Dynamical Considerations on a New Approach to the Many-Body Problem*

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In Part A, a further analysis is made of the collective coordinate Lagrangian first introduced in a previous paper. This Lagrangian, which replaces the physical Lagrangian, describes a set of fictitious harmonic oscillators whose masses and frequencies are established. We accomplish this by adding a term to the physical Lagrangian which, however, does not affect the equations of motion. The analysis is carried out by two distinct methods: comparison of Lagrangians and comparison of equations of motion. Both methods yield identical results.

In Part B, the difficult problem of representing the Dirac δ function by a finite number of terms is handled by the introduction of the d-function. A specific representation of this function is given, along with plausibility arguments that it satisfies the requirements of Part A. A brief analysis and summary of the manifold properties of the d-function is presented.

INTRODUCTION[1]

IN a preceding paper,[2] we have indicated how the use of collective coordinates is able to simplify the highly nonlinear equations of motion encountered in the many-body problem. The essential idea was that by the introduction of these coordinates, one may replace approximately the usual physical Lagrangian in coordinate space by a simple Lagrangian in collective coordinate space which can be regarded as that of a system of one-dimensional bounded harmonic oscillators. The requirements for the validity of this replacement were determined by a direct comparison with the true Lagrangian.

In this paper we shall first re-examine the justification for the description of the actual motion of N physical particles in a one-dimensional box of length L with periodic boundary conditions by means of the motion of N one-dimensional bounded harmonic oscillators. The conditions for the validity of the collective coordinate Lagrangian are fulfilled by choosing suitable fictitious masses f_k and frequencies ω_k of the collective coordinate harmonic oscillators. Next we indicate that the equations of motion for the physical particles obtained from the Lagrangian of the fictitious oscillators are a very close approximation to the equations obtained from the true Lagrangian. Such an analysis is meaningful and necessary because the approximate identity of the two Lagrangians does not in itself imply the approximate equivalence of the corresponding equations of motion, since the differentiations required in the transition from the Lagrangian to the equations of motion may introduce inordinately large errors.

In carrying through both the comparison of the Lagrangians and that of the equations of motion, use is again made of one's ability to approximate suitably the Dirac δ function by means of N fourier terms. Such an approximation to the Dirac δ function has been termed the "d-function" (see Paper I). The difficult problem of finding the d-function is treated in further detail in Part B. Highly plausible arguments for the existence of such a d-function, and indeed for the legitimacy of a specific representation which we exhibit, will be presented in Part B.

In both Parts A and B, we are required to keep in mind the physical nature of the potential which we would like to treat. It is characterized by a repulsive core with a width of the order of an angstrom, a shallow attractive well of several angstroms, and an amplitude of zero thereafter. An example of this is the Morse-type potential.

A. EVALUATION OF THE OSCILLATOR PARAMETERS

I. Comparative Analysis of the Lagrangians

In this section we shall compare the collective coordinate Lagrangian with the physical Lagrangian and so obtain the optimum values for the fictitious masses and frequencies of the oscillators.

We assume the Lagrangian in physical space to be of the form

$$L_x=\tfrac{1}{2}\sum_i m\dot{x}_i^2-\tfrac{1}{2}\sum_i\sum_{j\neq i}V(x_i-x_j). \tag{1}$$

However, for reasons which will soon be made evident, we desire to replace Eq. (1) by a new Lagrangian $\bar{L}_x$ whose physical consequences are the same as those of L_x. This can be accomplished by making use of a simple theorem pertaining to the Lagrangian equations of motion:

> If the equations of motion resulting from a Lagrangian L' are a consequence of those resulting from a Lagrangian L, then except for certain singular values of the constant K, the Lagrangian $\bar{L}=L-KL'$ and L yield equivalent equations of motion.

* Portions of this Paper were first presented at the Washington Meeting of the American Physical Society, April 1954 [Phys. Rev. 95, 624A (1954)].

