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Matrix diagonalization in the quantum anisotropic Kepler problem

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Abstract

In quantum chaos study, it is essential to study the statistical properties of energy levels of the system in order to unveil the quantum reflection of chaos. For this purpose we have to work out thousands of the energy levels. For the anisotropic Kepler problem a concrete method was devised by Wintgen et al. In this method a scaling parameter ϵ is introduced and the energy levels are calculated from the eigenvalues of a large size matrix at an in principle arbitrary choice of ϵ. However, in practice, the finite size effect caused by the truncation of the set of bases makes the matrix eigenvalues rather dependent on the value of ϵ. We propose a prescription which determines the most suitable choice of ϵ for a given matrix size and for given system parameters.

Keywords: quantum chaos, anisotropic Kepler problem, matrix diagonalization, level statistics.

1 Introduction

Nowadays systems which can be handled by experiments have reached nano-scale size and quantum theory analysis is required. However, most of these systems are classically non-integrable and the corresponding Schrödinger equation is not separable. Therefore one must rely on the numerical calculation to obtain approximate eigenvalues and various methods have been devised so far. It has been revealed that the statistics of the systems may be categorized into several distinct classes independent from the details of the systems. Only the symmetry property of the system is essential. For example, the nearest neighbour spacing distribution (NNSD) becomes Poisson when the system is integrable classically or the Wigner distribution when the system is chaotic. This is the way how the statistics of the quantum energy levels reflect the classical features of the system.

To this end it is desirable to explore a system which is suitable both for handling analytically in classical regime and computing the energy levels in the quantum regime. For this reason we focus our attention to the anisotropic Kepler problem (AKP). The AKP is a Kepler problem with the anisotropic mass tensor and it describes well the motion of the electron in a semiconductor. The classical theory of the AKP has been studied in detail in [1, 2] and it has been known that there is a one-to-one correspondence between an orbit and a binary sequence. In the quantum chaos study, the AKP was considered by Gutzwiller[3] which gave the foundation of the periodic orbit theory. The statistical approach are founded by Wigner, Mehta, Bohigas $\cdots$ and the numerical method is pioneered by Wintgen et al[4].

First detailed AKP energy level calculation was performed by Faulkner[5] and the lowest 27 levels are obtained with Rayleigh-Ritz method. However this is not sufficient because the level statistics require several thousands of levels in good accuracy. For this requirement a concrete and efficient method was devised by Wintgen et al[6]. In this method the energy levels are computed from the eigenvalues of a certain matrix which takes into account the scaling property of the AKP system and endowed with a scaling parameter ϵ. In principle this ϵ can be chosen arbitrary, but, in practice, the calculated energy levels rather depend on the choice of ϵ because only finite number of bases may be used. Therefore a good control of this behaviour is crucial to obtain the accurate energy levels.

We analyze the calculated energy levels and elucidate the systematics in them. We then propose a prescription how to obtain a large number of reliable energy levels by adjusting ϵ.

2 Scheme for calculations of the energy levels

The Hamiltonian of an electron in the three dimensional AKP is

$$H_0 - \frac{p_1^2 + p_2^2}{2m_\perp} + \frac{p_3^2}{2m_\parallel} - \frac{\epsilon^2}{\kappa\sqrt{q_1^2 + q_2^2 + q_3^2}} \qquad (1)$$

with the dielectric constant κ and the electron charge e. Here $\vec{q} = (q_1, q_2, q_3)$ is the position of the electron in Cartesian coordinates and $\vec{p} = (p_1, p_2, p_3)$ is the conjugate momentum. The $m_\perp$, $m_\parallel$ are the diagonal elements of the electronic mass tensor with the anisotropy $m_\perp < m_{\|}$. We use the units $a_0 = \hbar^2\kappa/m_\perp e^2$, $E_R = m_\perp e^4/2\hbar^2\kappa^2$, $t_0 = \hbar^3\kappa^2/m_\perp e^4$ for length, energy, time, respectively. With following dimensionless quantities

$$(x, y, z) = \frac{\vec{q}}{a_0},\ (p_x, p_y, p_z) = \frac{\vec{p}}{m_\perp a_0/t_0},\ H = \frac{H_0}{E_R}, \quad (2)$$

eq. (1) is rewritten as

$$H = p_x^2 + p_y^2 + \gamma p_z^2 - 2/r. \qquad (3)$$

Here $r = \sqrt{x^2 + y^2 + z^2}$ and $\gamma = m_\perp/m_\parallel < 1$ represents the mass anisotropy. For ordinary Kepler problem γ is unity and for the realistic cases 0.2079 (silicon), 0.05134 (germanium).

