2003:11

The valleys of shadow in Schrödinger landscape

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THE VALLEYS OF SHADOW IN SCHRODINGER LANDSCAPE

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ABSTRACT. The probability density function $|\psi(f)|^2$ is studied for the one-dimensional quantum particle whose motion is defined by the Schrödinger equation

$$\frac{\partial \psi}{\partial t} = \frac{1}{2\pi i} \frac{\partial^2 \psi}{\partial x^2}, \quad \psi(f; t, x) \bigg|_{t=0} = f(x),$$

with the periodic initial data $f$, $f(x + 1) \equiv f(x)$. For $f$ of the type $f_\varepsilon(x) := c(\varepsilon)e^{-\frac{|x|^2}{\varepsilon^2}}$, $\varepsilon$ a small positive parameter, $\langle x \rangle$ the distance from $x$ to the nearest integer, Daniel Dix conducted a numerical experiment of 3d-graphing the density $|\psi(f_\varepsilon; t, x)|^2$. Visually, the graph resembles a mountain landscape scarred by a peculiar discrete collection of deep rectilinear canyons, or “the valleys of shadow”. We prove that this phenomenon is common for a wide set of families of the initial data $\{f_\varepsilon\}$ such that the initial densities $\{|f_\varepsilon|^2\}$ approximate, as $\varepsilon \to 0$, the periodic Dirac’s delta-function: the Radon transformations of $|\psi(f_\varepsilon)|^2$ are indeed small on a definite collection of lines on the plane $(t, x)$. A complete description of such collections is established, and applications to Helmholtz equation are discussed.

AMS 2000 Subject classification: 35Q40, 11F27

Keywords: Schrödinger equation, density function, Gauss’ sums, Talbot effect.

0.1. **Free quantum particle with the periodic initial data.** Assume that the motion of the quantum particle is determined by the 0-potential Schrödinger equation with the periodic initial data condition:

$$\frac{\partial \psi}{\partial t} = \frac{1}{2\pi i} \frac{\partial^2 \psi}{\partial x^2}, \quad \psi(f; t, x) \bigg|_{t=0} = f(x) = \sum_{n \in \mathbb{Z}} \hat{f}_n e^{2\pi i nx}, \quad \hat{f}_n := \int_0^1 f(x) e^{-2\pi i nx} \, dx.$$

Via the Fourier method of separation of variables, the solution is given by

$$\psi(f; t, x) = \sum_{n \in \mathbb{Z}} \hat{f}_n e^{2\pi i (n^2 t + nx)}.$$

Fig. 1 (Daniel Dix) depicts “one quarter” of the graph of the probability density function $|\psi(f_\varepsilon; t, x)|^2$, see also (10) below, of finding the particle at the location $x$, at the fixed moment of time $t$. The initial data is the periodized (and $L^2$-normalized) Gauss bell function

$$f_\varepsilon(x) := c(\varepsilon) \sum_{n \in \mathbb{Z}} e^{-\frac{(x-n)^2}{\varepsilon}}, \quad c(\varepsilon) = \sqrt{\varepsilon} \sum_{n \in \mathbb{Z}} e^{-\pi n^2 \varepsilon}, \quad \varepsilon = 0.01.$$
Figure 1. The valleys of shadow

Apparently, the graph features a rugged “mountain landscape” scarred by a series of rather well-organized and deep rectilinear canyons, or “the valleys of shadow”\footnote{Even though I walk through the valley of the shadow of death, I will fear no evil, for you are with me; your rod and your staff, they comfort me. Psalm 23 of David.}. It will be shown that this feature is common for the densities $|\psi(f_x)|^2$ generated by $\sqrt{\delta}$-families of initial data $\{f_x\}$. By the definition, such a family consists of the functions whose moduli squares approximate,
as $\varepsilon \to 0$, the periodic Dirak’s delta-function, i. e.

$$\|f_\varepsilon\|_2^2 := \int_0^1 |f_\varepsilon(x)|^2 \, dx = 1, \quad \int_0^1 |f_\varepsilon(x)|^2 g(x) \, dx \to g(0), \quad \varepsilon \to 0$$

for every continuous function $g(x)$ of period 1. We consider the limiting properties of the densities $|\psi(f_\varepsilon)|^2$ generated by $\sqrt{\delta}$-families.