[1] This paper is a summary of a lengthy and detailed analysis which may be obtained at cost from the Department of Physics, Stevens Institute of Technology, Hoboken, New Jersey.

[2] G. J. Yevick and J. K. Percus, preceding paper [Phys. Rev. **101**, 1186 (1956)]. This paper will hereafter be referred to as Paper I.

The proof is left to the reader.

We employ this theorem in the following manner. As is well known, the acceleration of the center of mass of a system with the Lagrangian (1) is zero, i.e., $\sum\ddot{x}_i=0$. But this result may be obtained from an L' given by

$$L_x'=(\sum_i \dot{x}_i)^2. \quad (2)$$

It follows then that we may replace Eq. (1) by

$$\bar{L}_x=L_x-KL_x'$$
$$=\tfrac{1}{2}\sum_i m\dot{x}_i^2-K(\sum_i\dot{x}_i)^2-\tfrac{1}{2}\sum_i\sum_{j\neq i}V(x_i-x_j). \quad (3)$$

(The reader may verify that only the value $K=m/2N$ is singular.) As in previous work,[3] we assert that a suitable Lagrangian which takes the place of Eq. (3) is given by

$$L_q=\sum_{k\neq 0}\tfrac{1}{2}f_k(|\dot{q}_k|^2-\omega_k^2|q_k|^2)$$
$$+[N\sum_{k\neq 0}\tfrac{1}{2}\omega_k^2f_k-N(N-1)A/2], \quad (4)$$

where

$$q_k=\sum_i e^{ikx_i}. \quad (5)$$

It is readily seen that this is so if f_k, ω_k, A and K can be chosen such that

$$\sum_{k\neq 0}f_kk^2=m-2K \quad (6)$$

$$\sum_{i\neq j}(K+\sum_{k\neq 0}\tfrac{1}{2}f_kk^2e^{ik(x_i-x_j)})\dot{x}_i\dot{x}_j=0, \quad (7)$$

and

$$V(x_i-x_j)=\sum_{k\neq 0}\omega_k^2f_ke^{-ik(x_i-x_j)}+A. \quad (8)$$

Equation (6) can be solved exactly; Eq. (8) approximately because of the existence of N wave numbers k, and Eq. (7) only approximately irrespective of the finite number of wave numbers. As discussed in Paper I, the most effective method of using the finite number of k's is to introduce the d-function defined by

$$d(x-y)\equiv(1/L)+(1/L)\sum_{k\neq 0}d_ke^{ik(x-y)}, \quad (9)$$

where the k's are integral multiples of $k_0=2\pi/L$. If $d(x-y)$ is very narrow function we then have

$$V(y)\cong V_0+\sum_{k\neq 0}d_kV_ke^{-iky}, \quad (10)$$

where

$$V_k\equiv(1/L)\int_{-L/2}^{L/2}V(x)\exp(ikx)dx.$$

Since the particles never approach each other because of the assumed highly repulsive core (Fermi-Dirac statistics accentuates this), Eq. (7) will be closely satisfied if

$$K+\sum_{k\neq 0}\tfrac{1}{2}f_kk^2e^{ik(x_i-x_j)}\propto d(x_i-x_j). \quad (11)$$

We now observe the reason for including K in $\bar{L}_x$, for it provides the necessary constant term in Eq. (11). To within the approximations indicated, the solution to Eqs. (6), (7), and (8) now becomes trivial. We have

$$f_k=\frac{m}{\alpha N}\left(\frac{d_k}{k^2}\right),\quad \omega_k^2=\frac{\alpha Nk^2V_k}{m}, \quad (12)$$

and

$$K=m/2\alpha N,\quad A=V_0, \quad (13)$$

where α is defined by

$$\sum_k d_k\equiv\alpha N. \quad (14)$$

Equation (4) now becomes, in x-space, the following:

$$L_q=\tfrac{1}{2}m\sum_i\dot{x}_i^2+(mL/4\alpha N)\sum_i\sum_{j\neq i}d(x_i-x_j)\dot{x}_i\dot{x}_j$$
$$-(m/2\alpha N)(\sum_i\dot{x}_i)^2-$$
$$\sum_{i\neq j}\times(\sum_{k\neq 0}(1/L)V_kd_ke^{-ik(x_i-x_j)})+\text{const.} \quad (15)$$