In case of $\gamma = 1$ the shapes of bounded trajectories in the position space are all elliptical and hence each motion is regular. As the value of γ decreases from unity the motion changes to the quasi-regular motion. When γ is smaller than γ_c 8 9, the motion becomes chaotic and complicated. Because the AKP has such a controlling parameter γ of the degree of chaos in the classical regime it serves as a vital model to examine how the chaos in the classical regime governs the behavior of the system in the quantum regime.

We recapitulate the scheme devised by Wintgen et al. It is an all order calculation and in this point surpasses the perturbation method. The Schrodinger equation is

$$\left[\quad \triangle + (1 \quad \gamma)(\quad ^2 \quad z^2) \quad 2 \ r \right] \psi(r) = E\psi(r) \qquad (4)$$

For $\gamma \neq 1$ eq. (4) is not separable and we switch to a numerical way. For the bases, Sturumian functions in a spherical coordinates are de ned as

$$\begin{aligned} \langle r|n \ m\rangle &= \tfrac{1}{r}\phi_n(r;\lambda)Y_{\ m}(\theta \quad) \qquad (5) \\ \phi_n(r;\lambda) &= \sqrt{\tfrac{n!}{(2 \ +n+1)!}}e^{\ -\frac{r}{2}}(\lambda r)^{\ +1}L_n^{2\ +1}(\lambda r) \end{aligned}$$

Here n, , m are the radial, azimuthal, magnetic quantum numbers respectively and they are related to the principle quantum number n_p as $n_p = n + \ +1$. The $Y_{\ m}(\theta \quad)$ are the spherical harmonics, $L_n^{\alpha}(x)$ are the generalized Laguerre functions which satisfy a di erential equation $xL'' + (\alpha + 1 \quad x)L' + nL = 0$. When $\lambda = 2 \ n_p$, Sturumian functions are wave functions of hydrogen atom.

Using these bases the Schrodinger eq. (4) can be written as a matrix equation[6]:

$$\begin{aligned} \left[\ \lambda(\overrightarrow{\triangle}) + (1 \quad \gamma)\lambda(\ ^2 \quad \overrightarrow{z^2}) \quad 2(1 \ \overrightarrow{r}) \right] \psi \\ = (E \ \lambda)(\overrightarrow{\mathrm{Id}})\psi \end{aligned} \qquad (6)$$

Here $(1 \ \overrightarrow{r}) = (\langle n' \ 'm'|1 \ r|n \ m\rangle) = (\delta_{n \ n}\delta \quad \delta_{m \ m})$ is unit matrix. Other matrices have o diagonal elements which equal zero except for $' = \quad$ or $' = \quad + 2$; for instance elements of $(\overrightarrow{\mathrm{Id}})$ are

$$\begin{aligned} \langle n' \ 'm'|\mathrm{Id}|n \ m\rangle = (1 \ \lambda)\delta \quad \delta_{m \ m}[2(n + \quad + 1)\delta_{n \ n} \\ \sqrt{(n+1)(2 \ + n + 2)}\delta_{n \ n+1}] \end{aligned} \qquad (7)$$

