Spectral properties of three-dimensional quantum billiards with a pointlike scatterer

T. Shigehara
Computer Centre, University of Tokyo, Yayoi, Bunkyo-ku, Tokyo 113, Japan
and Department of Information and Computer Sciences, Faculty of Engineering, Saitama University, Shimo-Okubo, Urawa, Saitama 338, Japan

Taksu Cheon
Laboratory of Physics, Kochi University of Technology, Tosa Yamada, Kochi 782, Japan
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We examine the spectral properties of three-dimensional quantum billiards with a single pointlike scatterer inside. It is found that the spectrum shows chaotic (random-matrix-like) characteristics when the inverse of the formal strength $\overline{v}^{-1}$ is within a band whose width increases parabolically as a function of the energy. This implies that the spectrum becomes random-matrix-like at very high energy irrespective to the value of the formal strength. The predictions are confirmed by numerical experiments with a rectangular box. The findings for a pointlike scatterer are applied to the case for a small but finite-size impurity. We clarify the proper procedure for its zero-size limit which involves nontrivial divergence. The previously known results in one- and two-dimensional quantum billiards with small impurities inside are also reviewed from the present perspective. [S1063-651X(97)15606-9]

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I. INTRODUCTION

The quantum billiard with pointlike scatterers inside is a solvable model which still retains most of the interesting characteristics of nonintegrable quantum physics. The problem is based on obvious physical motivations. The billiard is a natural idealization of the particle motion in bounded systems. The one-electron problem in quantum dots is a possible setting which may be used as a single-electron memory, a promising computational device in the future. It is now possible to actually construct such structures with extremely pure semiconductors thanks to the rapid progress in the mesoscopic technology. However, real systems are not free from impurities which affect the electron motion inside. In the presence of a small amount of contamination, even a single-electron problem in bounded regions becomes unmanageable. The modeling of the impurities with pointlike scatterers is expected to make the problem easy to handle without changing essential physics, at least at low energy.

In spite of its seeming simplicity, the billiard problem with pointlike scatterers is known to possess several nontrivial properties. In two-dimensional billiards with a single pointlike scatterer, one observes phase reversion of wave function with the adiabatic rotation of the scatterer around certain points inside the billiard [1]. This can be regarded as the simplest manifestation of the geometrical phase or Berry phase [2,3]. Moreover, the two-dimensional quantum billiards with pointlike scatterers possess the properties of ultraviolet divergences, scale anomaly, and asymptotic freedom which are analogous to the ones found in quantum field theories [4]. Also, there is a problem of so-called *wave chaos* [5,6]; through its wavelike nature, the quantum particle can be diffracted by pointlike scatterers, which should have no effect on the classical motion of the particle [7–9].

A fundamental problem for quantum billiards with pointlike scatterers is to understand global behavior of the energy spectrum in the parameter space of particle energy z and the strength of the scatterers $\overline{v}$. In particular, statistical properties of the spectrum are important because they reflect the degree of complexity (regularity or chaos) of underlying dynamics. For two dimensions, the problem has already been examined in detail [10,11]. The chaotic spectrum (level statistics of random-matrix theory [12–14]) appears along the ''logarithmic strip'' in the parameter space $(z,\overline{v}^{-1})$. More precisely, the effects of a pointlike scatterer with formal strength $\overline{v}$ are most strongly observed in the eigenstates with an eigenvalue z such that

$$\frac{M}{2\pi}\ln\frac{z}{\Lambda}\simeq\overline{v}^{-1}, \tag{1}$$

where M is the mass of a particle moving in the billiard and Λ is an arbitrary mass scale. Equation (1) indicates that the maximal physical coupling is attained at the value of formal coupling that varies with the logarithmic dependence of the particle energy. This energy dependence is a manifestation of a phenomenon known as the scale anomaly, or the quantum mechanical breaking of scale invariance [15,16]: In two dimension, the physics is expected to be energy independent, since the kinetic term (Laplacian) and the zero-range interaction (a δ potential) are scaled in the same manner under a transformation of length scale. However, the quantization breaks a scale invariance, and as a result, the strong coupling region shifts with a logarithmic dependence of energy. The condition (1) also shows that, for any value of formal strength $\overline{v}$, the system approaches to the empty billiard when the energy increases. Thus the system possesses the property of the asymptotic freedom.

Quantum-mechanical billiard problems with pointlike scatterers inside can be defined for spatial dimension $d\leqslant 3$. Contrary to the two-dimensional case, spectral properties in three dimensions have been scarcely studied so far. The main

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purpose of this paper is precisely to fill this void. The logarithmic energy dependence of the strong coupling region observed in two dimensions has its origin in the energy independence of the average level density of the system. Since the level density is proportional to the square root of the energy in three dimensions, one expects substantially different spectral properties. In this paper, we find that this is indeed the case. It is shown that the value of formal strength which induces the maximal coupling is independent of the particle energy, whereas the width of the strip on which the strong coupling is attained broadens with square-root dependence of energy. This means that, in three dimensions, for any $\overline{v}$ $(\neq 0)$, the system exhibits chaotic spectra at the high energy limit.

Another objective of this paper is to relate the findings in the purely pointlike scatterers to the realistic situation of small but finite-size impurities. For the pointlike scatterers, the condition for the strong coupling also depends on the mass scale Λ which is introduced in the process of regularization. This reflects the fact that formal strength $\overline{v}$ does not have a direct relation to the observables as it stands. In order to clarify the physical meaning of $\overline{v}$, we begin by approximating a finite-range potential with a δ potential within a truncated basis. The size of the truncation depends on the range of potential. We then obtain a relation between the formal and bare strengths, the latter of which corresponds to the strength of the δ potential within the truncation. The relation enables us to apply the results for pointlike scatterers to finite-range cases. Moreover, it clarifies the proper procedure and physical meaning of the zero-size limit of the finite-size potential in an intuitive fashion.

The paper is organized as follows. In Sec. II, we deduce, from a general perspective without any assumption on the shape of billiards, the strong coupling condition in three-dimensional billiards under which the effect of a pointlike scatterer becomes substantial. In Sec. III, we consider the case for a small but finite-size scatterer. By examining a relation between the formal strength of the scatterer and the energy eigenstates of finite-size potential, we rewrite the condition for the strong coupling in terms of the observables. The previously known results for one and two dimensions are reviewed from the present point of view. We clarify the proper procedure and meaning of the zero-size limit of finite-size potential in one, two, and three dimensions. We test the predictions in Sec. II with the numerical calculations in Sec. IV. We look at the level statistics of rectangular box with a single pointlike scatterer inside. In particular, the case where the scatterer is located at the center of the box is examined in details. We summarize the present work in Sec. V.

II. CONDITION FOR STRONG COUPLING IN TERMS OF FORMAL STRENGTH

Consider a quantum particle of mass M moving in a three-dimensional billiard of volume V. The eigenvalues and eigenfunctions of this system are denoted by E_n and $\varphi_n(\vec{x})$;

$$-\frac{\nabla^2}{2M}\varphi_n(\vec{x})=E_n\varphi_n(\vec{x}) \quad (n=1,2,3,\ldots). \tag{2}$$

We impose the Dirichlet boundary condition to the wave functions φ_n at the billiard surface. The average level density at energy z has square-root energy dependence;

$$\rho_{\mathrm{av}}(z)=\frac{M^{3/2}V}{2^{1/2}\pi^2}\sqrt{z}. \tag{3}$$

Suppose that a single pointlike scatterer is placed at $\vec{x}=\vec{x}_0$ inside the billiard. Despite the simplicity of a contact interaction, the Schrödinger equation suffers from short-distance singularities at the location of the scatterer, which needs to be renormalized. This can be done in most mathematically satisfying fashion in the framework of the self-adjoint extension theory of a symmetric operator in functional analysis. Details are given elsewhere (see Ref. [11]). We just present the relevant results. Starting with the formulation of Zorbas [17], we obtain the equation for the eigenvalues of the system, z_n $(n=1,2,3,\ldots)$, as

$$\overline{G(z)}=\overline{v}^{-1}, \tag{4}$$

where

$$\overline{G(z)}\equiv\sum_{n=1}^{\infty}\varphi_n(\vec{x}_0)^2\left(\frac{1}{z-E_n}+\frac{E_n}{E_n^2+\Lambda^2}\right). \tag{5}$$

In Eq. (4), $\overline{v}$ is the formal strength of the pointlike scatterer and Λ in Eq. (5) is an arbitrary mass scale that arises in the renormalization. The formal strength $\overline{v}$ does not have a direct relation to physical observables as it stands. Its relation to physical strength of the scatterer is discussed later in Sec. III. Here we just mention the following two points: (1) To ensure the self-adjointness of the Hamiltonian for the system defined by Eq. (4), one has to take $\overline{v}$ to be independent of the energy, and (2) in the limit of $\overline{v}\rightarrow 0$, the system approaches the empty billiard.

