Numerical Evidence of Nano-scale One-dimensional Conservative System with GOE-type Quantum Level Statistics *

Mitsuyoshi Tomiya† and Shoichi Sakamoto
Department of Applied Physics, Seikei University, Musashino-shi,
Kichijouji-Kitamachi 3-3-1, Tokyo 180-8633, Japan

Naotaka Yoshinaga
Department of Physics, Saitama University, Shimo-okubo 255, Saitama-shi, Saitama 338-0825, Japan

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Quantum mechanics of one-dimensional time-independent system whose energy level statistics obeys the Gaussian ensemble is numerically studied. Recently the nano-size quantum dots and anti-dots made by the highly sophisticated fabrication process on the heterojunction structure of semiconductors often exhibit the anomalous physical behaviors. In order to understand them the study of the lower dimensional quantum electron transport from the viewpoint of quantum chaos is inevitably important. One-dimensional conserved systems are known to be integrable. However, at least numerically, it is also shown that we can construct the potential for the Schrödinger equation that reproduces a finite number of given energy levels of chaotic regime, e.g., the random matrix theory. In this work a potential is constructed numerically by the standard gradient method or by the inverse scattering method. The more energy levels of chaotic regime we take, the more complicated and finer the ripples of the potential become. The potential has fractal structure at high energy limit. [DOI: 10.1380/ejssnt.2003.175]

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I. INTRODUCTION

The vast varieties of the phenomena, i.e. super conductivity, super fluidity, semiconductor, Anderson localization and quantum Hall effect, etc., can not be explained without quantum mechanics.

Mesoscopic physic studies the phenomena in the range from submicron scale($10^{-1}$μm = $10^{-3}$m) down to nano scale($10^{-9}$m) where quantum mechanics rules instead of classical mechanics. Quantum chaos studies the microscopic or mesoscopic system which is classically chaotic has had the very close relation to mesoscopic physics. It has been observed the anomalous fluctuation of the magneto-resistance in the experiment of mesoscopic GaAs/AlGaAs heterojunction structure [1]. It is clearly different from usual fluctuation which is due to the impurity or the thermal noise. The two-dimensional electron plays important role.

Here we study one-dimensional (1D) time-independent system with a microscopic or mesoscopic particle, e.g. an electron, which has one degree freedom and one constant of motion the Hamiltonian $H = \text{const}$. Thus the one-dimensional system is integrable [2]. However, it was discovered that a numerical calculation could construct the potential of a Schrödinger equation which has eigenenergies of the finite dimensional Gaussian orthogonal ensemble (GOE) matrices about a decade ago [3]. The GOE represents the model of chaotic systems. It is known that the quantum levels of the classically chaotic systems follow the level statistics of the GOE very closely. Then the shape of the potential and the classical motion of the particle inside the potential will be our main concern.

One-dimensional Schrödinger equation with a potential

$$V(x) = \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi_i(x) = \epsilon_i \phi_i(x), \quad (1)$$

where the potential is yet to be constructed. Note that we put the dimensionless unit $m = \hbar = 1$. The coarse shape of the potential should be predicted as that of a harmonic oscillator, because the averaged density of states is set to be one. The shape is expected to have a complicated fine structure on top of the shape of the harmonic oscillator.

II. ONE-DIMENSIONAL SYSTEM AND QUANTUM CHAOS

Some people would say that quantum chaos is a study of a quantum system whose classical correspondence is chaotic. To observe quantum properties of the classically chaotic system, one of the most useful artillery is the quantum level statistics. The distribution of eigenenergies and the pattern of wave-functions, and etc. have the characteristically different signatures depending on whether the system is integrable or chaotic. However, the numerical calculation of wave-functions, which must be precise enough to see such properties, is far more difficult than the evaluation of eigen-energies.

The nearest level spacing distribution is one of the most known levels statistics. It is the collection of energy gaps between adjacent levels after unfolding, which implies to obtain unit density of states on average. This procedure is necessary to see a universal feature in various systems. Then the distribution becomes the Wigner distribution $P(s) = \frac{1}{\pi} \exp(-\frac{s^2}{4})$, if the system is the GOE-type chaotic system (Fig.1). Owing to the repulsion between quantum levels or the von Neumann-Wigner theorem [4], the chaotic system cannot have degenerate levels: $P(0) = 0$. On the other hand the integrable system obeys the Poisson distribution $P(s) = \exp(-s)$ since the

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†Corresponding author: tomiya@apm.seikei.ac.jp
integrate a system of two or more degrees of freedom allows the degeneracy of levels [5, 6].

The Bohigas, Giannoni and Schmit conjecture [7] is that “Spectra of time-reversal conservative systems whose classical analogs are K systems shows the same fluctuation properties as predicted by the GOE.” Most of examples support this conjecture. However, the aim of this work is to numerically construct the potential whose level statistics becomes indistinguishable from that of the GOE-type systems, in spite of 1D system.

