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Extraction of Accurate Frequencies from the Fast Fourier Transform Spectra

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The fast fourier transformation (FFT) is well known to be extremely fast and useful. However, its spectrum is quite often not accurate, because it is a discrete transformation and, further, the effect of finite range of sampling, the so-called Gibbs phenomenon, produces long tails. Here a very simple and efficient method to extract the accurate frequencies and the amplitudes of discrete spectra from FFT data is proposed. No window function is used in the present method. Indeed, our numerical examples show that the resultant frequencies and amplitudes are extremely accurate. © 1992 Academic Press, Inc.

I. INTRODUCTION

Quasi-periodic functions which are of the form

$$\phi(t) = \sum_{m \geqslant 0} C_m \cos(f_m t) + S_m \sin(f_m t) \quad (-\infty \leqslant t \leqslant \infty) \tag{1.1}$$

appear frequently in science and engineering. For example, in classical mechanics, coordinates and momenta of a particle in multiply periodic motions, such as molecular vibrations, can be represented as in the above expression [1]. Theoretically, the action–angle variables can be obtained by a certain procedure [2], in which the frequencies (f_m) and amplitudes (S_m and C_m), play essential roles. In principle, the continuous Fourier trasformation can reproduce these values from the time series data of $\phi(t)$. In practice, however, it is quite often required to extract them from a finite set of discrete sampling points with high accuracy and high speed. From the viewpoint of speed, the celebrated fast Fourier transformation (FFT) technique is almost exclusively used practically. However, the accuracy of the results by FFT is considerably limited, since FFT is not really a continuous integral transformation but a discrete one performed within a finite range. Therefore, if an actual frequency, say f_m, is located in between two frequencies which are given by FFT automatically, the FFT spectra at these sandwiching points oscillate violently with different signs. Furthermore, these peaks have long tails, which are due to sudden truncation of the series of sampling data (the so-called Gibbs phenomenon). An example of this situation is depicted in Fig. 1.

One of the methods to avoid the long-tail behavior is to apply the so-called window technique. It is well known that a bell-shaped window function, for instance, can well reduce the truncation effect [2, 3]. On the other hand, the data thus windowed are biased and the height of the spectral peaks is lowered. In order to suppress the tails and also to obtain accurate heights simultaneously, FFT is sometimes performed two times with different types of windows for each purpose. A recent and important example of the application of a window technique can be found in Ref. [2], which also briefly reviews the former works. It is also a usual practice to vary the length of sampling set to lead one of the FFT frequencies to come very close to a true frequency. These procedures are generally very tedious.

In this paper, I propose a method to obtain the accurate frequencies and amplitudes of quasi-periodic functions from their FFT spectra with no use of such a window function technique. The idea is very simple and its implementation and usage are extremely easy.

II. BASIC PROCEDURES

A. *FFT*

We consider a function having only two frequencies in Eq. (1.1) without loss of generality for the presentation of our procedure, namely,

$$\phi(t) = \phi_f(t) + \phi_g(t) \tag{2.1a}$$

with

$$\phi_f(t) = C_f \cos(ft) + S_f \sin(ft) \tag{2.1b}$$

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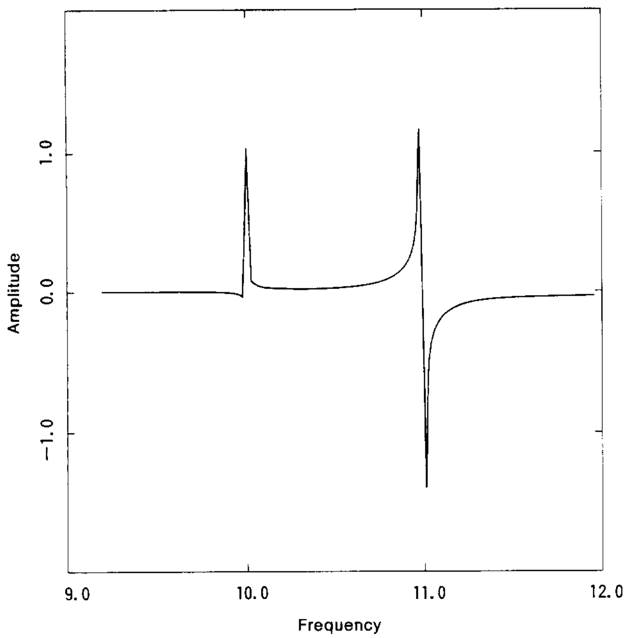