The second term of $\overline{G(z)}$ in Eq. (5) is independent of the energy z. It plays an essential role in making the problem well-defined; the infinite series in Eq. (5) does not converge without the second term. For spacial dimension $d\geqslant 4$, the summation in Eq. (5) diverges. This reflects the fact that the billiard problem with pointlike scatterers is not well-defined for $d\geqslant 4$ in quantum mechanics. Within any interval between two neighboring unperturbed eigenvalues, $\overline{G(z)}$ is a monotonically decreasing function that ranges over the whole real number. Therefore, Eq. (4) has a single solution on each interval. The eigenfunction corresponding to an eigenvalue z_n is written in terms of Green's function of the empty billiard as

$$\psi_n(\vec{x})\propto G^{(0)}(\vec{x},\vec{x}_0;z_n)=\sum_{k=1}^{\infty}\frac{\varphi_k(\vec{x}_0)}{z_n-E_k}\varphi_k(\vec{x}). \tag{6}$$

This shows that if a perturbed eigenvalue z_n is close to an unperturbed one E_n (or E_{n+1}), then the corresponding eigenfunction ψ_n is not substantially different from φ_n (or φ_{n+1}). Thus the disturbance by a pointlike scatterer is restricted to eigenstates with an eigenvalue around which $\overline{G(z)}$ has an inflection point. This is because each inflection point of $\overline{G(z)}$ is expected to appear, on average, around the midpoint on the interval between two neighboring unperturbed eigenvalues. Let $(\tilde{z},\overline{G(\tilde{z})})$ be one of such inflection points of $\overline{G(z)}$; $\tilde{z}\simeq(E_m+E_{m+1})/2$ for some m. In this case, the contributions on $\overline{G(\tilde{z})}$ from the terms with $n\simeq m$ cancel each other, and we can replace the summation in Eq. (5) by a principal integral with a high degree of accuracy;

$$\overline{G(\tilde{z})}\simeq\overline{g(\tilde{z})}\equiv\langle\varphi_n(\vec{x}_0)^2\rangle P\int_0^\infty\left(\frac{1}{\tilde{z}-E}+\frac{E}{E^2+\Lambda^2}\right)\times\rho_{\rm av}(E)dE, \tag{7}$$

where we have defined a continuous function $\overline{g(z)}$ which behaves like an interpolation of the inflection points of $\overline{G(z)}$. In Eq. (7), $\langle\varphi_n(\vec{x}_0)^2\rangle$ is the average value of $\varphi_n(\vec{x}_0)^2$ among various n. For a generic position of the scatterer, one has $\langle\varphi_n(\vec{x}_0)^2\rangle\simeq1/V$. Notice that $\overline{G(z)}\simeq\overline{g(z)}$ is valid only around the inflection points of $\overline{G(z)}$. Using an elementary indefinite integral

$$\int\left(\frac{1}{z-E}+\frac{E}{E^2+\Lambda^2}\right)\sqrt{E}dE=\sqrt{z}\ln\left|\frac{\sqrt{z}+\sqrt{E}}{\sqrt{z}-\sqrt{E}}\right|-\frac{1}{2}\sqrt{\frac{\Lambda}{2}}\ln\left(\frac{E+\sqrt{2\Lambda E}+\Lambda}{E-\sqrt{2\Lambda E}+\Lambda}\right)-\sqrt{\frac{\Lambda}{2}}\left\{\arctan\left(\sqrt{\frac{2E}{\Lambda}}+1\right)+\arctan\left(\sqrt{\frac{2E}{\Lambda}}-1\right)\right\} \tag{8}$$

for $z>0$, we obtain

$$\overline{G(\tilde{z})}\simeq-\frac{M^{3/2}\Lambda^{1/2}}{2\pi}. \tag{9}$$

The first term in Eq. (8), which depends on the energy z, disappears both at $E=0$ and $E=\infty$. As a result, the average value of $\overline{G(z)}$ at the inflection points is independent of the energy. Equation (9) indicates that the maximal coupling of a pointlike scatterer is attained with the formal strength $\bar{v}$ which satisfies

$$\bar{v}^{-1}\simeq-\frac{M^{3/2}\Lambda^{1/2}}{2\pi}. \tag{10}$$

The ''width'' of the strong coupling region can be estimated by considering a linearized eigenvalue equation. Expanding $\overline{G(z)}$ around $\tilde{z}$, we can rewrite Eq. (4) as

$$\overline{G(\tilde{z})}+\overline{G'}(\tilde{z})(z-\tilde{z})\simeq\bar{v}^{-1} \tag{11}$$

or

$$\overline{G'}(\tilde{z})(z-\tilde{z})\simeq\bar{v}^{-1}+\frac{M^{3/2}\Lambda^{1/2}}{2\pi}. \tag{12}$$

In order to ensure that the perturbed eigenvalue z_m is close to $\tilde{z}$, the range of $\bar{v}^{-1}+M^{3/2}\Lambda^{1/2}/2\pi$ has to be restricted to

$$\left|\bar{v}^{-1}+\frac{M^{3/2}\Lambda^{1/2}}{2\pi}\right|\lesssim\frac{\Delta(\tilde{z})}{2}, \tag{13}$$

where the width Δ is defined by

$$\Delta(\tilde{z})\equiv|\overline{G'}(\tilde{z})|\rho_{\rm av}(\tilde{z})^{-1}. \tag{14}$$

This is nothing but the variance of the linearized $\overline{G(z)}$ on the interval between the two unperturbed eigenvalues just below and above $\tilde{z}$ (see Fig. 1). The width can be estimated by the average level density at the energy under consideration as follows:

$$\begin{aligned}\Delta(\tilde{z})&=\sum_{n=1}^{\infty}\frac{\varphi_n(\vec{x}_0)^2}{(\tilde{z}-E_n)^2}\rho_{\rm av}(\tilde{z})^{-1}\\&\simeq\langle\varphi_n(\vec{x}_0)^2\rangle\sum_{n=1}^{\infty}\frac{2\rho_{\rm av}(\tilde{z})^{-1}}{\{(n-\frac{1}{2})\rho_{\rm av}(\tilde{z})^{-1}\}^2}\\&=\pi^2\langle\varphi_n(\vec{x}_0)^2\rangle\rho_{\rm av}(\tilde{z})\simeq\frac{M^{3/2}}{2^{1/2}}\sqrt{\tilde{z}}.\end{aligned} \tag{15}$$

We have implicitly assumed in Eq. (15) that the unperturbed eigenvalues are distributed with a mean interval $\rho_{\rm av}(\tilde{z})^{-1}$ in the whole energy region. This assumption is quite satisfactory, since the denominator of $\overline{G'}(z)$ is of the order of $(z-E_n)^2$, indicating that the summation in Eq. (15) converges rapidly.

We recognize from Eqs. (13) and (15) that the effects of a pointlike scatterer of formal strength $\bar{v}$ are substantial only in the eigenstates with eigenvalues z such that

$$\left|\bar{v}^{-1}+\frac{M^{3/2}\Lambda^{1/2}}{2\pi}\right|\lesssim\frac{\Delta(z)}{2}\simeq\frac{M^{3/2}}{2^{3/2}}\sqrt{z}. \tag{16}$$

The width Δ is proportional to the average level density, and as a result, it broadens with square-root energy dependence. This can be understood from another perspective, by considering a scale transformation of a heuristic Hamiltonian with a δ potential;

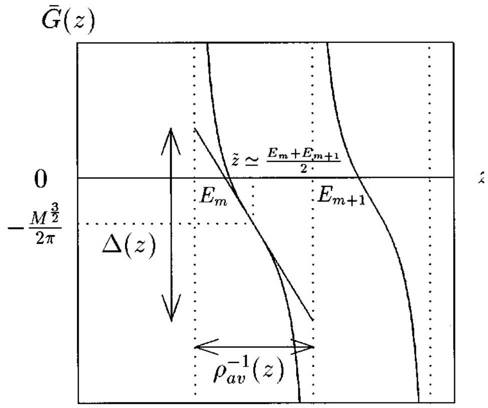

FIG. 1. Typical behavior of $\overline{G(z)}$ with mass scale $\Lambda=1$ in Eq. (5) and its linearized version is shown as a function of z. The latter is obtained by expanding $\overline{G(z)}$ at its inflection point $\tilde{z}$ on the interval $E_m<z<E_{m+1}$. The coordinate of the inflection point is given by $(\tilde{z},\overline{G(\tilde{z})})\simeq((E_m+E_{m+1})/2,-M^{3/2}/2\pi)$. Strong coupling is attained when $\bar{v}^{-1}$ takes a value within the range of the linearized function.

$$H=-\frac{\nabla^2}{2M}+v\,\delta(\vec{x}-\vec{x}_0). \tag{17}$$

Although the Hamiltonian (17) is not well defined in case of spatial dimension $d \geqslant 2$, we proceed further for the moment and return to this point in Sec. III. Under a scale transformation $\vec{x}\to\vec{x}/a$, the Hamiltonian (17) is transformed to

$$H\to a^2\left(-\frac{\nabla^2}{2M}+av\,\delta(\vec{x}-\vec{x}_0)\right). \tag{18}$$

Since the energy z scales as $z\to a^2 z$, the strength v which scales as $v\to av$ must have square-root energy dependence, which explains Eq. (16).

