Wave Chaos in Quantum Pseudointegrable Billiards

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Abstract—We clarify from a general perspective, the condition for the appearance of chaotic energy spectrum in quantum pseudointegrable billiards with a point scatterer inside.

I. Introduction

The quantum billiard with point scatterers is a quasi-exactly solvable model which is closely related to real systems. The billiards are a natural idealization of the particle motion in bounded systems. The single-electron problem in mesoscopic structures is now a possible setting, owing to the rapid progress in the mesoscopic technology. Real systems are, however, not free from impurities which affect the particle motion inside. In the presence of a small amount of contamination, even a single-electron problem becomes unmanageable. The modeling of the impurities with point scatterers makes the problem easy to handle without changing essential dynamics.

A fundamental problem for the billiards considered here is to understand global behavior of the energy spectrum in the parameter space of particle energy and the strength of the scatterers. In particular, statistical properties of the spectrum are important because they reflect the degree of complexity of underlying dynamics. It is widely believed that integrable systems obey Poisson statistics, while the predictions of the Gaussian Orthogonal Ensembles (GOE) describe chaotic systems. In this paper, we discuss the spectral properties of quantum billiards with a single point scatterer. It should be noticed that the nature of classical motion in such systems is pseudointegrable in the sense that unstable trajectories, which hit the point scatterer, are of measure zero. As a result, it is expected that the energy spectrum of a quantum analogue does not substantially differ from Poisson statistics. However, as shown in this paper, quantization induces the chaotic spectrum under a certain condition. This phenomenon might be called wave chaos because its origin is the wavelike nature of quantum dynamics. After deriving the eigenvalue equation with the help of self-adjoint extension theory in functional analysis, we discuss the statistical properties of the energy spectrum from a general perspective and deduce the condition for the appearance of chaotic spectrum in the quantum pseudointegrable system.

II. Formulation

We start from an empty billiard in spatial dimension \(d\), \(d = 1, 2, 3\). Let us consider a quantum point particle of mass \(M\) moving freely in a bounded region \(\Omega^{(d)}\). We impose the Dirichlet boundary condition such that wave functions vanish on the boundary of \(\Omega^{(d)}\). The eigenvalues and the corresponding normalized eigenfunctions are denoted by \(E_n\) and \(\varphi_n(\vec{x})\) respectively:

\[
H_0\varphi_n(\vec{x}) \equiv - \frac{\nabla^2}{2M} \varphi_n(\vec{x}) = E_n \varphi_n(\vec{x}).
\]

The Hamiltonian \(H_0\) is the kinetic operator in \(L^2(\Omega^{(d)})\) with domain \(D(H_0) = H^2(\Omega^{(d)}) \cap H_0^1(\Omega^{(d)})\) in terms of the Sobolev spaces. The Green’s function of \(H_0\) is given by

\[
G^{(0)}(\vec{x}, \vec{x}'; \omega) = \sum_{n=1}^{\infty} \frac{\varphi_n(\vec{x})\varphi_n(\vec{x}')}{\omega - E_n},
\]

The average level density is given by

\[
\rho_{av}^{(d)}(\omega) = \begin{cases} 
\frac{M^{1/2}\Omega^{(1)}}{2\pi^{1/2}} \frac{1}{\sqrt{\omega}}, & d = 1, \\
\frac{M^{1/2}\Omega^{(2)}}{\pi^{1/2}} \frac{1}{\sqrt{\omega}}, & d = 2, \\
\frac{M^{1/2}\Omega^{(3)}}{2\pi^{1/2}} \frac{1}{\sqrt{\omega}}, & d = 3,
\end{cases}
\]

where we denote the “volume” of \(\Omega^{(d)}\) by the same symbol. (For example, the area of a two-dimensional region \(\Omega^{(2)}\) is simply denoted by \(\Omega^{(2)}\).)

We now place a single point scatterer at \(\vec{x}_0\) inside the billiard. Naively, one defines the scatterer in terms of the \(d\)-dimensional Dirac’s delta function:

\[
H = H_0 + v\delta^{(d)}(\vec{x} - \vec{x}_0).
\]

However, the Hamiltonian \(H\) is not mathematically sound for \(d \geq 2\). It is easy to see that the eigenvalue equation of \(H\) is reduced to

\[
\sum_{n=1}^{\infty} \frac{\varphi_n(\vec{x}_0)^2}{\omega - E_n} = v^{-1}.
\]
Keeping Eq. (3) in mind, we realize that the infinite series in Eq. (4) does not converge for \( d \geq 2 \), since the average of the numerator (among many \( n \)) is energy-independent; \( \langle \varphi_n(\vec{x}_0)^2 \rangle \approx 1/\Omega^{(d)} \).