We observe that the coefficient of the $d(x_i-x_j)\dot{x}_i\dot{x}_j$ term is very small. Moreover $d(x_i-x_j)\dot{x}_i\dot{x}_j$ has an appreciable value only when x_i is very close to x_j which, of course, is a rare event since the highly repulsive core forbids this. Even when $x_i=x_j$, the contribution to Eq. (15) is only $m\dot{x}_i\dot{x}_j/4\alpha$, which is still small.

II. Dynamics of the Collective Coordinates

In this section we shall analyze the equations of motion obtained from our modified Lagrangian L_q [Eq. (15)] using real particle coordinates. Utilizing the same masses and frequencies as in Sec. I, we shall be able to both minimize the effect of velocity dependent *forces* and reproduce the approximately correct *forces* acting on the real particles.

Thus, this discussion explicitly reinforces our interpretation of the connection between the collective coordinate Lagrangian and the physical coordinate Lagrangian inasmuch as the methods of Secs. I and II are distinct.

The equations of motion resulting from Eq. (15) may be written, after elimination of the $\sum_j\ddot{x}_j$ term which appears, as

$$m\ddot{x}_i=\sum_j^{j\neq i}F(x_i-x_j)+\sum_j^{j\neq i}W_{ij}+\frac{1}{N(\alpha-1)}\sum_j\sum_{h\neq j}W_{hj}, \quad (16)$$

where

$$W_{ij}\equiv\dot{x}_j^2U'(x_i-x_j)-\ddot{x}_jU(x_i-x_j), \quad (17)$$

$$U(x)\equiv(m/\alpha N)(1+\sum_{k\neq 0}d_ke^{ikx}), \quad (18)$$

and

$$F(x)\equiv-\sum_k ikV_kd_ke^{ikx}. \quad (19)$$

Equation (17) must be compared with the exact equations of motion given by

$$m\ddot{x}_i=-\sum_j^{j\neq i}\partial V(x_i-x_j)/\partial x_i. \quad (20)$$

To within the d-function approximation, Eqs. (16) and (20) differ only by the W terms on the right-hand side

[3] See Sec. II of Paper I.

of Eq. (16). It must now be established that the velocity dependent forces which these terms represent are small compared to the correct interparticle forces.

To begin with, let us compare

$$V'(x_i-x_j)\leftrightarrow \dot{x}_j^2 U'(x_i-x_j). \tag{21}$$

If, for the sake of simplicity, we assume that the distribution of velocities is approximately Maxwellian, $\dot{x}_j^2$ is of the order of $\kappa T/m$, where κ is Boltzmann's constant and T the absolute temperature. We must then investigate

$$V'(x_i-x_j)\leftrightarrow(\kappa T/m)U'(x_i-x_j). \tag{22}$$

This comparison can be rewritten

$$\frac{V'(x_i-x_j)}{V(0)}\leftrightarrow\left(\frac{\kappa T}{V(0)}\right)\frac{U'(x_i-x_j)}{U(0)}. \tag{23}$$

To show that the right hand side of (23) is negligible compared to the left hand side, we first observe that without loss of generality in any molecular problem we can make $V(0)\approx 2000$ ev. Anticipating the results of Part B in which it is shown that we can approximate $V(x)$ by a finite fourier series, it follows that $\kappa T/V(0)$ is of the order of 10^{-5} at $T=300$ degrees absolute. (For small T this result is strengthened.) Moreover, we have chosen f_k and k^2 such that

$$\frac{U'(x_i-x_j)}{U(0)}=\frac{d'(x_i-x_j)}{d(0)}. \tag{24}$$

Since $d'(x)$ rapidly goes to zero, it follows that

$$\frac{U'(x_i-x_j)}{U(0)}\lesssim\frac{V'(x_i-x_j)}{V(0)}, \tag{25}$$

except for small values of the argument where, however, the system is unlikely to be. Thus the first term on the right-hand side of Eq. (17) is small compared to $F(x_i-x_j)$.