The findings in this section are summarized as follows:

(1) For a three-dimensional billiard, the effect of a pointlike scatterer on spectral properties is maximal when the formal strength of the scatterer satisfies $\bar{v}^{-1}\simeq -M^{3/2}\Lambda^{1/2}/2\pi$, irrespective to the energy z.

(2) The width Δ (or an allowable error in $\bar{v}^{-1}$ to look for the effect) increases with square-root energy dependence.

From these two, we conclude:

(3) For any value of formal strength ($\bar{v}\neq 0$), a pointlike scatterer tends to disturb a particle motion in billiards, as the particle energy increases; the physical strength increases proportional to the square-root of the energy. This makes a sharp contrast to the asymptotic freedom observed in two-dimensional billiards.

Before closing this section, we give a few words on the shape of the billiard. Our implicit assumption for the shape is that the average level density of the empty billiard is dominated by the volume term, which has a square-root dependence on energy. The assumption is justified for a generic three-dimensional billiard which has the same order of length scale in each direction, irrespective to a full detail of the shape of the billiard. If one length scale is substantially smaller than the other two, the surface term dominates the average level density in the low energy region. As a result, the spectral property at low energy is expected to change with the logarithmic energy-dependence which is specific to two dimensions [see Eq. (1)].

III. FORMAL, BARE, AND EFFECTIVE STRENGTHS

As stated in the previous section, $\bar{v}$ in Eq. (4) does not have a direct relation to physical observables as it stands. The main purpose of this section is to clarify the physical meaning of the formal strength $\bar{v}$. To this end, we relate the formal strength to a strength defined through a more realistic potential with small but finite range. The relation makes it possible to apply the findings in the previous section to the finite-size impurities. The previously published results in two dimension [11] and the well-known elementary results in one dimension are also reviewed from the present perspective.

We first point out that the definition of the formal strength is not unique. Indeed, Eq. (5) is not a unique candidate for $\overline{G(z)}$; it can be defined by any convergent series for $z\neq E_n$ which has a form

$$\overline{G(z)}=\lim_{N\to\infty}\sum_{n=1}^{N}\left(\frac{\varphi_n(\vec{x}_0)^2}{z-E_n}+f_n\right). \tag{19}$$

Here, f_n is an arbitrary quantity independent of the energy z, whereas it may depend, in general, on E_n and $\varphi_n(\vec{x}_0)$. The first term in the parenthesis on the right-hand side (RHS) in Eq. (19) does not converge as $N\to\infty$ in spatial dimension $d=2, 3$. This means that f_n should be taken as a counterterm which cancels the divergence of the first term. Once such a series $\{f_n\}$ is chosen, one can define an equation, $\overline{G(z)}=\gamma$, with an energy-independent constant γ. This gives a possible eigenvalue equation for the billiard with a pointlike scatterer of a certain fixed (energy-independent) coupling strength. It is obvious that, even with another choice of series, say $\{\tilde{f}_n\}$, the same eigenvalue equation can be reproduced by shifting the value of γ by $\Sigma_{n=1}^{\infty}(\tilde{f}_n-f_n)$. One possible choice of f_n is given by

$$f_n=\varphi_n(\vec{x}_0)^2\frac{E_n}{E_n^2+\Lambda^2} \tag{20}$$

with an arbitrary real number Λ ($\neq 0$). This choice along with the definition $\bar{v}\equiv 1/\gamma$ gives precisely the original eigenvalue problem Eqs. (4) and (5). Clearly, this $\bar{v}$ is a mathematical quantity whose physical interpretation is not immediately evident.

To reveal the meaning of the formal strength $\bar{v}$ in Eq. (4), we begin by approximating low-energy spectra (eigenvalues and eigenfunctions) of a finite-range potential by that of a zero-range interaction. Suppose that a small but finite-size scatterer of volume Ω is located at $\vec{x}=\vec{x}_0$ inside a three-dimensional billiard of volume V. We describe the scatterer in terms of a potential which has a constant strength on a region Ω;

$$U(\vec{x})=\begin{cases} U_0, & \vec{x}\in\Omega \\ 0, & \vec{x}\in V-\Omega, \end{cases} \tag{21}$$

where the regions of the potential and the outer billiard are denoted by the same symbols as the volumes. We assume that the scatterer has the same order of size, say R, in each spatial direction, and also assume that the volume of the scatterer is substantially smaller than that of the outer billiard; $\Omega \simeq R^3 \ll V$. In this case, the scatterer behaves as pointlike at low energy $z \ll E_{N(\Omega)}$, where $E_{N(\Omega)}$ is estimated as

$$E_{N(\Omega)} \simeq \frac{1}{MR^2} \simeq \frac{1}{M\Omega^{2/3}}. \tag{22}$$

Furthermore, the coupling of higher energy states than $E_{N(\Omega)}$ to the low-energy states is weak, since wave functions with wavelength shorter than R oscillate within the scatterer. This means that the low-energy states ($z \ll E_{N(\Omega)}$) can be described by the Hamiltonian in terms of a δ potential, Eq. (17), with the coupling strength

$$v \equiv U_0 \Omega, \tag{23}$$

together with *a basis truncated at* $E_{N(\Omega)}$. The truncation of basis is crucial for the present argument. In case of spatial dimension $d \geqslant 2$, a δ potential is not well-defined in the full unperturbed basis. This is clear from the fact that the summation in Eq. (24) diverges in the limit of $\Omega \to 0$ [hence as $N(\Omega) \to \infty$]. The finiteness of the scatterer introduces an ultraviolet cutoff in a natural manner, and as a result, the low-energy spectra can be reproduced by the Hamiltonian (17) within a suitably truncated basis.

In an analogy to the terminology of the field theories, we call the coupling v as the *bare strength*, since it appears as the coefficient of the δ potential within a given truncation [18]. The bare strength v can be related to formal strength $\overline{v}$ as follows. Within the truncated basis $\{\varphi_n(\vec{x});\ n=1,2,\ldots,N(\Omega)\}$, the eigenvalues of the Hamiltonian (17) are determined by

$$\sum_{n=1}^{N(\Omega)} \frac{\varphi_n(\vec{x}_0)^2}{z-E_n} = v^{-1}. \tag{24}$$

Inserting Eq. (24) into Eq. (4) with Eq. (5), we obtain

$$\overline{v}^{-1} = v^{-1} + \sum_{n=1}^{N(\Omega)} \varphi_n(\vec{x}_0)^2 \frac{E_n}{E_n^2+\Lambda^2} + \sum_{n=N(\Omega)+1}^{\infty} \varphi_n(\vec{x}_0)^2 \left(\frac{1}{z-E_n} + \frac{E_n}{E_n^2+\Lambda^2} \right). \tag{25}$$

Equation (25) gives an exact relation between formal and bare strengths. In order to have further insight on Eq. (25), we take an average for $\varphi_n(\vec{x}_0)^2$ among various n, $\langle \varphi_n(\vec{x}_0)^2 \rangle \simeq 1/V$, and replace the remaining summations on the RHS by integrals. We then have

$$\overline{v}^{-1} \simeq v^{-1} + \langle \varphi_n(\vec{x}_0)^2 \rangle \left\{ \int_0^{E_{N(\Omega)}} \frac{E}{E^2+\Lambda^2} \rho_{\rm av}(E)\, dE + \int_{E_{N(\Omega)}}^{\infty} \left(\frac{1}{z-E} + \frac{E}{E^2+\Lambda^2} \right) \rho_{\rm av}(E)\, dE \right\}. \tag{26}$$

