From the smoothness of the initial state to that of the autocorrelation function

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Drawing principles from Fourier analysis, we argue that for a generic system, the smoother an initial state is, the faster its decomposition coefficients with respect to the eigenstates of the system decay, and in turn result in a sufficiently smooth autocorrelation functions, leading to a series of oscillating terms. Thus, we understand the periodic cusps of the autocorrelation functions in the quench dynamics of a Bloch state, which was observed previously [Zhang and Yang, EPL 114, 60001 (2016)].

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In quantum dynamics, a fundamental quantity is the autocorrelation function, which measures the recurrence (or survival) of an initial state. Let the Hamiltonian of the system be $H$, and the initial state be $|\psi_0\rangle$. The autocorrelation function associated with this particular state is defined as the overlap between it and its time-evolved state $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$.

$$A(t) = \langle \psi_0 | \psi(t) \rangle = \langle \psi_0 | e^{-iHt} | \psi_0 \rangle.$$  (1)

So, $|A|^2$ is the ratio of the initial state in the time-evolved state. This makes it the quantity of primary interest in quantum decay. Introducing the eigenstates $|\phi_n\rangle$ and the corresponding eigenenergies $\{E_n\}$ of $H$, we have

$$A(t) = \sum_{n=1}^{\infty} |c_n|^2 e^{-iE_nt},$$  (2)

where the coefficients

$$c_n = \langle \phi_n | \psi_0 \rangle.$$  (3)

From the point of view of Fourier analysis, here two procedures working in opposite directions are involved. First, in the forward direction, the initial state is decomposed with respect to the orthonormal basis $\{|\phi_n\rangle\}$, and the coefficients $c_n$ are obtained; then, in the backward direction, the autocorrelation function is constructed as a Fourier series with $\{c_n\}$ being the coefficients.

Now, we note that in Fourier analysis, a general principle is that the smoothness of a function is linked to the rate of decay of its Fourier coefficients—the smoother the function is, the faster the Fourier coefficients decay. While this principle can only be appropriately understood in terms of rigorous theorems (see below for some), it is in agreement with the intuition that to fit a jump or a cusp we need fast oscillating terms.

By this principle, an initial state sufficiently smooth will yield a series $\{c_n\}$ decaying sufficiently fast, which in turn will lead to a sufficiently smooth autocorrelation function in time. On the contrary, an initial state with jumps or cusps will yield a series decaying relatively slow, and in turn result in an autocorrelation function less smooth.

In the following, we take the infinite square well potential to illustrate this point.

By choosing proper units, we can assume that the well is on the interval $(0, \pi)$, and the Hamiltonian is $H = -\frac{d^2}{dx^2}$. The eigenstates and eigenenergies are then $(n \geq 1)$

$$\phi_n = \sqrt{\frac{2}{\pi}} \sin nx, \quad E_n = n^2.$$  (4)

For given arbitrary initial state $\psi$, the decomposition $\psi = \sum_n c_n \phi_n$ can be carried out by calculating the coefficients $c_n$ as

$$c_n = \int_0^\pi dx \phi_n(x) \psi(x).$$  (5)

To make use of ready-made results in Fourier analysis, we define the odd function $\tilde{\psi}$ on $(-\pi, \pi)$,

$$\tilde{\psi}(x) = \begin{cases} \psi(x), & 0 < x < \pi, \\ -\psi(-x), & -\pi < x < 0, \end{cases}$$  (6)

and then extend it to the whole axis by periodicity. On $(-\pi, \pi)$, (a complete orthogonal basis is

$$\left\{ \frac{1}{\sqrt{2\pi}} e^{inx}, n \in \mathbb{Z} \right\}.$$  (7)

Let the expansion of $\tilde{\psi}$ with respect to this basis be

$$\tilde{\psi}(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} d_n e^{inx}.$$  (8)

Then it is ready to check that

$$c_n = \frac{i}{2} (d_n - d_{-n}).$$  (9)

Therefore, the problem reduces to the standard problem of the decay rate of the Fourier coefficients of the function $\tilde{\psi}$ in the standard basis $e^{inx}/\sqrt{2\pi}$. For the latter, several useful theorems are well-known.

**Theorem 1** If $f$ is $2\pi$-periodic and $f^{(k-1)}$ absolutely continuous on $[0, 2\pi]$, $f(x) \sim \sum_n d_n e^{inx}/\sqrt{2\pi}$, then $d_n = O(1/n^k)$ as $|n| \to \infty$. 

