# On the convergence of the Rayleigh ansatz for hard-wall scattering on arbitrary periodic surface profiles



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# On the convergence of the Rayleigh ansatz for hard-wall scattering on arbitrary periodic surface profiles

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**Abstract.** The plane-wave ansatz for the scattered waves is convergent only if, roughly speaking, the surface profile is (i) not too deep and (ii) sufficiently smooth. This convergence is investigated for general one-dimensional corrugations by means of an asymptotic analysis. The results are explicitly given for a three-term Fourier series and for analytic approximations to linear profiles with discontinuous slopes. A relation between the convergence and the maximal curvature is established for triangular corrugations, and used for the definition of a pseudoinvariant which is slowly varying for various corrugation profiles.

## 1. Introduction

The scattering of waves from a corrugated surface was first studied by Rayleigh using a plane-wave ansatz. This so-called Rayleigh hypothesis is only valid if the periodic corrugation is not too steep. Petit and Cadilhac (1966) were the first to prove that the Rayleigh ansatz diverges for a sinusoidal corrugation, when the ratio depth to period $2h/a > 0.1425$. Later, Millar (1969, 1971) proved that this is exactly the limit of convergence, and that below this limit the Rayleigh hypothesis is valid. In 1978, Hill and Celli used an asymptotic evaluation of the scattering amplitudes to discuss the convergence of the plane-wave ansatz to the solution of the Helmholtz equation. They found the limit of the two-dimensional sinusoidal profile to be $2h/a = 0.592$. Van den Berg and Fokkema (1979) investigated the convergence for gratings with periodic profiles exhibiting discontinuous slopes by using analytic approximations with finite Fourier series. In a later paper (van den Berg and Fokkema 1980) they extended these results to non-periodic profiles as given by a perturbation in a plane surface.

The purpose of this paper is (1) to show that the same conditions for convergence found by Hill and Celli can be derived from the eikonal approximation of the scattering problem; (2) to use the approach of Hill and Celli to explain the influence of the different profile parameters on the convergence limit for some typical profile functions; (3) to find a convergence parameter (other than $h/a$) allowing estimation of the convergence limit from Fourier coefficients and/or simple geometrical characteristics like the minimum radius of curvature or the maximal amplitude of the corrugation. Though an exact criterion for the limit of the convergence cannot be proved, a rough estimate is possible since a nearly constant or slowly varying convergence parameter, a pseudoinvariant, can be defined.

  

## 2. Definitions and mathematical preliminaries

The wavefunction $\psi(\boldsymbol{R}, z)$ with $\boldsymbol{R}=(x, y)$ should satisfy the Helmholtz equation

$$\Delta\psi + k^2\psi = 0, \tag{2.1}$$

where $k=\omega/c$ is the wavevector. According to a hard-wall potential at the corrugated surface $z=D(\boldsymbol{R})$, the wavefunction has to vanish on the boundary

$$\psi(\boldsymbol{R}, D(\boldsymbol{R})) = 0. \tag{2.2}$$

By superposition of plane waves, the solution is

$$\psi(\boldsymbol{R}, z) = \exp(\mathrm{i}\boldsymbol{K}_i \cdot \boldsymbol{R} + ik_{iz}z) + \sum_{\boldsymbol{G}} A_G \exp(\mathrm{i}\boldsymbol{K}_G \cdot \boldsymbol{R} + ik_{Gz}z), \tag{2.3}$$

with $\boldsymbol{k}_i = (\boldsymbol{K}_i, k_{iz})$, the incident $k$-vector decomposed into a component $\boldsymbol{K}_i$ parallel to the (asymptotic) surface and one perpendicular to it, $k_{iz}$. The sum goes over all scattered waves numbered by the reciprocal surface lattice vector $\boldsymbol{G}$, with $k$-vector $\boldsymbol{k}_G = (\boldsymbol{K}_G, k_{Gz})$ and beam amplitude $A_G$. In order to guarantee surface periodicity

$$\psi(\boldsymbol{R} + \boldsymbol{R}_n, z) = \exp(\mathrm{i}\boldsymbol{K}_i \cdot \boldsymbol{R}_n)\psi(\boldsymbol{R}, z), \tag{2.4}$$

(2.3) becomes

$$\psi(\boldsymbol{R}, z) = \exp(\mathrm{i}\boldsymbol{K}_i \cdot \boldsymbol{R})\left(\exp(\mathrm{i}k_{iz}z) + \sum_{\boldsymbol{G}} A_G \exp(\mathrm{i}\boldsymbol{G} \cdot \boldsymbol{R} + ik_{Gz}z)\right), \tag{2.5}$$

and the boundary condition is

$$\sum_{G} A_G \exp(\mathrm{i}G \cdot \boldsymbol{R} + \mathrm{i}k_{Gz}D(\boldsymbol{R})) = -\exp(-\mathrm{i}k_{0z}D(\boldsymbol{R})), \tag{2.6}$$

where, because of $|k_i| = |k_G|$ and $\boldsymbol{k}_G = \boldsymbol{K}_i + \boldsymbol{G}$,

$$k_{Gz} = \begin{cases} [k_i^2 - (\boldsymbol{K}_i + \boldsymbol{G})^2]^{1/2} & \text{for } |\boldsymbol{K}_i + \boldsymbol{G}| < k_i, \text{ i.e. in the Ewald sphere EW,} \\ \mathrm{i}[(\boldsymbol{K}_i + \boldsymbol{G})^2 - k_i^2]^{1/2} & \text{outside EW.} \end{cases} \tag{2.7}$$

Since the sum in (2.5) extends over infinitely many $G$-vectors, the scattered beams with real $k_{Gz}$ and the evanescent waves for $z \to +\infty$ with imaginary $k_{Gz}$, its convergence is, in general, an open question.