FIG. 1. The cosine-FFT spectrum for $\phi(t) = \cos(10.0\,t) + 2.0\sin(11.0\,t)$: One of the discretized frequencies given by FFT happens to be extremely close to 10.0, and, correspondingly, a single sharp peak is produced. On the other hand, the sine component in $\phi(t)$ is detected even in the cosine transformation with a large amplitude oscillation which is accompanied by long tails.

and

$$\phi_g(t) = C_g \cos(gt) + S_g \sin(gt). \tag{2.1c}$$

The frequencies f and g are assumed not very close to each other throughout the present paper. The cosine-FFT and sine-FFT are usually defined as

$$F_c(k) = \frac{2}{N} \sum_{j=0}^{N-1} \cos\left(\frac{2\pi kj}{N}\right) [\phi_f(j\,\Delta t) + \phi_g(j\,\Delta t)] \tag{2.2}$$

and

$$F_s(k) = \frac{2}{N} \sum_{j=1}^{N-1} \sin\left(\frac{2\pi kj}{N}\right) [\phi_f(j\,\Delta t) + \phi_g(j\,\Delta t)] \tag{2.3}$$

with

$$\Delta t = T/N, \tag{2.4}$$

where T and N are the sampling length and number, respectively.

By inserting Eqs. (2.1) in Eqs. (2.2) and (2.3), we have

$$\begin{aligned} F_c(k) = {} & A_{cc}(k, f)\, C_f + A_{cs}(k, f)\, S_f \\ & + A_{cc}(k, g)\, C_g + A_{cs}(k, g)\, S_g \end{aligned} \tag{2.5}$$

and

$$\begin{aligned} F_s(k) = {} & A_{sc}(k, f)\, C_f + A_{ss}(k, f)\, S_f \\ & + A_{sc}(k, g)\, C_g + A_{ss}(k, g)\, S_g. \end{aligned} \tag{2.6}$$

The definitions of the above functions, such as $A_{sc}(k, f)$, are obvious. For example,

$$A_{cs}(k, f) = \frac{2}{N} \sum_{j=0}^{N-1} \cos\left(\frac{2\pi kj}{N}\right) \sin(fj\,\Delta t). \tag{2.7}$$

It is obvious that if nonlinear parameters f and g are known, linear parameters C_f, S_f, C_g, and S_g can be determined by various types of linear equations such as Eqs. (2.5) and (2.6).

B. *Approximate Evaluation of FFT*

FFT is a very fast approximation to the true Fourier transformation. Here we invert the standpoint: The true Fourier transformation is viewed as an approximation to FFT. Let us rewrite Eq. (2.2) as follows:

$$F_c(k) = \frac{2}{T} \sum_{j=0}^{N-1} \cos\left(\frac{2\pi kj}{T}\,\Delta t\right) [\phi_f(j\,\Delta t) + \phi_g(j\,\Delta t)]\,\Delta t. \tag{2.8}$$

