Efficiently filling domains in Kähler manifolds with quantum states

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Motivating problems from quantum mechanics

Let M be a Riemann surface and let $D \subset M$ be a bounded domain in M. How do you fill D with quantum states with minimal spill-over into $M \backslash D$?

In Kähler quantization of a Kähler manifold (M, ω), a quantum state with Planck constant $\frac{1}{k}$ is an L^2-normalized holomorphic section $s \in H^0(M, L^k)$ of the kth power of a positive Hermitian line bundle $(L, h) \to (M, \omega)$.

This is the 'Bargmann-Fock' or 'Berezin-Toeplitz' holomorphic representation of quantum mechanics. It is basic to the Landau theory of electrons in a magnetic field. Holomorphic 'sections' are called lowest Landau levels. We wish to fill D with 1-particle states in the LLL.

Problem: how to fill a domain with quantum states?

We assume the states $s_{k,j}$ are orthogonal. Roughly speaking, we want the *density profile*

$$\frac{1}{N}\sum_{j=1}^{N}|s_{k,j}(z)|^2_{h^k} \simeq \mathbf{1}_D$$

to be approximately equal to the characteristic function $\mathbf{1}_D$ of D. Here, h is the Hermitian metric on the line bundle L Of course, we cannot literally have $\frac{1}{N}\sum_{j=1}^{N}|\psi_j(z)|^2 = \mathbf{1}_D$ but the LHS should interpolate between 1 and 0.

There are a number of inequivalent ways in which this question could be formulated mathematically.

Coherent states and discrete configurations

A key role in Kähler analysis is played by the Bergman(= Szego) kernel $\Pi_{h^k}(z, w)$ associated to a Hermitian metric h on L. If we fix the second slot at z_0 and L^2-normalize we obtain a coherent state

$$\Phi_{h^k}^{z_0}(z) := \frac{\Pi_{h^k}(z, z_0)}{\sqrt{\Pi_{h^k}(z_0, z_0)}}$$

"centered" at z_0. It is a kind of highly peaked Gaussian state of width $k^{-\frac{1}{2}}$ and height $\sqrt{k}^m$ in dimension m.

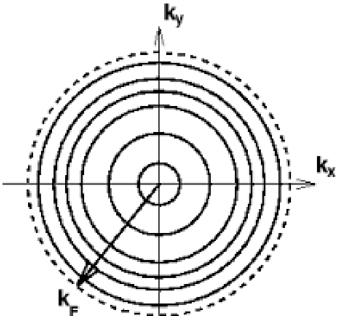
A first thought is to try to pack D with coherent states centered at a discrete configuration of points. But this seems to be impossible for most domains.

Unit disc

Let $M = \mathbb{CP}^1$ and $L = \mathcal{O}(1)$. Then $H^0(\mathbb{CP}, \mathcal{O}(k))$ is the space of homogeneous holomorphic polynomials of degree k in 2 variables: $z_1^{\alpha} z_2^{k-\alpha}$. In the affine chart $\mathbb{C}$ let D be the disc of radius R^2. We choose the quantum to be

$$\psi_{k,j}(z) = \sqrt{k}\frac{(\sqrt{k}z)^j}{\sqrt{j!}} e^{-k|z|^2/2}, \;\; j \leq R.$$

The jth is a transverse Gaussian state centered on the circle of radius $\sqrt{j}$.



What is this graph?

In the disc case,

$$\frac{1}{N}\sum_{j=1}^{N} |\psi_{k,j}(z)|^2_{h^k} \simeq \mathbf{1}_D$$

is radial and has the following graph (the Gaussian Erf function):

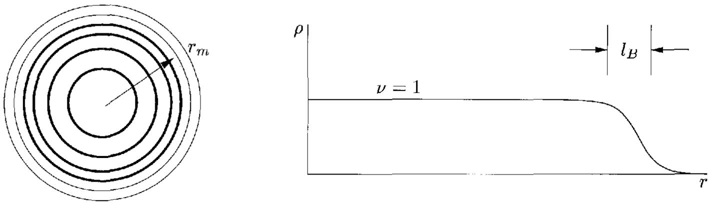


FIG. 7.11. The density profile of the $\nu = 1$ droplet, where the first m levels (represented by the thick lines) are filled.

