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The valleys of shadow in Schrödinger landscape

K.I. Oskolkov

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Department of Mathematics
University of South Carolina

THE VALLEYS OF SHADOW IN SCHRÖDINGER LANDSCAPE

K.I.OSKOLKOV

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

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

with the periodic initial data f, $f(x+1) \equiv f(x)$. For f of the type $f_\varepsilon(x) := c(\varepsilon)e^{-\frac{\langle x\rangle^2}{\varepsilon}}$, ε – 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 Dirack'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
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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:

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

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

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

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

$$f_\varepsilon(x) := c(\varepsilon)\sum_{n\in\mathbb{Z}} e^{-\frac{\pi(x-n)^2}{\varepsilon}} \left(= c(\varepsilon)\sqrt{\varepsilon}\sum_{n\in\mathbb{Z}} e^{-\pi n^2\varepsilon}e^{2\pi i n x}\right), \quad \varepsilon = 0.01.$$

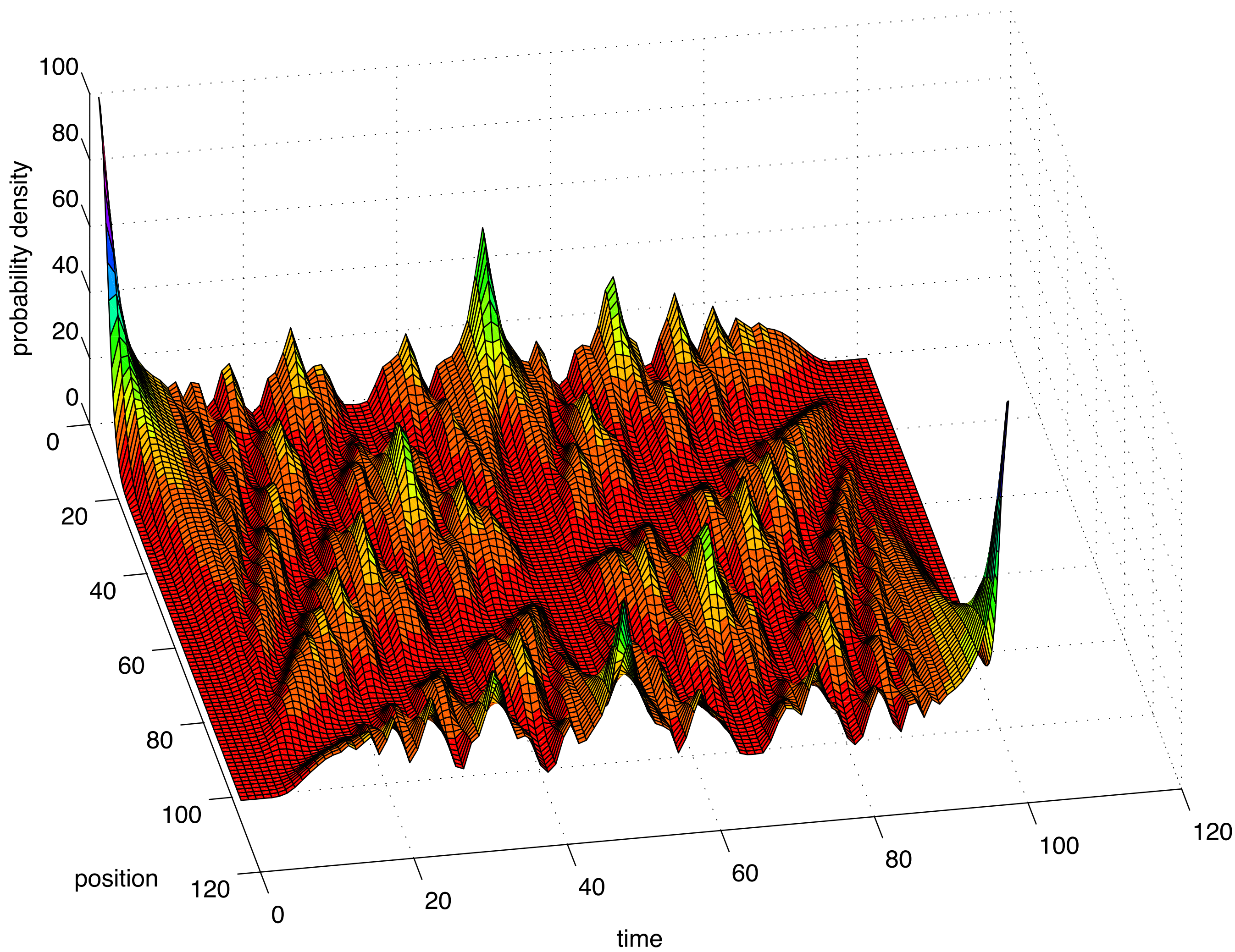

FIGURE 1. The valleys of shadow

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"[1]. It will be shown that this feature is common for the densities $|\psi(f_\varepsilon)|^2$ generated by $\sqrt{\delta}$-*families* of initial data $\{f_\varepsilon\}$. By the definition, such a family consists of the functions whose moduli *squares* approximate,