Next, let us consider the second term on the right hand side of Eq. (17) and compare it with $F(x_i-x_j)$. This term may be evaluated by iteration of Eq. (16), but since only an estimate of error is required we shall consider just the first step in the iteration. That is, in the term $\ddot{x}_j U(x_i-x_j)$ we may choose $\ddot{x}_j=(1/m)\times\sum_h^{h\neq j}F(x_j-x_h)$. Hence we compare

$$\sum_j^{j\neq i} F(x_i-x_j)\leftrightarrow\frac{1}{m}\sum_j^{j\neq i}\sum_h^{h\neq j} F(x_j-x_h)U(x_i-x_j). \tag{26}$$

Let

$$\sum_h^{h\neq j} F(x_j-x_h)\equiv G(x_j), \tag{27}$$

then (26) becomes

$$G(x_i)\leftrightarrow(1/m)\sum_j^{j\neq i} U(x_i-x_j)G(x_j). \tag{28}$$

We note that in the second expression $j\neq i$, so that $U(x_i-x_j)/m\neq U(0)/m$ for any term. Now if x_j approaches x_i then since $U(0)/m\approx 1$, it is conceivable that a term in the right hand sum is of the same order of magnitude as $G(x_i)$ itself. This, however, is not possible because even if x_i is close enough to x_j to feel the full effect of the repulsive core, we have already presumably chosen $U(x)/m$ to be essentially zero in this region.

By means of the comparisons Eqs. (21) and (28), we have demonstrated that

$$\sum_j^{j\neq i} W_{ij}\ll\sum_j^{j\neq i} F(x_i-x_j). \tag{29}$$

There still remains the problem of showing that the rightmost term in Eq. (16) is small compared to $\sum F(x_i-x_j)$. Since

$$\sum_j\sum_{h\neq j} W_{hj}\lesssim N\sum_j^{j\neq i} W_{ij}, \tag{30}$$

(in absolute value) it will be sufficient to show that $1/(\alpha-1)$ is not large compared to 1. Clearly, if $\alpha\approx 1$, $1/(\alpha-1)$ becomes very large and the correction term may be enormous, whereas for $\alpha>1.5$, $1/(\alpha-1)$ is less than 2, which is quite satisfactory. It is no accident that K corresponding to $\alpha\approx 1$ is precisely the singular case which was noted following Eq. (3).

Since the d-function obtained by choosing $\Delta k=k_0$ and $d_k=1$ yields an $\alpha=1+1/N$, we conclude that serious difficulties may be encountered unless one selects a d-function with gap frequencies. This is, in fact, the problem which we propose to discuss in Part B of this paper.

Let us summarize this section by pointing out that the requirements for making the velocity-dependent forces negligible in the exact equations of motion, as well as reproducing the correct potential, are essentially the requirements needed to satisfy conditions I, II, and III in Paper I. The fundamental idea in each case is to make the velocity potential have a small nonzero value only well within the repulsive core of the physical potential so that it is never felt.

