Nonintegrable Deformation of Integrable Three-Body Problem

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Abstract

Three-body problem on a circle interacting through a Guassian potential is solved both classically and quantum mechanically. The Poincaré section of the classical system is analyzed for various potential widths, energies and initial conditions and it is shown that the system is chaotic when the energy is comparable to the potential height while it is regular for energies much smaller or larger than the potential height. In quantum mechanics, the energy spectrum of three bosons is considered. A three-boson system with the δ-function potential is solved exactly by the Bethe Ansatz method. Then the δ-function potential is replaced by a Gaussian potential. The eigenvalue problem of the three-body Schrödinger equation is solved by diagonalizing the Hamiltonian with symmetrized plane-wave basis. The change of the level statistics is studied as the width σ and the energy E are varied. It is found that there exists a region in the σ-E plane where the level statistics is given by the Wigner distribution, which indicates the chaotic behavior in the underlying classical system. This is also confirmed by studying the Brody parameter of the level statistics.

keywords: integrable system, nonintegrable system, level statistics, Bethe Ansatz

1 Introduction

Quantum chaos is an interesting and important subject in contemporary physics [1, 2, 3]. There are several definitions of quantum chaos in the literature, among which we adopt one that a quantum mechanical system exhibits quantum chaos when the classical counterpart is chaotic. Quantum chaos so far studied has been realized by (1) special boundary conditions, such as a particle in the Sinai's billiard or the stadium

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billiard [4, 5, 6], by (2) special choices of the metric, such as a particle in a constant negative curvature space [7, 8], or by (3) a judicious choice of an interaction potential [9].

In the present paper, we propose another possibility of quantum chaos, namely, a three-boson system on a circle interacting with a Gaussian two-body potential. This is quite a simple system but has never been studied in the light of quantum chaos, so far as the authors know.

The rest of the paper is organized as follows. The next Section is devoted to the analysis of the classical system. We first define the problem and solve the Hamilton equations of motion using the symplectic integration method. We obtain the Poincaré sections for various potential widths and system energies. In Section III, we solve the quantum-mechanical three-body problem in which the particles are interacting through the δ-function potential. This system is exactly solvable by the Bethe Ansatz method. There are three quantum numbers and the system is completely integrable. The level statistics of this system is studied and is shown to obey the Poisson distribution. In Section IV, the δ-function potential is replaced by a Gaussian potential with the width σ. The exact solution of this system is not known so far and the system is conjectured to be nonintegrable. The Schrödinger equation is solved by writing the Hamiltonian in the plane-wave basis and then diagonalizing it. The number of the basis being finite, this calculation is variational in nature. The change of the level statistics is studied in Section V as the width σ is varied from zero to finite values. It is shown that if the width is large enough the potential is almost constant and the system becomes essentially free. For small σ, however, the spectrum exhibits level repulsion characteristic of a nonintegrable system. The final Section is devoted to Summary. There are two Appendices, the first of which explains the symplectic integration method used in Section II while the second is devoted to the detailed derivation of the matrix element introduced in Section IV.

We will use the unit in which $\hbar = 2m = 1$, m being the particle mass.

2 Classical Theory

In the present Paper we consider a three-body system on a circle. The Hamiltonian is taken to be

$$H = \sum_{i=1}^{3} p_i^2 + V_\sigma(x_1, x_2, x_3) \tag{1}$$

where the second term is the potential energy given explicitly as

$$\begin{aligned} & V_\sigma(x_1, x_2, x_3) \\ &= \sum_{i<j} v_\sigma(x_i - x_j) \\ &= \sum_{i<j} \frac{2c}{(2\pi)^{1/2}\sigma} \sum_{m\in\mathbf{Z}} \exp\left[-\frac{(x_i - x_j - mL)^2}{2\sigma^2}\right] \end{aligned} \tag{2}$$

where $x_i \in [0, L)$. The parameter $c > 0$ denotes the strength of the repulsive potential while $\sigma \geq 0$ is the potential width. Since the system is defined on a circle, the coordinate x_i is identified with $x_i + L$. The summation over m makes the potential periodic over the interval $[0, L]$, namely

$$\begin{aligned} V_\sigma(x_1 + L) &= V_\sigma(x_1),\ V_\sigma(x_2 + L) = V_\sigma(x_2), \\ V_\sigma(x_3 + L) &= V_\sigma(x_3)\ . \end{aligned}$$

Figure 1 shows the potential profiles $v_\sigma(x)$ for several choices of σ. Note that the potential is essentially constant ($\simeq 6c$) for $\sigma > 0.5$.

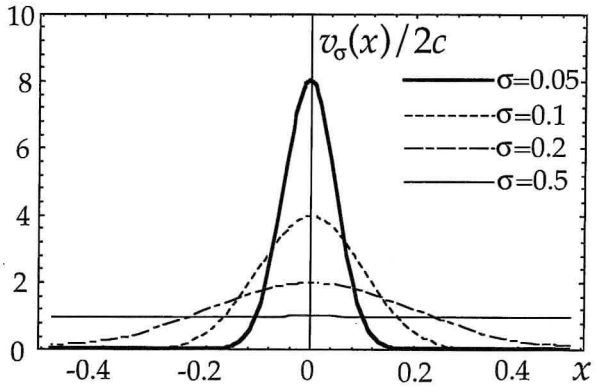

Figure 1: Potential profile v_σ for $\sigma = 0.05, 0.1, 0.2$ and 0.5.

Before we start our analysis, let us consider the case $\sigma = 0$. The potential becomes the δ-function in this limit. Then the particle is free between two consecutive collisions and exchange their momenta on each collision. Suppose the particles are numbered as 1, 2 and 3. Then the trajectory in this case is exactly the same as that for a free system except that the particle labels are exchanged on each collision. Thus it is not difficult to predict the particle positions at any time in the future and the system becomes completely integrable.

We now consider the general Hamiltonian (1) with Eq. (2). Let us introduce the following coordinate transformation

$$\begin{aligned} X &= \frac{1}{3^{1/2}}(x_1 + x_2 + x_3) \\ Y &= \frac{1}{2^{1/2}}(x_1 - x_2) \\ Z &= \frac{1}{6^{1/2}}(x_1 + x_2 - 2x_3)\,. \end{aligned} \tag{3}$$

The center-of-mass coordinate X, which is clearly conserved, decouples from the rest of the coordinates. Thus one may put, without loss of generality, $X = 0$ and the corresponding momentum $P_X = 0$. The Hamiltonian is now written in terms of the relative coordinates as

$$\begin{aligned} H &= P_Y^2 + P_Z^2 \\ &\quad + \frac{2c}{(2\pi)^{1/2}\sigma} \sum_{m\in\mathbf{Z}} \left[\exp\left(-(2^{1/2}Y - mL)^2/2\sigma^2\right)\right. \\ &\quad + \exp\left(-(2^{1/2}Y + 6^{1/2}Z - 2mL)^2/8\sigma^2\right) \\ &\quad \left. + \exp\left(-(2^{1/2}Y - 6^{1/2}Z - 2mL)^2/8\sigma^2\right)\right]\,. \end{aligned} \tag{4}$$

Once the total energy E is fixed, the independent degrees of freedom may be taken Y, Z and P_Y for example. Figure 2 shows the three-body potential in Eq. (4) for $\sigma = 0.1$ as a function of Y and Z.