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Integrating by parts, we have
\begin{align*}
d_n &= \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dx f(x) e^{-inx} \\
&= \frac{1}{\sqrt{2\pi}} \left[ f(x) e^{-inx} \right] \bigg|_{-\pi}^{\pi} + \frac{1}{in} \int_{-\pi}^{\pi} dx f'(x) e^{-inx} \\
&= \frac{1}{in\sqrt{2\pi}} \int_{-\pi}^{\pi} dx f'(x) e^{-inx}.
\end{align*}

Here in the second line, because of the periodicity of the integrand, the boundary contributions cancel. Iterating gives
\begin{equation}
d_n = \frac{1}{(in)^k \sqrt{2\pi}} \int_{-\pi}^{\pi} dx f^{(k)}(x) e^{-inx}.
\end{equation}

We then have
\begin{equation}
|d_n| \leq \frac{1}{n^k \sqrt{2\pi}} \int_{-\pi}^{\pi} dx |f^{(k)}(x)|.
\end{equation}

**Theorem 2** If $f$ is of bounded variation on $[0, 2\pi]$, $f(x) \sim \sum_n d_n e^{inx}/\sqrt{2\pi}$, then $d_n = O(1/n)$ as $|n| \to \infty$.

A very short proof of this theorem was given by Taibleson in Ref. [5].

**Theorem 3** If $f$ is $2\pi$-periodic, $f^{(k-1)}$ absolutely continuous on $[0, 2\pi]$, and $f^{(k)}$ is of bounded variation, $f(x) \sim \sum_n d_n e^{inx}/\sqrt{2\pi}$, then $d_n = O(1/n^{k+1})$ as $|n| \to \infty$.

This is just a combination of the two previous theorems. Applying theorem 2 to the integral in (11), we get one more factor of $1/n$.

With these theorems in hand, we proceed to three concrete states, namely
\begin{align*}
\psi_1 &= \sqrt{\frac{3}{\pi^3}} (\pi - x), \\
\psi_2 &= \sqrt{\frac{12}{\pi^2}} \left( \frac{\pi}{2} - \left| x - \frac{\pi}{2} \right| \right), \\
\psi_3 &= \sqrt{\frac{30}{\pi^5}} (\pi - x).
\end{align*}

They are illustrated in Fig. 1. These states are chosen in the order of increasingly smooth. It is easily seen that the extend function $\psi_1$ has a jump at $x = 0$. The function $\psi_2$ is continuous, but its first derivative has jumps at $x = \pm \frac{\pi}{2}$. As for $\psi_3$, its first derivative is still continuous but its second derivative has a jump at $x = 0$. All these functions and their derivatives are of bounded variation.

Therefore, by theorem 3 we expect that their Fourier coefficients $c_n$ are on the order of $O(1/n)$, $O(1/n^2)$, and $O(1/n^3)$, respectively. Indeed, by straightforward calculation, we get
\begin{align*}
\psi_1 &= \sum_{n=1}^{\infty} \frac{\sqrt{6}}{n\pi} \phi_n, \\
\psi_2 &= \sum_{n=1}^{\infty} \frac{4\sqrt{3}}{n^2\pi} \sin \frac{n\pi}{2} \phi_n, \\
\psi_3 &= \sum_{n=1}^{\infty} \frac{4\sqrt{15}}{n^3\pi^3} (1 - (-1)^n) \phi_n.
\end{align*}

We can then form the autocorrelation functions as
\begin{align*}
A_1(t) &= \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{e^{-ln^2t}}{n^2}, \\
A_2(t) &= \frac{96}{\pi^4} \sum_{n \geq 1, n \in \text{odd}} \frac{e^{-ln^2t}}{n^4}, \\
A_3(t) &= \frac{960}{\pi^6} \sum_{n \geq 1, n \in \text{odd}} \frac{e^{-ln^2t}}{n^6}.
\end{align*}

By Weierstrass’ test [4], we see that the three series all converge uniformly on $\mathbb{R}$ and thus the three functions are all continuous. The problem is to what extent they are differentiable. For $A_1$, tentative term-by-term differentiation generates a series converging nowhere, which suggests its poor differentiability. This is supported by its plot in Fig. 2(a), where we see that both the real and the imaginary part of $A_1$ are zigzag on minute scales. Indeed, the imaginary part of $A_1$ is proportional to the Riemann function,
\begin{equation}
R(t) = \sum_{n=1}^{\infty} \sin \frac{n^2t}{\pi^2}.
\end{equation}

Riemann conjectured that this function is nowhere differentiable. In 1916, Hardy proved that it is indeed not differentiable when $t$ is an irrational multiple of $\pi$ [3]. But the problem was completely solved only much later. Around 1969, Gerver proved that $R(t)$ is differentiable when $t = \frac{p\pi}{q}$ with $p$ and $q$ being odd integers, and not differentiable elsewhere [4, 5]. Hence, we know that $A_1$ is differentiable at most at countably many points.