It will now be shown that the eikonal approximation (Garibaldi *et al* 1975) applied to very large $G$-vectors (in contrast to its usual application range with $\boldsymbol{G} \in \mathrm{EW}$) gives the correct asymptotic solution. The eikonal approximation is

$$A_G = A^{-1} \int_{(A)} \mathrm{d}R \exp[-\mathrm{i}\boldsymbol{G} \cdot \boldsymbol{R} - \mathrm{i}(k_{Gz} + k_{0z})D(\boldsymbol{R})], \tag{2.8}$$

where the integral should be extended symmetrically over the unit cell; any other choice gives only an arbitrary phase factor for $A_G$, which is irrelevant for the intensities (scattering probabilities)

$$P_G = (k_{Gz}/k_{0z})|A_G|^2. \tag{2.9}$$

According to the conservation of the particle currents, the unitarity condition, i.e. $\Sigma_G P_G = 1$, should be fulfilled.

## 3. Evaluation of the asymptotic scattering amplitudes from the eikonal integral

The double sum of the scattered waves $\psi_{sc}$ has to be convergent for the Rayleigh ansatz to hold. Its asymptotic parts depend on the direction $\boldsymbol{g}=\boldsymbol{G}/G$, since in the double sum $\boldsymbol{G}$ goes to infinity, i.e. $\boldsymbol{G}=\boldsymbol{g}G$ with $G\rightarrow+\infty$. The eikonal integral is evaluated as an integral over the complex variables $x$ and $y$ by the saddle-point method. It has to be extended to the complex plane with $x=x_1+\mathrm{i}x_2$ and $y=y_1+\mathrm{i}y_2$, where $x_1$, $y_1$ are the real and $x_2$, $y_2$ the imaginary parts of $x$, $y$. For simplicity, we consider a rectangular surface lattice with lattice constants $a_1$ and $a_2$. Because of the integrand periodicity, the complex line integral

$$\int \mathrm{d}x=\int_{\substack{x_2=0\\(x_1=-a_1/2)}}^{\infty}\mathrm{d}(\mathrm{i}x_2)=\int_{\substack{x_2=0\\(x_1=a_1/2)}}^{\infty}\mathrm{d}(\mathrm{i}x_2) \tag{3.1}$$

and analogously for $\int \mathrm{d}y$. Therefore, the path of integration from $-a_1/2$ to $a_1/2$ in $x$ can be extended to a U-like shape in the complex $x$-plane with $-a_1/2$, $a_1/2$ being the basis of the U-like path. The U-shaped path has to go to $-\infty$ or $\infty$, if $G_x$ is positive or negative, respectively, to define a convergent integral, since $\exp[-\mathrm{i}G_x(x_1+\mathrm{i}x_2)]=\exp(-\mathrm{i}G_xx_1+G_xx_2)$ has to go to zero. The same holds for the complex integral in the complex $y$-plane.

Because of the regularity of the integrand (entire function), these U-shaped ways can be deformed and eventually be guided through the saddle points of the integrand. For large $G$, the eikonal integral becomes

$$A_G=\int_C \mathrm{d}x\,\mathrm{d}y\exp[F_G(x,y)], \tag{3.2}$$

$$F_G(x,y)=(-\mathrm{i}\boldsymbol{g}\cdot\boldsymbol{R}+D(\boldsymbol{R}))G+F_0(x,y), \tag{3.3}$$

$$F_0(x,y)=(\boldsymbol{g}\cdot\boldsymbol{K}_{\shortparallel}-\mathrm{i}k_{0z})D(\boldsymbol{R}), \tag{3.4}$$

where use has been made of $k_{Gz}\sim\mathrm{i}(G+(\boldsymbol{K}_{\shortparallel},\boldsymbol{g}))+\mathrm{O}(1/G)$ following from (2.7) for large $G$.

The saddle points are given by the condition of stationary phase, i.e.

$$G^{-1}\,\partial F_G/\partial\boldsymbol{R}=(-\mathrm{i}\boldsymbol{g}+\partial D/\partial\boldsymbol{R})=0, \tag{3.5}$$

defining a set of complex solutions $\boldsymbol{R}^s$ $(s=1,2,\ldots,S)$ depending on $\boldsymbol{g}$, the asymptotic direction.

