)) = 2$$

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To construct the local solution $\tilde{\varphi}$ with the aforementioned properties, the key tool is the Cauchy-Kowalewsky theorem.

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Second: using the inverse localization lemma we construct an eigenfunction ψ of the harmonic oscillator (for any large enough eigenvalue) whose localization in the ball of radius $\lambda^{-1/2}$ is C^1-close to φ in B.

Third: the structural stability of $\tilde{\Phi}(L)$ implies that $\psi^{-1}(0)$ contains a number of components diffeomorphic to L. Notice that this diffeomorphism Φ is the composition of $\tilde{\Phi}$ and a rescaling $x \to \lambda^{-1/2}x$.

Final remark: the hydrogen atom

An analogous theorem holds for the eigenfunctions $\psi \in H^1(\mathbb{R}^3, \mathbb{C})$ of the hydrogen atom:

$$\Big(\Delta + \frac{2}{|x|} + \lambda\Big)\psi = 0\,.$$

The eigenvalues are $\lambda = -1/n^2$ with n a positive integer, and their multiplicity is n^2. In this case the highly excited eigenfunctions correspond to eigenvalues that are close to 0.

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Let $L \subset \mathbb{R}^3$ be a finite link. Then there is a positive constant E_0 such that, for any Coulomb eigenvalue $\lambda > -E_0$, there exist a complex-valued eigenfunction ψ of energy λ and a diffeomorphism $\Phi : \mathbb{R}^3 \to \mathbb{R}^3$ such that $\Phi(L)$ is a union of structurally stable connected components of the nodal set $\psi^{-1}(0)$.

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Although the proof of this result goes along the same lines as the proof for the harmonic oscillator, a key technical difficulty concerns estimates for the Green's function of the operator $\Delta + 2/|x|$.

Thanks a lot for your attention!