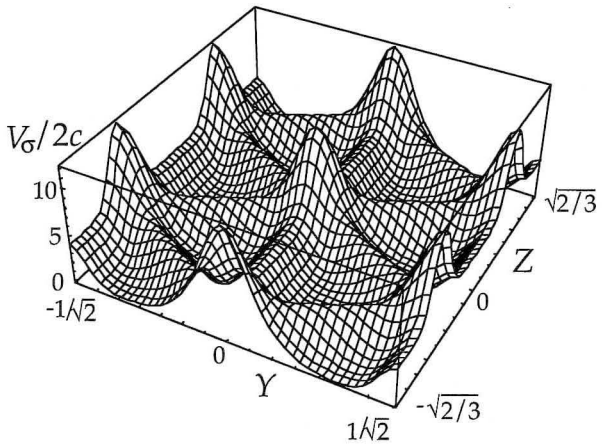

Figure 2: three-body potential with $\sigma = 0.1$ as a function of Y and Z. The peak at the center is the point where the three particles meet.

The above Hamiltonian cannot be solved exactly and one has to resort to certain numerical analysis. Here we employ the symplectic integration method outlined in Appendix A. This scheme is ideal for our purpose since it (almost) conserves the total energy

without an accumulation of errors for an arbitrary duration of time. In our calculation we employed the fourth-order symplectic method. If the infinitesimal time step is denoted by τ, there exists a "Hamiltonian" $\tilde{H}$ which is exactly conserved and differs from H by $\mathcal{O}(\tau^4)$. Accordingly if τ is sufficiently small, the variation of the energy is negligible.

In actual computation, only a finite number of terms are kept in the m-summation. This is because the domains of the coordinates are restricted within

$$\begin{aligned} X &\in \left[0, 3^{1/2}L\right), \\ Y &\in \left(-2^{-1/2}L, 2^{-1/2}L\right), \\ Z &\in \left(-(2/3)^{1/2}L, (2/3)^{1/2}L\right). \end{aligned} \tag{5}$$

Therefore, the summand with a large m is exponentially small compared to the terms with small m. It is important to realized that the coodinates X, Y and Z have to be normalized so that they remain in the above domain. This is done by carrying out the inverse transformation $(X, Y, Z) \to (x_1, x_2, x_3)$, then normalize x_i by adding (or subtracting) mL, $(m \in \mathbf{Z})$ so that all of x_i stay in the interval $[0, L)$. Then one transforms $\{x_i\}$ back to (X, Y, Z). This procedure is repeated at each step of the symplectic time evolution.

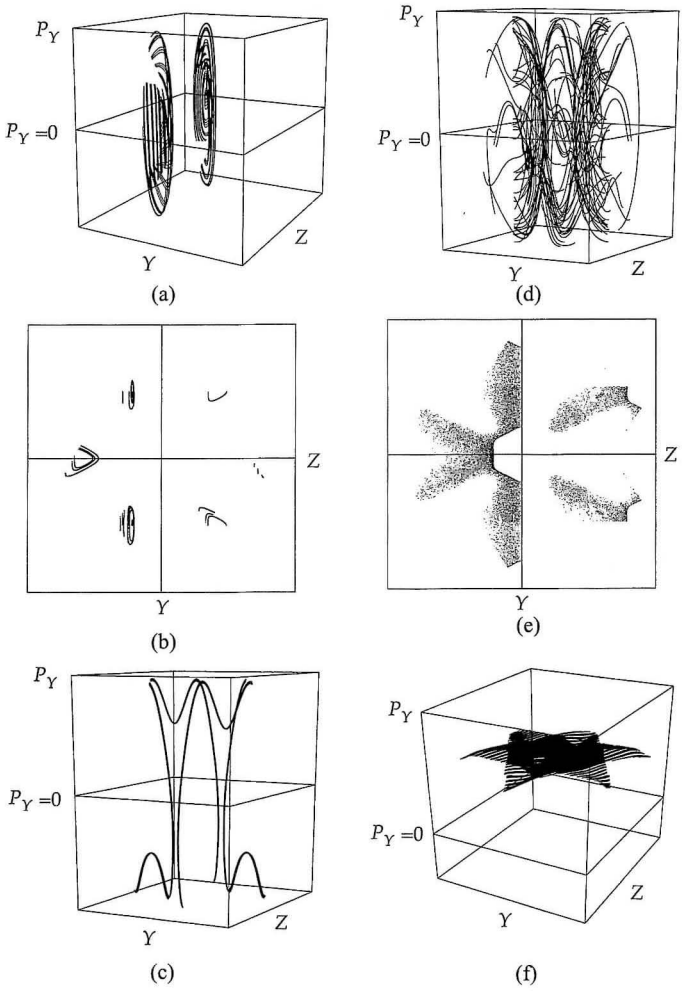

Figure 3: Phase space trajectories and corresponding Poincaré section with $L = 1, c = 10^3, \sigma = 0.1$ and several choices of the total energy E. (a) is a phase space trajectory and (b) is the Poincaré section both for $E = 10^3$. (c) is a regular trajectory while (d) is a chaotic trajectory both for $E = 10^4$. The Poincaré section for this energy is given in (e). (f) is the trajectory for $E = 2\times10^5$. The coordinates Y and Z satisfy $-2^{-1/2} < Y < 2^{-1/2}$ and $-(2/3)^{1/2} < Z < (2/3)^{1/2}$ in all the figures while the scale of P_Y is arbitrary.

Figures 3 are the trajectoris and Poincaré sections with $L = 1$, $c = 10^3$, $\sigma = 0.1$ and several choices of the total energy E. (We have chosen a large potential strength c to make the difference of the energy levels of an interacting system and those of a free system manifest in the corresponding quantum theory, see Sections III and IV.) Figure 3 (a) shows the trajectories in the (Y, Z, P_Y)-space for $E = 10^3$, which is much smaller than the height $2c/\left((2\pi)^{1/2}\sigma\right) \sim 7980$ of the two-body potential. The corresponding Poincaré section is given in Fig.3 (b). It is impossible for two particles to exchange their positions after collision in this case. Similarly, Fig.3 (c), (d) and (e) show the trajectories and the Poincaré section for $E = 10^4$, which is slightly above the potential height. The trejectory (c) is regular while (d) is chaotic. If the total energy E is much larger than the potential height, the particles do not detect the existence of the potential and the system becomes almost free. Figure 3 (f) is the phase space trajectory for $E = 2 \times 10^5$. It is seen that the motion tends to be confined on a fixed P_Y-plane as the energy increases. This is because the energy is approximately given by $E = P_Y^2 + P_Z^2$ in this region and both P_Y and P_Z are approximately conserved separately. For these high energies it is very difficult to obtain the Poincaré sections across the $P_Y = 0$ plane since the momentum P_Y hardly changes the signature.