Because of a rotational symmetry about z axis the elements of matrix included in eq. (6) are all proportional to $\delta_{m \ m}$. By these properties eq. (6) is transformed to standard eigenvalue problem as

$$\begin{aligned} \overrightarrow{M}\psi &= (2 \ \lambda)\psi \\ \overrightarrow{M} &= \quad (\overrightarrow{\triangle}) + (1 \quad \gamma)(\ ^2 \quad \overrightarrow{z^2}) + \epsilon(\overrightarrow{\mathrm{Id}}) \end{aligned} \qquad (8)$$

and $\epsilon = \quad E \ \lambda^2 < 0$. Here the matrix $\overrightarrow{M}$ is an $N \times N$ symmetric matrix. It is block diagonal in the sense that $' = \quad + 2$ or and $m' = m$. Whole energy levels are obtained by putting together the levels which calculated from each sector. Hereafter we consider only the even and $m = 0$ sector. Then if we want eigenvalues for the states with the principle quantum number n_p up to N_p with this restriction the matrix size N must be $(N_p + 1)^2$ 4. We should add that $\overrightarrow{M}$ is banded and sparse. By solving (8) for the eigenvalues 2 λ_is ($i = 1 \quad N$) the energy levels are in turn determined as $E_i = \quad \epsilon\lambda_i^2$. Supposing that we choose another value for the parameter ϵ of the matrix $\overrightarrow{M}$, the eigenvalues 2 λ_is will be accordingly changed and the physical energies will be kept invariant. However in practice the number of available bases is limited; we cannot help truncating the number of bases. Then the above ideal scaling becomes only approximate.

3 Results (The most suitable choice of ϵ)

As the truncation condition we adopt $N_p = 177$. The matrix size N of our sector is 7921. This is the largest size among all sectors. We present in Fig. 1 the results of diagonalizing eq. (8) for energy levels at various values of ϵ. The parameter γ is decreased through 18 panels from 0 9 down to 0 05. Instead of the energy levels E_is ($i = 1$ for ground state) we depict

$$f_i = \quad 1 \ (4\sqrt{\gamma}E_i) \quad i = 1 \ 2 \quad 7921 \qquad (9)$$

which are appropriately stretched so that $f_i = i$ and the average spacing $\delta f_i \quad f_{i+1} \quad f_i$ should be theoretically unity [1]. The curves of f_is are expected to be all parallel and their spacings are expected to be unity. However, at a glance one nds that the curves are all simultaneously deformed. Especially the deformation from the constant line is remarkable for small γ (extremely large spacing) and for small $|\epsilon|$ (anomalous accumulation of f_i curves). This dependence is not physical but an error which should be considered as the weak point of the matrix method. The remedy for this problem is our task discussed below.

Accordingly we have to select the part of calculated energy levels that we can trust. We propose a prescription to select 'good results' for each ϵ based on two criteria.

This concerns with the global property of levels. To check this, the whole $f_i(\epsilon)$s are divided into ensembles, $\mathcal{F}_n = \ f_i(\epsilon)|200(n \ 1) < i \quad 200n$, $(n = 1 \quad 39)$, and the average of spacings $\langle \delta f_i \rangle_n$ is calculated for each ensemble $\mathcal{F}_n$ varying ϵ with inclement $\Delta\epsilon = 0 \ 01$. In Fig. 1 we show the region on the $f \quad \epsilon$ plane where the deviation of $\langle \delta f_i \rangle_n$ from unity is 0.05 or less. It is connected and convex and we depict the boundary by a solid curve.

($\gamma < 8 \ 9$) This concerns

[1] The cumulative mean density of levels of our sector should obey Thomas-Fermi formula[4],