Under a condition that Δt is "sufficiently" small, the above sum is evaluated approximately by an integral

$$F_c(k) \cong \frac{2}{T} \int_0^T dt \cos\left(\frac{2\pi kt}{T}\right) [\phi_f(t) + \phi_g(t)], \tag{2.9}$$

which is simply a return to the continuous Fourier transform. This integral can be evaluated exactly, the result being

$$\begin{aligned} F_c(k) = {} & \frac{C_f}{T} \frac{\sin(fT)}{f - 2\pi k/T} + \frac{C_f}{T} \frac{\sin(fT)}{f + 2\pi k/T} \\ & - \frac{S_f}{T} \frac{\cos(fT) - 1}{f - 2\pi k/T} - \frac{S_f}{T} \frac{\cos(fT) - 1}{f + 2\pi k/T} \\ & + \frac{C_g}{T} \frac{\sin(gT)}{g - 2\pi k/T} + \frac{C_g}{T} \frac{\sin(gT)}{g + 2\pi k/T} \\ & - \frac{S_g}{T} \frac{\cos(gT) - 1}{g - 2\pi k/T} - \frac{S_g}{T} \frac{\cos(gT) - 1}{g + 2\pi k/T}. \end{aligned} \tag{2.10}$$

In a similar way, sine-FFT is also evaluated as

$$F_s(k) = \frac{C_f}{T}\frac{\cos(fT)-1}{f-2\pi k/T} - \frac{C_f}{T}\frac{\cos(fT)-1}{f+2\pi k/T} + \frac{S_f}{T}\frac{\sin(fT)}{f-2\pi k/T} - \frac{S_f}{T}\frac{\sin(fT)}{f+2\pi k/T} + \frac{C_g}{T}\frac{\cos(gT)-1}{g-2\pi k/T} - \frac{C_g}{T}\frac{\cos(gT)-1}{g+2\pi k/T} + \frac{S_g}{T}\frac{\sin(gT)}{g-2\pi k/T} - \frac{S_g}{T}\frac{\sin(gT)}{g+2\pi k/T}. \tag{2.11}$$

In Eqs. (2.10) and (2.11), the oscillatory behavior shown in Fig. 1 is quite apparent. Before proceeding, let us confirm that in these expressions f, g, C_f, and S_f are unknown, while $F_c(k)$ and $F_s(k)$ are known as the FFT spectra.

C. *First Guess of the Frequencies*

We assume that the true frequency f is located in the range

$$\frac{2\pi}{T}K < f < \frac{2\pi}{T}(K+1), \tag{2.12}$$

where K is one of k's. Such K can be easily found by inspecting FFT spectra or its power. The sudden change of the sign of $F_c(k)$ in the k-coordinate is helpful to find the K. Then the far dominant term in Eq. (2.10) for $k = K$ is

$$F_c(K) \approx \frac{1}{T}\frac{C_f \sin(fT) - S_f[\cos(fT)-1]}{f-2\pi K/T} \tag{2.13}$$

and that for $k = K+1$,

$$F_c(K+1) \approx \frac{1}{T}\frac{C_f \sin(fT) - S_f[\cos(fT)-1]}{f-2\pi(K+1)/T}. \tag{2.14}$$

The other terms are very small. In addition, we have assumed that T is chosen so that $\sin(fT)$ is not very small.

Although both C_f and S_f are unknown at this moment, they are cancelled out by taking the ratio of Eqs. (2.13) and (2.14) such that

$$X_c = \frac{F_c(K+1)}{F_c(K)} \tag{2.15}$$

and f is given in turn as

$$f \approx \frac{2\pi K}{T} - \frac{2\pi}{T}\frac{X_c}{1-X_c}. \tag{2.16}$$

Thus we can make a first guess of f. The similar procedure can be carried out using the sine-FFT data. We have observed that the difference between the two guesses is generally very small and accordingly we adopt the simple average of them hereafter. Moreover, our numerical experience has shown that the f value thus guessed is already fairly close to the exact one. The same procedure can be carried out independently for the frequency g.

D. *First Guess of the Amplitudes* (*Linear Equation Method*)

Now that the first guess of the frequencies have been obtained, it is almost straightforward to calculate the amplitudes, since these are linear parameters and FFT is a linear transformation. For completeness, we list below three methods that are applied in our practical calculation.