The reason for the chaotic behavior when E is of the order of the potential height is easily understood. In this energy range the total energy is distributed among three particles and the relative energy may or may not exceed the potential height when two particles collide. Accordingly it is very difficult to predict whether the particles pass through or reflect each other after a particular collision. If, on the other hand, the total energy is much smaller than the potential height, particles never exchange their positions. If the total energy is much larger than the potential height the potential energy may be negligible and the particles are almost free. Thus in the latter two cases, the motion is expected to be regular. The phase space trajectories and the Poincaré sections in Fig.3 confirm our claim.

3 Quantum Three-Body Problem with δ-Function Potential

Now let us turn to the quantum theory. Consider three bosons on a circle with the circumference L interacting through δ-function repulsive potentials. The Hamiltonian of this system is given by

$$H_0 = -\sum_{i=1}^{3} \partial_i^2 + 2c \sum_{i<j} \delta(x_i - x_j) \qquad (6)$$

where $x_i \in [0, L)$. This potential is obtained from Eq. (2) by taking the limit $\sigma \to 0$. The periodic boundary condition implies $\psi(x_i + L) = \psi(x_i)$ $(1 \leq i \leq 3)$ and the bosonic symmetry requires that the wave function be symmetric under the exchange of x_i and x_j.

The spectrum of the above Hamiltonian is completely solvable by the Bethe Ansatz method. By applying the method to the present case, we obtain the total energy

$$E = \sum_{i=1}^{3} k_i^2 \qquad (7)$$

where the quasi-momenta or the "rapidities" k_i are

determined by the conditions

$$\begin{aligned} k_1 L &= 2\pi n_1 - 2\left[\tan^{-1}\left(\frac{k_1-k_2}{c}\right) + \tan^{-1}\left(\frac{k_1-k_3}{c}\right)\right] \\ k_2 L &= 2\pi n_2 - 2\left[\tan^{-1}\left(\frac{k_2-k_3}{c}\right) + \tan^{-1}\left(\frac{k_2-k_1}{c}\right)\right] \\ k_3 L &= 2\pi n_3 - 2\left[\tan^{-1}\left(\frac{k_3-k_1}{c}\right) + \tan^{-1}\left(\frac{k_3-k_2}{c}\right)\right]. \end{aligned} \tag{8}$$

In the above equations, n_i are mutually distinct integers. (The above conditions do not require the mutual difference. However the wave function identically vanishes when $n_i = n_j$, $(i \neq j)$.) The above equations also show that the spectrum is determined by the combination cL except for the overall normalization given by L. Note also that k_i are determined by the quantization conditions (8) and are different from the free ones $k_i = 2\pi n_i/L$. Accordingly Eq. (7) takes the interaction into account, although it looks as if it were the total energy of a free system. The quantum numbers k_i are conserved since the particles simply exchange k_i under a collision. Thus the Hamiltonian (6) is completely integrable.

The study of the N-body system interacting through the δ-potentials has concentrated on the thermodynamic limit $N \to \infty$ so far [10]. Here, in contrast, we take $N = 3$ as above and concentrate on the individual energy levels and their level statistics. Before we proceed further, we specify the relevant Hilbert space of our analysis to avoid degeneracies due to the symmetry of the problem. Our system being interacting through two-body potentials, the total momentum

$$K_G = \sum_{i=1}^{3} k_i = \frac{2\pi}{L}\sum_{i=1}^{3} n_i \tag{9}$$

is a good quantum number and the Hilbert space $\mathcal{H}$ is divided into a direct sum of subspaces indexed by K_G,

$$\mathcal{H} = \bigoplus_{K_G} \mathcal{H}_{K_G}. \tag{10}$$

In other words, the Hamiltonian is block diagonal and the matrix elements between states with different K_G vanish. If the total momentum K_G is introduced, the energy E is separated into the center-of-mass motion and the relative motion as

$$E = \frac{K_G^2}{3} + \epsilon, \tag{11}$$

where the first term is the center-of-mass energy and $\epsilon = \sum_i k_i^2 - (\sum_i k_i)^2/3$ is the energy of the relative motion. Since we are interested only in the relative motion, the trivial contribution from the center of mass motion must be subtracted. Here, without loss of generality, we can restrict ourselves within the subspace $\mathcal{H}_0$ where the total momentum K_G vanishes and the total energy solely comes from the relative motion. This choice is also consistent with our classical analysis in Section II, where we have put $X = P_X = 0$.

Even within the subspace $\mathcal{H}_0$, we should not take all the vectors $|n_1, n_2, n_3\rangle$ such that $\sum_i n_i = 0$. We rather have to take the following symmetries into account.

(1) The Bose symmetry; namely the vector is invariant under the interchange of n_i and n_j. In other words, the wave functions belong to the symmetric representation A_1 of the permutation group S_3.

Therefore we fix the ordering as $n_1 > n_2 > n_3$ for example.
(2) The parity; under the map $\{n_i\} \to \{-n_i\}$, the rapidities change as $\{k_i\} \to \{-k_i\}$ and hence the energy $E = \sum_i k_i^2$ is left invariant. This degeneracy is removed if we keep states with even parity only. For example, from $|2,1,-3\rangle$ a parity even state $|+\rangle = \frac{1}{2^{1/2}}(|2,1,-3\rangle + |3,-1,-2\rangle)$ is obtained. The parity odd state

$$|-\rangle = \frac{1}{2^{1/2}}(|2,1,-3\rangle - |3,-1,-2\rangle)$$

should be discarded.

In summary, our choice of the set $\{n_i\}$ satisfies

$$n_i \in \mathbf{Z},\ n_1 + n_2 + n_3 = 0,\ n_1 > n_2 > n_3 \qquad (12)$$

and the states must be parity even.

Now we are ready to study the level statistics of the Hamiltonian (6). We have taken $L = 1$ and $c = 10^3$ in our computation. As mentioned before, the energy levels are determined by the combination cL and we are free to put $L = 1$. We have chosen a large potential strength c since $\tan^{-1}[(k_i - k_j)/c]$ in Eq. (8) is very close to $\pi/2$ for large $k_i - k_j$ unless c is small so that the larger eigenvalue becomes almost identical to the free one. We have solved the Bethe Ansatz equations (8) numerically for $-200 \leq n_i \leq 200$. The number density is approximately constant with the average $\rho_0 = 0.0039$ in the interval $D \equiv \{\epsilon | 4 \times 10^5 < \epsilon < 2 \times 10^6\}$. If the eigenvalues are sorted in an increasing order, the level spacing is defined by the difference of the two neighboring levels, $s_n \equiv \epsilon_{n+1} - \epsilon_n$. Figure 4 shows the level spacing distribution $P(s)$ of the present spectrum taken over the range D. Also shown in Fig.4 is the Poisson distribution function

$$P(s) = \rho_0 e^{-\rho_0 s}. \qquad (13)$$

The agreement between our numerical result and the above distribution function is obvious. This is the consequence of the "theorem" by Berry and Tabor [11] claiming that any completely integrable system with more than two degrees of freedom, except harmonic oscillators, has exponential level spacing distribution.