To handle the divergence, a scheme for renormalization is called for. One of the most satisfying schemes is given by the self-adjoint extension theory of functional analysis [6]. We first consider in \( L^2(\Omega^{(d)}) \) the nonnegative operator

\[
H_{\vec{x}_0} = -\frac{\nabla^2}{2M} + \epsilon_0(\Omega^{(d)} - \vec{x}_0)
\]

with its closure \( \hat{H}_{\vec{x}_0} \) in \( L^2(\Omega^{(d)}) \). Namely, we restrict \( D(H_0) \) to the functions which vanish at the location of the point scatterer. By using integration by parts, it is easy to prove that the operator \( \hat{H}_{\vec{x}_0} \) is symmetric (Hermitian). But it is not self-adjoint. Indeed, the equation

\[
\hat{H}_{\vec{x}_0}^* \psi_\omega(\vec{x}) = \omega \psi_\omega(\vec{x}), \quad \psi \in D(\hat{H}_{\vec{x}_0}^*)
\]

has a solution for \( Im \omega \neq 0 \) [6]:

\[
\psi_\omega(\vec{x}) = G^{(0)}(\vec{x}, \vec{x}_0; \omega), \quad \vec{x} \in \Omega^{(d)} - \vec{x}_0
\]

indicating

\[
D(\hat{H}_{\vec{x}_0}) = D(H_{\vec{x}_0}) \oplus N(\hat{H}_{\vec{x}_0} - \omega) \oplus N(\hat{H}_{\vec{x}_0}^* - \omega)
\]

\[
\neq D(\hat{H}_{\vec{x}_0}),
\]

where \( N(A) \) is the kernel of an operator \( A \). Since \( \hat{H}_{\vec{x}_0} \) has the deficiency indices \((1, 1)\), \( \hat{H}_{\vec{x}_0} \) has one-parameter family of self-adjoint extensions \( H_\theta \) [6]:

\[
D(H_\theta) = \{ f | f = \varphi + c(\psi_{\Lambda A} + e^{i\theta} \psi_{-\Lambda A});
\varphi \in D(H_{\vec{x}_0}), c \in C, 0 \leq \theta < 2\pi \},
\]

\[
H_\theta f = \hat{H}_{\vec{x}_0} \varphi + i\Lambda c(\psi_{\Lambda A} + e^{i\theta} \psi_{-\Lambda A}),
\]

where \( \Lambda > 0 \) is an arbitrary mass scale. With the aid of Krein’s formula, we can write down the Green’s function for the Hamiltonian \( H_\theta \) as

\[
G_\theta(\vec{x}, \vec{x}; \omega) = G^{(0)}(\vec{x}, \vec{x}; \omega)
+
G^{(0)}(\vec{x}, \vec{x}_0; \omega)T_\theta(\omega)G^{(0)}(\vec{x}_0, \vec{x}; \omega).
\]

The transition matrix \( (T_\theta) \) is calculated by

\[
T_\theta(\omega) = \frac{1 - e^{i\theta}}{(\omega - i\Lambda)c_{\Lambda}(\omega) - e^{i\theta}(\omega + i\Lambda)c_{-\Lambda}(\omega)},
\]

where

\[
c_{\pm\Lambda}(\omega) = \int_{\Omega^{(d)}} G^{(0)}(\vec{x}, \vec{x}_0; \omega)G^{(0)}(\vec{x}, \vec{x}_0; \pm i\Lambda) d\vec{x}.
\]

Using the resolvent equation, we have

\[
T_\theta(\omega) = (v_\theta^{-1} - G(\omega))^{-1},
\]

where

\[
v_\theta^{-1} = \Lambda \cot \frac{\theta}{2} \sum_{n=1}^{\infty} \varphi_n(\vec{x}_0)^2 E_n^2 + \Lambda^2;
\]

\[
G(\omega) = \sum_{n=1}^{\infty} \varphi_n(\vec{x}_0)^2 \left( \frac{1}{\omega - E_n} + \frac{E_n}{E_n^2 + \Lambda^2} \right).
\]