Method A. A simple way to obtain the amplitudes is by making use of Eqs. (2.5) and (2.6). It is assumed that g satisfies

$$\frac{2\pi}{T}L < g < \frac{2\pi}{T}(L+1). \tag{2.17}$$

Further let K' be either one of K and $K+1$, which is closer to f in the sense of Eq. (2.12), and similarly choose L' in Eq. (2.17). Then by putting $k = K'$ and $k = L'$ in Eqs. (2.5) and (2.6), we have simultaneous linear equations, the number of which is equal to that of the unknown. In our example, that is

$$\begin{bmatrix} A_{cc}(K',f) & A_{cs}(K',f) & A_{cc}(K',g) & A_{cs}(K',g) \\ A_{sc}(K',f) & A_{ss}(K',f) & A_{sc}(K',g) & A_{ss}(K',g) \\ A_{cc}(L',f) & A_{cs}(L',f) & A_{cc}(L',g) & A_{cs}(L',g) \\ A_{sc}(L',f) & A_{ss}(L',f) & A_{sc}(L',g) & A_{ss}(L',g) \end{bmatrix} \begin{bmatrix} C_f \\ S_f \\ C_g \\ S_g \end{bmatrix} = \begin{bmatrix} F_c(K') \\ F_s(K') \\ F_c(L') \\ F_s(L') \end{bmatrix}. \tag{2.18}$$

Thus the first guess of the amplitudes can be obtained. The matrix elements in Eq. (2.18) can be evaluated through the expressions as in Eq. (2.7). Alternatively, they can be approximated by the integral representation as in Eq. (2.9). For example, the approximation of $A_{cs}(K, f)$ is obtained as a coefficient of C_f in Eq. (2.10) by comparing Eqs. (2.5) and (2.10). From this approximation, it is seen that if fT and/or gT are very close to an integer multiple of 2π and k is not properly chosen, the matrix $\{A_{sc}\}$ becomes nearly singular. This was already pointed out below Eq. (2.14). The above method based on Eq. (2.18) is convenient in that the matrix $\{A_{sc}\}$ and the vector $\{F_c\}$ are decoupled more or less to each frequency region as the functions of k. For example, the off-diagonal terms $A_{sc}(K', g)$'s in Eq. (2.18) are all small if f and g are sufficiently separated. This fact will lead to an iterative method to solve Eq. (2.18) locally at each frequency part as will be described in Subsection IIF.

Method B. A major drawback of Eq. (2.18) is, however, that the evaluation of $\{A_{sc}\}$ is a little time consuming and, moreover, certain error is expected to arise: Remember that the values of f and g to be put in $\{A_{sc}\}$ are approximate ones, which were obtained in the preceding subsection. Even if both f and g are reasonably good, $\sin(ft)$ and $\cos(ft)$, for example, deviate from the exact values as t becomes large and, correspondingly, this takes place as j becomes large in Eq. (2.7). A very simple way to circumvent this is to use the initial data $\{\phi(j\,\Delta t) \mid j=1, 2, ..., N\}$ directly. We have the equations

$$\cos(fj\,\Delta t)\,C_f + \sin(fj\,\Delta t)\,S_g + \cos(gj\,\Delta t)\,C_g + \sin(gj\,\Delta t)\,S_g = \phi(j\,\Delta t) \qquad (2.19)$$

for $j=0, 1, ..., N-1$. Here again f and g are only approximated quantities. Equations (2.19) can be inverted to obtain the amplitudes, where the j's have to be chosen to be small enough, and the resultant linear equations should be made mutually independent.