The transition from 1 to 0 at the 'edge' or boundary of ∂D_R is asymptotically Erf.

Erf

The Erf function,

$$Erf(x) = \int_{-\infty}^{x} e^{-s^2/2} \frac{ds}{\sqrt{2\pi}},$$

is the cumulative distribution function of the Gaussian. This interpolates from 0 to 1 (left to right). We also use $Erf(x) = \int_x^{\infty} e^{-s^2/2} \frac{ds}{\sqrt{2\pi}}$ for the interpolation 1 to 0.

The usual Gaussian error function $\mathrm{erf(x)} = (2\pi)^{-1/2} \int_{-\mathrm{x}}^{\mathrm{x}} \mathrm{e}^{-\mathrm{s}^2/2} \mathrm{ds}$ is related to Erf by $\mathrm{Erf(x)} = \frac{1}{2}(1 + \mathrm{erf}(\frac{\mathrm{x}}{\sqrt{2}}))$.

Bergman kernels on positive line bundles

We now give the precise definitions. Denote by $H^0(M, L^k)$ the space of holomorphic sections of the kth power of a positive Hermitian holomorphic line bundle $L \to M$ over a Kähler manifold (M, ω). The Hermitian metric is denoted by h and in a local frame e_L it is denoted by $|e_L(z)|_h^2 = e^{-\varphi}$. Positive Hermitian means that $i\partial\bar{\partial} \log h = \omega$ is a Kähler form. The Szego projector

$$\Pi_{h^k} : L^2(M, L^k) \to H^0(M, L^k)$$

is the orthogonal projection with respect to the inner product

$$\langle s_1, s_2 \rangle := \int_M (s_1(z), s_2(z))_{h^k} \frac{\omega^m}{m!}.$$

The Schwartz kernel of $\Pi_{h^k}(z, w)$ relative to the volume form $\frac{\omega^m}{m!}$ is known as the semi-classcial Bergman kernel or Szego kernel.

Density of states

In terms of an orthonormal basis $\{s_{k,j}\}$,

$$\Pi_{h^k}(z,w) = \sum_{j=1}^{N_k} s_{k,j}(z)\overline{s_{k,j}(w)}.$$

Here, $N_k = \dim H^0(M, L^k)$. If we set $z = w$ and take the Hermitian norm, we get the DOS (density of states),

$$\Pi_{h^k}(z) = \sum_{j=1}^{N_k} |s_{k,j}(z)|^2_{h^k} \simeq k^m(1 + \frac{a_1}{k} + \cdots).$$

Partial Bergman kernels

Consider a subspace $\mathcal{S}_k \subset H^0(M, L^k)$. Let $d_k = \dim \mathcal{S}_k$. The associated partial Bergman kernel is the projection operator

$$\Pi_{h^k, \mathcal{S}_k} : H^0(M, L^k) \to \mathcal{S}_k.$$

If $\{s_{k,j}\}_{j=1}^{d_k}$ is an orthonormal basis of $\mathcal{S}_k$ then

$$\Pi_{h^k, \mathcal{S}_k}(z, w) = \sum_{j=1}^{d_k} s_{k,j}(z) \overline{s_{k,j}(w)}.$$

The associated DOS (Density of states) is

$$\Pi_{h^k, \mathcal{S}_k}(z) = \sum_{j=1}^{d_k} |s_{k,j}(z)|^2_{h^k}.$$

More precise statement of our problem

Suppose $D \subset M$ is a domain in a kahler manifold M^m of dimension m. Problem: Construct a subspace $\mathcal{S}_k(D) = Span\{s_j^k\}_{j=1}^{d_{k,D}}$ such that the partial DOS satisfies,

$$k^{-m} \sum_{j=1}^{d_{k,D}} |s_j^k(z)|_{h^k} \simeq C_m k^m \mathbf{1}_D(z). \tag{1}$$

Here, $\mathbf{1}_D$ is the characteristic function of D. Also, $d_{k,D} = \dim \mathcal{S}_k$.