The asymptotic value of the eikonal integral therefore becomes

$$A_G\sim\sum_s\int_{C_s}\mathrm{d}x\,\mathrm{d}y\exp\left[F_G(\boldsymbol{R}^s)+\tfrac{1}{2}\left(\sum_{\alpha,\beta=1}^{2}\frac{\partial^2F_G}{\partial R_\alpha\,\partial R_\beta}\bigg|_{\boldsymbol{R}^s}(R_\alpha-R_\alpha^s)(R_\beta-R_\beta^s)\right)\right], \tag{3.6}$$

where the integration path has to be led along $C_s$, the valley-to-valley path through the saddle point. The main contribution comes from the close vicinity of $\boldsymbol{R}^s$ only. The remaining Gauss integral is easily found to be

$$\int_{C_s}\mathrm{d}x\,\mathrm{d}y\exp(\tfrac{1}{2}[\ \ ])=\left(\frac{-2\pi}{\partial^2F_G/\partial x^2}\right)^{1/2}\left(\frac{-2\pi}{\partial^2F_G/\partial y^2-(\partial^2F_G/\partial x\partial y)^2/(\partial^2F_G/\partial x^2)}\right)^{1/2}. \tag{3.7}$$

If

$$\mathrm{Re}(\partial^2 F_G/\partial x^2) < 0, \tag{3.8}$$

$$\mathrm{Re}[\partial^2 F_G/\partial y^2 - (\partial^2 F_G/\partial x \partial y)^2/(\partial^2 F_G/\partial x^2)] < 0, \tag{3.9}$$

the conditions of $C_s$ to be a valley-to-valley path through the saddle point $\boldsymbol{R}^s$ are fulfilled.

Apart from a factor (3.7), the different saddle points contribute to a geometrical series by its exponential term $\exp[F_G(R^s)]$. The term with the largest $\mathrm{Re} F_G(\boldsymbol{R}^s)$, i.e. for $s = d$ with

$$\max \mathrm{Re}\ F_G(\boldsymbol{R}^s) = \mathrm{Re}\ F_G(\boldsymbol{R}^d), \tag{3.10}$$

gives the dominant saddle point $\boldsymbol{R}^d$. Therefore the eikonal integral for large $G$ yields

$$A_G \sim \exp[F_G \cdot (\boldsymbol{R}^d)] \frac{2\pi}{|[(\partial^2 F_G/\partial x^2)(\partial^2 F_G/\partial y^2) - (\partial^2 F_G/\partial x \partial y)^2]_{\boldsymbol{R}=\boldsymbol{R}^d}|^{1/2}}, \tag{3.11}$$

where the phase factor is defined up to an irrelevant sign in front of the square root. Inserting this result into (2.5) gives, for the asymptotical ($G \gg 1$) part of the scattered wavefunction,

$$\psi_{\mathrm{sc}} \sim \exp(\mathrm{i}\boldsymbol{K}_i \cdot \boldsymbol{R}) \sum_{\boldsymbol{G}}{}' \frac{\text{constant}}{G} \exp[(-\mathrm{i}\boldsymbol{g} \cdot \boldsymbol{R}^d + D(\boldsymbol{R}^d))G$$
$$+ (\boldsymbol{g} \cdot \boldsymbol{K}_t - \mathrm{i}k_{0z}) D(R^d) + \mathrm{i}\boldsymbol{G} \cdot \boldsymbol{R} - Gz] \tag{3.12}$$

which is majorised, apart from a $G$-independent factor, by the series

$$\sum_{\boldsymbol{G}}{}' \text{constant} \exp(-\mathrm{i}\boldsymbol{g} \cdot \boldsymbol{R}^d + D(\boldsymbol{R}^d) - D_{\min})G \tag{3.13}$$

for all $z > D_{\min}$, the absolute minimum of $D$, i.e. in the whole range of the solution. The prime on the sum indicates that finite $\boldsymbol{G}$ are omitted, i.e. only the asymptotical contributions, which are responsible for convergence, have to be taken. The Rayleigh ansatz is therefore convergent if the majorant converges, i.e. if

$$\mathrm{Re}(D(R^d) - \mathrm{i}\boldsymbol{g} \cdot R^d - D_{\min}) \leq 0. \tag{3.14}$$

The convergence limit is given by the equality sign in (3.14), since the sum (3.12) then becomes divergent for all $\boldsymbol{R}$.

The conditions for convergence of the Rayleigh ansatz are given by (3.5) defining the saddle point $\boldsymbol{R}^s$ ($s = 1, 2, \ldots, S$), by (3.10) defining the dominant saddle point $\boldsymbol{R}^d$, contributing most to the integral, and by (3.14) defining the convergence limit. These equations are identical to the ones given by Hill and Celli (1978) indicating that the eikonal formula yields the correct scattering amplitudes in the limit of large $\boldsymbol{G}$ vectors.

Since the saddle points $\boldsymbol{R}^s(\boldsymbol{g})$ are complex and depend on $\boldsymbol{g}$, the following symmetry relation holds:

$$\boldsymbol{R}^s(-\boldsymbol{g}) = (\boldsymbol{R}^s(\boldsymbol{g}))^*, \tag{3.15}$$

i.e. it is generally sufficient to consider only the range $g_x > 0$, which simplifies the problem considerably. It is also possible to use the symmetry of the lattice for further simplification. In a square lattice with $\boldsymbol{g} = (\cos\gamma, \sin\gamma)$ for example, $\gamma$ can be restricted to the range $(0, \pi/4)$. Since the saddle points depend on $\gamma$, the dominancy may change from one saddle point to another if $\gamma$ is varied.

In order to find the convergence limit, it is expedient to look for a maximal multiplier $H$, the convergence factor of a class of similar profiles

$$D(\mathbf{R}) = hd(\boldsymbol{R}), \tag{3.16}$$

where $d(\boldsymbol{R})$ is a suitably normalised unit form of the corrugation function, and $h>0$. Without corrugation, i.e. for the plane surface with $h=0$, there is only a specular beam, and the convergence is trivial. If $h$ becomes larger, more $G$-terms are involved in the sum, and in particular the spread of $A_G$ becomes larger, which finally leads to a limit of convergence given by (3.5), (3.10) and (3.14).