Method C. In many physical problems, one has to treat anharmonic problems, where fundamental frequencies are accompanied by many harmonics. In such a case, it is often that the number of harmonics to be included is not known clearly, since the high harmonics tend to have diminishing amplitudes. For these problems, the above methods A and B do not always work, because the truncated components can generate numerical instability and, thereby, large error. Here we assume that the fundamental frequencies f and g are associated with some harmonics mf and ng, where $m=1, 2, ...,$ and $n=1, 2, ...$ Then we can construct a least-squares procedure by minimizing the functional

$$\sum_i \Big[\phi(t_i) - \sum_m \{C_{mf}\cos(mft_i) + S_{mf}\sin(mft_i)\} - \sum_n \{C_{ng}\cos(ngt_i) + S_{ng}\sin(ngt_i)\} \Big]^2, \qquad (2.20)$$

where t_i are sampling points which should be selected among the short time data and make the resultant linear equations nonsingular. One of these simultaneous linear equations is then, for instance,

$$\sum_i \cos(m'ft_i) \Big[\sum_m \{C_{mf}\cos(mft_i) + S_{mf}\sin(mft_i)\} - \sum_n \{C_{ng}\cos(ngt_i) + S_{ng}\sin(ngt_i)\} \Big] = \sum_i \cos(m'ft_i)\,\phi(t_i) \qquad (m'=1, 2, ...). \qquad (2.21)$$

E. *Decoupling of the Tail Effects (Improvement of the Frequencies)*

We have now the first estimate of amplitudes, which can in turn be made use of in order to improve the first guess of the frequencies. We remember that the frequencies have been estimated through Eqs. (2.15) and (2.16), in which the original (raw) spectral data of FFT were adopted. However, each peak in a FFT spectrum is contaminated by long tails extended from the other peaks. Let us look at the FFT spectrum at $F_c(K)$, that is,

$$F_c(K) \approx \frac{1}{T}\frac{C_f\sin(fT) - S_f[\cos(fT)-1]}{f-2\pi K/T} + \frac{2}{N}\sum_{j=0}^{N-1}\cos\left(\frac{2\pi Kj}{N}\right) \times \{C_g\cos(gj\,\Delta t) + S_g\sin(gj\,\Delta t)\}. \qquad (2.22)$$

The second term in the right-hand side forms the tail extended from frequency g. The magnitude of the tail is not necessarily small in general, since it looks like

$$\frac{C_g}{T}\frac{\sin(gT)}{g-2\pi K/T} + \frac{C_g}{T}\frac{\sin(gT)}{g+2\pi K/T} - \frac{S_g}{T}\frac{\cos(gT)-1}{g-2\pi K/T} - \frac{S_g}{T}\frac{\cos(gT)-1}{g+2\pi K/T} \qquad (2.23)$$

and thus its range is very long, just like the Coulomb potential. It is a trivial work to remove the effect of the tail in Eq. (2.22) and, thus, we obtain the purer spectrum, for instance,

$$F'_c(K) = F_c(K) - \frac{2}{N}\sum_{j=0}^{N-1}\cos\left(\frac{2\pi Kj}{N}\right) \times [C_g\cos(gj\,\Delta t) + S_g\sin(gj\,\Delta t)], \qquad (2.24)$$

which should be returned to Eq. (2.15) to refine the frequencies.

The renewed frequencies are again inserted into Eq. (2.18), Eq. (2.19), or Eq. (2.21) to improve the amplitudes. This entire process should be iterated until a convergence is attained.

F. *The Iteration Method for the Amplitudes*

When we treat a spectrum composed of many peaks, the matrices and vectors in Eq. (2.18) become large. To avoid this, we can solve Eq. (2.18) in an iterative manner: Going back to Eqs. (2.10) and (2.11), we can set up the following linear equations for the amplitudes associated with the frequency f;