III. NUMERICAL METHODS

The next question is what are the characteristic properties of the potential which has the GOE-type level statistics. We apply two kinds of numerical methods to reproduce the 1D ”chaotic” potential. The iterative numerical method which was already used in Ref. 2 is based on the standard gradient method [8]. Also the method of the inverse scattering theory is applied. Formally it can construct the potential which produces given eigen-energies exactly and successively from the ground state [8–10].

The GOE-type spectrum that we use here is obtained by diagonalizing a 500 × 500 real symmetric random matrix and by unfolding the levels. The unfolding is done with the formula

\[ e_{i+1} - e_i = (E_{i+1} - E_i)\rho(E_i), \]

where \( E_i \) are the eigen-values of the matrix, \( e_i \) are the unfolding ones, and \( \rho(E_i) \) is the smoothed level density [3]. Thus, after unfolding, the averaged density of states becomes one as that of the harmonic oscillator \( V(x) = x^2/2 \).

If we look at higher energy region, the ripples of the potential are expected to become larger and more winding.

A. Standard Gradient Method

The standard gradient method is not only practical and simple, but also powerful enough to create the potential for more than 500 given eigen-energies [3]. However, we always need to concern about the precision of the calculation that we carry out, because it is essentially an approximation method.

Let us give the sequence of the finite number of unfolded GOE eigen-energies \( e_i (i = 1, 2, ..., N) \) from the ground state. Also let us denote the \( N \)-eigen-energies by solving the Schrödinger equation eq.(1) by \( e_i (i = 1, 2, ..., N) \). The standard gradient method adjusts the potential \( V(x) \) to minimize

\[ F[V(x)] = \sum_{i=1}^{N} (e_i - e_{\text{new}}(x))^2. \]

The functional derivative of \( F \) with respect to \( V(x) \) is obtained

\[ \frac{\delta F}{\delta V(x)} = 2 \sum_{i=1}^{N} (e_i - e_{\text{old}}(x)) \phi_i^2(x), \]

where \( \phi_i(x) \) represents the normalized eigen-function for the \( i \)-th state. Then the iterative search

\[ V_{\text{new}}(x) = V_{\text{old}}(x) - 2e \sum_{i=1}^{N} (e_i - e_{\text{new}}(x)) \phi_i^2(x). \]

leads us asymptotically to the potential with \( e_i (i = 1, 2, ..., N) \). Note that \( e \) is a small constant which ensures \( F[V_{\text{new}}(x)] < F[V_{\text{old}}(x)] \). Numerically the Schrödinger equation is solved on lattice points whose differences are sufficiently small. Here we use the Numerov method and eq.(5) should be written as

\[ V_{\text{new}}(n) = V_{\text{old}}(n) - 2e \sum_{i=1}^{N} (e_i - e_{\text{new}}(n)) \phi_i^2(n), (1 \leq n \leq M), \]

and \( n \) is the label of the lattice points and \( M \) is the total number of the lattice points.

B. Inverse Scattering Method

The inverse scattering method is essentially the exact method by definition. However, the calculation is almost impossible when the number of eigen-energies to be reproduced becomes larger because of the rapid growth of

\[ \text{FIG. 1: The nearest neighbor level spacing distribution of 500 eigen-energies that are adopted for the potential construction.} \]

\[ \text{FIG. 2: Errors of fitted energy levels } e_i - e_{\text{old}} \text{ plotted with respect to } i. \]
FIG. 3: The constructed potential $V(x)$ for reproducing 500 energy levels of the GOE matrix. From the definition (5) the potential must be symmetric $V(x) = V(-x)$. (a) $V(x)$ is plotted in whole range $0 \leq x \leq 40$. (b) $V'(x)$ is plotted for $0 \leq x \leq 10$ to show its details.

FIG. 4: The constructed potential $V(x)$ for reproducing 100 energy levels of the GOE matrix. From the definition (5) the potential must be symmetric $V(x) = V(-x)$. (a) $V(x)$ is plotted in whole range $0 \leq x \leq 40$. (b) $V(x)$ is plotted for $0 \leq x \leq 10$ to show its details.

CPU time or the required precision of the variables in the middle of the program, or the demand for the vast size of memory space. This method needs no initial potential such as the harmonic oscillator and no iterative approximation.

The inverse scattering method can construct the exact potential that has given levels from the ground state. The method we apply has to put the finite value of the potential at $x \to \pm \infty$: $V_{\infty}$ [9–12]. This is a major difference from the standard gradient method.