The constant \( v_\theta \) is a coupling constant of the point scatterer, the value of which ranges over the whole real number as one varies \( 0 \leq \theta < 2\pi \). It follows from Eq. (14) that the eigenvalues of \( H_\theta \) are determined by

\[
G(\omega) = v_\theta^{-1}.
\]

On any interval \( (E_n, E_{n+1}) \), \( G \) is a monotonically decreasing function of \( \omega \) that ranges over the whole real number. This means that Eq. (17) has a single solution on each interval for \( v_\theta \). The eigenfunction of \( H_\theta \) corresponding to an eigenvalue \( \omega_n \) is given by

\[
\psi_n(\vec{x}) \propto G^{(i)}(\vec{x}, \vec{x}_0; \omega_n).
\]

### III. Condition for Strong Coupling

#### A. \( d = 1 \)

In one dimension, each infinite series on RHS in Eq. (16) converges separately. Thus, if we set

\[
v^{-1} = v_\theta^{-1} - \sum_{n=1}^{\infty} \varphi_n(\vec{x}_0)^2 \frac{E_n}{E_n^2 + \Lambda^2},
\]

Eq. (13) is reduced to Eq. (6): A somewhat complicated argument above leads us to the well-known result with Dirac’s delta. In the following, we consider Eq. (6), the LHS of which is denoted by \( G^{(1)}(\omega) \).

To obtain each solution of Eq. (6), a numerical task is needed in general. However, since our main purpose lies in the statistical properties of spectrum, we proceed further by introducing some approximations without losing the essence, while still keeping loss of generality minimal [6]. The first is that the value of \( \varphi_n^2(\vec{x}_0)^2 \) is replaced by its average among many \( n \).

\[
\varphi_n(\vec{x}_0)^2 \simeq \langle \varphi_n(\vec{x}_0)^2 \rangle = 1/\Omega^{(1)}.
\]

Since the statistics is taken within a large number of, sometimes thousands of eigenstates, Eq. (16) is quite satisfactory. Keeping \( |\varphi_n(\vec{x}_0)|^2 \simeq 1/\sqrt{\Omega^{(d)}} \) in mind, we recognize from Eq. (16) with Eq. (6) that if \( \omega_m \simeq E_m \) (or \( E_{m+1} \)) for some \( m \), then \( \psi_m \simeq \varphi_m \) (or \( \varphi_m \)), implying that only \( \psi_m \) with an eigenvalue \( \omega_m \simeq (E_m + E_{m+1})/2 \) is distorted by a point scatterer. For such \( \omega_m \), since the contributions on the summation of \( G^{(d)} \) from the terms with \( n \simeq m \) cancel each other, \( G^{(d)} \) can be estimated by a principal integral:

\[
G^{(d)}(\omega_m) \approx g^{(d)}(\omega_m), \quad \omega_m \simeq \frac{E_m + E_{m+1}}{2},
\]

1 With some minor modifications if necessary, a major part of the argument here is applicable to higher dimensions. We thus explicitly signify “\( d = 1 \)” only for the assertions specific to one dimension.
where we have defined a continuous function $g^{(d)}(\omega)$ of $\omega$ which behaves like an interpolation of the inflection points of $G^{(d)}$. Inserting Eq. (3) into Eq. (22) and using the elementary indefinite integral

$$
\int \frac{dE}{(E-E_0)^{\frac{1}{2}}} = \frac{1}{\sqrt{\omega}} \ln \left| \frac{\sqrt{\omega + \sqrt{E}}}{\sqrt{\omega - \sqrt{E}}} \right|
$$

(23)

for $\omega > 0$, we obtain for $\omega_m \simeq (E_m + E_{m+1})/2$

$$
G^{(d)}(\omega_m) \simeq 0, \quad d = 1,
$$

(24)
indicating that the maximal coupling of a point scatterer is attained when the strength $\nu$ satisfies

$$
\nu^{-1} \simeq 0, \quad d = 1,
$$

(25)
which is going well with our intuition.