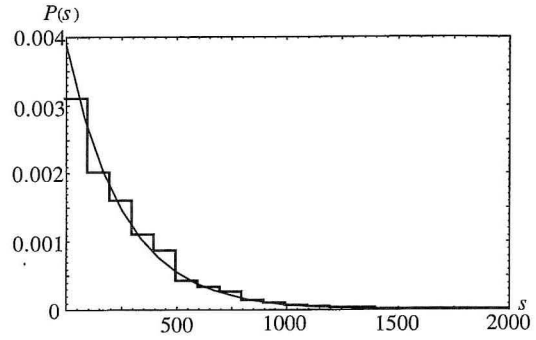

Figure 4: Level spacing distribution of the spectrum of the quantum three-body system with the δ-function potential.

4 Quantum Three-Body Problem with Gaussian Potential

Having analyzed the integrable three-body problem, we now consider the deformation of the δ-function potential to Gaussian potentials and solve the deformed Schrödinger equation. So far as the authors know, this problem has not been solved exactly and we have to resort to numerical computations. In the present Paper we write the Hamiltonian with respect to the (symmetrized) plane-wave basis and then diagonalize it. The number of the plane waves is, of course, finite, which amounts to truncate our Hilbert space. Therefore our approach is considered to be variational.

Let us consider the Hamiltonian

$$H = -\sum_{i=1}^{3} \partial_i^2 + \sum_{i<j} v_\sigma(x_i - x_j) \qquad (14)$$

where v_σ is given by Eq. (2) and $x_i \in [0, L)$ is the particle position of the i-th particle on a circle of the circumference L. Since the total momentum is conserved, the Hilbert space $\mathcal{H}$ is again decomposed into subspaces of a definite total momentum K_G as

$$\mathcal{H} = \bigoplus_{K_G} \mathcal{H}_{K_G}.$$

Without loss of generality, we may choose the subspace $\mathcal{H}_0$ as in the previous Section and analyze the spectrum of the Hamiltonian within this subspace. Let us write the Hamiltonian with respect to the symmetrized plane waves, which are made of one-particle plane waves of the form

$$\langle x|k\rangle = \frac{1}{L^{1/2}} e^{ikx}, \; k = \frac{2\pi n}{L}, \qquad (15)$$

where n is an integer. After symmetrizing three one-particle states, we have the basis $\langle x_1, x_2, x_3|k_1, k_2, k_3\rangle$ which takes the following form
(i) If $k_i \neq k_j$, $i \neq j$, then

$$\langle x_1, x_2, x_3|k_1, k_2, k_3\rangle = \frac{1}{(3!L^3)^{1/2}} \sum_P \exp\left[i(k_1 x_{P1} + k_2 x_{P2} + k_3 x_{P3})\right], \qquad (16)$$

where P is the permutation of three indices.
(ii) If two of k_i's are identical, $k_1 \neq k_2 = k_3 \equiv k$ say, the basis is given by

$$\begin{aligned}\langle x_1, x_2, x_3|k_1, k, k\rangle &= \frac{1}{(3L^3)^{1/2}} \left\{e^{i(k_1 x_1 + k(x_2+x_3))} + e^{i(k_1 x_2 + k(x_3+x_1))} + e^{i(k_1 x_3 + k(x_1+x_2))}\right\} \\ &= \frac{1}{(3L^3)^{1/2}} \left\{e^{ik(-2x_1+x_2+x_3)} + e^{ik(x_1-2x_2+x_3)} + e^{ik(x_1+x_2-2x_3)}\right\} \qquad (17)\end{aligned}$$

where use has been made of the relation $k_1 + 2k = 0$.
(iii) If $k_1 = k_2 = k_3 \equiv k$, we have

$$\langle x_1, x_2, x_3|k, k, k\rangle = \frac{1}{L^{3/2}} e^{ik(x_1+x_2+x_3)}. \qquad (18)$$

Since $\sum_i k_i = 3k = 0$, the only basis of this form is $k_1 = k_2 = k_3 = 0$.

The choice of the basis vectors is similar to that employed in the previous Section with proper modifications. That is, if we write $k_i = 2\pi n_i/L$, the ket $|k_1, k_2, k_3\rangle$ has to satisfy, besides the identity $\sum n_i = 0$, the following conditions.
(1) $n_i \in \mathbf{Z}$ and they are ordered in such a way that $n_1 \geq n_2 \geq n_3$. There is no reason to reject the possibility $n_i = n_j$ any more.
(2) To avoid degeneracies between a state and its mirror reflection, we keep even-parity states only. Namely, instead of $|2, 1, -3\rangle$ and $|3, -1, -2\rangle$ say, we only keep the combination

$$|+\rangle = \frac{1}{2^{1/2}} \left(|2, 1, -3\rangle + |3, -1, -2\rangle\right). \qquad (19)$$

(We occasionally write $|n_1, n_2, n_3\rangle$ instead of $|k_1, k_2, k_3\rangle$ to avoid writing ubiquitous $2\pi/L$. Which notation is employed should be clear from the context.)

Now we are ready to evaluate the matrix elements of the Hamiltonian (14). Let us define the sets $K = \{k_1, k_2, k_3\}$ and $K' = \{k_1', k_2', k_3'\}$ and the kets $|K\rangle = |k_1, k_2, k_3\rangle$ and $|K'\rangle = |k_1', k_2', k_3'\rangle$. The ki-

netic term is easily found to be

$$\langle K'|\left(-\sum_{i=1}^{3}\partial_i^2\right)|K\rangle = \delta_{K,K'}\sum_{i=1}^{3}k_i^2, \qquad (20)$$

where the $\delta_{K,K'}$ is unity if K is equal to K' as a set and is zero if $K \neq K'$.