As for $A_2$ and $A_3$, term-by-term differentiation is legitimate for once and twice, respectively, as the resultant series, apart from some constant coefficients, are essentially
\begin{equation}
D(t) = \sum_{n \geq 1, n \in \text{odd}} \frac{e^{-ln^2t}}{n^4}.
\end{equation}
which is uniformly convergent on \( \mathbb{R} \). However, further differentiation seems impossible, as hinted by the plot of \( D \) (see Fig. 3) and by its similarity with the Riemann function.

Hence, in accordance with the increasing smoothness of the initial state \( \psi_1 \), the autocorrelation functions \( A_i \) \((1 \leq i \leq 3)\) are increasingly smooth. See Fig. 2 for comparison.

An objection might be that the state \( \psi_1 \) is not a legitimate state of the infinite square potential. Indeed, it does not vanish at \( x = 0 \), and as can be seen from (14a), its energy is infinite. However, there exist legitimate states approximating it to arbitrary precision. For example, by truncating the series in (14a) at the fifth term, we get a totally valid state

\[
\psi_4 \propto \sum_{n=1}^{5} \frac{\sqrt{6}}{n\pi} \phi_n. \tag{18}
\]

This state, as shown in the inset of Fig. 3, resembles the state \( \psi_1 \), but avoids its difficulty by satisfying the boundary condition. As a neighbor of \( \psi_1 \) in the Hilbert space, its autocorrelation function \( A_4(t) \), which is a truncation of the \( A_i(t) \) series in (15), retains the zigzag features of the latter to a good extent.

In conclusion, by drawing mathematical results from Fourier analysis, we have gained some insight into quantum dynamics. The point is that we should pay attention to the decay rate of the coefficients \( |c_n|^2 \). Their decay behavior on the one hand reflects the smoothness of the initial state and on the other hand determines that of the autocorrelation function.

Some remarks are in order.

First, in our discussion, we have tacitly assumed that all the eigenstates are bound states. But it is conceivable that similar relations hold when some or all of the eigenstates are extended.

Second, in the infinite square well case, it is the Fourier theory in the narrow sense that takes a part. For other systems, the eigenstates are different, and the Fourier expansion is in a board sense. But in many cases, the “smoothness means fast decay” principle still hold [5].

Third, while here we have taken a toy model to illustrate our point, the idea is actually relevant in more realistic problems. Actually, now we understand the periodic cusps of the autocorrelation function in the quench dynamics of a Bloch state \([\text{[7]}\). In that problem, the autocorrelation function \( A_\alpha(t) = e^{-i\alpha t}B(t) \), with \( \alpha \) some non-integral real number and \( B(t) \) defined by the series

\[
B(t) = \sin^2 \frac{\pi \alpha}{\pi^2} \sum_{n \in \mathbb{Z}} \frac{e^{-int}}{(n + \alpha)^2}. \tag{19}
\]

Here the weight coefficients \( |c_n|^2 = \sin^2(\pi\alpha)/[\pi^2(n + \alpha)^2] \) decay like \( 1/n^2 \). Because of this slow decay rate, by theorem [8], the \( 2\pi \)-periodic function \( B(t) \) cannot be continuously differentiable. Indeed, it has the closed expression

\[
B(t) = \left(1 - \frac{1 - e^{-2\pi\alpha t}}{2\pi t}\right) e^{i\alpha t}, \quad 0 \leq t \leq 2\pi, \tag{20}
\]

and show cusps when \( t \) is an integral multiple of \( 2\pi \).

Finally, we should note that the link between autocorrelation function and Fourier analysis was noted decades ago by Krylov and Fock [11]. Later, Khalfin borrowed...
 FIG. 4. (Color online) Real and imaginary parts of the autocorrelation function of the state $\psi_4$ in (18), which is illustrated in the inset. Compare the curves with those in Fig. 2(a).

the Paley-Wiener theorem, which is again a reflection of the principle, in the latter to study the former, and came to the important conclusion that exponential decay at all time is impossible for a realistic system with a spectrum bounded from below [12]. As the field of Fourier analysis is full of profound results, we have reasons to believe that the field of quantum dynamics can continually benefit from it.

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