The “width” of the strong coupling region (allowable error of $\nu^{-1}$ in Eq. (25)) is estimated by considering a linearized eigenvalue equation. Expanding $G^{(d)}$ at $\omega_m \simeq (E_m + E_{m+1})/2$, we can rewrite the eigenvalue equation as

$$
G^{(d)'}(\omega_m)(\omega - \omega_m) \simeq -G^{(d)}(\omega_m).
$$

(26)
In order that Eq. (26) has a solution $\omega \simeq \omega_m$, the range of RHS has to be restricted to

$$
\left| \frac{\omega - \omega_m}{G^{(d)}(\omega_m)} \right| \leq \frac{\Delta^{(d)}(\omega_m)}{2},
$$

(27)

$$
\Delta^{(d)}(\omega_m) \equiv \left| G^{(d)'}(\omega_m) \rho^{(d)}_{av}(\omega_m)^{-1},
$$

(28)

where we have defined the width $\Delta^{(d)}(\omega)$ which is nothing but the average variance of the linearized $G^{(d)}$ on the interval $(E_m, E_{m+1})$. Using the approximation (26), the value of $\left| G^{(d)'}(\omega_m) \right|$ can be estimated as follows;

$$
\left| G^{(d)'}(\omega_m) \right| = \sum_{n=1}^{\infty} \left( \frac{\varphi_n(x_0)}{\omega_m - E_n} \right)^2 \simeq \left( \frac{\varphi_n(x_0)^2}{(n - \frac{1}{2}) \rho^{(d)}_{av}(\omega_m)^{-1}} \right)^2 \simeq \frac{2}{\left(2n - 1 \right)^2} \left( \frac{\varphi_n(x_0)^2}{\rho^{(d)}_{av}(\omega_m)^{-1}} \right)^2
$$

$$
= \frac{4}{\varphi_n(x_0)^2} \rho^{(d)}_{av}(\omega_m)^{-2} \sum_{n=1}^{\infty} \frac{1}{(2n - 1)^2}
$$

$$
= \frac{\pi^2 \varphi_n(x_0)^2 \rho^{(d)}_{av}(\omega_m)^{-2}}{\pi^2}
$$

(29)
The second equality follows from the approximation that the unperturbed eigenvalues are distributed with a mean interval $\rho^{(d)}_{av}(\omega_m)^{-1}$ in the whole energy region. This assumption is quite satisfactory, since the denominator of $G^{(d)'}(\omega)$ is of the order of $(\omega - E_n)^2$ indicating that the summation in Eq. (29) converges rapidly. From Eqs. (3) and (24) for $d = 1$, we obtain

$$
\Delta^{(1)}(\omega_m) \simeq \frac{\pi M^{1/2}}{2^{1/2}} \frac{1}{\sqrt{\omega_m}},
$$

(30)
which is inversely proportional to square root of the energy $\omega$. We can summarize the finding in one dimension as follows; The effect of a point scatterer of coupling strength $\nu$ is substantial only in the eigenstates with eigenvalue $\omega$ such that

$$
|\nu| < \frac{\Delta^{(1)}(\omega)}{2} \simeq \frac{\pi M^{1/2}}{2^{1/2}} \frac{1}{\sqrt{\omega}}.
$$

(31)

### B. $d = 2, 3$

It is easy to apply the argument above to higher dimensions. Since each series on RHS in Eq. (16) diverges when summed separately for $d = 2, 3$, we have to resort to Eq. (17). As a result, Eq. (23) is replaced by

$$
g^{(d)}(\omega) = \langle \varphi_n(x_0)^2 \rangle P \int_0^{\infty} \frac{\Lambda^{(d)}(E) dE}{\omega - E}, \quad d = 2, 3.
$$

(32)

Using the elementary indefinite integrals,

$$
\int \left( \frac{1}{\omega - E} + \frac{E}{E^2 + \Lambda^2} \right) dE = -\ln \left| \frac{\omega - E}{\sqrt{E^2 + \Lambda^2}} \right|
$$

(33)

$$
\int \left( \frac{1}{\omega - E} + \frac{E}{E^2 + \Lambda^2} \right) \sqrt{E} dE = \sqrt{\omega} \ln \left( \frac{\sqrt{\omega} + \sqrt{E}}{\sqrt{\omega} - \sqrt{E}} \right)
$$

$$
\frac{1}{2} \sqrt{\Lambda} \ln \left( \frac{E + \sqrt{2\Lambda E} + \Lambda}{E - \sqrt{2\Lambda E} + \Lambda} \right)
$$

$$
- \sqrt{\Lambda} \left\{ \arctan \left( \frac{2E}{\Lambda} + 1 \right) + \arctan \left( \frac{2E}{\Lambda} - 1 \right) \right\},
$$