Using Eq. (3), along with elementary integrals

$$F_1^{(3)}(z,E) \equiv \int \frac{\sqrt{E}}{z-E}\, dE = \sqrt{z} \ln \left| \frac{\sqrt{z}+\sqrt{E}}{\sqrt{z}-\sqrt{E}} \right| - 2\sqrt{E}, \quad (z>0), \tag{27}$$

$$F_2^{(3)}(E) \equiv \int \frac{E}{E^2+\Lambda^2} \sqrt{E}\, dE = 2\sqrt{E} - \frac{1}{2}\sqrt{\frac{\Lambda}{2}} \ln \left(\frac{E+\sqrt{2\Lambda E}+\Lambda}{E-\sqrt{2\Lambda E}+\Lambda} \right) - \sqrt{\frac{\Lambda}{2}} \left\{ \arctan\left(\sqrt{\frac{2E}{\Lambda}}+1 \right) + \arctan\left(\sqrt{\frac{2E}{\Lambda}}-1 \right) \right\}, \tag{28}$$

we can rewrite Eq. (26) as

$$\overline{v}^{-1} \simeq v^{-1} - \frac{M^{3/2}\Lambda^{1/2}}{2\pi} - \frac{M^{3/2}}{2^{1/2}\pi^2} F_1^{(3)}(z, E_{N(\Omega)}). \tag{29}$$

In Eq. (27), the first term on the RHS is negligible in case of $z \ll E$. Hence, at low energy $z \ll E_{N(\Omega)}$, we have

$$\overline{v}^{-1} \simeq v^{-1} - \frac{M^{3/2}\Lambda^{1/2}}{2\pi} + \frac{2^{1/2}M^{3/2}}{\pi^2} \sqrt{E_{N(\Omega)}}. \tag{30}$$

The third term on the RHS in Eq. (30) diverges as $E_{N(\Omega)}$ increases. This is exactly the same divergence which we observe in the summation in Eq. (24) [or Eq. (19)] with opposite sign. This ensures the convergence of $\overline{G}(z)$ in Eq. (5). Using Eq. (22), we arrive at

$$\overline{v}^{-1} \simeq v^{-1} - \frac{M^{3/2}\Lambda^{1/2}}{2\pi} + \frac{2^{1/2}M}{\pi^2 \Omega^{1/3}}. \tag{31}$$

In order to reproduce a zero-range scatterer with a fixed formal strength $\overline{v}\ (\neq 0)$, the RHS of Eq. (31) needs to converge as Ω shrinks. This means that, for small Ω, v should take a form

$$v(\Omega) = 1 \Big/ \left(-\frac{C}{\Omega^{1/3}} + r(\Omega) \right). \tag{32}$$

The first term in the denominator is a counterterm that cancels the divergence of the third term on the RHS in Eq. (31);

$$C \simeq \frac{2^{1/2}M}{\pi^2}. \tag{33}$$

[More precisely, C should be taken to cancel the divergence which appears in the summation in Eq. (24).] The remnant quantity $r(\Omega)$ in the denominator is a regular function which converges as $\Omega \to 0$. In the zero-size limit, the finite-size scatterer shrinks into a pointlike one with formal strength

$$\overline{v}^{-1} \simeq r(0) - \frac{M^{3/2}\Lambda^{1/2}}{2\pi}. \tag{34}$$

In terms of the potential height U_0, Eq. (32) is rewritten as

$$\begin{aligned} U_0(\Omega) &= 1/(-C\Omega^{2/3} + r(\Omega)\Omega) \\ &= 1/(-C\Omega^{2/3} + r(0)\Omega + o(\Omega)). \end{aligned} \tag{35}$$

Since C is positive, we obtain

$$\begin{cases} v(\Omega) \to -0, \\ U_0(\Omega) \to -\infty, \end{cases} \quad \text{as } \Omega \to 0. \tag{36}$$

Equation (36) indicates that the potential has to be negative in the zero-size limit, irrespective to a form of $r(\Omega)$. This is consistent with the fact that a pointlike scatterer with an arbitrary formal strength $\overline{v}\ (\neq 0)$ sustains a single eigenstate with an eigenvalue smaller than E_1. A seemingly plausible limit, $\Omega \to 0$ along with keeping $U_0\Omega$ constant, is not allowable in the case of three dimensions; such a limit induces too strong a potential to define a quantum mechanical Hamiltonian for a pointlike scatterer. Notice that Eq. (36) does not exclude a possibility of strong repulsion $U_0 \gg 0$ on a small-size region $\Omega \neq 0$. Indeed, Eq. (32) [or Eq. (35)] does not impose any restriction on v (or U) for any *finite* Ω. As long as Ω is finite, one can reproduce even a strong repulsion by taking $r(\Omega)$ as slightly larger than $C/\Omega^{1/3}$. Such $r(\Omega)$ is, in general, a very large positive quantity which diverges to $+\infty$ when Ω shrinks into the zero size together with positively fixed U_0.

Combining the findings in the current and previous sections, we can deduce the condition for the strong coupling for a finite-size scatterer. Inserting Eq. (30) or Eq. (31) into Eq. (16), we obtain

$$\left| v^{-1} + \frac{2^{1/2}M^{3/2}}{\pi^2}\sqrt{E_{N(\Omega)}} \right| \lesssim \frac{\Delta(z)}{2} \tag{37}$$

or

$$\left| v^{-1} + \frac{C}{\Omega^{1/3}} \right| \lesssim \frac{\Delta(z)}{2} \tag{38}$$

for $z \ll E_{N(\Omega)}$. Equation (38) indicates that $v^{-1} \simeq -C/\Omega^{1/3}$ is the condition for the strong coupling, and hence that the effects of a finite-size scatterer at low energy most strongly appear when it is weakly attractive, namely, when the bare strength v is slightly negative. In the zero-size limit, the condition (38) is equivalent to

$$|r(0)| \lesssim \frac{\Delta(z)}{2}. \tag{39}$$

Equation (39) shows that it is the inverse of $r(0)$ that represents a direct measure of coupling strength of the zero-size limit of a scatterer. This naturally leads us to a definition of the *effective strength* of a pointlike scatterer by

$$v_{\text{eff}} \equiv 1/r(0). \tag{40}$$

Using the effective strength v_{eff}, we can rewrite Eq. (39) as

$$|v_{\text{eff}}^{-1}| \lesssim \frac{\Delta(z)}{2}. \tag{41}$$

It can be observed from Eq. (34) that, if the origin of $\overline{v}^{-1}$ axis is shifted to the strong coupling value $-M^{3/2}\Lambda^{1/2}/2\pi$, the formal strength $\overline{v}$ is identical to v_{eff}. We can also say that v_{eff}^{-1} is a ''distance'' to the strong coupling value $v^{-1} \simeq -C/\Omega^{1/3}$, which is, in general, a large negative quantity for small Ω. Inserting Eqs. (15), (23), and (33) into Eq. (38), we have

$$\left| \frac{1}{U_0\Omega} + \frac{2^{1/2}M}{\pi^2\Omega^{1/3}} \right| \lesssim \frac{M^{3/2}}{2^{3/2}}\sqrt{z}. \tag{42}$$

Equation (42) is the condition for the strong coupling in terms of the ''observables;'' at low energy where a finite-size scatterer can be approximated by a pointlike one ($z \ll 1/M\Omega^{2/3}$), a particle of mass M moving in three-dimensional billiards is most strongly coupled to a finite-size ($\simeq \Omega$) scatterer of potential height U_0 under the condition (42). [As seen from the arguments above, the coefficients of $\Omega^{-1/3}$ and $\sqrt{z}$ in Eq. (42) are not exact, but they are of the order of, or approximately, the values in Eq. (42).]