Related literature: P. R. Holland [14], Chapter 6, Section 6.5; D. Bohm [7], Chapter 10, Section 10.10 (p. 207), W. Heisenberg[13].

0.2. “Schrödinger approximation” of the Helmholtz equation. We follow here some lines of the paper [16], and the references therein.

Consider the boundary value problem posed for the Helmholtz equation:

$$\left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2} + \left(\frac{2\pi}{\lambda}\right)^2 \right) \varphi = 0, \quad \varphi(f; z, x) \bigg|_{z=0} = f(x) = \sum_n \hat{f}_n e^{\frac{2\pi inx}{\lambda}},$$

$$\hat{f}_n = \int_0^a f(x) e^{-\frac{2\piinx}{\lambda}} \, dx,$$

$\lambda$ - the wave length, $a$ - the period of the optical image on the boundary, which is a flat screen, $z$ - the distance along the optical axis, i. e. in the direction perpendicular to the screen; $z_T := \frac{a^2}{\lambda}$ - Talbot [20] distance; $\gamma := \frac{\lambda}{a}$. Introduce the dimensionless variables

$$\eta := \frac{x}{a}, \quad \zeta := \frac{z}{z_T} = \frac{z\lambda}{a^2}.$$

Then, using the Fourier method of separation of variables, we obtain the exact solution:

$$\varphi(f; \zeta, \eta) = \sum_{n\in\mathbb{Z}} \hat{f}_n e^{2\pi i(\mu_n \zeta + mn)}, \quad \mu_n := \sqrt{1 - \left(\frac{n\gamma}{\gamma^2}\right)^2}.$$

[16] suggests the following approximation of the exact solution of the Helmholtz equation by that of Schrödinger equation. Both steps, especially the second of them, require a serious mathematical scrutiny, currently unavailable.

1) For $n > 1/\gamma$, the factors $e^{2\pi i\mu_n \zeta} := e^{-2\pi i|\mu_n|k}$, are exponentially small as $n \to \infty$, and the appropriate terms of the series can be disregarded.

2) For $n \leq 1/\gamma$, the exact values of $\mu_n$ can be replaced by just two terms of Taylor’s expansion which generates an “approximation” of the solution of the problem (4) by that of (1):

$$\mu_n \approx \gamma^2 - \frac{n^2}{2}, \quad \tilde{\varphi}(\zeta, \eta) = e^{2\pi i\gamma^{-2}\zeta} \sum_{n\in\mathbb{Z}} \hat{f}_n e^{\pi i(-n^2\zeta + 2mn)}.$$

0.3. The valleys of shadow, and the Wigner function. Let us establish the following $(0 \lor 1 \lor 2)$-alternative for the limits of Radon transformations of the densities:

\[
\lim_{\varepsilon \to 0} \int_0^1 |\psi(f; t, -Nt + \xi)|^2 \, dt \begin{cases} 
0 & (a) \\
1 & (b) \\
2 & (c)
\end{cases}
\]

where an integer $N$ and a real number $\xi$ are fixed, and $\{f_\varepsilon\}$ is a $\sqrt{\delta}$-family of the initial data for the problem (1). Relations (6(b),(c)) mean that the average densities $|\psi(f_\varepsilon)|^2$ are not small, as $\varepsilon \to 0$, on the line $L_N(\xi) := \{(t, x) : Nt + x = \xi\}$. Of a special interest are the lines where (6(a)) is true, i.e. the densities are small in the mean. These lines represent the “valleys of the shadow”.

**Theorem 1.** Assume that $\{f_\varepsilon\}$ is a $\sqrt{\delta}$-family, $N$ an integer, $\xi$ - a real number. Then (6(b)) is true for each line $L_N(\xi)$ such that $2\xi$ is not an integer.

If all initial data $\{f_\varepsilon\}$ are even functions, then (6(a)) is true if and only if $\xi = 1/2$ and $N$ is odd; (6(c)) is true if and only if either $\xi = 0$, or $\xi = 1/2$ and $N$ is even.