$$N(E) = -1 \ (4\sqrt{\ }E) \qquad (10)$$

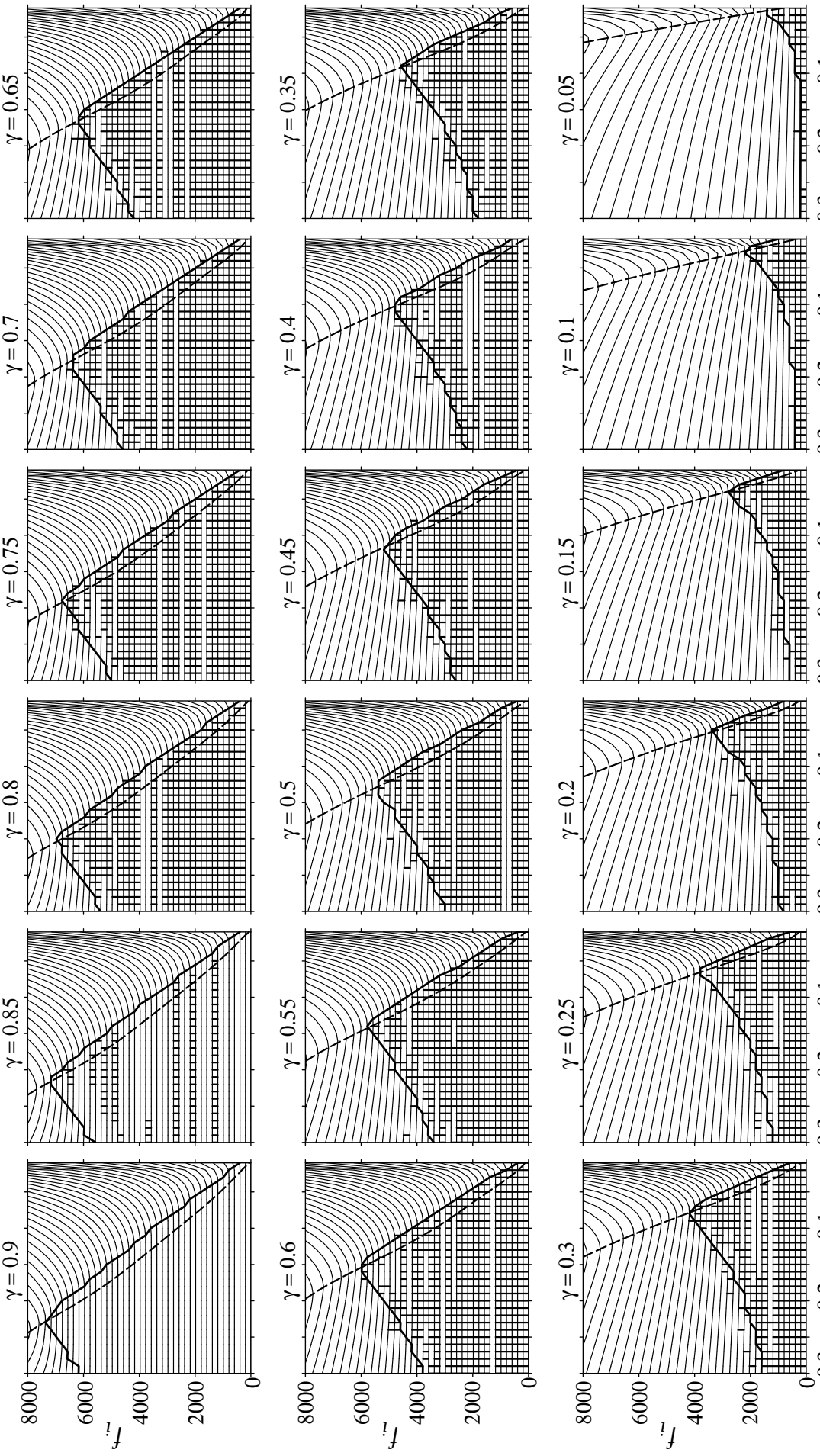

Fig. 1: Variation of $f_i =$ 1 $(4\sqrt{\gamma}E_i)$ with ϵ. N_p =177, i = 1 $N = 7921$, =even, m=0. Diagonalization is performed for each of $\epsilon =$ 0 01 0 02 0 3. Dashed curves connect the minimum points of f_i. Solid curve single out the region where the condition $|\langle \delta f_i \rangle_n$ 1| 0 05 is satis ed(see text). In this region levels are reliable from the viewpoint of criterion A. Vertical lines show regions of $\langle (\delta f_i \quad \langle \delta f_i \rangle_n)^2 \rangle_n$ 0 3. In these regions levels are reliable from the viewpoint of criterion B. The regions allowed by critera A and B agree well.