The effective strength of a pointlike scatterer can be defined in two dimensions in a similar manner. However, an energy-dependent correction is needed in this dimension. One possible way to show this is to follow the arguments in the previous and present sections. Reference [11] has taken this path. Instead, we here take an alternative manner which makes it easy to understand the origin of the energy dependence specific to two dimensions. We begin by reexamining the condition for the strong coupling in three dimensions, Eq. (16), in terms of the δ potential with a truncated basis. We start by rewriting Eq. (16) as

$$|\overline{v}^{-1} - \overline{g}(z)| \lesssim \frac{\Delta(z)}{2}, \tag{43}$$

where $\overline{g}(z)$ is defined in Eq. (7). Recall that it behaves like an interpolation of the inflection points of $\overline{G}(z)$ in Eq. (5). The energy dependence of $\overline{g}(z)$ is expected to be small. Indeed, we have $\overline{g}(z) \simeq -M^{3/2}\Lambda^{1/2}/2\pi$ from Eq. (9), irrespective to the energy z. This indicates that Eq. (43) is equivalent to the condition (16). Inserting Eqs. (7) and (26) into the condition (43), we obtain

$$\left| v^{-1} - \langle \varphi_n(\vec{x}_0)^2 \rangle P \int_0^{E_{N(\Omega)}} \frac{\rho_{\rm av}(E)}{z-E} dE \right| \lesssim \frac{\Delta(z)}{2}. \tag{44}$$

This is the condition for the eigenvalue equation Eq. (24) to have a solution z around some inflection point of the LHS in Eq. (24). Using Eqs. (3) and (27), we have

$$\left| v^{-1} - \frac{M^{3/2}}{2^{1/2}\pi^2} F_1^{(3)}(z, E_{N(\Omega)}) \right| \lesssim \frac{\Delta(z)}{2}. \tag{45}$$

Equation (45) is identical to Eq. (37) for $z \ll E_{N(\Omega)}$. Notice that $F_1^{(3)}(z,0) = 0$, namely, the lower bound does not contribute on the principal integral.

Let us now consider a two-dimensional analogue of the finite-range potential (21); it takes a constant value U_0 on a finite-size region of area Ω and zero everywhere else. The bare strength v is defined by $v = U_0 \Omega$ as in three dimensions. Then, one can deduce an analogous formula to Eq. (44) in two dimensions. A crucial difference in two and three dimensions lies in the energy dependence of the average level density. For the billiard with area S, it is given by $\rho_{\rm av} = MS/2\pi$, according to Weyl's formula. Since $\rho_{\rm av}$ is independent of energy in two dimensions, the analogue of Eq. (44) is estimated by

$$F_1^{(2)}(z,E) \equiv \int \frac{dE}{z-E} = -\ln\frac{|z-E|}{\Lambda}, \tag{46}$$

instead of Eq. (27). Using $\langle \varphi_n(\vec{x}_0)^2 \rangle \simeq 1/S$ for a generic position of the scatterer, we obtain

$$\left| v^{-1} - \frac{M}{2\pi} (F_1^{(2)}(z, E_{N(\Omega)}) - F_1^{(2)}(z,0)) \right| \lesssim \frac{\Delta}{2}, \tag{47}$$

namely,

$$\left| v^{-1} - \frac{M}{2\pi} \left(\ln\frac{z}{\Lambda} - \ln\frac{E_{N(\Omega)} - z}{\Lambda} \right) \right| \lesssim \frac{\Delta}{2}. \tag{48}$$

Here, the width Δ is estimated in a similar manner as in Eq. (15);

$$\Delta \simeq \pi^2 \langle \varphi_n(\vec{x}_0)^2 \rangle \rho_{\rm av} \simeq \frac{\pi M}{2}, \tag{49}$$

which is independent of the energy z. The condition (48) is identical to Eq. (51) in Ref. [11], apart from a minor change in the definition of the width Δ in the RHS. In two dimension, $F_1^{(2)}(z,0)$ does not vanish and indeed has a logarithmic dependence on energy. This is the crucial difference from the three-dimensional case. At low energy $z \ll E_{N(\Omega)} \simeq 1/M\Omega$, we have

$$\left| v^{-1} - \frac{M}{2\pi} \left(\ln\frac{z}{\Lambda} + \ln(M\Lambda\Omega) \right) \right| \lesssim \frac{\Delta}{2}. \tag{50}$$

Equation (50) indicates that as Ω shrinks, v should behave like

$$v(\Omega) = 1 \Big/ \left(\frac{M}{2\pi} \ln(M\Lambda\Omega) + r(\Omega) \right), \tag{51}$$

where $r(\Omega)$ is a regular function which converges in the zero-size limit, $\Omega \to 0$. The first term in the denominator ensures that the logarithmic divergence disappears in Eq. (50). Inserting Eq. (51) into Eq. (50), we obtain, in the zero-size limit, a two-dimensional analogue of Eq. (39);

$$\left| r(0) - \frac{M}{2\pi} \ln\frac{z}{\Lambda} \right| \lesssim \frac{\Delta}{2}. \tag{52}$$

This indicates that one can define the effective strength of the pointlike scatterer by

$$v_{\rm eff}(z) \equiv 1 \Big/ \left(r(0) - \frac{M}{2\pi} \ln\frac{z}{\Lambda} \right). \tag{53}$$

Equation (52) now reads

$$|v_{\rm eff}(z)^{-1}| \lesssim \frac{\Delta}{2}. \tag{54}$$

Equation (54) with Eq. (53) embodies the logarithmic strip of wave chaos that is the condition for the strong coupling in two dimensions. By comparing this to Eq. (1), we obtain

$$\overline{v}^{-1} \simeq r(0). \tag{55}$$

The effective strength $v_{\rm eff}$ can be regarded as the direct measure of coupling strength of the scatterer, as in three dimensions, and its inverse, $v_{\rm eff}^{-1}$, is a ''distance'' to a logarithmic curve of the strong coupling limit. The logarithmic energy dependence in $v_{\rm eff}$ exhibits a specific feature in two dimensions. It comes from nonvanishing $F_1^{(2)}(z,0)$ which can be regarded as the origin of scale anomaly in a formalistic sense. Equation (51) shows

$$\begin{aligned} U_0(\Omega) &= 1 \Big/ \left(\frac{M\Omega}{2\pi} \ln(M\Lambda\Omega) + r(\Omega)\Omega \right) \\ &= 1 \Big/ \left(\frac{M\Omega}{2\pi} \ln(M\Lambda\Omega) + r(0)\Omega + o(\Omega) \right). \end{aligned} \tag{56}$$

Hence we obtain

$$\begin{cases} v(\Omega) \to -0, \\ U_0(\Omega) \to -\infty, \end{cases} \quad \text{as } \Omega \to 0. \tag{57}$$

This is consistent with the fact that a pointlike scatterer supports a single eigenstate with an eigenvalue smaller than E_1, irrespective to the value of formal strength $\overline{v}$ $(\neq 0)$. The condition for the strong coupling in two dimensions is rewritten in a comparable form with experiment. Inserting $v=U_0\Omega$ as well as Eq. (49) into Eq. (50), we obtain

$$\left|\frac{1}{U_0\Omega}-\frac{M}{2\pi}\ln(zM\Omega)\right|\lesssim\frac{\pi M}{4} \tag{58}$$

for $z\ll 1/M\Omega$. An arbitrary mass scale Λ disappears from Eq. (58). Similarly to the three-dimensional case, the effects of a finite-size scatterer at low energy $z\ll 1/M\Omega$ appear most strongly when it is weakly attractive [11].

Our treatment is also applicable to one-dimensional case. We end this section by showing that all the standard results in the elementary textbooks on quantum mechanics for one-dimensional δ function is recovered in our formalism. In one dimension, one can define a δ potential (of strength v) with the full unperturbed basis. The summation on the LHS in Eq. (24) is convergent in the limit of $N(\Omega)\to\infty$, since the average level density is inversely proportional to square root of energy;

$$\rho_{\mathrm{av}}(z)=\frac{M^{1/2}L}{2^{1/2}\pi}\frac{1}{\sqrt{z}} \tag{59}$$

for one-dimensional billiards with width L. The condition for the strong coupling is given by an equation formally identical to Eq. (44);

$$\left|v^{-1}-\langle\varphi_n(x_0)^2\rangle P\int_0^\infty\frac{\rho_{\mathrm{av}}(E)}{z-E}dE\right|\lesssim\frac{\Delta(z)}{2}, \tag{60}$$

where $\langle\varphi_n(x_0)^2\rangle\simeq 1/L$ and the width is given by

$$\Delta(z)\simeq\pi^2\langle\varphi_n(x_0)^2\rangle\rho_{\mathrm{av}}\simeq\frac{\pi M^{1/2}}{2^{1/2}}\frac{1}{\sqrt{z}}. \tag{61}$$