If all initial data $\{f_\varepsilon\}$ are odd functions, then (6(a)) is true if and only if either $\xi = 0$, or $\xi = 1/2$ and $N$ is even; (6(c)) is true if and only if $\xi = 1/2$ and $N$ is odd.

**Proof.** For a periodic $f(x)$, and an integer $N$, let us introduce the $N$th Wigner function:

\[
W_N(f; \xi) := \int_0^1 f(\xi + x) f^*(\xi - x) e^{-2\pi i N x} \, dx, \quad \xi \in \mathbb{R},
\]

cf. [14], Section 8.4.3 (p. 357).

**Lemma 1.** Let $N$ be an integer, $\xi \in \mathbb{R}$, and $\psi(f; t, x)$ - the solution of (1). Then

\[
\int_0^1 |\psi(f; t, -Nt + \xi)|^2 \, dt = \|f\|^2_2 + W_N(f; \xi).
\]

Indeed, we have

\[
|\psi(f; t, x)|^2 = \sum_{(m, n) \in \mathbb{Z}^2} \hat{f}_n \hat{f}_m^* e^{2\pi i (n^2 - m^2) t + (n-m)x}.
\]

Therefore

\[
\int_0^1 |\psi(f; t, -Nt + \xi)|^2 \, dt = \int_0^1 \left( \sum_{(m, n) \in \mathbb{Z}^2} \hat{f}_n \hat{f}_m^* e^{2\pi i (n^2 - m^2) t + (n-m)(-Nt+x)} \right) \, dt
\]

\[
= \sum_{(n-m)(n+m-N)=0} \hat{f}_n \hat{f}_m^* e^{2\pi i (n-m)\xi} = \sum_{n \in \mathbb{Z}} |\hat{f}_n|^2 + \sum_{n \in \mathbb{Z}} \left( \hat{f}_n e^{2\pi i \xi} \right) \left( \hat{f}_{N-n} e^{2\pi i (N-n)\xi} \right)^*.
\]

From here, the relation (6) follows by the Parseval’s identity

\[
\int_0^1 f(x) g^*(x) \, dx = \sum_{n \in \mathbb{Z}} \hat{f}_n \hat{g}_n^*.
\]
and the following correspondence between functions and the Fourier coefficients:
\[ \{ \hat{f}_n e^{2\pi i n \xi} \} \leftrightarrow \{ f(x + \xi) \}, \quad \{ \hat{f}_{-n} e^{2\pi i (N-n) \xi} \} \leftrightarrow \{ f(\xi - x) e^{2\pi i N \xi} \}. \]

Now let us assume that \( \{ f_\varepsilon \} \) is \( \sqrt{\delta} \)-family. Then it is easy to see (by application of the Cauchy inequality) that if \( 2\xi \) is not an integer, then for each fixed integer \( N \)
\[ |W_N(f_\varepsilon, \xi)| \leq \int_0^1 |f_\varepsilon(\xi + x)f_\varepsilon(\xi - x)| \, dx \to 0, \quad \varepsilon \to 0, \]
and (6.2) follows from (7).

Therefore, it remains to consider the cases \( \xi = 0 \) and \( \xi = 1/2 \). We have
\[ W_N(f; 0) = \int_0^1 f(x) f^*( -x) e^{-2\pi i N \xi} \, dx, \]
\[ W_N(f; 1/2) = \int_0^1 f(1/2 + x) f^*(1/2 - x) e^{-2\pi i N \xi} \, dx = (-1)^N \int_0^1 f(x) f^*(-x) e^{-2\pi i N \xi} \, dx. \]

Therefore, if \( \{ f_\varepsilon \} \) is a \( \sqrt{\delta} \)-family, and all \( f_\varepsilon \) are even functions, then
\[ \lim_{\varepsilon \to 0} W_N(f_\varepsilon; 0) = 1, \quad \lim_{\varepsilon \to 0} W_N(f_\varepsilon; 1/2) = (-1)^N; \]
on the contrary, if all \( f_\varepsilon \) are odd functions, then
\[ \lim_{\varepsilon \to 0} W_N(f_\varepsilon; 0) = -1, \quad \lim_{\varepsilon \to 0} W_N(f_\varepsilon; 1/2) = (-1)^{N+1}. \]

This and the application of (7) complete the proof of the theorem.