Let us now turn to the the potential term $\langle K'|V_\sigma|K\rangle$. We first note that the potential term vanishes identically unless at least one of k_i' is equal to one of k_j. This is clear from the observation that our potential is a two-body one and the third particle is just a "spectator" during the collision of the first two. Therefore we first have to evaluate the two-body matrix element

$$\begin{aligned}
&\tilde{v}_\sigma(k_1', k_2'; k_1, k_2) \\
&\equiv \langle k_1', k_2'|v_\sigma(x_1 - x_2)|k_1, k_2\rangle \\
&= \langle k_1', k_2'|\frac{2c}{(2\pi)^{1/2}\sigma}\sum_{m\in\mathbf{Z}} e^{-(x_1-x_2-mL)^2/2\sigma^2}|k_1, k_2\rangle \\
&= \frac{2c}{(2\pi)^{1/2}L^2\sigma}\sum_m \int_0^L dx_1 \int_0^L dx_2 e^{-i(k_1'x_1+k_2'x_2)} \times e^{-(x_1-x_2-mL)^2/2\sigma^2} e^{i(k_1x_1+k_2x_2)}. \qquad (21)
\end{aligned}$$

The above matrix element is obtained after straightforward but tedious calculation given in Appendix B. It takes a very simple form,

$$\tilde{v}_\sigma(k_1', k_2'; k_1, k_2) = \frac{2c}{L}\delta_{\Delta K,0}\exp\left[-\frac{1}{8}(\sigma\Delta k)^2\right], \qquad (22)$$

where $\Delta k \equiv (k_1 - k_2) - (k_1' - k_2')$ is the change of the relative momentum while $\Delta K \equiv (k_1 + k_2) - (k_1' + k_2')$ is the change of the total momentum. If we write $k_i = 2\pi n_i/L$ and $k_i' = 2\pi n_i'/L$, Δk becomes

$$\Delta k = \frac{2\pi}{L}(n_1 - n_2 - n_1' + n_2'). \qquad (23)$$

Since $\tilde{v}_\sigma(k_1', k_2'; k_1, k_2)$ depends only on Δk and not on individual k's, this matrix element will be written as $\tilde{v}_\sigma(\Delta k)$. Note that the combination of the integers in Eq. (23) is always even, which follows from the momentum conservation $\Delta K = 2\pi(n_1 + n_2 - n_1' - n_2')/L = 0$. Note that $v_\sigma(\Delta k) \equiv 1$ if the potential is the δ-function (i.e., $\sigma = 0$).

We finally obtained the matrix element of the potential term in the case of $k_1 \neq k_2 \neq k_3 \neq k_1$, for example,

$$\begin{aligned}
&\langle K'|2c\sum_{i<j} v_\sigma(x_i - x_j)|K\rangle \\
&= \frac{2c}{6}\sum_P \left[\tilde{v}_\sigma(\Delta k_{12})\delta_{k_3', k_{P3}}\right. \\
&\quad \left. + \tilde{v}_\sigma(\Delta k_{23})\delta_{k_1', k_{P1}} + \tilde{v}_\sigma(\Delta k_{31})\delta_{k_2', k_{P2}}\right] \qquad (24)
\end{aligned}$$

where $\Delta k_{ij} \equiv (k_{Pi} - k_{Pj}) - (k_i' - k_j')$.

5 Deformation of Spectrum and Level Statistics

Quantum three-body systems with a family of two-body potentials parametrized by σ have been analyzed in Sections III and IV. In the present Section, we study the deformation of the spectrum as σ is var-

ied. We have diagonalized the Hamiltonian according to the prescription described in Section IV by introducing 2116 basis vectors, which corresponds to $|n| \leq 90$.

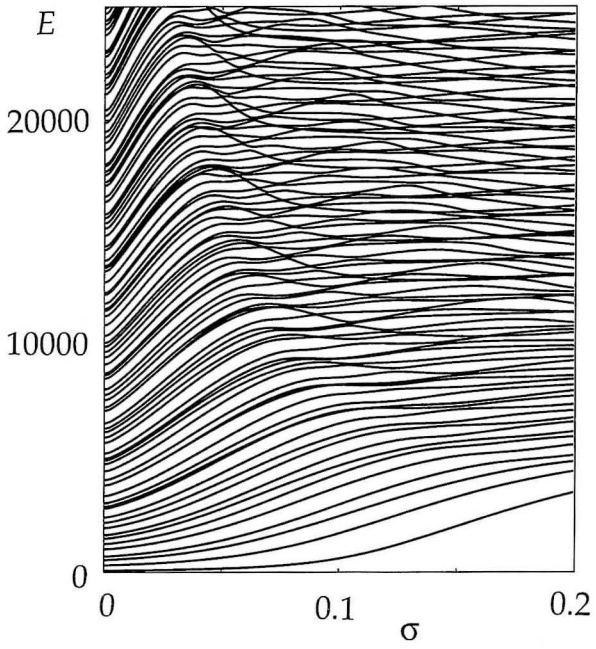

Figure 5: Spectral profile as a function of σ. Only low-lying levels are plotted with a restricted range of σ for clarity.

Figure 5 shows the spectral profile as a function of σ in a restricted region of the σE-plane. In the following calculations, we have kept only the lowest 800 eigenvalues among 2116 ones. These low-lying eigenvalues should have enough accuracy unless σ is very close to zero. (The matrix elements do not decay as $\Delta k \to \infty$ for $\sigma = 0$ so that all the basis vectors mix with each other as noted in the previous Section.) We have taken $\sigma = 0.01$, which is the "worst" case in our analysis, and evaluated the lowest 800 eigenvalues by reducing the number of basis vectors to 1681, which corresponds to $|n| \leq 80$, and then compared these eigenvalues with those obtained with 2116 basis vectors. The average level spacing for the 800 levels is approximately 256, while the change in the energy level is merely less than 0.9. Therefore we conclude that these eigenvalues have enough precision to analyze the level statistics. The spectrum becomes flat above $\sigma \simeq 0.5$ since all the matrix elements $\tilde{v}_\sigma(\Delta k)$ vanish for $\sigma > 0.5$ except for $\Delta k = 0$, for which $v_\sigma(0) = 1$, see Eq. (22). Therefore the Hamiltonian is equivalent to a free Hamiltonian with a constant potential $6c$ in this range of σ. Figure 6 are a close-up of the spectral profile shown in Fig.5. Note that level repulsions are observed at many places.

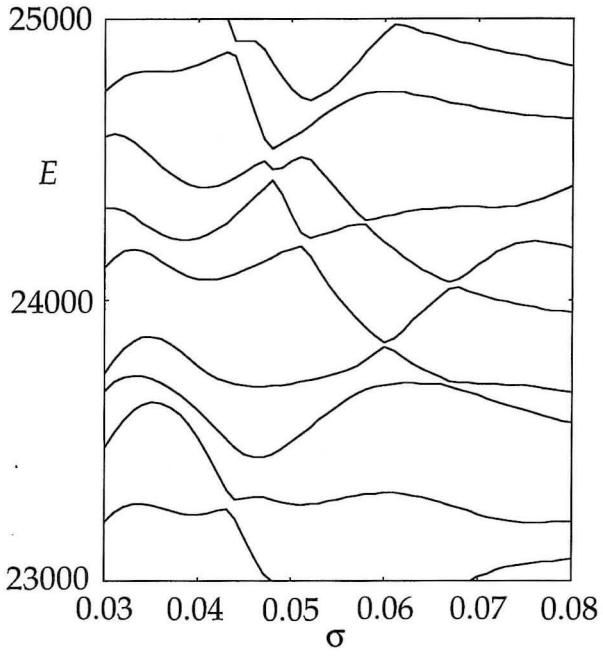

Figure 6: Close-up of the spectral profile. Observe the ubiquitious level repulsion.