In principle, it would be possible, instead of (3.16), to discuss the convergence as a function of the coefficients of a general Fourier series of $D(\boldsymbol{R})$, but in this case it is difficult to see the entirety of solutions and the range in which the Fourier coefficients are allowed to vary.

We want to discuss the one-dimensional case in more detail in the next sections.

## 4. Explicit convergence conditions for one-dimensional profiles

The corrugation function is assumed to be of the form (3.16), (with $x$ instead of $\boldsymbol{R}$), and

$$d(x) = \sum_{n=1}^{N} \left( \alpha_n \cos\frac{2\pi nx}{a} + \beta_n \sin\frac{2\pi nx}{a} \right) \tag{4.1}$$

with $\alpha_1 = 1$, $\beta_1 = 0$, since a constant is irrelevant for scattering and the lowest sine term can be absorbed by translational invariance. Supposing $g = 1$, the conditions for $h$ become ($' = \mathrm{d}/\mathrm{d}x$: $x = x_1 + \mathrm{i}x_2$)

$$F(x_1, x_2) = \operatorname{Re} d'(x) = 0, \tag{4.2}$$

$$\operatorname{Im} d'(x) = 1/h, \tag{4.3}$$

$$h \operatorname{Re} d(x) + x_2 = \max, \tag{4.4}$$

$$G(x_1, x_2) = x_2 \operatorname{Im} d'(x) + \operatorname{Re} d(x) - d_{\min} \leqslant 0. \tag{4.5}$$

Since $\operatorname{Im} d'(x)$ is odd and $\operatorname{Re} d(x)$ even in $x_2$, (4.5) defines symmetric saddle points $x_1 \pm \mathrm{i}x_2$. Figure 1 shows the unit corrugation $d(x)$ for $\alpha_2 = 0.1$, $\beta_2 = 0.2$, $\alpha_3 = 0.3$, and $\beta_3 = 0.4$ and below the complex $x$-plane, with the curves $F=0$ (broken) and $G=0$ (full). The saddle points are their intersections, and additionally there exists an isolated point solution for $x_1^0 = x_{\min}$, the position of the absolute minimum of $d(x)$, and $x_2^0 = 0$. More details on the curves $F=0$ and $G=0$ are discųssed in the appendix. For $G>0$, the U-shaped contour opens to $-\mathrm{i}\infty$, and the saddle points will be connected by the deformed contour. Equations (4.2), (4.3) and (4.5) give solutions $x^s$, $h^s$ for $s = 1, 2, 3$ with $G_1 h^1 = 0.14$, $G_1 h^2 = 0.23$ and $G_1 h^3 = 0.37$, where $G_1$ is the primitive reciprocal lattice vector. Using (4.4), it can easily be seen that $s = 1$ gives the dominant solution, i.e. $H = h^1$. As shown in van den Berg and Fokkema (1979), the smallest $h^s$ belongs to the dominant saddle point, i.e.

$$H = h^d = \min_s h^s. \tag{4.6}$$

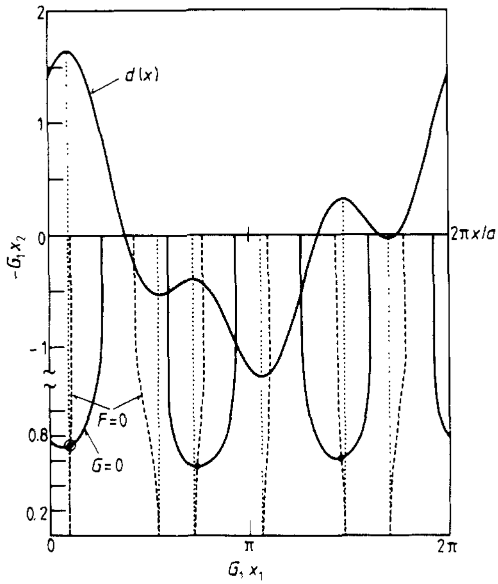


**Figure 1.** A corrugation with Fourier coefficients $(1, 0)$, $(0.1, 0.2)$, $(0.3, 0.4)$ (upper half) and the curves $F = 0$ (broken) and $G = 0$ (full) with saddle points at intersections in the complex $x$-plane (lower half). The leftmost saddle is dominant and $G_1 = 2\pi/a$.

The number of saddle points $S$ increases with $N$, the number of Fourier terms in the corrugation, and it seems that $S = N$.

In § 5, we introduce convergence parameters, which hopefully vary slowly for various profiles.

## 5. Examples of one-dimensional profiles

Our method, which applies to all corrugations, will be used for Fourier series with $N = 2$ rather generally. In case (a), we assume $\beta_2 = 0$, in case (b), $\alpha_2 = 0$, and for the general case (c), we give a table for the values $-1 < \alpha_2 < 1$ and $0 < \beta_2 < 1$ in intervals of 0.2.