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[1] *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.

as $\varepsilon \to 0$, the periodic Dirack's delta-function, i. e.

$$\|f_\varepsilon\|_2^2 := \int_0^1 |f_\varepsilon(x)|^2\, dx = 1, \quad \int_0^1 |f_\varepsilon(x)|^2 g(x)\, dx \to g(0), \quad \varepsilon \to 0 \tag{3}$$

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:

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

$$\hat{f}_n = \int_0^a f(x)\, e^{-\frac{2\pi i n x}{a}}\, dx, \tag{4}$$

λ – 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:

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

[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 $e^{2\pi i \mu_n \zeta} := e^{-2\pi|\mu_n|\zeta}$, 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 μ_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):

$$\mu_n \approx \gamma^{-2} - \frac{n^2}{2}, \quad \tilde{\varphi}(\zeta, \eta) = e^{2\pi i \gamma^{-2}\zeta} \sum_{n\in Z} \hat{f}_n e^{\pi i(-n^2\zeta + 2n\eta)}. \tag{5}$$

Related literature: [16], [1] – [6], [8], [15], [19] – [21].

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

$$\lim_{\varepsilon \to 0} \int_0^1 |\psi(f_\varepsilon; t, -Nt+\xi)|^2 \, dt = \begin{cases} 0 & \text{(a)} \\ 1 & \text{(b)} \\ 2 & \text{(c)} \end{cases} \tag{6}$$

where an integer N and a real number ξ 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, ξ - a real number. Then (6,(b)) is true for each line $L_N(\xi)$ such that 2ξ 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 Nth 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*

$$\int_0^1 |\psi(f;t,-Nt+\xi)|^2 \, dt = \|f\|_2^2 + W_N(f;\xi). \tag{7}$$

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

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

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

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:

$$\left\{\hat{f}_n e^{2\pi i n\xi}\right\} \longleftrightarrow \{f(x+\xi)\}, \quad \left\{\hat{f}_{N-n}\, e^{2\pi i(N-n)\xi}\right\} \longleftrightarrow \{f(\xi-x)e^{2\pi iNx}\}.$$

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 2ξ is not an integer, then for each fixed integer N

$$|W_N(f_\varepsilon,\xi)| \le \int_0^1 |f_\varepsilon(\xi+x)f_\varepsilon(\xi-x)|\, dx \to 0, \quad \varepsilon \to 0,$$

and (6,b) follows from (7).

Therefore, it remains to consider the cases $\xi = 0$ and $\xi = 1/2$.We have

$$W_N(f;0) = \int_0^1 f(x)f^*(-x)\, e^{-2\pi iNx}\, dx,$$
$$W_N(f;1/2) = \int_0^1 f(1/2+x)f^*(1/2-x)\, e^{-2\pi iNx}\, dx = (-1)^N \int_0^1 f(x)f^*(-x)\, e^{-2\pi iNx}\, dx.$$

Therefore, if $\{f_\varepsilon\}$ is a $\sqrt{\delta}$-family, and all f_ε 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_ε 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

$$\frac{1}{T}\int_0^T |\psi(f;t,-Nt+\xi)|^2\, dt = \|f\|_2^2 + \frac{1}{T} \sum_{(m,n)\in\mathbb{Z}^2, m\neq n} \hat{f}_n \hat{f}_m^* \frac{e^{2\pi i(n-m)(n+m-N)T}-1}{(n-m)(n+m-N)} e^{2\pi i(n-m)\xi}.$$

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

$$\left| \sum_{(m,n)\in\mathbb{Z}^2, m\neq n} \hat{f}_n \hat{f}_m^* \frac{e^{2\pi i(n-m)(n+m-N)T}-1}{(n-m)(n+m-N)} e^{2\pi i(n-m)\xi} \right| \le \frac{c\|f\|^2}{\langle N\rangle},$$

so that if the slope N is non-integral we have $\mathcal{E}_N(f,\xi) = 1$. On the other hand, for the lines $L_N(\xi)$ with the integral slope, the values of $\mathcal{E}_N(f,\xi)$ 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 φ of the Helmholtz equation (4), avoiding the mathematically dubious "approximation" step (4):

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

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

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

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

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

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 Dirack's periodic δ-functions:

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

$$\psi\left(f;\frac{a}{q},x\right) = \sum_{k=1}^{q} G\left(\frac{a}{q},\frac{k}{q}\right) f\left(x-\frac{k}{q}\right). \tag{8}$$

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

$$G\left(\frac{a}{q},\frac{k}{q}\right) = \frac{1}{q}\sum_{n=1}^{q} e^{\frac{2\pi i n^2 a}{q}} e^{\frac{2\pi i n k}{q}}.$$

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])

$$\sqrt{q}\left|G\left(\frac{a}{q},\frac{k}{q}\right)\right| = \begin{cases} 1 & \text{if } q \equiv 1 \pmod 2, \\ \frac{1+(-1)^{aQ+k}}{\sqrt{2}} & \text{if } q \equiv 0 \pmod 2,\ Q := \frac{q}{2}, \end{cases} \tag{9}$$

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*)

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

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

$$\|\vartheta_\varepsilon\|_1 := \int_0^1 |\vartheta_\varepsilon(x)|\, dx = \int_0^1 \vartheta_\varepsilon(x)\, dx = 1.$$

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)

$$f_\varepsilon(x) := c(\varepsilon)\vartheta_\varepsilon(x), \quad c(\varepsilon) = \left(\sum_{n\in\mathbb{Z}} e^{-2\pi\varepsilon n^2}\right)^{-\frac{1}{2}} = \vartheta_{2\varepsilon}^{-\frac{1}{2}}(0) = (2\varepsilon)^{\frac{1}{4}} + O\left(e^{-\frac{a}{\varepsilon}}\right),\ \varepsilon \to 0.$$

The exact initial data functions ϑ_ε, f_ε can be with a very high accuracy substituted by one single term of the series

$$\vartheta_\varepsilon(x) = \sqrt{\frac{1}{\varepsilon}} e^{-\frac{\pi\langle x\rangle^2}{\varepsilon}} + O\left(e^{-\frac{a}{\varepsilon}}\right), \quad f_\varepsilon(x) = \sqrt[4]{\frac{2}{\varepsilon}} e^{-\frac{\pi\langle x\rangle^2}{\varepsilon}} + O\left(e^{-\frac{a}{\varepsilon}}\right),\ \varepsilon \to 0,$$

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:

$$|\psi(f_\varepsilon; t, x)|^2 = \sum_{n\in\mathbb{Z}} e^{-\frac{\pi\varepsilon n^2}{2}} e^{-\frac{\pi\langle 2(nt+x)\rangle^2}{2\varepsilon}} - 2 \sum_{n\equiv 1 \bmod 2} e^{-\frac{\pi\varepsilon n^2}{2}} e^{-\frac{2\pi\langle nt+x+1/2\rangle^2}{\varepsilon}} + O\left(e^{-\frac{a}{\varepsilon}}\right). \tag{10}$$

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

$$\begin{aligned} |\Theta_\varepsilon(t,x)|^2 &= \sum_{(m,n)\in\mathbb{Z}^2,\ m\equiv n \bmod 2} e^{-\frac{\pi\varepsilon}{2}(m^2+n^2)} e^{2\pi i(mnt+mx)} \\ &= \sum_{n\equiv 0 \bmod 2} e^{-\frac{\pi\varepsilon n^2}{2}} A(nt+x) + \sum_{n\equiv 1 \bmod 2} e^{-\frac{\pi\varepsilon n^2}{2}} B(nt+x), \end{aligned}$$

where

$$A(x) := \sum_{m\equiv 0 \bmod 2} e^{-\frac{\pi\varepsilon m^2}{2}} e^{2\pi i m x} = \vartheta_{2\varepsilon}(2x) = \sqrt{\frac{1}{2\varepsilon}} e^{-\frac{\pi\langle 2x\rangle^2}{2\varepsilon}} + O\left(e^{-\frac{a}{\varepsilon}}\right) ;$$

$$B(x) := \sum_{m\equiv 1 \bmod 2} e^{-\frac{\pi\varepsilon m^2}{2}} e^{2\pi i m x} = \frac{1}{2}\left(\vartheta_{\frac{\varepsilon}{2}}(x) - \vartheta_{\frac{\varepsilon}{2}}(x+\frac{1}{2})\right) = \vartheta_{2\varepsilon}(2x) - \vartheta_{\frac{\varepsilon}{2}}(x+\frac{1}{2})$$

$$= \sqrt{\frac{1}{2\varepsilon}} e^{-\frac{\pi\langle 2x\rangle^2}{2\varepsilon}} - \sqrt{\frac{2}{\varepsilon}} e^{-\frac{2\pi\langle x+1/2\rangle^2}{\varepsilon}} + O\left(e^{-\frac{a}{\varepsilon}}\right),$$

and the approximate representation (10) follows.

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