B. PRODUCT REPRESENTATION OF d-FUNCTION

I. Introductory Remarks

We have already indicated in Part A that the problem of representing the physical potential as well as minimizing the velocity dependent potential depends on a suitable approximation for the Dirac δ function, using only N Fourier terms. As a prototype for the d-function, although admittedly a poor one for our purposes, let us write down what one would naively obtain by utilizing the minimum mean square approximation to the Dirac δ function and assuming equally spaced frequencies. This function is given by

$$d(x)=\frac{1}{L}\sum_{k=-Nk_0/2}^{Nk_0/2} e^{ikx}=\frac{\sin[\frac{1}{2}(N+1)k_0x]}{L\sin(\frac{1}{2}k_0x)}, \quad (30)$$

We observe that the first zero of $d(x)$ occurs at $(N-1)k_0x/2=\pi$ or $x=L/N$. But for the case of gases with $L=1$ cm and $N\approx 10^7$ this $d(x)$ obliterates the details of the potential and obviously cannot be used. Moreover, in Part A, the above case, which corresponds to $\alpha=1$, has been shown to lead to serious difficulties.

One can show that expression (30) may equally well be obtained by choosing the frequencies k as having a random distribution between $-Nk_0/2$ and $+Nk_0/2$. Following this lead, we may then assume a distribution of frequencies between $-\infty$ and ∞ but with a probability distribution other than uniform. This results in an expectation value of the d-function which possesses all the desired properties. While the corresponding minimization of the standard deviation of the function does not seem to have an easy solution, evidence has been obtained[1] that this is not an insurmountable obstacle.

The major conclusions to be drawn from a more detailed analysis, not presented here for lack of space, are the following:

(a) It is necessary to utilize frequencies higher than $Nk_0/2$ to obtain a narrow d-function.

(b) The distribution of frequencies needed to achieve (a) must have a random nature which is evidenced by the appearance of numerous gaps since all frequencies must be integral multiples of k_0.

(c) It is not appropriate to have equal coefficients for all Fourier terms.

(d) The probability methods mentioned above indicate the justification for the existence of a suitable d-function which we shall now construct explicitly in Sec. II.

II. Product Representation

Drawing inspiration from the conclusions of the preceding section, we shall now indicate a plausible d-function which appears to be suitable for representing a periodic $V(x)$. Its main characteristic is the extreme narrowness of its central lobe. Another advantage is that $\alpha\neq 1$.

Consider the case where $\Delta k=k_0$; then Eq. (30) can be written in the following form (assuming that $N=3^r-1$).

$$d(x)=\frac{1}{L}\frac{\sin[\frac{1}{2}(N+1)k_0x]}{\sin(\frac{1}{2}k_0x)}=\frac{1}{L}\sum_{j=-N/2}^{N/2}\exp(ijk_0x)$$

$$=(1/L)\prod_{i=0}^{r-1}[1+2\cos(3^ik_0x)]\equiv d_r(x). \quad (31)$$

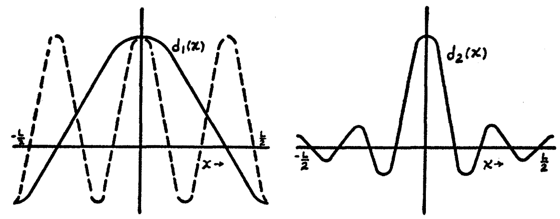

FIG. 1. Development of a d-function: (a) The first state $d_1(x)=1+2\cos(k_0x)$; the next factor $1+2\cos(3k_0x)$ is indicated by the dashed curve. (b) The second stage $d_2(x)$ results from multiplying the curves of Fig. 1(a).

The product form of the d-function [henceforth referred to as $d_r(x)$] is instructive from a geometrical point of view because it shows how the d-function approximates a δ function. The first factor produces a peak at $x=0$ and is -1 at $x=L/2$.

The next factor $[1+2\cos(3k_0x)]$ narrows the central lobe [this is indicated in Fig. 1(a) by a dashed line]. The product of these is given in Fig. 1(b). We observe that succeeding factors produce a more and more narrow central lobe and that side lobes are successively reduced.