with the local property of levels. Recall that in the region with $\gamma < 8\ 9$ the system is classically chaotic and hence the quantum levels must show repulsion. Here the NNSD is Wigner-like and the mean squared deviation (MSD) of level spacings is $4\ \pi\quad 1\quad 0\ 273$ for the ideal Wigner distribution. On the other hand for $\gamma > 8\ 9$ the distribution is expected to be Poisson and the MSD is unity. Based on this theoretical expectation we set a condition that MSD must be 0.3 or less with a tolerance of 10% in the regions with $\gamma < 8\ 9$. We indicate in Fig. 1 by vertical lines the regions where this condition is met. For $\gamma = 0\ 9 (> 8\ 9)$ (the rst panel) there is naturally no region of repulsion. For other panels with $\gamma < 8\ 9$ the B allowed region remarkably agrees with the A allowed region. Fig. 1 succinctly shows this and strongly guarantees our prescription.

We list a few interesting observations in items.

(i) N_p is restricted by the computational ability. Thus one has to choose the best value of ϵ (ϵ_{max}) which gives the largest number of reliable levels. This ϵ_{max} can be read o from the crest of the convex curve in each panel of Fig.1. Now let us turn our eyes to the dashed curve. This connects the minimum points of $f_i(\epsilon)$ curves and hence the $f_i(\epsilon)$s below this curve at given ϵ are maximally compressed. Now if one follows this line downwards until one reaches the region allowed by the criterion A, remarkably one always meets the crest of the boundary curve. This is natural because at this time the compression reaches for the rst time to the extent $\langle \delta f_i \rangle_n \simeq 1$ and this implies the crest, at which the maximum number of $f_i(\epsilon)$s are contained below the curve.

(ii) Fig. 2 shows the relationship between γ and ϵ_{max}. Data points clearly follow a linear line well described by $\epsilon_{max} \simeq (\ 1\ 4)\gamma$.

(iii) Fig. 3 shows the ratio (R_{eff}) of the number of levels which satisfy the criteria at $\epsilon = \epsilon_{max}$ to number of whole levels N (=7921) is plotted as a function of γ. This relation is well described by $R_{eff} \simeq \sqrt{\gamma}$ with about 1% error for coe cient. From this we can estimate that the e ciency of determining reliable levels in the realistic cases of silicon or germanium is about 30% and 15% respectively.

These observations do not change even if we analyze smaller set of levels with $N_p = 75 (N = 1444)$ instead of $N_p = 177 (7921)$. These regularities seem re ecting the e ect of truncating the set of bases.

4 Conclusions

In this article we have recapitulated the vital matrix method[4]. The relations between the calculated energy levels and the scaling parameter ϵ is elucidated in Fig. 1 and a prescription how to select suitable ϵ regions is presented. The best ϵ (ϵ_{max}) and the ratio of reliable levels (R_{eff}) are estimated for various γ and it is observed that they follow simple rules (Fig. 2, 3). The results in this article guarantee the reliability of the matrix method and provide us with a prescription

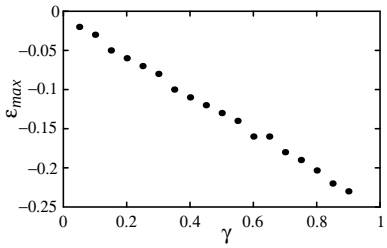

Fig. 2: The ϵ_{max} vs. γ.

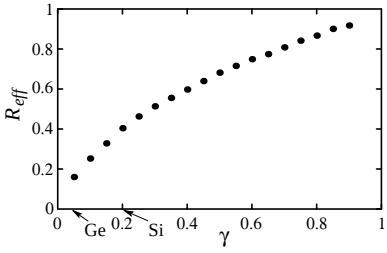

Fig. 3: Ratio of reliable levels vs. γ.

to increase the e ciency of the calculation.

Finally we comment on the subjects we are working with. Some random matrix model for an extended Gaussian orthogonal ensembles was constructed[7] and it was shown that the AKP may be treated within it. We are extensively studying this issue and will present elsewhere the relationship between γ values and the matrix-model temperatures. Armed by our prescription we will furthermore examine the multifractality of wave functions of the AKP.

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