$$\begin{bmatrix} \dfrac{\sin(fT)}{fT-2\pi K}+\dfrac{\sin(fT)}{fT+2\pi K} & -\dfrac{\cos(fT)-1}{fT-2\pi K}-\dfrac{\cos(fT)-1}{fT+2\pi K} \\ \dfrac{\cos(fT)-1}{fT-2\pi K}-\dfrac{\cos(fT)-1}{fT+2\pi K} & \dfrac{\sin(fT)}{fT-2\pi K}-\dfrac{\sin(fT)}{fT+2\pi K} \end{bmatrix} \begin{bmatrix} C_f \\ S_f \end{bmatrix} = \begin{bmatrix} F'_c(K) \\ F'_s(K) \end{bmatrix}, \qquad (2.25)$$

where F'_c and F'_s are the spectra in which the tail effects have been subtracted as in Eq. (2.22). The similar set of equations can be set up for each frequency. In the calculation of the purified spectra F', however, the amplitudes should have been known beforehand. Thus the procedure should be carried out iteratively.

III. NUMERICAL EXAMPLES

Here we present two simple, but not necessarily easy, examples to show how the method works.

EXAMPLE I. The first example is confined to only two frequency cases for the sake of simplicity, although our procedure and program are general. The iteration procedure from Subsection IIC to IIE has been performed. The matrix $\{A_{sc}\}$ has been evaluated directly with Eq. (2.7). The sample functions are chosen to be exactly the same form as in Eq. (2.1). One is

$$\phi_1 = \cos(5.5\,t) + 2.0\sin(11.0\,t),$$

where two frequencies are far apart and the other is

$$\phi_2 = \cos(10.5\,t) + 2.0\sin(11.0\,t)$$

which has relatively close frequencies, in which the tails have stronger magnitude.

Δt, T, and N are varied. The standard values of Δt here is 0.1, which is not very small compared with the shortest period in the above trigonometric functions involved, that is, about 0.571. The standard value of N here is 2048 (2^{11}). This is a small-scale FFT. In short, our examples are set so that the conditions are not exceptionally good, or rather, relatively worse than the usual applications of FFT. The resolution of frequency in FFT is

$$\Delta f = \frac{2\pi}{T} = \frac{2\pi}{N\,\Delta t}. \qquad (3.1)$$

For our standard values of Δt and N, Δf is about 0.030680, which means the resolution of frequency by the present FFT is up to the first decimal point below zero.

The convergence has been judged when the successive improvement of the frequencies does not exceed 10^{-13}. The number of iterations was generally about five to 10. Since the first guess of the frequencies and amplitudes are not *relatively* good, the second iteration improves their values significantly. The convergence after the second iteration is, hence, slow.

The results are shown in Table I. Method A is referred to a procedure using Eq. (2.18), and B to that based on Eq. (2.19). As seen in the table, the results obtained are generally very good. In particular, the accuracy of the frequencies is far beyond the FFT resolution mentioned above.

On the other hand, the accuracy of the amplitude is not as good as that of the frequencies. In particular, Method A reproduces the amplitudes rather poorly as noted in subsection IID. Method B, which is faster, gives better results as anticipated.

In Eq. (2.9), the sum has been approximated by the integral. This must be crucial. Hence the result depends on how small Δt can be chosen. On the other hand, if we let Δt become smaller with keeping N constant, Δf becomes larger in accordance with Eq. (3.1), which in turn means that the dominance by the single term in Eq. (2.13) is deteriorated. Thus the better results are expected only when N is increased simultaneously. We choose $\Delta t = 0.05$ and $N = 4096 = 2^{12}$. As seen in Table I, the errors both in the frequencies and amplitudes have been reduced by a factor of about 2.