We know, however, that $d_r(x)$ cannot be a good δ-function for our problem because the width of the central lobe for a given physical situation is too wide and washes out the details of the potential. It now suggests itself to use the form of Eq. (31) to construct a modified δ function which can be made more narrow at the expense of raising the side lobes to some extent. It is this δ function which we believe can suitably represent the potential. Consider the following:

$$d_r(x)=(1/L)\prod_{i=0}^{r-1}[1+f\cos(3+\epsilon)^ik_0x], \quad (32)$$

where f will be approximately 2, and by $(3+\epsilon)^i$ we mean the nearest integer thereto; f and ϵ are to be determined.

First a few obvious remarks:

$$\int_{-L/2}^{L/2} d_r(x)dx=1. \quad (33)$$

Moreover, qualitatively the geometrical appearance does not change significantly from that of the preceding analysis, with the exception that the central lobe is much narrower because of the higher maximum frequency which is present.

If

$$f=(2+\epsilon), \quad (34)$$

then the area underneath the central lobe is approximately 1. To see this, we observe that the width of the principal lobe is given by $1+(2+\epsilon)\cos(3+\epsilon)^{r-1}k_0x=0$, or $(3+\epsilon)^{r-1}k_0x\approx 2\pi/3$, a full width of $\sim 2L/(3+\epsilon)^r$;

but the amplitude at $x=0$ is $(3+\epsilon)^r/L$ so that the area of the principal lobe ≈ 1. The same choice of f leads to $d_r(0)=(3+\epsilon)^r/L$ which is the value at zero of a $\bar{d}_r$ whose maximum frequency is the same as the maximum frequency in $d_r(x)$, a fact which will be of some importance in the sequel.

We also note that

$$\alpha=(3+\epsilon)^r/N^r \approx \exp(r\epsilon/3). \tag{35}$$

We further observe from the above analysis that the ratio of the widths of the central lobe for $\epsilon\neq 0$ and $\epsilon=0$ is given by

$$3^r/(3+\epsilon)^r=1/\alpha \cong \exp(-r\epsilon/3). \tag{36}$$

Let us now consider what happens when $N, L\rightarrow\infty$ such that the density $n=N/L$ remains constant. The width of the central lobe is $2L/(3+\epsilon)^r$, but we have seen that $N\approx 3^r$; therefore the width becomes

$$2L/N^{\ln(3+\epsilon)/\ln 3}=(1/n)N^{-\epsilon/\ln 3}. \tag{37}$$

This goes to zero as $N\rightarrow\infty$ even if ϵ is a slowly decreasing function of r.

The problem arises as to whether the side lobes decrease sufficiently so that $d_r(x)$ actually approaches $\delta(x)$ as $r\rightarrow\infty$. Recalling the dependence of L and N on r, we rewrite Eq. (32) as

$$d_r(x)=n\prod_{i=0}^{r-1}\left[\tfrac{1}{3}+\tfrac{1}{3}f\cos((3+\epsilon)^i 2\pi nx/3^r)\right], \tag{38}$$

which may be recast into the interative form

$$d_{r+1}(x)=\left[\tfrac{1}{3}+\tfrac{1}{3}f\cos(2\pi nx/3^{r+1})\right]d_r((1+\epsilon/3)x). \tag{39}$$

We note from Eq. (39) that $d_{r+1}(x)$ is, except for a slight scale shift, a multiple of $d_r(x)$; moreover, the multiplying factor is predominantly less than unity, so that *all side lobes do tend to approach zero.* However, even if the above were rigorously true, it would not be sufficient to guarantee the efficacy of the resulting d-function because there may nonetheless exist regions for which the total area under the curve does not approach zero. A detailed argument indicating that this difficulty does not arise is presented in the Appendix.

We thus conclude that by the use of gaps in the wave number spectrum, it is possible to construct a suitable approximation to the Dirac δ function employing only $N=nL$ Fourier terms *if* we allow L to become sufficiently large. This validates the analysis made in Part A.

III. The Nature of Fourier Coefficients and Frequencies of the d-Function

We present without proof a summary of some typical results[1] emanating from various techniques for analyzing the d-function.