Let us briefly consider the following ergodic characteristic of the density \( |\psi(f_\varepsilon)|^2 \) on a line \( L_N(\xi) \) with a non integral, slope \( N \):
\[ \mathcal{E}_N(f, \xi) := \lim_{T \to \infty} \frac{1}{T} \int_0^T |\psi(f; t, -Nt + \xi)|^2 \, dt. \]

We have
\[ \frac{1}{T} \int_0^T |\psi(f; t, -Nt + \xi)|^2 \, dt = \|f\|^2 + \frac{1}{T} \sum_{(m,n) \in \mathbb{Z}^2, m \neq n} \hat{f}_n \hat{f}_m \frac{e^{2\pi i (n-m)(n+m-N)T} - 1}{(n-m)(n+m-N)} e^{2\pi i (n-m)\xi}. \]

Since \( N \) is non-integral, there are no “small denominators” in the double sum on the right. Moreover, since
\[ \frac{1}{(n-m)(n+m-N)} = \frac{1}{2m-N} \left( \frac{1}{n-m} - \frac{1}{n+m-N} \right), \]
it is plausible that this sum can be estimated using the known property of the Hilbert matrix, as follows
\[ \left| \sum_{(m,n) \in \mathbb{Z}^2, m \neq n} \hat{f}_n \hat{f}_m \frac{e^{2\pi i (n-m)(n+m-N)T} - 1}{(n-m)(n+m-N)} e^{2\pi i (n-m)\xi} \right| \leq \frac{\|f\|^2}{\langle N \rangle}, \]
so that if the slope $N$ is non-integral we have $E_N(f, \xi) = 1$. On the other hand, for the lines $L_N(\xi)$ with the integral slope, the values of $E_N(f, \xi)$ are given by the relations (6).

This type of characteristic seems to be promising also in the consideration of the valleys of shadow for the solution $\varphi$ of the Helmholtz equation (4), avoiding the mathematically dubious “approximation” step (4):

$$
\frac{1}{T} \int_0^T |\varphi(f; \zeta, -N\zeta + \xi)|^2 d\zeta = \|f\|_2^2 + \frac{1}{T} \sum_{(m,n)\in \mathbb{Z}^2, m \neq n} \hat{f}_n \hat{f}_m \frac{e^{2\pi i \Delta(n,m,N)T}}{\Delta(n, m, N)} e^{2\pi i (n-m)\xi}
$$

where

$$
\Delta(n, m, N) := \mu_n - \mu_m - (n - m)N.
$$

The author intends to address the elaboration of this idea in the future.

0.4. Talbot effect, and the Gauss’ sums interpretation. Let us consider the formal series

$$
\Theta_0(t, x) := \sum_{n \in \mathbb{Z}} e^{2\pi i n^2 t + nx}
$$

as limit for $\varepsilon \to 0_+$, of

$$
\Theta_\varepsilon(t, x) := \sum_{n \in \mathbb{Z}} e^{-\pi n^2 \varepsilon} e^{2\pi i (n^2 t + nx)} , \quad \varepsilon > 0.
$$

Obviously, $\Theta_0(t, x)$ represents the formal Green’s function of the problem (1), see (2), i. e.

$$
\psi(f; t, x) = \int_0^1 \Theta_0(t, x - y) f(y) dy.
$$

G.H. Hardy and J.E. Littlewood [12] (see also [11], pp. 67 – 112) thoroughly studied the summability properties of $\Theta_0(t, x)$, and established that if $t$ is an irrational number, then $\Theta_0(t, x)$ is not summable by any of the Cesaro means.