Figure 2 represents the complex $x$-plane for case (a) (full curve) and case (b) (broken curve). Since $D$ is invariant for $x \rightarrow -x$, if $\beta$ is replaced by $-\beta$, the saddle point in cases (b) and (c) will be symmetric with respect to the ordinate. There is no symmetry of this kind for case (a), but the saddle points are purely imaginary for $\alpha > \alpha_c = -0.030\,67$, and for $\alpha < \alpha_c$ they become complex, tending for $\alpha \rightarrow \pm\infty$ to a value which corresponds to a lattice with half the lattice constant when compared with the Millar (1969, 1971) value $\alpha = \beta = 0$.

In figure 3, the dimensionless convergence factor $\kappa = G_1 H$, the relative corrugation amplitude (RCA)

$$\rho = (D_{\max} - D_{\min})/a = (d_{\max} - d_{\min})H/a \tag{5.1}$$

and the normalised convergence parameters (NCP) $\kappa_0$, $\kappa_1$, $\rho_1$ and $\rho_2$ are presented as functions of $\alpha_2$ or $\beta_2$—all for the dominant saddle point. The latter are defined by

$$\kappa_l = \sigma_l \kappa, \tag{5.2}$$

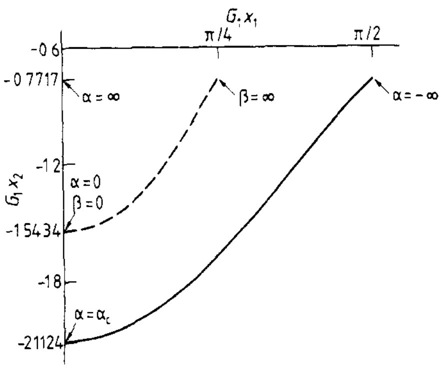


**Figure 2.** The saddle points in the complex $x$-plane for $N=2$ with (a) $\alpha_2=\alpha$, $\beta_2=0$ (full), and for (b) $\alpha_2=0$, $\beta_2=\beta$ (broken); the latter is symmetric for $\beta\to-\beta$ with respect to the ordinate.

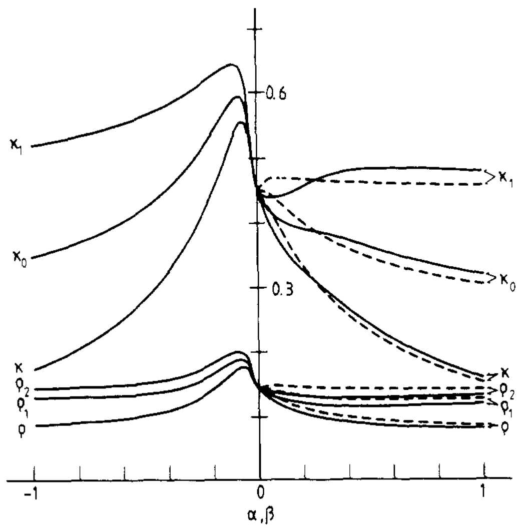


**Figure 3.** The dominant convergence parameters $\kappa$, $\rho$ and their normalised forms $\kappa_0$, $\kappa_1$, $\rho_1$, and $\rho_2$ as a function of $\alpha_2=\alpha$ for case (a) (full curves), or as a function of $\beta_2=\beta$ for case (b) (broken curves).

$$\rho_l=(\sigma_l/\sigma_{l-1})\rho, \tag{5.3}$$

where

$$\sigma_l=\sum_{n=1}^{N} n^l(|\alpha_n|+|\beta_n|) \tag{5.4}$$

extends over all Fourier coefficients of the corrugation function (4.1). As mentioned earlier, the curves are symmetric as a function of $\beta$ (broken), whereas as a function of $\alpha$ (full), they exhibit a maximum $\rho_m=0.176\,52$ for $\alpha_m=-0.064\,55$. These symmetry properties are well understood by the shapes of the profiles, which in case (b) lead to the same profiles for $\beta\to-\beta$, when also $\theta_i\to-\theta_i$ is replaced. In case (a), the saddle

**Table 1.** The convergence parameters for a profile $d(x) = \cos 2\pi x/a + \alpha_2 \cos 4\pi x/a + \beta_2 \sin 4\pi x/a$. The first six columns are $\alpha_1$, $\beta_1$, $\alpha_2$, $\beta_2$, and the maximum and minimum of $d(x)$. Columns 7 and 8 give the dominant (complex) saddle point, and the last six the convergence factor $\kappa = G_1 H$, the relative corrugation amplitude $\rho$, and some of their normalised versions $\kappa_l$ and $\rho_l$, eventually multiplied with the primitive reciprocal lattice vector $G_1 = 2\pi/a$.