So far, the only approach which works is to define spectral partial Bergman kernels.

Toeplitz quantization of a Hamiltonian

Let us assume $D = \{z \in M : 0 \leq H(z) \leq E\}$ for some Hamiltonian $H : M \to \mathbb{R}$.

The quantization of H is the self-adjoint zeroth order Toeplitz operator

$$\hat{H}_k := \Pi_{h^k}(\frac{1}{i2\pi k}\nabla_\xi + H)\Pi_{h^k} : H^0(M, L^k) \to H^0(M, L^k). \qquad (2)$$

Here, $\Pi_{h^k} : L^2(M, L^k) \to H^0(M, L^k)$ is the orthogonal (Bergman) projection, $\xi = \xi_H$ is the Hamilton vector field of H, ∇_ξ is the Chern covariant deriative on sections, and H acts by multiplication.

Spectral subspaces and spectral partial Bergman kernels

Let $\{\mu_{k,j}\}_{j=1}^{N_k}$ denote the eigenvalues of $\hat{H}_k$ and denote the eigenspaces by

$$V_k(\mu_{k,j}) := \{s \in H^0(M, L^k) : \hat{H}_k s = \mu_{k,j} s\}. \tag{3}$$

Given an interval $[E_1, E_2]$, denote the corresponding spectral subspace by $\mathcal{H}_{[E_1,E_2]}$:

$$\mathcal{S}_k := \mathcal{H}_{k:[E_1,E_2]} := \bigoplus_{\mu_{k,j} \in H^{-1}([E_1,E_2])} V_{\mu_{k,j}} \tag{4}$$

Spectral partial Bergman kernels are the corresponding orthogonal projections

$$\Pi_{h^k,[E_1,E_2]} : H^0(M, L^k) \to \mathcal{H}_{k:[E_1,E_2]}. \tag{5}$$

Adapting a Hamiltonian to a domain

We return to our problem: Find a subspace $\mathcal{S}_k(D)$ whose sections efficiently fill up D, i.e. for which the DOS is as close as possible to $\mathbf{1}_D$.

This problem does not have a unique solution as formulated. Given D there exist many functions $H : M \to \mathbb{R}$ so that

$$D = \{z : E_1 \leq H(z) \leq E_2\}.$$

Any choice will solve the problem reasonably well.

Spectral partial Density of States

Given D, we pick H so that $D = H^{-1}[E_1, E_2]$, and let the partial Bergman kernels be the spectral projections

$$\Pi_{h^k,[E_1,E_2]} : H^0(M, L^k) \to \mathcal{H}_{k:[E_1,E_2]}. \tag{6}$$

A simple result is that as $k \to \infty$,

$$k^{-m}\Pi_{h^k,[E_1,E_2]}(z, z) \to \mathbf{1}_{H^{-1}[E_1,E_2]}$$

and thus "fills the domain $H^{-1}[E_1, E_2]$ with lowest Landau levels". Thus, the partial density of states $k^{-m}\mathbf{1}_{[E_1,E_2]}(\hat{H}_k)(z, z)$ essentially equals 1 in $H^{-1}([E_1 E_2])$ and zero in the complement, giving a reasonable notion of "filling" the 'lowest Landau level' in the region $H^{-1}([E_1, E_2])$.

Efficient filling result

The following result uses only standard techniques:

Theorem

Let $(L, h) \to (M, \omega)$ be a polarized Kähler manifold, and D be any open domain of M with smooth boundary $\mathcal{C} = \partial D$, and $\mathcal{F} = M \backslash \overline{D}$. Let $H \in C^\infty(M)$ be such that $D = H^{-1}[E_1, E_2]$, and let $\mathcal{S}_k = \mathcal{H}_{k:[E_1,E_2]} :\subset H^0(M, L^k)$. Then,

$$\left(\frac{\Pi_{k,\mathcal{S}_k}}{\Pi_k}\right)(z) = \begin{cases} 1 & \text{if } z \in D \\ 0 & \text{if } z \in \mathcal{F} \end{cases} \mod O(k^{-\infty}), \quad \forall z \in M \backslash \mathcal{C}.$$

Interface result

We would like to study the interface asymptotics at $\partial D = \{H = E_1\} \cup \{H = E_2\}$ of the spectral partial Bergman kernels for the intervals $[E_1, E_2]$.