On the other hand, if $t$ is a rational number, $t = \frac{a}{q}$, $(a, q) = 1$, then the series $\Theta_0(t, x)$ is summable, say, by the $(C, 1)$-means (and consequently, by the Gaussian method, because it is stronger) to the linear combination of shifted Dirac’s periodic $\delta$-functions:

$$
(C, 1) \Theta_0 \left( \frac{a}{q}, x \right) = \lim_{\varepsilon \to 0} \Theta_\varepsilon \left( \frac{a}{q}, x \right) = \sum_{k=1}^q G \left( \frac{a}{q}, \frac{k}{q} \right) \delta \left( x - \frac{k}{q} \right),
$$

(8)

$$
\psi \left( f; \frac{a}{q}, x \right) = \sum_{k=1}^q G \left( \frac{a}{q}, \frac{k}{q} \right) f \left( x - \frac{k}{q} \right).
$$

where $G \left( \frac{a}{q}, \frac{k}{q} \right)$ are the discrete Fourier transforms of the factors $e^{2\pi i n \varepsilon}$:

$$
G \left( \frac{a}{q}, \frac{k}{q} \right) = \frac{1}{q} \sum_{n=1}^q e^{2\pi i n \frac{a}{q}} e^{2\pi i n \frac{k}{q}}.
$$
The complex numbers $G$ are the complete Gauss’ sums. Their moduli are determined by the relations (see e.g. [18]), p. 183, formulas (1.3), and also [17])

\[
\sqrt{q} \left| G \left( \frac{a}{q}, \frac{k}{q} \right) \right| = \begin{cases} 
1 & \text{if } q \equiv 1 \pmod{2}, \\
\frac{1+i(-1)^{q+1}}{\sqrt{q}} & \text{if } q \equiv 0 \pmod{2}, \quad Q := \frac{q}{2},
\end{cases}
\]

and one has

\[
\sum_{k=1}^{q} \left| G \left( \frac{a}{q}, \frac{k}{q} \right) \right|^2 = 1.
\]

The relation (8) means, that for the rational moments of time parameter $t = \frac{a}{q}$, the solution of the problem (1) is a $q$-term linear combination of the shifted initial data function $f$. This implies that if the “original image” $f$ is supported “in a narrow interval”, of the length $l << 1$, and $q \leq \frac{1}{l}$ then the solution operator reproduces $q$ scaled non-overlapping copies of this image on the period. This is presumably the essence of the Talbot self-imaging effect, cf.[20], [16], in the classical and electromagnetic optics.

The following is the interpretation of the “valleys of the shadow” via the Gauss’ sums.

Every line $L_N(1/2) = \{(t,x) : Nt + x = 1/2\}$, with an odd slope $N$, avoids “hitting a delta-function”, i.e. does not pass through any rational point on $\mathbb{R}^2$ with a non-zero factor $G$ in (8). In the other words, if a rational point $\left( \frac{a}{q}, \frac{k}{q} \right)$, $(a,q) = 1$, belongs to such a line, then

\[
G \left( \frac{a}{q}, \frac{k}{q} \right) = 0.
\]

Indeed, assume that $(t,x) = \left( \frac{a}{q}, \frac{k}{q} \right) \in L_N(1/2)$, and $N = 2m + 1$, $m \in \mathbb{Z}$. Then

\[
(2m + 1)t + x = \frac{(2m + 1)a + k}{q} = \frac{1}{2}.
\]

It follows that

\[
2((2m + 1)a + k) = q.
\]

Clearly, this relation is not possible if $q$ is an odd number. On the other hand, if $q$ is even, $q = 2Q$, then we have

\[
(2m + 1)a + k = Q,
\]

and $a$ is an odd number, because $(a, 2Q) = 1$. Therefore, if $Q$ is an even number, $k$ has to be odd, so that on this case $aQ + k$ is odd. On the contrary, if $Q$ is odd, then then $k$ has to be even, so that the sum $aQ + k$ is odd in this case, as well, and the equality $G \left( \frac{a}{q}, \frac{k}{q} \right) = 0$ follows from (9).
0.5. **The Gauss’ bell initial data.** Let us consider the periodized Gauss bell function (known also as the Jacobi’s elliptic theta-function)

\[ \vartheta_{\varepsilon}(x) := \sum_{n \in \mathbb{Z}} e^{-\pi \varepsilon n^2} e^{2\pi i n x} = \frac{1}{\sqrt{\varepsilon}} \sum_{n \in \mathbb{Z}} e^{-\pi (\varepsilon n)^2} \]

as the initial data in the problem (1), and denote \( \psi(\vartheta_{\varepsilon}, t, x) := \Theta_{\varepsilon}(t, x) \). Note, that \( \vartheta_{\varepsilon} \) is not normalized in \( L^2 \), but is such in \( L^1 \):

\[ \| \vartheta_{\varepsilon} \| := \int_0^1 |\vartheta_{\varepsilon}(x)| \, dx = \int_0^1 \vartheta_{\varepsilon}(x) \, dx = 1. \]