The Fourier coefficients of $d_r(x)$ are related to wave number density [normalized such that $\rho(k)=1$ when $\Delta k=k_0$] by the reciprocal relation

$$d_k\rho(k)\approx 1. \tag{40}$$

This can be interpreted by choosing for $d_r(x)$ a Fourier series with $\Delta k=k_0$ and constant Fourier coefficients between $-k_{\max}$ to $+k_{\max}$, and then causing the Fourier terms to coalesce in bunches.

Some typical forms for the density of wave numbers for the product representation are as follows:

$$\rho(k)\approx(k/k_0)^{-\epsilon/3\ln 3}, \tag{41}$$

$$\rho(k)\approx\frac{1}{(12\pi\alpha)^{\frac{1}{2}}}\frac{1}{b_{r-2}}\left\{\exp-\frac{3}{4\alpha}\left(\frac{k}{b_{r-2}}\right)^2+\exp\left[-\frac{3}{4\alpha}\left(\frac{k-b_{r-1}}{b_{r-2}}\right)^2\right]+\exp\left[-\frac{3}{4\alpha}\left(\frac{k+b_{r-1}}{b_{r-2}}\right)^2\right]\right\}. \tag{42}$$

Other forms involve discontinuous functions.

Another result concerns the evaluation of gap series sums of the form $\sum_{\{k\}}f(k,d_k,\rho_k)$, where $\{k\}$ denotes the set of available wave-numbers. It can be shown that for slowly varying f, one may as a reasonable approximation choose both ρ_k and d_k as constant

$$\rho_k=1/\alpha \quad\text{and}\quad d_k\approx\alpha \tag{43}$$

for the range $-N\alpha k_0/2\leq k\leq N\alpha k_0/2$.

The above results, while possessing intrinsic interest, are actually needed in the analytical description of physical phenomena by means of collective coordinates. As an example of what we mean, the partition function and the various thermodynamic quantities derived from it depend explicitly on d_k. A further analysis will be presented in a succeeding paper.

APPENDIX. LIMITING VALUE OF THE d-FUNCTION

In this appendix we present a plausibility argument for the transition of the d-function into the Dirac δ function as $r\rightarrow\infty$. Consider the expression

$$I_r(a)=\int_{-\infty}^{\infty}d_r(x)\exp(-a^2x^2/4)dx. \tag{1}$$

If $I_r(a)=1$ as $r\rightarrow\infty$ for any value of a then it is reasonably clear that $d_r(x)\rightarrow\delta(x)$. This appears to be a valid criterion for a δ function. First, we write $d_r(x)$

in the following form:

$$d_r(x)=n(\tfrac{2}{3}f)^r\prod_{i=0}^{r-1}\cos(\tfrac{1}{2}b_ix+\tfrac{1}{2}\beta)\cos(\tfrac{1}{2}b_ix-\tfrac{1}{2}\beta),\quad(2)$$

where

$$b_i=[(3+\epsilon)^i]2\pi n/3^r=[(3+\epsilon)^i]k_0,\quad(3)$$

and

$$\cos\beta\equiv 1/f.\quad(4)$$

Since

$$\cos x=\tfrac{1}{2}(\exp ix+\exp -ix)=\tfrac{1}{2}\sum_\epsilon e^{i\epsilon x},\quad(5)$$

where ϵ runs over the set $\{-1,1\}$, $d_r(x)$ is given by

$$d_r(x)=n(\tfrac{1}{6}f)^r\sum_{\{\epsilon_j,\eta_j\}}\exp[i\sum_j\tfrac{1}{2}(\epsilon_j+\eta_j)b_jx]\times\exp[i\sum_j\tfrac{1}{2}(\epsilon_j-\eta_j)\beta].\quad(6)$$