The principal integral in Eq. (60) can be estimated with the use of

$$F_1^{(1)}(z,E)\equiv\int\frac{1}{(z-E)\sqrt{E}}dE=\frac{1}{\sqrt{z}}\ln\left|\frac{\sqrt{z}+\sqrt{E}}{\sqrt{z}-\sqrt{E}}\right|,\quad (z>0). \tag{62}$$

Since we have $F_1^{(1)}(z,0)=F_1^{(1)}(z,\infty)=0$, we get

$$|v^{-1}|\lesssim\frac{\Delta(z)}{2}. \tag{63}$$

Therefore, in one dimension, the strong coupling with a pointlike scatterer is reached when the bare strength v is large. The property is energy independent (no scale anomaly). Since the width becomes narrow as the energy increases, the effect of a pointlike scatterer with any (finite) bare strength disappears in the high energy limit. The bare strength v is identical to the effective strength v_{eff} in one dimension. They are related to the formal strength by

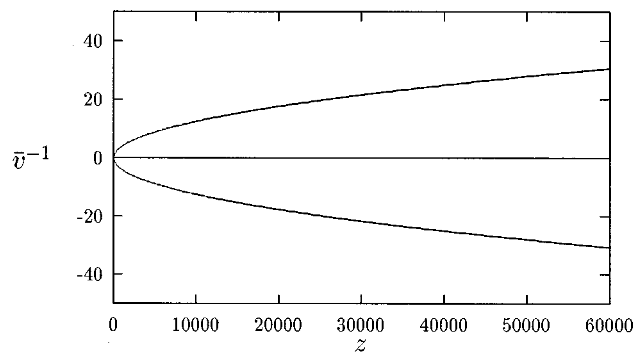

FIG. 2. Plot of $\overline{v}^{-1}=-M^{3/2}/2\pi\pm\Delta(z)/2$. The effects of a pointlike scatterer on the energy spectrum are expected to appear in the eigenstates in the region between both curves.

$$v^{-1}=v_{\mathrm{eff}}^{-1}=\overline{v}^{-1}-\sum_{n=1}^{\infty}\varphi_n(x_0)^2\frac{E_n}{E_n^2+\Lambda^2}. \tag{64}$$

In contrast to two and three dimensions, no divergent quantity appears in the definition of effective coupling. In analogy to the similar situation in quantum field theories, one might call this property of one-dimensional pointlike scatterer as *super-renormalizability*. A pointlike scatterer of bare strength v is obtained as the zero-size limit of a finite-range (Ω) potential with height $U_0\equiv v/\Omega$ in a natural manner. In order to ensure $v\neq 0$, U_0 should behave like

$$U_0(\Omega)=1/(r(\Omega)\Omega), \tag{65}$$

where $r(\Omega)$ is regular in the zero-size limit. Since no singular term appears in $v(\Omega)^{-1}$ at $\Omega\to 0$ limit, the usual zero-size limit, in which the product $U_0\Omega$ is kept constant, is attained by keeping $r(\Omega)$ constant as Ω varies. Thus one obtains a pointlike object with the bare strength

$$v=1/r(0). \tag{66}$$

We may conclude from the current perspective that it is an accidental fortune of super-renormalizability that has enabled the simple formulation of the one-dimensional Dirac δ function with a straightforward limiting procedure.

IV. NUMERICAL EXAMPLE

We have revealed, in Sec. II, the condition for the appearance of the effects of a pointlike scatterer in three-dimensional quantum billiards. It has been applied to the low-energy spectrum in case of a small but finite-size scatterer in Sec. III. In this section, the predictions are confirmed by examining statistical properties of quantum spectrum. We restrict ourselves to the exactly pointlike case. Even in this case, the numerical burden of handling very large number of basis states is quite heavy, and a smart trick is required to overcome it.

We take a rectangular box as an outer billiard. We also assume the Dirichlet boundary condition such that wave functions vanish on the boundary. The mass scale is set to $\Lambda=1$ in the following. Fixing the value of Λ makes all parameters dimensionless. The eigenvalues E_n and eigenfunctions $\varphi_n(\vec{x})$ in Eq. (5) are given by rearranging the triple-indexed eigenvalues and eigenfunctions in ascending order of energy;

$$E_{n_x n_y n_z}=\frac{\pi^2}{2M}\left\{\left(\frac{n_x}{l_x}\right)^2+\left(\frac{n_y}{l_y}\right)^2+\left(\frac{n_z}{l_z}\right)^2\right\}, \tag{67a}$$

$$\varphi_{n_x n_y n_z}(\vec{x})=\sqrt{\frac{8}{V}}\sin\frac{n_x\pi x}{l_x}\sin\frac{n_y\pi y}{l_y}\sin\frac{n_z\pi z}{l_z}$$

$$(n_x,n_y,n_z=1,2,3,\ldots). \tag{67b}$$

The mass of a particle and the side lengths of the billiard are assumed to be $M=1/2$ and $(l_x,l_y,l_z)=(1.0471976, 1.1862737, 0.8049826)$, respectively. In this choice of the side lengths, the volume of the billiard is $V=1$. We calculate $\overline{G(z)}$ on the interval between E_m and E_{m+1} by

$$\overline{G(z)}\simeq\langle\varphi_n(\vec{x}_0)^2\rangle\int_{E_1}^{E_{m-2000}}\left(\frac{1}{z-E}+\frac{E}{E^2+1}\right)\rho_{\mathrm{av}}(E)dE+\sum_{n=m-2000}^{m+2000}\varphi_n(\vec{x}_0)^2\left(\frac{1}{z-E_n}+\frac{E_n}{E_n^2+1}\right)$$
$$+\langle\varphi_n(\vec{x}_0)^2\rangle\int_{E_{m+2000}}^{\infty}\left(\frac{1}{z-E}+\frac{E}{E^2+1}\right)\rho_{\mathrm{av}}(E)dE. \tag{68}$$

When $m<2000$, the first integral is discarded and the lower bound of the summation is replaced by $n=1$ in Eq. (68). The integral in Eq. (68) is easily calculated by using Eq. (8). The approximation by Eq. (68) serves to reduce numerical burden considerably, keeping a sufficient numerical accuracy.

For a moment, we restrict ourselves to the case where the scatterer is placed at the center of the billiard. In this case, $\langle\varphi_n(\vec{x}_0)^2\rangle=\varphi_n(\vec{x}_0)^2=8/V$, which is eight times larger than the average value for generic cases. However, Eq. (16) is still valid, since only one-eighth of the whole unperturbed states, namely, that with even parity in each direction are affected by the scatterer $(n_x,n_y,n_z=1,3,5,\ldots)$. The solid curves in Fig. 2 represent $\overline{v}^{-1}=-M^{3/2}/2\pi\pm\Delta(z)/2$. According to the condition (16) (with $\Lambda=1$), the effects of a pointlike scatterer are expected to appear mainly in the eigenstates in the region between both curves. This is in fact the case as observed in Figs. 3 and 4, where the nearest-neighbor level spacing distribution $P(S)$ is displayed for various nonnegative values of $\overline{v}^{-1}$ in two energy regions: $z_{100}\sim z_{3100}$ in Fig. 3 and $z_{17000}\sim z_{20000}$ in Fig. 4, respectively. We have numerically confirmed that the sign reversion of $\overline{v}^{-1}$ does not change the qualitative behavior of the distribution in both energy regions. Figures 3 and 4 show that the case of $\overline{v}^{-1}=-M^{3/2}/2\pi=-0.056269769\simeq 0$ is closest to the Wigner distribution (solid line). It is numerically observed that the second moment of $P(S)$ is given by $\int_0^\infty P(S)S^2dS\simeq 1.5$ for $\overline{v}^{-1}=0$, irrespective to the energy. This indicates that $P(S)$ is Wigner-like in the whole energy region for $v^{-1}\simeq -M^{3/2}/2\pi$. As $\overline{v}^{-1}$ increases, $P(S)$ tends to approach the Poisson distribution (dotted line). However, its rate depends on the energy. While $P(S)$ becomes intermediate in shape between the Poisson and Wigner distributions at $\overline{v}^{-1}\simeq 10$ in Fig. 3, such distribution appears at $\overline{v}^{-1}\simeq 30$ in Fig. 4. This can be easily understood from Fig. 2; the value of $-M^{3/2}/2\pi+\Delta(z)/2$ is 11.3 at $z_{1600}=8303.96$, and 25.7 at $z_{18500}=42508.80$, respectively. These values can be considered as the upper bound of $\overline{v}^{-1}$ for inducing a Wigner-like shape in $P(S)$ at each energy region. With $\overline{v}^{-1}$ beyond the bound, the system is not substantially different from the empty billiard, and as a result, $P(S)$ resembles the Poisson distribution. In Fig. 5, the spectral rigidity $\Delta_3(L)$ is shown for various values of $\overline{v}^{-1}$. The average is taken in the same energy region as in Fig. 3. We can see the gradual shift to Poisson statistics (dotted line) as $\overline{v}^{-1}$ increases. Beyond $\overline{v}^{-1}\simeq 20$, the value of $\Delta_3(L)$ is close to the Poisson prediction, $L/15$. There still exists an appreciable difference from random-matrix prediction (solid line) even for the strong-coupling limit $(\overline{v}^{-1}=-M^{3/2}/2\pi\simeq 0)$. A similar tendency has been reported in two-dimensional cases [10]. This can be understood from the fact that the range of the nth perturbed eigenvalue is restricted to the region between nth and $(n+1)$th unperturbed ones in case of a single pointlike scatterer. As a result, the number of perturbed eigenstates on a certain energy interval does not differ largely from the number of unperturbed ones in the same region. This restriction does not apply to the case of multiple number of pointlike scatterers. We can therefore expect that the increase of the number of scatterers makes the energy spectrum more rigid. For two-dimensional rectangular billiard, a recent calculation corroborate this argument [4].