| $\alpha_1$ | $\beta_1$ | $\alpha_2$ | $\beta_2$ | $d_{max}$ | $d_{min}$ | $G_1x_1$ | $G_1x_2$ | $\kappa$ | $\rho$ | $\kappa_0$ | $\kappa_1$ | $\rho_1$ | $\rho_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.0 | 0.0 | −1.0 | 0.0 | 1.1250 | −2.0000 | 1.4544 | −0.8936 | 0.1734 | 0.0863 | 0.3468 | 0.5202 | 0.1294 | 0.1438 |
| 1.0 | 0.0 | −0.8 | 0.0 | 0.9563 | −1.8000 | 1.4297 | −0.9210 | 0.2052 | 0.0900 | 0.3693 | 0.5334 | 0.1300 | 0.1454 |
| 1.0 | 0.0 | −0.6 | 0.0 | 0.8083 | −1.6000 | 1.3917 | −0.9643 | 0.2510 | 0.0962 | 0.4016 | 0.5523 | 0.1323 | 0.1487 |
| 1.0 | 0.0 | −0.4 | 0.0 | 0.7125 | −1.4000 | 1.3244 | −1.0429 | 0.3229 | 0.1086 | 0.4521 | 0.5813 | 0.1396 | 0.1568 |
| 1.0 | 0.0 | −0.2 | 0.0 | 0.8000 | −1.2000 | 1.1673 | −1.2324 | 0.4482 | 0.1427 | 0.5378 | 0.6274 | 0.1664 | 0.1834 |
| 1.0 | 0.0 | 0.0 | 0.0 | 1.0000 | −1.0000 | 0.0000 | −1.5434 | 0.4477 | 0.1425 | 0.4477 | 0.4477 | 0.1425 | 0.1425 |
| 1.0 | 0.0 | 0.2 | 0.0 | 1.2000 | −0.8000 | 0.0000 | −1.0917 | 0.3253 | 0.1035 | 0.3903 | 0.4554 | 0.1208 | 0.1331 |
| 1.0 | 0.0 | 0.4 | 0.0 | 1.4000 | −0.7125 | 0.0000 | −0.9556 | 0.2664 | 0.0896 | 0.3730 | 0.4796 | 0.1152 | 0.1294 |
| 1.0 | 0.0 | 0.6 | 0.0 | 1.6000 | −0.8083 | 0.0000 | −0.9006 | 0.2192 | 0.0840 | 0.3507 | 0.4822 | 0.1155 | 0.1298 |
| 1.0 | 0.0 | 0.8 | 0.0 | 1.8000 | −0.9562 | 0.0000 | −0.8710 | 0.1848 | 0.0811 | 0.3326 | 0.4804 | 0.1171 | 0.1309 |
| 1.0 | 0.0 | 1.0 | 0.0 | 2.0000 | −1.1250 | 0.0000 | −0.8525 | 0.1593 | 0.0792 | 0.3185 | 0.4778 | 0.1188 | 0.1320 |
| 1.0 | 0.0 | −1.0 | 0.2 | 1.2368 | −2.0159 | 1.3600 | −0.8953 | 0.1665 | 0.0862 | 0.3662 | 0.5661 | 0.1332 | 0.1470 |
| 1.0 | 0.0 | −0.8 | 0.2 | 1.0907 | −1.8189 | 1.3149 | −0.9217 | 0.1935 | 0.0896 | 0.3870 | 0.5805 | 0.1344 | 0.1493 |
| 1.0 | 0.0 | −0.6 | 0.2 | 0.9734 | −1.6232 | 1.2462 | −0.9610 | 0.2293 | 0.0948 | 0.4127 | 0.5961 | 0.1369 | 0.1531 |
| 1.0 | 0.0 | −0.4 | 0.2 | 0.9099 | −1.4300 | 1.1309 | −1.0225 | 0.2759 | 0.1028 | 0.4415 | 0.6070 | 0.1413 | 0.1588 |
| 1.0 | 0.0 | −0.2 | 0.2 | 0.9401 | −1.2422 | 0.9143 | −1.1137 | 0.3258 | 0.1132 | 0.4561 | 0.5864 | 0.1455 | 0.1635 |
| 1.0 | 0.0 | 0.0 | 0.2 | 1.0687 | −1.0687 | 0.5521 | −1.1548 | 0.3336 | 0.1135 | 0.4003 | 0.4670 | 0.1324 | 0.1459 |
| 1.0 | 0.0 | 0.2 | 0.2 | 1.2422 | −0.9401 | 0.2935 | −1.0534 | 0.2897 | 0.1006 | 0.4056 | 0.5214 | 0.1294 | 0.1453 |
| 1.0 | 0.0 | 0.4 | 0.2 | 1.4300 | −0.9099 | 0.1872 | −0.9637 | 0.2441 | 0.0909 | 0.3906 | 0.5370 | 0.1250 | 0.1405 |
| 1.0 | 0.0 | 0.6 | 0.2 | 1.6232 | −0.9734 | 0.1364 | −0.9113 | 0.2066 | 0.0854 | 0.3719 | 0.5372 | 0.1233 | 0.1379 |
| 1.0 | 0.0 | 0.8 | 0.2 | 1.8189 | −1.0907 | 0.1072 | −0.8797 | 0.1774 | 0.0821 | 0.3547 | 0.5321 | 0.1232 | 0.1369 |
| 1.0 | 0.0 | 1.0 | 0.2 | 2.0159 | −1.2368 | 0.0882 | −0.8593 | 0.1546 | 0.0800 | 0.3401 | 0.5256 | 0.1237 | 0.1365 |
| 1.0 | 0.0 | −1.0 | 0.4 | 1.3733 | −2.0624 | 1.2764 | −0.8920 | 0.1565 | 0.0856 | 0.3755 | 0.5945 | 0.1355 | 0.1486 |