The interface occurs in a tube around ∂D of width $k^{-\frac{1}{2}}$. For small enough $\delta > 0$, there exists an embedding $\Phi : \mathcal{C} \times (-\delta, \delta) \to M$ with the properties $\Phi(z, 0) = z$, $\mathrm{dist}(\Phi(z, t), \mathcal{C}) = |t|$ and $\Phi(z, t) \in D$ if and only if $t > 0$,

Theorem

With the same notation as in above. then

$$\Phi^* \left(\frac{\Pi_{k,\mathcal{S}_k}}{\Pi_k} \right) (z, \frac{t}{\sqrt{k}}) = Erf(t) + O(k^{-1/2}), \quad \forall z \in \mathcal{C}, t \in \mathbb{R}$$

where $Erf(t)$ is the Gaussian error function.

Discussion

- There is no canonical choice of H given D except perhaps $\mathbf{1}_D$. There are recent somewhat related results on the Toeplitz operator $\Pi_{h^k} \mathbf{1}_D \Pi_{h^k}$ but (apparently) restricted to its spectrum rather than to pointwise asymptotics of the DOS.

- The theorem above is part of a series of results involving two types of localization for the DOS of a Toeplitz operator $\hat{H}_k$: we can localize in the spectrum, i.e. to eigenvalues $\mu_{k,j} \in I_k$ for any interval I_k; or we can localize in M. Thus we may consider $\Pi_{h^k, I_k}(z)$ for z in a region Ω_k.

Idea of Proof: Three types of smooth sums over eigenvalues

The eigenvalue problem is $\hat{H}_k s_{kj} = \mu_{kj} s_{kj}$. There are several 'localization scales' that may be studied rigorously:

- Energy range localization: $\sum_{j:\mu_{k,j}\in P_0} f(\mu_{k,j} - E)\Pi_{k,j}(z,z)$;
- Interface localization: $\sum_{j:\mu_{k,j}\in P_0} f(\sqrt{k}(\mu_{k,j} - E))\Pi_{k,j}(z,z)$, with $z = F^{\beta/\sqrt{k}}(z_0)$ with $H(z_0) = E$.
- Energy level localization: $\sum_{j:\mu_{k,j}\in P_0} f(k(\mu_{k,j} - E))\Pi_{k,j}(z,z)$;

The 'sharp versions' use characteristic functions $f = \mathbf{1}_{[E_0,E_1]}$. Tauberian arguments bridge smooth and sharp asymptotics.

Ideas of proof

Given a function $f \in \mathcal{S}(\mathbb{R})$ (Schwartz space) one defines

$$f(\hat{H}_k) = \int_{\mathbb{R}} \hat{f}(\tau) e^{i\tau \hat{H}_k} d\tau, \tag{7}$$

to be the operator on $H^0(M, L^k)$ with the same eigensections as $\hat{H}_k$ and with eigenvalues $f(\mu_{k,j})$. Thus, if $s_{k,j}$ is an eigensection of $\hat{H}_k$, then

$$f(\hat{H}_k)\hat{s}_{k,j} = f\left(\mu_{k,j}\right)\hat{s}_{k,j} \tag{8}$$

Partial Bergman kernels

Given an interval $[E_1, E_2] \subset P_0 = H(M)$ the subspace (4) is defined as the range of $f(\hat{H}_k)$ where $f = \mathbf{1}_{[E_1,E_2]}$ and the partial density of states is given by the metric contraction of the kernel,

$$\Pi_{|kP}(z, z) = f(\hat{H}_k)(z, z) = \sum_{j:\mu_{k,j} \in P} \Pi_{\mu_{k,j}}(z, z). \tag{9}$$