One-dimensional Schrödinger equation

$$\left( \frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) - V_{\infty} \right) \phi(x, \zeta) = \zeta^2 \phi(x, \zeta)$$  \hspace{1cm} (7)

has two independent Jost solutions with asymptotic conditions

$$\phi_1(x, \zeta) \sim \exp(i\zeta x) \text{ as } x \to +\infty, \hspace{1cm} (8a)$$
$$\phi_2(x, \zeta) \sim \exp(-i\zeta x) \text{ as } x \to -\infty. \hspace{1cm} (8b)$$

From the two solutions a meromorphic function can be constructed as

$$\Phi(x, \zeta) = a^{-1}(\zeta) \phi_2(x, \zeta) \exp(i\zeta x) \text{ for } \Im \zeta > 0; \hspace{1cm} (9a)$$
$$= \phi_1^*(x, \zeta^*) \exp(i\zeta x) \text{ for } \Im \zeta < 0, \hspace{1cm} (9b)$$

where $a^{-1}(\zeta)$ is just the transmission coefficient. If there are $N$ bound states of energies $E_n$ and wave-functions $\psi_n(x)$, from the singularity argument [9, 10] the meromorphic function (9) may be expressed as

$$\Phi(x, \zeta) = 1 + i \sum_{n=1}^{N} c_n e^{-\kappa_n x} \frac{1}{\zeta - i\kappa_n} \psi_n(x), \hspace{1cm} (10)$$

where $\kappa_n^2 = 2(V_{\infty} - E_n)$ and $c_n^2 = 2\kappa_n \prod_{q \neq n} \left| \frac{\kappa_n + \kappa_q}{\kappa_n - \kappa_q} \right|$. The asymptotic behavior of the bound states should be

$$\psi_n \sim c_n e^{-\kappa_n x} \equiv \lambda_n(x) \text{ at } x \to +\infty. \hspace{1cm} (11)$$

Thus, at $\zeta = -i\kappa_m$, $\Phi(x, \zeta)$ is proportional to the bound state wave-function

$$\Phi(x, -i\kappa_m) = \psi_m(x)/\lambda_m(x). \hspace{1cm} (12)$$
From eqs. (4) and (6) we obtain a system of $N$ linear equations for $N$ wave-functions $\psi_n(x)$, which may be represented as

$$\sum_{n=1}^{N} A_{mn} \psi_n = \lambda_n, \quad (13)$$

where the matrix $A$ is defined by

$$A_{mn} = A(x)_{mn} = \delta_{mn} + \frac{\lambda_m(x) \lambda_n(x)}{\kappa_m + \kappa_n}. \quad (14)$$

Finally the meromorphic function can be obtained from the matrix $A$ as

$$\Phi(x, \zeta) = 1 + \sum_{m,n=1}^{N} \frac{i \lambda_m}{\zeta - i \kappa_m} (A^{-1})_{mn} \lambda_n. \quad (15)$$

Then the exact potential that has $N$ bound states may be formally recovered from

$$V(x) = V_\infty - 2 \frac{d^2}{dx^2} \ln D(x), \quad (16)$$

where

$$D(x) = \det A(x). \quad (17)$$

This formula is also used for this work.

IV. RESULTS AND DISCUSSION

The potential with 500 GOE type eigen-levels is constructed numerically by a standard gradient method. The GOE type eigen-energies clearly follow the Wigner distribution (Fig.1). The interval difference of the lattice points is put $\Delta = 0.001$ to solve the Schrödinger equation (1) by the Numerov method in the whole range of the computation $0 \leq x \leq 50$. Therefore the number of lattice points are $M = 50001$. More than 100 mesh points are set to describe each oscillation on the potential. The average error between the reproduced eigen-energies and the target GOE energies $\epsilon_i^* - \epsilon_i$ is $2.2 \times 10^{-8}$ and the standard deviation is 0.0033 (Fig.2), which is much smaller than the previous work [3].

The resulting potential $V(x)$ is shown in Fig.3. As expected, the course averaged shape is a harmonic oscillator and oscillating ripples are on it. The oscillation has larger amplitude and finer structure near the origin: $x \approx 0$. The more target eigen-energies we use, the wider range of the potential has the oscillation. The potential for $N = 100$ is also shown in Fig.4. From eq.(6), we always use $N$ eigen-functions of the present potential to improve the eigen-energies reconstruction. Therefore, according to the range that is from the origin up to the same distance from the classical turning point, the potential can be modified. The amplitude of the ripples becomes larger and its structure is finer when $N$ is larger.

If we add one more level to the potential that is once sufficiently converged for $n$-levels, the convergence of the calculation suddenly becomes bad. It means that the shapes of the potentials with $n$-levels and with $(n+1)$-levels from the ground states are remarkably different.

Contrary to usual classical Hamiltonian systems, there cannot exit the shortest period from the consequence of the semi-classical argument, if the system completely reproduces the chaotic levels of the RMT [5]. If its density of states is unfolded and its average density is independent of energy, the coarse averaged shape of the potential is just a harmonic oscillator and the potential has peculiar ripples on it (Fig.3, 4). The more energy levels of chaotic regime we take, the more complicated and the finer these ripples become. It implies that the potential has fractal structure at high energy limit.