Now let us leave the spectrum and turn to the level spacing distribution or the level statistics. It is ex-

pected that the level statistic is exponential for $\sigma = 0$ and for sufficiently large σ ($\sigma > 0.5$). This is because the system is integrable for $\sigma = 0$ and almost free for $\sigma > 0.5$. It is interesting to study the level statistics in the intermediate region, $0 < \sigma < 0.5$. We may be inspired from the Poincaré sections of the classical system and expect that the level statistics obeys the Wigner distribution if the system energy is of the order of the potential height and the exponential distribution if it is much smaller or larger than the potential height.

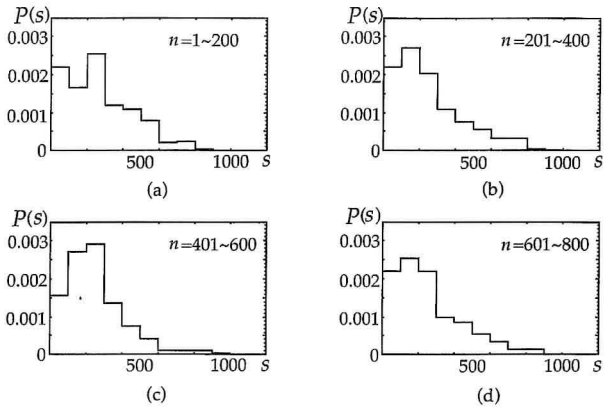

Figure 7: Level statistics of the three-body system with a Gaussian potential with $\sigma = 0.01$.

We consider the three-boson system with $L = 1$ and $c = 10^3$ as before. The local level statistics for $\sigma = 0.01$ are given in Fig.7. They clearly indicate that the level statistics is exponential if the total energy is much smaller or larger than the potential height $2c/\left((2\pi)^{1/2}\sigma\right)$. If, on the other hand, the total energy is of the order of the potential height, the level statistics is well approximated by the Wigner distribution

$$P(s) = \frac{\pi}{2}\rho_0^2 s \exp(-\frac{\pi}{4}\rho_0^2 s^2). \tag{25}$$

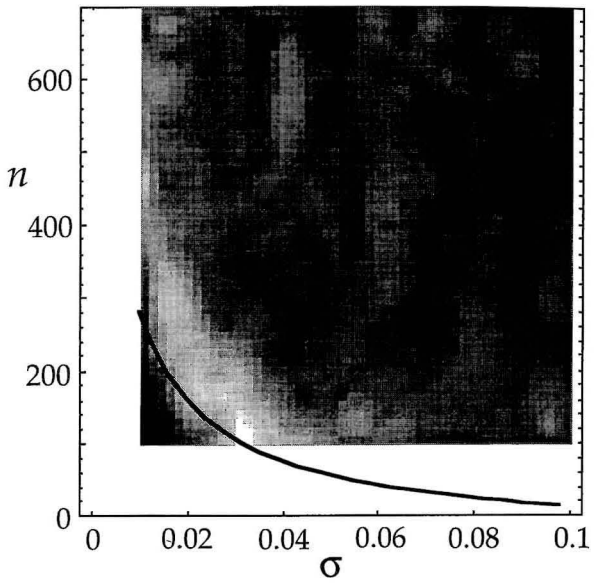

Figure 8: Density plot of the Blody parameter as a function of the potential width σ and the level number n. The curve denotes the two-body potential height.

It is interesting to fit our distributions to the Brody distribution [12]

$$P(s,\alpha) = as^\alpha \exp(-bs^{\alpha+1}) \tag{26}$$

with

$$\begin{aligned} a &= (\alpha+1)\left[\Gamma\left(\frac{\alpha+2}{\alpha+1}\right)\right]^{\alpha+1}, \\ b &= \left[\Gamma\left(\frac{\alpha+2}{\alpha+1}\right)\right]^{\alpha+1}. \end{aligned} \tag{27}$$

The Brody parameter α measures the deviation of the given distribution from the exponential distribution. Namely, the Brody distribution with $\alpha = 0$ reduces to the Poisson distribution, while $\alpha = 1$ to the Wigner distribution. Figure 8 is the density plot of the Blody parameter as a function of σ and the level number n of the energy eigenvalue E_n. THe lighter spot shows the parameter α is closer to 1 while the darker spot

closer to 0. We can see that the most chaotic region ($\alpha \simeq 1$) is where the energy is slightly above the potential height, which justifies our observation mentioned above.

6 Summary

We have studied a three-body system interacting with a repulsive δ-function potential or Gaussian potentials both classically and quantum mechanically. Our main concern is how the characteristics change when the potential is deformed from the integrable δ-function potential to the nonintegrable Gaussian potential. The degree of chaoticity depends on the potential width and the energy. When the energy is comparable to the potential height, the system shows a chaotic behavior in both classical mechanics and quantum mechanics. The degree of the chaotic behavior can be recognized from the Poincaré section of the classical trajectories and the nearest-neighbor level statistics in quantum mechanics. When the energy is much smaller or larger than the potential height, the system behaves quite regularly, which can be seen from the regular Poincaré section and Poisson distribution of the level statistics. This is because the available classical phase space is limited or the quantum mechanical wave function is localized for small energies, while the particles can move almost freely for large energies. Therefore we conclude that our model shows a variety of phenomena depending on the potential width and the energy, although it is simple enough to analyze both classically and quantum mechanically.

We are grateful to Haruo Yoshida for expalining us the symplectic integration method. One of the authors (MN) would like to thank Katsuhiro Nakamura for fruitful discussions. We also thank Akio Ohno for assistance in some numerical computations in the earlier stage of the present work.

A Symplectic Integration Method

Here the relevant aspects of the symplectic integration method are summarized since we believe that this method is not very popular among general readers.