Up to now, we have placed a pointlike scatterer at a specific position, namely, the center of the rectangular box. We next show the level statistics for the case of a generic location for the pointlike scatterer. In Fig. 6, we show the nearest-neighbor level spacing distribution $P(S)$ for a box with a scatterer located at $\vec{x}_0=(0.5129731, 0.5489658, 0.3342914)$. The formal coupling is chosen to be $\overline{v}^{-1}=0$.

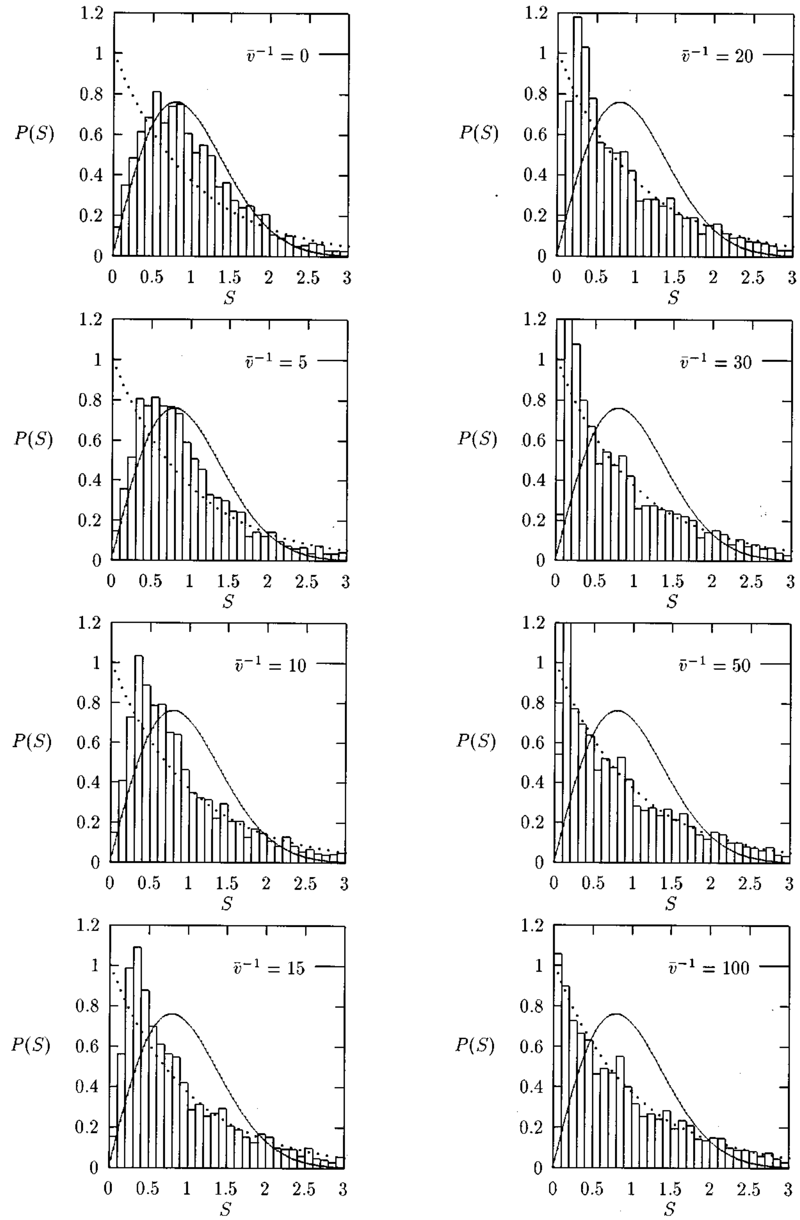

FIG. 3. The nearest-neighbor level spacing distribution $P(S)$ is shown for various values of $\overline{v}^{-1}$ in case of the scatterer being located at the center of the rectangular solid. The statistics are taken within the eigenvalues between $z_{100}=1307.95$ and $z_{3100}=12932.70$. (The eigenvalues are numbered by taking into account only the eigenstates with even parity in each direction.) The solid (dotted) line is the Wigner (Poisson) distribution.

Although a nearly maximal coupling is expected to be attained with this value of $\overline{v}^{-1}$, the level repulsion is rather weak and the observed $P(S)$ is considerably different from the Wigner distribution. This can be understood by considering the state dependence of $\varphi_n(\vec{x}_0)^2$. In case that the scatterer is placed at the center, the value of $\varphi_n(\vec{x}_0)^2$ is independent of the unperturbed states: $\varphi_n(\vec{x}_0)^2=8/V$ for even parity states in each direction. This ensures a smooth change of the value of $\overline{G(z)}$ at the successive inflection points. For a generic position of the scatterer, however, the value of $\varphi_n(\vec{x}_0)^2$ changes nearly at random as n varies, causing a considerable fluctuation of the inflection points of $\overline{G(z)}$. As a result, it frequently happens that successive unperturbed states are not substantially affected by the scatterer even with the strong coupling value of the formal strength. It should be also noticed that, for the generic position of the scatterer, the width of strong coupling is substantially smaller than its average estimate given in Eq. (16). This can be understood as follows. Define the width for the nth state by

$$\Delta_n(z)\equiv\pi^2\varphi_n(\vec{x}_0)^2\rho_{\mathrm{av}}(z) \tag{69}$$

with $z\simeq z_n\simeq E_n$. Since $\varphi_n(\vec{x}_0)^2$ ranges from 0 to $8/V$ as n varies, the width $\Delta_n(z)$ fluctuates between 0 and $8\Delta(z)$ for a generic $\vec{x}_0$. Since its average is given by $\Delta(z)$, it frequently occurs that $\Delta_n(z)$ is substantially smaller than $\Delta(z)$ for successive n. This also explains why the coupling of the pointlike scatterer is rather weak for the generic case. [For the case that the scatterer is located at the center, we have $\Delta_n(z)=\Delta(z)$, irrespective to the unperturbed states.] Clearly, a successive existence of the eigenstates unaffected by the scatterer is a specific feature of a single-scatterer case. As the number of scatterers increases, such tendency disappears because only in very rare occurrence, none of the scatterers has a substantial influence on successive unperturbed eigenstates, as long as the coupling