To obtain the \( L^2 \)-normalized data, as in (3), we take (in the sequel, \( a \) denotes strictly positive absolute constants, whose numerical values can be different on different occasions)

\[ f_{\varepsilon}(x) := a(\varepsilon) \vartheta_{\varepsilon}(x), \quad c(\varepsilon) = \left( \sum_{n \in \mathbb{Z}} e^{-2\pi \varepsilon n^2} \right)^{-1} = \vartheta_{2\varepsilon}^{-1}(0) = \left( 2 \varepsilon \right)^{-\frac{1}{2}} + O \left( e^{-\frac{\varepsilon}{2}} \right), \quad \varepsilon \to 0. \]

The exact initial data functions \( \vartheta_{\varepsilon}, f_{\varepsilon} \) can be with a very high accuracy substituted by one single term of the series

\[ \vartheta_{\varepsilon}(x) = \sqrt{\frac{1}{\varepsilon} e^{-\pi \varepsilon x^2}} + O \left( e^{-\frac{\varepsilon}{2}} \right), \quad f_{\varepsilon}(x) = \sqrt{\frac{2}{\varepsilon} e^{-\pi \varepsilon x^2}} + O \left( e^{-\frac{\varepsilon}{2}} \right), \quad \varepsilon \to 0, \]

where \( \langle x \rangle \), as above, denotes the distance from \( x \) to the nearest integer.

Let us establish the following approximate representation of the density \( |\psi(f_{\varepsilon})|^2 \) as a sum of Gauss-bell ridge functions:

\[ |\psi(f_{\varepsilon}; t, x)|^2 = \sum_{n \in \mathbb{Z}} e^{-\pi \varepsilon n^2} e^{-\pi (2nt + x)^2 / 2\varepsilon} - \sum_{n \equiv 1 \text{ mod } 2} 2 e^{-\pi \varepsilon n^2} e^{-2\pi \varepsilon (nt + x)} + O \left( e^{-\frac{\varepsilon}{2}} \right). \]

By (2) we have

\[ |\Theta_{\varepsilon}(t, x)|^2 = \sum_{(m, n) \in \mathbb{Z}^2} e^{-\pi \varepsilon (m^2 + n^2)} e^{2\pi i (m-n)(m+n)t + (m-n)x}. \]

Let us introduce the new variables of summation \( m - n \to m, \ m + n \to n \) in the double sum on the right. Then we obtain

\[ |\Theta_{\varepsilon}(t, x)|^2 = \sum_{(m, n) \in \mathbb{Z}^2, m \equiv n \text{ mod } 2} e^{-\pi \varepsilon (m^2 + n^2)} e^{2\pi i (m+n)t + mx} = \sum_{n \equiv 0 \text{ mod } 2} e^{-\pi \varepsilon n^2} A(nt + x) + \sum_{n \equiv 1 \text{ mod } 2} e^{-\pi \varepsilon n^2} B(nt + x), \]
where
\[
A(x) := \sum_{m \equiv 0 \mod 2} e^{-\frac{m^2}{2}} e^{2\pi i m x} = \varphi_{2\varepsilon}(2x) = \sqrt{\frac{1}{2\varepsilon}} e^{-\frac{\varepsilon(x+1/2)^2}{2}} + O\left(e^{-\varepsilon}\right); \\
B(x) := \sum_{m \equiv 1 \mod 2} e^{-\frac{m^2}{2}} e^{2\pi i m x} = \frac{1}{2} \left(\varphi_{\varepsilon}(x) - \varphi_{\varepsilon}(x + \frac{1}{2})\right) = \varphi_{2\varepsilon}(2x) - \varphi_{\varepsilon}(x + \frac{1}{2})
\]

and the approximate representation (10) follows.

References