Let us consider a Hamiltonian of the form

$$H(p,q) = T(p) + V(q), \tag{28}$$

with arbitrary degrees of freedom. If the coordinates q and the momenta p are written collectively as $z = (q,p)$, the Hamiltonian equations of motion are written as

$$\frac{dz}{dt} = \{z, H(z)\}, \tag{29}$$

where the curly bracket denotes the Poisson bracket. Suppose G is some physical quantitiy. If a linear differential operator D_G acting on $F(z)$ is defined by

$$D_G F(z) \equiv \{F, G\},$$

Eq. (29) can be rewritten as

$$\frac{dz}{dt} = D_H z. \tag{30}$$

Since $D_H F(z) = \{F, T+V\} = D_T F + D_V F = (D_T + D_V)F$, the time evolution of z from $t = 0$ to $t = \tau > 0$ is formally given by

$$z(\tau) = [\exp(\tau D_H)]z(0) = \exp[\tau(D_T + D_V)]z(0). \tag{31}$$

The above equation is just a replacement of the original differential equation (29) and is difficult to evaluate in general since D_T and D_V do not commute. An essential observation in the present method is that the action of the operator $\exp(\tau D_T)$ or $\exp(\tau D_V)$ is evaluated with no difficulty. For example, $z(\tau) = \exp(\tau D_T)z(0)$ is a solution whose Hamiltonian is given by $H = T(p)$ and written explicitly as

$$q(\tau) = q(0) + \tau \frac{\partial T}{\partial p}, \;\; p(\tau) = p(0). \tag{32}$$

Simlarly, $\exp(\tau D_V)$ corresponds to the Hamiltonian $H = V(q)$ and the solution is a staight line

$$q(\tau) = q(0), \;\; p(\tau) = p(0) - \tau \frac{\partial V}{\partial q}. \tag{33}$$

It is easily verified that these solutions represent symplectic evolutions, namely they preserve the symplectic strucuture $\omega \equiv \sum dp_i \wedge dq_i$. Accordingly the combined transformation

$$z(\tau) = \exp(\tau D_T)\exp(\tau D_V)z(0) \tag{34}$$

is also symplectic. It should be noted that the combined evolution corresponds to that of the original Hamiltonian up to the first order in τ since

$$e^{\tau(A+B)} = e^{\tau A}e^{\tau B} + \mathcal{O}(\tau^2) \tag{35}$$

Written explicitly, Eq. (34) is

$$q' = q + \tau \left(\frac{\partial T}{\partial p}\right)_{p=p}, \; p' = p - \tau \left(\frac{\partial V}{\partial q}\right)_{q=q'}. \tag{36}$$

There is a conserved quantity $\tilde{H}$, which differs from H by $O(\tau)$, associated with the above evolution. Suppose operators X and Y do not commute. Then an operator Z defined by $e^X e^Y = e^Z$ is found, from Baker-Campbell-Hausdorff formula, as

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}([X,[X,Y]] + [Y,[Y,X]]) + \cdots,$$

where $[X, Y] \equiv XY - YX$. If this formula is applied to the present problem, we obtain

$$e^{\tau D_T} e^{\tau D_V} = \exp\left[\tau D_T + \tau D_V + \frac{1}{2}[\tau D_T, \tau D_V] + \frac{1}{12}([\tau D_T, [\tau D_T, \tau D_V]] + [\tau D_V, [\tau D_V, \tau D_T]]) + \cdots\right]. \quad (37)$$

If we put $h = T$ and $g = V$ in the Jacobi identity

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$$

the operators in Eq. (37) are written as

$$[D_T, D_V] = D_{\{V,T\}}$$
$$[D_T, [D_T, D_V]] = [D_T, D_{\{V,T\}}] = D_{\{\{V,T\},T\}}$$
$$\cdots$$

Therefore, the L.H.S. of Eq. (37) is written in terms of a single exponential operator as

$$\begin{aligned} e^{\tau D_T} e^{\tau D_V} &= \exp\left[\tau D_T + \tau D_V + \frac{\tau^2}{2} D_{\{V,T\}} + \frac{\tau^3}{12}(D_{\{\{V,T\},T\}} + D_{\{\{T,V\},V\}}) + \cdots\right] \\ &= \exp\left[\tau D_{(T+V+\frac{\tau}{2}\{V,T\}+\frac{\tau^2}{12}(\{\{V,T\},T\}+\{\{T,V\},V\})+\cdots}\right] \\ &= \exp\left[\tau D_{\tilde{H}}\right], \end{aligned} \quad (38)$$

where

$$\tilde{H} \equiv T + V + \frac{\tau}{2}\{V, T\} + \frac{\tau^2}{12}(\{\{V, T\}, T\} + \{\{T, V\}, V\}) + \cdots. \quad (39)$$

We finally found the conserved quantity $\tilde{H}$ whose time evolution is given *exactly* by Eq. (36). The difference between H and $\tilde{H}$ being $O(\tau)$, the error in the energy remains of the order of τ.

A natural extension of the above observation is to find $\tilde{H}_n$ which differs from H by $O(\tau^n)$,

$$\tilde{H}_n = H + \tau^n H_n + O(\tau^{n+1}).$$

As a result, the error in the energy remains within $O(\tau^n)$. Such an extension is called the higher order symplectic integration method. This is realized by approximating Eq.(35) by a product of exponential operators in such a way that the error is $O(\tau^{n+1})$. Namely we write

$$e^{\tau(D_T+D_V)} = \prod_{i=1}^{k} e^{c_i \tau D_T} e^{d_i \tau D_V} + \mathcal{O}(\tau^{n+1}) \quad (40)$$

where $k > 0$ is an interger which depends on a given positive interger n. The coefficients $(c_i,\ d_i)$ are fixed so that they satisfy the above equation. This can be done by expanding the both sides of Eq.(40) in τ and compare the coefficients of each term up to τ^n.

When $n = 1$, we find $c_1 = 1, d_1 = 1$ $(k = 1)$ recovering Eq.(36). For $n = 2$ the matching of the coefficients requires $k = 2$ and

$$\begin{cases} c_1 + c_2 = 1 \\ d_1 + d_2 = 1 \\ c_1^2 + 2c_1c_2 + c_2^2 = 1 \\ d_1^2 + 2d_1d_2 + d_2^2 = 1 \\ c_1d_1 + c_1d_2 + c_2d_2 = \dfrac{1}{2} \\ c_2d_1 = \dfrac{1}{2}, \end{cases}$$

from which we obtain $c_1 = c_2 = \frac{1}{2}, d_1 = 1, d_2 = 0$. As a result, the second order symplectic intergration method yields

$$z(\tau) = e^{\frac{1}{2}\tau D_T} e^{\tau D_V} e^{\frac{1}{2}\tau D_T} z(0). \tag{41}$$

More explicitly, they are

$$q^* = q + \frac{\tau}{2}\left(\frac{\partial T}{\partial p}\right)_{p=p},\ p' = p - \tau\left(\frac{\partial V}{\partial q}\right)_{q=q^*},\ q' = q^* + \frac{\tau}{2}\left(\frac{\partial T}{\partial p}\right)_{p=p'}. \tag{42}$$