| 1.0 | 0.0 | −0.8 | 0.4 | 1.2484 | −1.8735 | 1.2188 | −0.9142 | 0.1777 | 0.0883 | 0.3908 | 0.6040 | 0.1364 | 0.1506 |
| 1.0 | 0.0 | −0.6 | 0.4 | 1.1549 | −1.6891 | 1.1372 | −0.9436 | 0.2029 | 0.0918 | 0.4058 | 0.6087 | 0.1377 | 0.1531 |
| 1.0 | 0.0 | −0.4 | 0.4 | 1.1090 | −1.5125 | 1.0176 | −0.9805 | 0.2304 | 0.0961 | 0.4146 | 0.5989 | 0.1388 | 0.1553 |
| 1.0 | 0.0 | −0.2 | 0.4 | 1.1280 | −1.3501 | 0.8455 | −1.0164 | 0.2527 | 0.0997 | 0.4044 | 0.5560 | 0.1371 | 0.1540 |
| 1.0 | 0.0 | 0.0 | 0.4 | 1.2147 | −1.2147 | 0.6353 | −1.0244 | 0.2569 | 0.0993 | 0.3597 | 0.4625 | 0.1277 | 0.1435 |
| 1.0 | 0.0 | 0.2 | 0.4 | 1.3501 | −1.1280 | 0.4517 | −0.9911 | 0.2402 | 0.0947 | 0.3843 | 0.5284 | 0.1302 | 0.1464 |
| 1.0 | 0.0 | 0.4 | 0.4 | 1.5125 | −1.1090 | 0.3299 | −0.9453 | 0.2143 | 0.0894 | 0.3857 | 0.5572 | 0.1291 | 0.1444 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.0 | 0.0 | 0.6 | 0.4 | 1.6891 | −1.1549 | 0.2541 | −0.9079 | 0.1885 | 0.0853 | 0.3769 | 0.5654 | 0.1280 | 0.1422 |
| 1.0 | 0.0 | 0.8 | 0.4 | 1.8735 | −1.2484 | 0.2050 | −0.8810 | 0.1659 | 0.0824 | 0.3650 | 0.5641 | 0.1274 | 0.1406 |
| 1.0 | 0.0 | 1.0 | 0.4 | 2.0624 | −1.3733 | 0.1712 | −0.8619 | 0.1471 | 0.0804 | 0.3530 | 0.5589 | 0.1273 | 0.1397 |
| 1.0 | 0.0 | −1.0 | 0.6 | 1.5272 | −2.1362 | 1.2061 | −0.8855 | 0.1450 | 0.0846 | 0.3771 | 0.6092 | 0.1366 | 0.1490 |
| 1.0 | 0.0 | −0.8 | 0.6 | 1.4204 | −1.9588 | 1.1437 | −0.9026 | 0.1610 | 0.0866 | 0.3863 | 0.6117 | 0.1371 | 0.1504 |
| 1.0 | 0.0 | −0.6 | 0.6 | 1.3440 | −1.7894 | 1.0615 | −0.9226 | 0.1782 | 0.0889 | 0.3920 | 0.6059 | 0.1373 | 0.1516 |
| 1.0 | 0.0 | −0.4 | 0.6 | 1.3085 | −1.6323 | 0.9542 | −0.9436 | 0.1947 | 0.0911 | 0.3894 | 0.5841 | 0.1367 | 0.1519 |
| 1.0 | 0.0 | −0.2 | 0.6 | 1.3225 | −1.4948 | 0.8206 | −0.9595 | 0.2065 | 0.0926 | 0.3716 | 0.5368 | 0.1337 | 0.1495 |
| 1.0 | 0.0 | 0.0 | 0.6 | 1.3873 | −1.3873 | 0.6730 | −0.9613 | 0.2089 | 0.0922 | 0.3342 | 0.4595 | 0.1268 | 0.1426 |
| 1.0 | 0.0 | 0.2 | 0.6 | 1.4948 | −1.3225 | 0.5359 | −0.9461 | 0.2009 | 0.0901 | 0.3617 | 0.5224 | 0.1301 | 0.1455 |
| 1.0 | 0.0 | 0.4 | 0.6 | 1.6323 | −1.3085 | 0.4267 | −0.9219 | 0.1862 | 0.0872 | 0.3725 | 0.5587 | 0.1307 | 0.1453 |
| 1.0 | 0.0 | 0.6 | 0.6 | 1.7894 | −1.3440 | 0.3464 | −0.8976 | 0.1693 | 0.0844 | 0.3724 | 0.5755 | 0.1304 | 0.1440 |
| 1.0 | 0.0 | 0.8 | 0.6 | 1.9588 | −1.4204 | 0.2881 | −0.8771 | 0.1528 | 0.0822 | 0.3666 | 0.5805 | 0.1301 | 0.1427 |
| 1.0 | 0.0 | 1.0 | 0.6 | 2.1362 | −1.5272 | 0.2451 | −0.8609 | 0.1379 | 0.0804 | 0.3586 | 0.5793 | 0.1299 | 0.1417 |
| 1.0 | 0.0 | −1.0 | 0.8 | 1.6932 | −2.2333 | 1.1487 | −0.8774 | 0.1336 | 0.0835 | 0.3740 | 0.6143 | 0.1371 | 0.1488 |
| 1.0 | 0.0 | −0.8 | 0.8 | 1.6009 | −2.0687 | 1.0863 | −0.8900 | 0.1453 | 0.0849 | 0.3779 | 0.6105 | 0.1371 | 0.1496 |
| 1.0 | 0.0 | −0.6 | 0.8 | 1.5371 | −1.9149 | 1.0093 | −0.9034 | 0.1572 | 0.0864 | 0.3772 | 0.5973 | 0.1367 | 0.1500 |
| 1.0 | 0.0 | −0.4 | 0.8 | 1.5082 | −1.7763 | 0.9161 | −0.9156 | 0.1676 | 0.0876 | 0.3687 | 0.5698 | 0.1354 | 0.1494 |