The fractal dimension of the shape of the potential is evaluated, using the box counting method [13]. If the po-
potential is just a harmonic oscillator, its fractal dimension is one. Certainly it means that the shape is not fractal. Fig.5 shows that fractal dimension is 1.7... and in the range where the box size is too small, the dimension reduces to one discontinuously. Its bending point becomes clearer, if we apply the potential that more precisely reproduces eigen-energies. In the middle of the reproduction process, the rough shape is quickly constructed. However, the detail of the ripples, especially in the local minima and maxima, their shapes are not sharp enough to reproduce the given eigen-energies. The precise detail of the potential is reconstructed only slowly. The larger number of the eigen-energies is to reproduced, the slower the process becomes. The bending point moves to the range where the size of boxes used to count the dimension is smaller. This time it means that larger number of eigen-energies we use, more finer ripples exists on the shape of the potential as the Fourier analysis tells us [8]. It also implies that the potential of the chaotic eigen-energies at \( N \to \infty \) becomes completely fractal. The finer ripples allow the shorter periodic orbits to be confined in them at any given energy. Then the level statistics becomes indistinguishable from the GOE [5].

The gradient method is essentially a numerical approximation approach and the most important thing to be concerned is the CPU time to reach the required precision of the computation.

It needs less time to reach the required precision of the computation compared to the inverse scattering method. The standard gradient method has the tendency that the two consecutive levels with a very small energy gap have poor precisions. The lower energy level is a bit too low and the higher energy is a bit too high. The calculation of these levels determines the precision of our work.

On the other hand, the inverse scattering method is a successful method to reconstruct the potential with a relatively small number of the energy levels, if the shape of the potential is preferably smooth [9–12]. It is not true for very winding potential as our model. We have found that even the shape near the origin \((x = 0)\) varies rapidly, increasing the number of the target levels from the ground levels. Even though, from rough inspection the higher level wave-function would have larger contribution near the classical turning point than around the origin.

The inverse scattering theory is the exact one and is good at the theoretical analysis, e.g., the analytical approach to the solutions of the KdV equation, e.t. [8–10]. Equation (16) is formally an exact solution. However, its numerical evaluation is surprisingly difficult. The more GOE energy levels we set, the higher precision setting of program variable, or the longer CPU time, or the more tremendous mount of memory space it requires. Increasing \( N \), it becomes beyond the realization rapidly. Even if any effort can save the program, it can be easily compensated as \( N \) increases. Thus eq.(16) is unlikely to be available for \( N \geq 16 \).

The shape of the potential is determined considerably at a fairly early stage of the potential. The rest of CPU time is necessary to match the calculated levels precisely to the target spectrum, especially to two adjacent levels with small energy gap. During the calculation, the shape of the potential becomes shaper at the top and the bottom of the ripples. It might be able to explained from the view point of the semi-classical approximation. The classical orbits that are confined in the ripple valleys would make the level repulsion weaker to allow specific energy gaps to be smaller.

We find the almost same winding potential even by the two completely different numerical methods (the standard gradient method and the inverse scattering method), if the calculations sufficiently converge (Fig.6). We also check the convergence, changing the parameters \( \epsilon \) and \( \Delta x \). Note that both methods create symmetric potentials with respect to the origin. Thus the fractal structure is the fundamental nature of our 1D system. Finer ripples can create the local minima of the potential here and there, where smaller classical orbits can exist. It explains the relation between the non-existence of the shortest orbit in the chaotic system and our 1D system is allowed to be "near" chaotic.

V. CONCLUSION

We have constructed the 1D time-independent potential with the unfolded GOE type levels from the ground state up to the 500th state. The shape of potential turns out to be the harmonic oscillator with the plentiful oscillations. The amplitude of the oscillations is larger and finer, when we use a larger number of eigen-energies. Numerical extrapolation to adopt higher energy levels leads to the fractal structure of the potential. We expect that the potential would be continuous, yet not differentiable everywhere when the number of energy levels becomes infinite. It implies that the 1D mesoscopic system would possibly exhibits the quantum chaotic behavior in its physical quantities. Due to the limitation of the fabrication technique of the mesoscopic scale today, if the system has nano scale ripples on its potential, its spectral statistics may seems to belong to chaotic system. Even if the ripples are not strictly fractal, they could be winding enough to
make the experimental results show the quantum chaotic level statistics, as our numerical results. Our numerically reconstructed potential also just seems fractal in some finite range of the measuring scale, adopting finite reasonable number of chaotic eigenvalues. It is also found that the potential should be unique, even if we use two different methods with completely different theoretical foundations.

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