For $n = 4$, the matching conditions are

$$\begin{cases} c_1 + c_2 + c_3 + c_4 = 1 \\ d_1 + d_2 + d_3 + d_4 = 1 \\ c_2d_1 + c_3(d_1 + d_2) + c_4(d_1 + d_2 + d_3) = \dfrac{1}{2} \\ c_2d_1^2 + c_3(d_1 + d_2)^2 + c_4(d_1 + d_2 + d_3)^2 = \dfrac{1}{3} \\ c_2d_1^3 + c_3(d_1 + d_2)^3 + c_4(d_1 + d_2 + d_3)^3 = \dfrac{1}{4} \\ c_1^2d_1 + (c_1 + c_2)^2d_2 + (c_1 + c_2 + c_3)^2d_3 + (c_1 + c_2 + c_3 + c_4)^2d_4 = \dfrac{1}{3} \\ c_1^3d_1 + (c_1 + c_2)^3d_2 + (c_1 + c_2 + c_3)^3d_3 + (c_1 + c_2 + c_3 + c_4)^3d_4 = \dfrac{1}{4} \\ c_1c_2d_1^2 + c_1c_3(d_1 + d_2)^2 + c_1c_4(d_1 + d_2 + d_3)^2 + c_2c_3d_2^2 + c_2c_4(d_2 + d_3)^2 + c_3c_4d_3^2 = \dfrac{1}{12}. \end{cases}$$

Here we have taken $k = 4$. A solution to the above equations was found by Forest and Ruth [13, 14] as,

$$c_1 = c_4 = \frac{1}{2(2 - 2^{1/3})},\ c_2 = c_3 = \frac{1 - 2^{1/3}}{2(2 - 2^{1/3})}$$
$$d_1 = d_3 = \frac{1}{2 - 2^{1/3}},\ d_2 = \frac{-2^{1/3}}{2 - 2^{1/3}},\ d_4 = 0. \tag{43}$$

If we note that c_i and d_i are related as

$$c_1 = \frac{d_1}{2}, c_2 = \frac{d_1 + d_2}{2}, c_3 = \frac{d_2 + d_3}{2}, c_4 = \frac{d_3}{2} \tag{44}$$

the R.H.S. of Eq.(40) is written explicitly as

$$\begin{aligned} S_4(\tau) &\equiv e^{c_1\tau D_T} e^{d_1\tau D_V} e^{c_2\tau D_T} e^{d_2\tau D_V} e^{c_3\tau D_T} e^{d_3\tau D_V} e^{c_4\tau D_T} \\ &= e^{\frac{d_1}{2}\tau D_T} e^{d_1\tau D_V} e^{\frac{d_1}{2}\tau D_T} e^{\frac{d_2}{2}\tau D_T} e^{d_2\tau D_V} e^{\frac{d_2}{2}\tau D_T} e^{\frac{d_3}{2}\tau D_T} e^{d_3\tau D_V} e^{\frac{d_3}{2}\tau D_T}. \end{aligned} \tag{45}$$

If we write the second order evolution operator as

$$S_2(\tau) \equiv e^{\frac{1}{2}\tau D_T} e^{\tau D_V} e^{\frac{1}{2}\tau D_T}, \tag{46}$$

Eq.(45) is written in terms of S_2 as

$$S_4(\tau) = S_2(d_1\tau) S_2(d_2\tau) S_2(d_1\tau). \tag{47}$$

Thus the fourth order symplectic integration method is equivalent to three consecutive second order integrations.

B Matrix Elements of the Potential Energy

Here we sketch the derivation of the matrix element (22). Consider the integral

$$I \equiv \sum_m \int_0^L dx_1 \int_0^L dx_2 e^{-i(k_1' x_1 + k_2' x_2)} e^{-(x_1 - x_2 + mL)^2/2\sigma^2} e^{i(k_1 x_1 + k_2 x_2)}$$

which appears in Eq.(21). Let us make the change of variables

$$\begin{aligned} X &\equiv \frac{1}{2}(x_1 + x_2),\ x \equiv x_1 - x_2, \\ \Delta K &\equiv (k_1 + k_2) - (k_1' + k_2'),\ \Delta k \equiv (k_1 - k_2) - (k_1' - k_2') \end{aligned}$$

and write the above integral as

$$\sum_m \int_{-L}^{L} dx \int_{|x|/2}^{L-|x|/2} dX e^{i\Delta KX} e^{i\Delta kx/2-(x+mL)^2/2\sigma^2}.$$

Note here that the momentum conservation requires $\Delta K = 0$. In fact it is not difficult to show that the integral vanishes if $\Delta K = 2\pi N/L \neq 0$ and $\Delta k = 2\pi n/L$.

Thus we write

$$\begin{aligned} I &= \delta_{\Delta K,0} \sum_m \int_0^L dx 2(L-x) \cos\left(\frac{\Delta k}{2}x\right) e^{-(x+mL)^2/2\sigma^2} \\ &= 2\delta_{\Delta K,0} \sum_m \int_{mL}^{mL+L} dy[(m+1)L-y] e^{-y^2/(2\sigma^2)} \cos\left(\frac{\Delta k}{2}y - \frac{\Delta k}{2}mL\right) \end{aligned}$$

where $y \equiv x + mL$. Here we find from $\Delta K = 0$ that $\Delta k = 2(k_1 - k_1') = 4\pi n/L$, $(n \in \mathbf{Z})$ and hence

$$\cos\left(\frac{\Delta k}{2}y - \frac{\Delta k}{2}mL\right) = \cos\frac{\Delta k}{2}y.$$

Substituting this into the above integral, we find

$$\begin{aligned} I &= 2\delta_{\Delta K,0}\left[\sum_m (m+1)L \int_{mL}^{mL+L} dx \cos\left(\frac{\Delta k}{2}x\right) e^{-x^2/2\sigma^2} - \int_{-\infty}^{\infty} dx x \cos\left(\frac{\Delta k}{2}x\right) e^{-x^2/2\sigma^2}\right] \\ &= 2\delta_{\Delta K,0} \sum_m (m+1)L \int_{mL}^{mL+L} f(x)dx, \end{aligned}$$

where $f(x) \equiv e^{-x^2/2\sigma^2}\cos(\Delta kx/2)$. Then it follows that

$$\begin{aligned} I &= 2\delta_{\Delta K,0}\left(\sum_{m=-\infty}^{-1} + \sum_{m=0}^{\infty}\right)(m+1)L \int_{mL}^{mL+L} f(x)dx \\ &= 2\delta_{\Delta K,0}L\left[\sum_{m'=0}^{\infty}(-m')\int_{m'L}^{m'L+L} dy\, f(y) + \sum_{m=0}^{\infty}(m+1)\int_{mL}^{mL+L} dx\, f(x)\right] \\ &= 2\delta_{\Delta K,0}L\int_0^{\infty} dx f(x), \end{aligned}$$

where $m' = -m-1$ and $y = -x$. Thus we finally obtain

$$I = 2\delta_{\Delta K,0}L\int_0^{\infty} dx e^{-x^2/2\sigma^2}\cos\frac{\Delta k}{2}x = \delta_{\Delta K,0}L(2\pi)^{1/2}\sigma e^{-\sigma^2\Delta k^2/8}. \tag{48}$$

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