For a smooth test function f, it is the metric contraction of the Schwartz kernel of $f(\hat{H}_k)$ at $z = w$, is given by

$$f(\hat{H}_k)\hat{\Pi}_{h^k}(\hat{z}, \hat{w})|_{z=w} = \sum_{j:\mu_{k,j} \in P_0} f(\mu_{k,j})\, \Pi_{\mu_{k,j}}(z, z). \tag{10}$$

Interface result for smoothed partial Bergman kernel

Theorem

Let ω be a C^∞ Kähler metric, and let H be a C^∞ Hamiltonian. Fix $E \in H(M)$, and let $z = F^{\beta/\sqrt{k}} z_0$ for some $z_0 \in H^{-1}(E), \beta \in \mathbb{R}$, and let $f \in C_b(\mathbb{R})$. Then there exists a complete asymptotic expansion,

$$\sum_{j:\mu_{k,j}\in P_0} f(\sqrt{k}(\mu_{k,j}-E))\Pi_{k,j}(F^{\beta/\sqrt{k}}z_0) \simeq k^m I_m(f,E)+k^{m-\frac{1}{2}} I_{m-\frac{1}{2}}(f,E)+\cdot$$

in descending powers of $k^{\frac{1}{2}}$, with leading coefficient

$$[I_m(f,E) = \lim_{k\to\infty} k^{-m} \sum_{j:\mu_{k,j}\in P_0} f(\sqrt{k}(\mu_{k,j}-E))\Pi_{k,j}(F^{\beta/\sqrt{k}}z_0)$$

$$= \int_{-\infty}^{\infty} f(x) e^{-\frac{1}{2}\left(\frac{2x\sqrt{\pi}}{|\nabla_H|}-\beta\frac{|\nabla H|}{\sqrt{\pi}}\right)^2} \frac{2dx}{\sqrt{2|\nabla H|(z_0)}}.$$

The propagator

The propagator is the unitary group,

$$U_k(t) = \exp ikt\hat{H}_k.$$

IMPORTANT: note the k in the exponent. This makes it a dynamical Toeplitz operator, i.e. a Fourier integral operator. A key point is that there exists a parametrix for the propagator in terms of the Bergman kernel and the Hamiltonian flow of H:

Proposition

$\hat{U}_k(t,x,y)$ is a semi-classical Fourier integral operator. There exists an analytic symbol $\sigma_{k,t}$ so that if $\pi(x) = z$,

$$\begin{aligned} U_k(t,z,z) &= \hat{U}_k(t,x,x) := \hat{\Pi}_k(\hat{g}^{-t})^* \sigma_{k,t} \hat{\Pi}_k(x,x) \\ &= \hat{\Pi}_k e^{2\pi ik\int_0^t H(\exp s\xi_H(z))ds} (\exp t\xi_H^h)^* \sigma_{k,t} \hat{\Pi}_k(x,x). \end{aligned} \tag{11}$$

Expression for interface asymptotics

Let F^t be the gradient flow of H. The smoothed interface asymptotics thus amount to the asymptotics of the dilated sums,

$$\sum_j f(\sqrt{k}(\mu_{k,j} - E))\Pi_{k,j}(F^{\beta/\sqrt{k}}(z_0))$$

$$= \int_{\mathbb{R}} \hat{f}(t) e^{-iE\sqrt{k}t} \hat{\Pi}_{h^k} \sigma_{kt} (\hat{g}^t)^* \hat{\Pi}_{h^k} (F^{\beta/\sqrt{k}}(z_0)) dt$$

where $z_0 \in \partial D = H^{-1}(E_1)$ and where $\hat{f} \in L^1(\mathbb{R})$, so that the integral on the right side converges. We employ the Boutet-de-Monvel-Sjostrand parametrix to give an explicit formula for the right side.