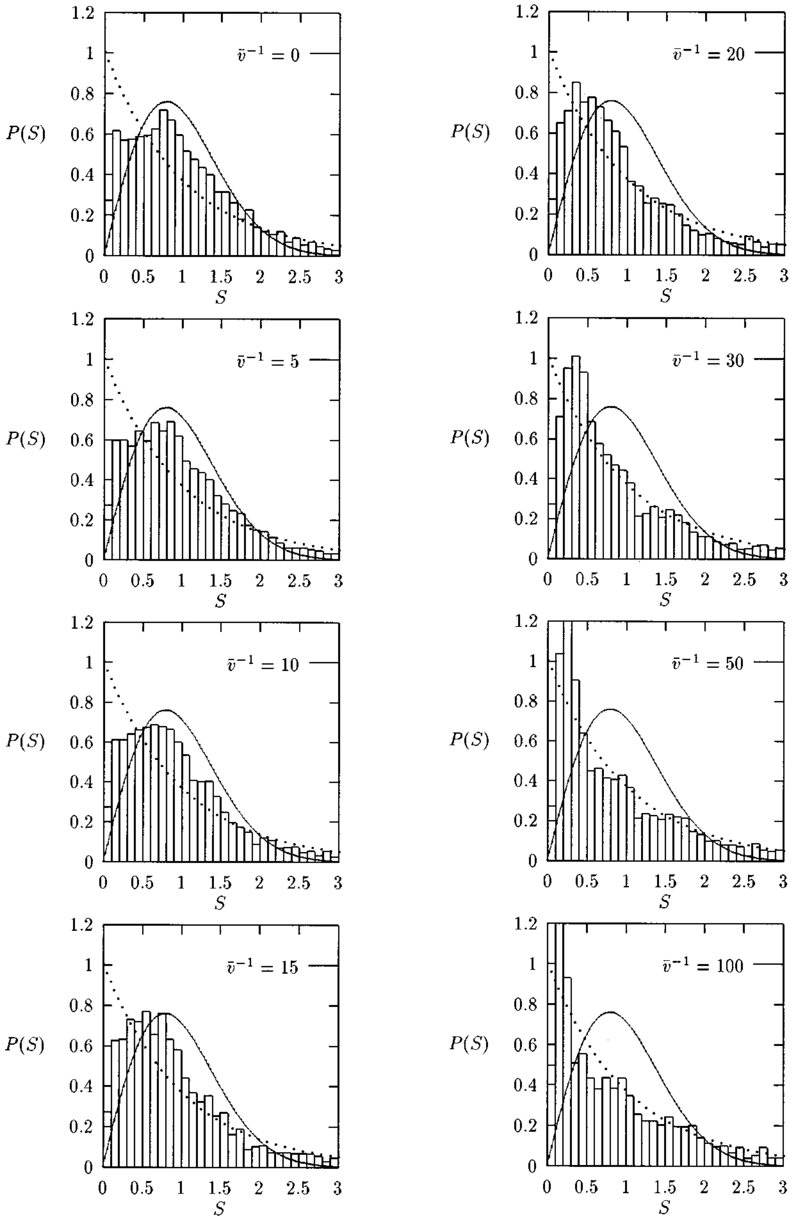

FIG. 4. Same as Fig. 3 except for the energy region between $z_{17000}=40184.77$ and $z_{20000}=44767.02$.

strength of each scatterer satisfies the condition (16). Again, for two-dimensional cases, numerical results support this assertion [4].

V. CONCLUSION

To conclude the paper, we summarize the findings in the previous sections. Equation (16) in Sec. II is precisely the necessary condition for the appearance of wave chaos for three-dimensional pseudointegrable billiards with pointlike scatterers. The condition is essentially different from that for two dimensions. Whereas it is described by a logarithmically energy-dependent strip with an energy-independent width in two dimensions, it is characterized by a parabola with a symmetric axis parallel to the energy axis in three dimensions. This implies that in three-dimensional billiards, the effect of the pointlike scatterer is stronger in the higher energy region. The numerical experiments using the rectangular box confirm the assertion that even a single pointlike scatterer brings about wave chaos under the predicted condition, although the precise amount of the effect depends on the location of the scatterer.

Since the condition for wave chaos, Eq. (16) is described in terms of the formal strength $\overline{v}$ of the pointlike scatterer, it is not directly applicable to the case for realistic finite-size impurities. For this in mind, we have examined a relation between formal strength $\overline{v}$ of the pointlike scatterer and the bare strength v of the finite-size potential which is defined in a natural way as the product of height and volume of the constant potential on a finite-size region. The relation between $\overline{v}$ and v also makes clear how one should take a zero-size limit to obtain a pointlike object with a given formal strength. It is shown that v^{-1} has an inverse cubic-root divergence in $\Omega\rightarrow 0$ limit in three dimension. It is also shown that one can use a regular part of v^{-1} [$r(\Omega)$ in Eq. (32)] as a direct measure of the coupling strength of a small scatterer. In other words, the inverse of the regular part corresponds to the effective strength of the scatterer. Since the

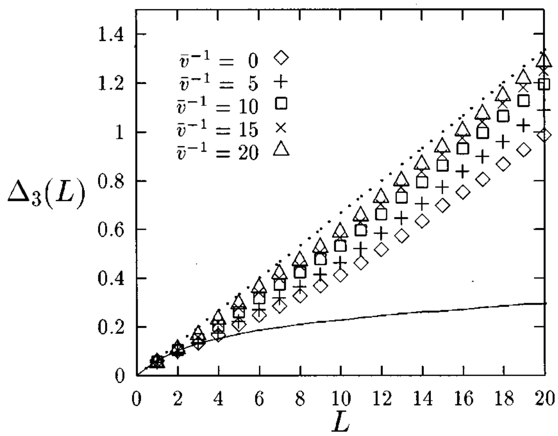

FIG. 5. The spectral rigidity $\Delta_3(L)$ is shown for various values of $\overline{v}^{-1}$ in the energy region between $z_{100}=1307.95$ and $z_{3100}=12932.70$. The scatterer is located at the center of the billiard. The solid (dotted) line is the prediction of random-matrix (Poisson) statistics.

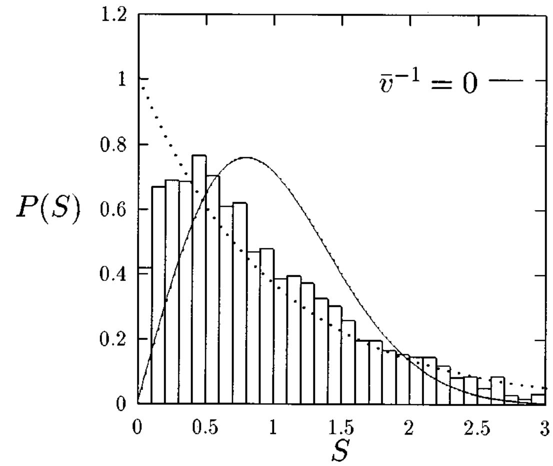

FIG. 6. The nearest-neighbor level spacing distribution $P(S)$ is shown for $\overline{v}^{-1}=0$ in case of the scatterer being located at a generic position in the rectangular solid. The statistics are taken within the eigenvalues between $z_{100}=415.81$ and $z_{3100}=3503.68$. The solid (dotted) line is the Wigner (Poisson) distribution.

coefficient of the singular part of v^{-1} is negative, wave chaos is expected to appear at low energy in case of weak attraction.

We have reviewed the previously known results in two dimensions from the present perspective. Similarly to the three dimensional case, the inverse of the bare coupling v^{-1} has to contain a singularity as a function of the size of the scatterer, and the regular part of v^{-1} plays a central role in determining the effective coupling strength. There is a crucial difference, however. In two dimensions, a logarithmically energy-dependent correction term is required to define the effective strength. The existence of the energy-dependent term results in a peculiar feature for two dimensions, namely, the scale anomaly. Its origin is identified as the z dependence of $F_1^{(2)}(z,E=0)$ in Eq. (46) for two dimensions. There is no corresponding term for three (and one) dimensions.

A few words on the relevance of our results to the billiard problem with more generic boundary shapes are in order. By placing small obstacles along the boundary and around the edges of the rectangular billiard considered here, one can construct systems which approxiamte billiards of various boundary shapes. Therefore, from our rather special example with a pointlike scatterer, we might hope to obtain some insight into the generic quantum billiard problem both in two and three dimensions. At the same time, extreme care has to be taken when one deals with the high energy limit and discuss the relevance of the asymptotic behaviors found in our examples to the generic case. This becomes evident by considering the fact that infinite numbers of obstacle are needed to simulate a given boundary shape at short wave length.

In a sense, the current work amounts to the search of a sensible zero-size limit of small obstacles in the quantum mechanics of general spatial dimension. Apart from the case of one dimension, where super-renormalizability guarantees the existence of trivial limit (δ function), one encounters a subtle balance of divergence and renormalizability, which results in nontrivial properties of coupling strengths. We hope that we have persuaded the readers that the model of the billiards with pointlike scatterer is a valid, mathematically sound, and practically useful idealization of the quantum system with small impurities. We also hope that the predictions in this paper are to be checked through the experiments in the laboratories. In particular, Eqs. (42) and (58) for three and two dimensions, respectively, can be directly tested, since they are stated in an experimentally controllable form. Recent progress of microwave techniques with macroscopic devices [19–22] offers a possible opportunity.

ACKNOWLEDGMENTS

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