(34)

we obtain for $\omega_m \simeq (E_m + E_{m+1})/2$

$$
G^{(d)}(\omega_m) \simeq \left\{ \begin{array}{ll}
\frac{M}{2\pi} \ln \frac{\omega_m}{\Lambda}, & d = 2, \\
\frac{M^{3/2}}{2\pi^{1/2}} \sqrt{\omega_m}, & d = 3.
\end{array} \right.
$$

(35)

The width $\Delta^{(d)}(\omega)$ is estimated by Eq. (28) with Eq. (24). Using Eq. (3), we find

$$
\Delta^{(d)}(\omega_m) \simeq \left\{ \begin{array}{ll}
\frac{\pi M}{2\pi^{1/2}} \sqrt{\omega_m}, & d = 2, \\
\frac{M^{3/2}}{2\pi^{1/2}} \sqrt{\omega_m}, & d = 3.
\end{array} \right.
$$

(36)

From Eq. (27) with $\nu$ replaced by $\nu^*$, we realize that the strong coupling is attained under the condition

$$
|\nu^*| \leq \frac{\pi M}{2\pi} \ln \frac{\omega_m}{\Lambda} \leq \frac{\pi M}{4}, \quad d = 2, (37)
$$

$$
|\nu^*| + \frac{M^{3/2} \Lambda^{1/2}}{2\pi} \leq \frac{M^{3/2}}{2^{1/2} \sqrt{\omega_m}}, \quad d = 3. \quad (38)
$$
IV. Numerical Example

We consider a quantum particle with mass $M = 1/2$ moving in a three-dimensional rectangular box with side-lengths $(l_x, l_y, l_z) = (1.047, 1.186, 0.8049)$ and hence $\Omega^{(3)} = 1$. The mass scale is set to $\Lambda = 1$. A single point scatterer is placed at the center of the billiard. We take into account only the states with even parity in each direction, since the others are unaffected by the scatterer in this case. Fig.1 shows, for $v_\theta^{-1} = 0, 10$ and 30, the nearest-neighbor level spacing distribution $P(S)$, which is defined such that $P(S)dS$ is the probability to find the spacing between any two neighboring eigenstates in the interval $(S, S + dS)$. (The average spacing is normalized to one.) Generic integrable systems obey the Poisson distribution $P(S) = \exp(-S)$ (dotted line), while chaotic systems are described by the GOE prediction $P(S) = \pi S/2 \times \exp(-\pi S^2/4)$ (solid line). The statistics is taken within $\omega_{1000} \sim \omega_{2100}$ in Fig.1 ($\omega_{1600} = 8304$). According to Eq.(38), the most strong coupling is attained for $v_\theta^{-1} = M^{1/2} \Lambda^{1/2}/2\pi = -0.05626$. As $v_\theta^{-1}$ increases, $P(S)$ tends to approach the Poisson prediction. For $v_\theta^{-1} \simeq \Delta^{(3)}(\omega_{1600})/2 = 11.3$, $P(S)$ is expected to be intermediate in shape between Poisson and GOE. The value can be considered as the upper bound of $v_\theta^{-1}$ for inducing a GOE-like shape in this energy region. With $v_\theta^{-1}$ beyond the bound, the system is not substantially different from the empty billiard, and as a result, $P(S)$ resembles to the Poisson distribution. These features are successfully reproduced in Fig.1.

V. Conclusion

We have discussed the condition for the appearance of chaotic spectrum in the quantum pseudointegrable billiards with a single point scatterer inside. Chaotic spectrum appears if the conditions (63), (67) and (68) are satisfied for dimension $d = 1, 2, 3$, respectively. In two dimension, the condition is described by a logarithmically energy-dependent strip with a constant width, indicating that the system recovers integrability in the high energy limit for any $v_\theta$. In three dimension, the spectrum shows GOE-like nature when $v_\theta^{-1}$ is within a band whose width increases parabolically as a function of the energy. This implies that the spectrum becomes chaotic at high energy for any $v_\theta$, which makes a clear contrast with two dimension.

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Fig. 1. $P(S)$ for $v_\theta^{-1} = 0, 10, 30$. The solid (dotted) line is GOE prediction (Poisson distribution).