Hence,

$$I_r(a)=n\left(\frac{f}{6}\right)^r\frac{2\sqrt{\pi}}{a}\sum_{\{\epsilon_j,\eta_j\}}\exp\{-[\sum_j(\epsilon_j+\eta_j)b_j/2a]^2\}\times\exp[i\sum_j\tfrac{1}{2}(\epsilon_j-\eta_j)\beta].\quad(7)$$

Let us now define a j_0 such that $b_{j0}=a$. Such a j_0 exists since as $r\to\infty$, we may assume that b_0 decreases to zero and b_{r-1} increases to ∞. We observe that

$$[\sum(\epsilon_j+\eta_j)b_j/2a]^2\sim(b_{j'}/a)^2,\quad(8)$$

where j' is the highest j for which $\epsilon_j+\eta_j\neq 0$; the reason for this is that

$$\left|\sum_{j=0}^{j'-1}\tfrac{1}{2}(\epsilon_j+\eta_j)b_j\right|\lesssim\sum_{j=0}^{j'-1}b_j<b_{j'}/2+\epsilon.$$

If $j'\geq j_0$, then $\exp-(b_{j'}/a)^2$ is negligible and we can neglect such terms. Therefore only terms for which $\epsilon_j+\eta_j=0$ whenever $j\geq j_0$ contribute to the sum.

On the other hand, if $j'<j_0$ then

$$\exp-(b_{j'}/a)^2\approx 1.\quad(9)$$

We conclude that

$$I_r(a)=\frac{2n\sqrt{\pi}}{a}\left(\frac{f}{6}\right)^r\Big(\sum_{\{\epsilon_j,\eta_j\}}^{j<j_0}\exp[i\sum_j\tfrac{1}{2}(\epsilon_j-\eta_j)\beta]\Big)$$

$$\times\Big(\sum_{\{\epsilon_j\}}\exp(i\sum\epsilon_j\beta\Big)=\frac{2n\sqrt{\pi}}{a}\left(\frac{f}{6}\right)^r\Big[\prod_{j<j_0}\Big(\sum_{\epsilon_j}\exp(i\epsilon_j\beta/2)\Big)$$

$$\times\Big(\sum_{\eta_j}\exp(-i\eta_j\beta/2)\Big)\Big(\prod_{j\geq j_0}\sum_{\epsilon_j}\exp(i\epsilon_j\beta)\Big),$$

or

$$I_r(a)=(2n\sqrt{\pi}/a)(f/6)^r\times[2\cos(\beta/2)]^{2j_0}[2\cos\beta]^{r-j_0}.\quad(10)$$

Recalling that $\cos\beta=1/f$, it follows that $\cos\beta/2=[(f+1)/2f]^{\frac{1}{2}}$ and $a=b_{j0}=(3+\epsilon)^{j_0}n2\pi/3^r$. Equation (10) becomes

$$I_r(a)=\frac{2n\sqrt{\pi}3^r}{2\pi n(3+\epsilon)^{j_0}}\left(\frac{f}{6}\right)^r2^{j_0}\left(\frac{f+1}{f}\right)^{j_0}2^{r-j_0}f^{j_0-r}$$

$$=\frac{1}{\sqrt{\pi}}\left(\frac{f+1}{3+\epsilon}\right)^{j_0}.\quad(11)$$

If $f=2+\epsilon$ then $I_r(a)$ is independent of a. Due to the crudity of the analysis, the value of $I_r(a)$ is 0.6 rather than 1.

The above discussion makes plausible our belief that by the use of gaps, we are able to construct a suitable representation of the Dirac δ function, using only N frequencies.

We should like to point out briefly that the specific choice of b_j which we have utilized is a special case of a more general situation in which, however, f is a function of j as well. It is again necessary for $(b_{j+1}/b_j)>3$ in order to improve (31). With b_j subject only to this condition, the preceding analysis Eqs. (1) to (11) can be easily carried through in precisely the same manner providing only that one chooses

$$1+f_j=b_{j+1}/b_j.\quad(12)$$