EXAMPLE II. This example has been taken from a realistic physical problem. Let us consider a classical Hamiltonian for the Morse oscillator, namely,

$$H = \frac{p^2}{2} + (1 - e^{-q})^2, \qquad (3.2)$$

TABLE I

The Frequencies and Amplitudes Extrated from the FFT Spectra

Methods[a]	f	C_f	S_f	g	C_g	S_g
ϕ_1						
Exact	5.500000	1.000000	0.000000	11.000000	0.000000	2.000000
A[b]	5.500069	0.990846	0.006965	11.000004	−0.000806	1.999547
A[c]	5.500035	0.995401	0.003507	11.000002	−0.000400	1.999776
B[b]	5.500069	1.000005	0.000018	11.000006	−0.000005	1.999991
B[c]	5.500034	1.000002	0.000010	11.000003	−0.000002	1.999995
ϕ_2						
Exact	10.500000	1.000000	0.000000	11.000000	0.000000	2.000000
A[b]	10.500061	0.990914	0.006258	11.000001	−0.000243	1.999885
A[c]	10.500030	0.995432	0.003152	11.000001	−0.000103	1.999953
B[b]	10.500055	1.000108	0.000072	11.000016	−0.000107	1.999928
B[c]	10.500027	1.000057	0.000032	11.000008	−0.000057	1.999968

[a] Method A is based on Eq. (2.18), while B is based on Eq. (2.19).
[b] $\Delta t = 0.1$, $N = 2^{11}$, $\Delta f = 0.030680$.
[c] $\Delta t = 0.05$, $N = 2^{12}$, $\Delta f = 0.030680$.

where q is a coordinate in configuration space and p is its conjugate momentum. In order to calculate the action variable I,

$$I = \frac{1}{2\pi} \oint p\, dq, \tag{3.3}$$

we have defined a function $B'(t)$ [4]

$$B'(t) = \frac{1}{2}\left[\{q(t) - q(0)\} \frac{dp(t)}{dt} + \{p(t) - p(0)\} \frac{dq(t)}{dt} \right] \tag{3.4}$$

along a classical trajectory (the solution of the Hamilton canonical equations of motion). It can be shown [4] that $B'(t)$ can be represented as

$$B'(t) = a + \omega \sum_{m=1} m[b_m \cos(m\omega t) - c_m \sin(m\omega t)], \tag{3.5}$$

where ω is the fundamental frequency of the oscillating motion. Since the Morse potential is highly anharmonic, $B'(t)$ in Eq. (3.5) involves many harmonics. Then the action variable I can be represented in terms of the Fourier data such that

$$I = -\sum_{m=1} m b_m. \tag{3.6}$$

The entire theory for the action–angle variables will be given elsewhere [4].

This time, we have carried out the larger scale FFT, that is, $N = 16384$ (2^{14}), and $T = 12500.513$ ($\Delta t = 0.762971$), so that the resolution of the present FFT is about ($\Delta f =$) 0.00050. The amplitudes have been determined by Method C of Section IID. Some 20 harmonics have been observed in the power spectrum of $B'(t)$. In the present calculation, the harmonics up to the 90th have been taken into account just for the safety in Eq. (2.21). The number of the sampling points for the least-squares procedure in Eq. (2.21) is 190, which is also sufficiently large. We picked up five energy points, each of which corresponds to the exactly quantized energy [2a].

The convergence of the iterated procedure to remove the tail effect is much faster than that of the first example, presumably because the size of the FFT here is much larger. This is shown in Table II, where the fundamental frequencies obtained at each iteration are displayed. For all energies the convergence has been attained in three iterations.

In Table III, these values, together with the resultant action variables based on Eq. (3.6), are compared with the exact values, which happen to be available in analytical expressions [5]. The accuracy of our procedure for extracting the frequencies from the FFT data is remarkably good. The minor exceptions are the action variables I_B at $E = 0.879101$ and $E = 0.969812$. (Note that the dissociation limit is $E = 1.0$.) Closer examination has revealed that this is simply because the present FFT with $N = 2^{14}$ was too small to reproduce the very high harmonics having finite amplitudes. The errors are extremely small anyway.