Boutet de Monvel-Sjostrand parametrix

The projections Π_{h^k} onto $H^0(M, L^k)$ lift to projections $\hat{\Pi}_{h_k}$ on the principal S^1 bundle $\partial D_h^* \subset L^*$ where $D_h^* = \{(z, \lambda) : |\lambda|_{h_z} < 1\}$. This is a strictly pseudo-convex domain in L^*. The sum $\Pi = \sum_{k \geq 0} \hat{\Pi}_{h_k}$ is the true Szego kernel

$$\hat{\Pi} : L^2(\partial D_h^*) \to H^2(\partial D_h^*)$$

onto boundary values of holomorphic functions on D_h^*

Near the diagonal in $\partial D_h^* \times \partial D_h^*$, the Boutet de Monvel-Sjostrand parametrix is:

$$\hat{\Pi}(x, y) = \int_0^\infty e^{-\sigma\psi(x,y)} \chi(x, y) s(x, y, \sigma) d\sigma + \hat{R}(x, y). \tag{12}$$

Here, $\chi(x, y)$ is a smooth cutoff to the diagonal; $s(x, y, \sigma)$ is a semi-classical symbol of order $m = \dim_{\mathbb{C}} M$.

Osculating Bargmann Fock representations

At each $z \in M$ there is an osculating Bargmann-Fock or Heisenberg model associated to $(T_z M, J_z, h_z)$. We denote the model Heisenberg Bergman kernel on the tangent space by

$$\Pi^{T_z M}_{h_z, J_z}(u, \theta_1, v, \theta_2) : L^2(T_z M) \to \mathcal{H}(T_z M, J_z, h_z) = \mathcal{H}_J. \qquad (13)$$

In K-coordinates with respect to a K-frame,

$$\Pi^{T_z M}_{h_z, J_z}(u, \theta_1, v, \theta_2) = \pi^{-m} e^{i(\theta_1 - \theta_2)} e^{u \cdot \bar{v} - \frac{1}{2}(|u|^2 + |v|^2)}$$

$$= \pi^{-m} e^{i(\theta_1 - \theta_2)} e^{i \Im u \cdot \bar{v} - \frac{1}{2}(|u - v|^2}$$

Note that $\Im u \cdot \bar{v} = \omega(u, v)$.

Linearization approximation

[Shiffman-Z, 2007] [Z. Lu-Shiffman 2015]

PROPOSITION

In K-coordinates in a K-frame at z,

$$\hat{\Pi}_{h^k}(\hat{g}^{\frac{t}{\sqrt{k}}} z, z) \simeq k^m e^{2\pi t H(z)} \Pi^{T_z M}_{J_z, h_z}(t\xi_H, 0, 0, 0) \left(1 + k^{-1} A_t + \cdots\right).$$

PROPOSITION

In K-coordinates in a K-frame at z,

$$\hat{U}_k(t/\sqrt{k}, z, \theta, z, \theta) \;=\; k^m e^{2\pi i t \sqrt{k} H(z))} e^{-|t\xi_H(z)|^2}[1 + O(k^{-\frac{1}{2}})]$$

Putting it together

Lemma

$$\sum_j f\sqrt{k}(\mu_{k,j} - E))\Pi_{k,\mu_{k,j}}(F^{\frac{u}{\sqrt{k}}} z_0, F^{\frac{u}{\sqrt{k}}} z_0)$$

$$= \int_{\mathbb{R}} \hat{f}(t) e^{-iE\sqrt{k}t} \hat{U}_k(t/\sqrt{k}, F^{\frac{u}{\sqrt{k}}} z_0, g^{\frac{u}{\sqrt{k}}} F^{\frac{u}{\sqrt{k}}} z_0) dt$$

$$= k^m \int_{-\infty}^{\infty} \hat{f}(t) e^{2\pi i t\sqrt{k} H(z))} e^{-iE\sqrt{k}t} e^{-|t\xi_H(z)|^2}\, dt\, [1 + O(k^{-\frac{1}{2}})] \,,$$

By the Plancherel formula,

$$k^{-m} \sum_{j=1}^{d_k} f(\sqrt{k}(\mu_{k,j} - E))\Pi_{k,j}(z_k, z_k)$$

$$= \int_{-\infty}^{\infty} f(x) e^{-\frac{1}{2}\left(\frac{2x\sqrt{\pi}}{|\nabla H(z_k)|} - \beta \frac{|\nabla H(z_k)|}{\sqrt{\pi}}\right)^2} \frac{2dx}{\sqrt{2|\nabla H(z_0)|}} + O(k^{-1/2}.$$