Martens and Ezra [2a] have performed FFT calculation over $q(t)$ and $p(t)$ for the same Morse potential with their own window technique. Some of their resultant frequencies, of which energies are slightly different from those of Table III, are referred to in Table IV, along with the exact

TABLE II

The Convergence of the Iterated Procedure to Remove the Tail Effect

Energy	$n = 1^a$	$n = 2^a$	$n = 3^a$
0.243902	1.2297138	1.2297138	1.2297138
0.516154	0.98371325	0.98371325	0.98371325
0.727889	0.73771371	0.73771373	0.73771373
0.879109	0.49171319	0.49171313	0.49171313
0.969812	0.24571486	0.24571470	0.24571470

[a] The fundamental frequencies in the nth iteration.

TABLE III

The Frequencies and Action Variables for the Morse Oscillator

Energy(E)	$\omega_{\text{exact}}{}^a$	$\omega_B{}^b$	$I_{\text{exact}}{}^c$	$I_B{}^d$
0.243902	1.229714	1.229714	0.184500	0.184500
0.516154	0.983713	0.983713	0.430500	0.430500
0.727889	0.737714	0.737714	0.676500	0.676500
0.879109	0.491713	0.491713	0.922500	0.922507
0.969812	0.245715	0.245715	1.168498	1.168500

Note. The amplitudes have been determine by Method C, Eq. (2.21).

[a] Exact frequency $\omega(E) = [2(1-E)]^{1/2}$, Ref. [5].

[b] Approximate frequencies through the FFT data of 2^{14} sampling points. The resolution of the present FFT is 0.000503.

[c] Exact action variable $I(E) = 2^{1/2}[1 - (1-E)^{1/2}]$, Ref. [5].

[d] Approximate action variables through the FFT data, Eq. (3.6).

TABLE IV

The Fundamental Frequencies with the Window Technique [a]

Energy(E)	$\omega_{\text{exact}}{}^b$	$\omega_{\text{ME}}{}^a$
0.243903	1.229713	1.229711
0.516156	0.983711	0.983711
0.727895	0.737706	0.737708
0.879119	0.491693	0.491691
0.969816	0.245699	0.245700

[a] The results by Martens and Ezra, Ref. [2a].

[b] The exact frequencies obtained with an analytical expression as in Table III.

values. Their accuracy is also very good, although some deviations are found in the last decimal place, and our results are actually exact in this level. Unfortunately, however, this comparison is not complete, since our experience about the practical labor for window technique is limited. In fact, it is this expected complication in manipulating the standard window technique that have driven us to devise the new practical method. In conclusion, except for a procedure for coding a computer program of the process described in Section II, which is really easy, the frequencies and amplitudes are computed simply and very accurately with our proposed method.

IV. CONCLUDING REMARKS

We have proposed an efficient and simple idea to extract the frequencies and amplitudes of a quasi-periodic function from FFT spectra. FFT is performed only once without use of any window function. The numerical results have been found very accurate. One of the most annoying parts of the numerical procedure of FFT is the selection of window functions. This shortcoming has been improved [2] by finding the standard windows. Although the window technique can avoid the truncation effect (the Gibbs phenomenon), still accurate frequencies are not obtained, unless the true frequencies happen to coincide with the grid point provided by FFT. To improve the situation, one either has to take a very long time (T in Eq. (3.1)) of sampling points to reduce Δf (then a very large scale FFT is required if high frequency is necessary), or FFT should be repeatedly performed varying T so as to adjust a grid point of FFT to the true frequency (almost no hope for many frequency case). Interpolation method may be useful in this context. As far as we know, these delicate practices seem to demand some perception and experience, and thus are not appropriate for automated procedure. We hope that the present method can relax this situation in part.

We have described our iterative procedure for extracting from FFT data both frequencies and amplitudes. It is stressed, however, that the single application of Eq. (2.16) already leads to much more accurate frequencies beyond FFT resolution. Thus even Eq. (2.16) alone can provide a good approximation scheme.

Finally, the present procedure has been devised in a study of onset of Hamilton chaos. Its theoretical aspect and numerical examples will be presented elsewhere [6].

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