| 1.0 | 0.0 | −0.2 | 0.8 | 1.5193 | −1.6591 | 0.8088 | −0.9235 | 0.1745 | 0.0883 | 0.3490 | 0.5235 | 0.1324 | 0.1471 |
| 1.0 | 0.0 | 0.0 | 0.8 | 1.5710 | −1.5710 | 0.6951 | −0.9237 | 0.1760 | 0.0880 | 0.3168 | 0.4576 | 0.1271 | 0.1422 |
| 1.0 | 0.0 | 0.2 | 0.8 | 1.6591 | −1.5193 | 0.5866 | −0.9153 | 0.1716 | 0.0868 | 0.3432 | 0.5149 | 0.1302 | 0.1447 |
| 1.0 | 0.0 | 0.4 | 0.8 | 1.7763 | −1.5082 | 0.4926 | −0.9013 | 0.1628 | 0.0851 | 0.3581 | 0.5534 | 0.1315 | 0.1451 |
| 1.0 | 0.0 | 0.6 | 0.8 | 1.9149 | −1.5371 | 0.4162 | −0.8854 | 0.1515 | 0.0832 | 0.3636 | 0.5758 | 0.1318 | 0.1446 |
| 1.0 | 0.0 | 0.8 | 0.8 | 2.0687 | −1.6009 | 0.3559 | −0.8705 | 0.1397 | 0.0816 | 0.3631 | 0.5866 | 0.1318 | 0.1437 |
| 1.0 | 0.0 | 1.0 | 0.8 | 2.2333 | −1.6932 | 0.3086 | −0.8576 | 0.1283 | 0.0802 | 0.3591 | 0.5900 | 0.1317 | 0.1429 |
| 1.0 | 0.0 | −1.0 | 1.0 | 1.8675 | −2.3492 | 1.1024 | −0.8690 | 0.1227 | 0.0824 | 0.3682 | 0.6137 | 0.1373 | 0.1483 |
| 1.0 | 0.0 | −0.8 | 1.0 | 1.7869 | −2.1975 | 1.0426 | −0.8782 | 0.1315 | 0.0834 | 0.3682 | 0.6049 | 0.1370 | 0.1486 |
| 1.0 | 0.0 | −0.6 | 1.0 | 1.7323 | −2.0583 | 0.9723 | −0.8871 | 0.1398 | 0.0843 | 0.3635 | 0.5871 | 0.1362 | 0.1486 |
| 1.0 | 0.0 | −0.4 | 1.0 | 1.7080 | −1.9357 | 0.8914 | −0.8946 | 0.1467 | 0.0851 | 0.3521 | 0.5574 | 0.1347 | 0.1477 |
| 1.0 | 0.0 | −0.2 | 1.0 | 1.7172 | −1.8345 | 0.8023 | −0.8989 | 0.1511 | 0.0854 | 0.3324 | 0.5137 | 0.1320 | 0.1457 |
| 1.0 | 0.0 | 0.0 | 1.0 | 1.7602 | −1.7602 | 0.7098 | −0.8986 | 0.1520 | 0.0852 | 0.3041 | 0.4561 | 0.1278 | 0.1420 |
| 1.0 | 0.0 | 0.2 | 1.0 | 1.8345 | −1.7172 | 0.6203 | −0.8934 | 0.1494 | 0.0845 | 0.3287 | 0.5080 | 0.1305 | 0.1441 |
| 1.0 | 0.0 | 0.4 | 1.0 | 1.9357 | −1.7080 | 0.5391 | −0.8846 | 0.1437 | 0.0833 | 0.3449 | 0.5462 | 0.1320 | 0.1448 |
| 1.0 | 0.0 | 0.6 | 1.0 | 2.0583 | −1.7323 | 0.4690 | −0.8739 | 0.1361 | 0.0821 | 0.3538 | 0.5715 | 0.1326 | 0.1446 |
| 1.0 | 0.0 | 0.8 | 1.0 | 2.1975 | −1.7869 | 0.4105 | −0.8631 | 0.1275 | 0.0809 | 0.3570 | 0.5866 | 0.1328 | 0.1441 |
| 1.0 | 0.0 | 1.0 | 1.0 | 2.3492 | −1.8675 | 0.3622 | −0.8531 | 0.1188 | 0.0797 | 0.3565 | 0.5941 | 0.1329 | 0.1435 |

points occur in pairs $(x, -x)$ because of $d(-x) = d(x)$. Since the corrugation for $\alpha \to -\alpha$ changes in essence, e.g. becomes flatter in the maximum (for $-\frac{1}{4} < \alpha < 0$), the convergence parameters should also change.

Table 1 represents the values of the absolute extrema of $d(x)$, the position of the dominant saddle point $2\pi x^s/a$ for $s = d = 1$, and the convergence parameters $\kappa$ and $\rho$. The last four columns give the NCPS $\kappa_0$, $\kappa_1$, $\rho_1$ and $\rho_2$ defined above. It can be seen that $\rho_2$, in particular, behaves nearly like a constant, when the ratio of maximum to minimum is considered for the last six columns. In order to have a measure which is nearly independent of the scale, the quantities $\kappa_l$ and $\rho_l$ have been introduced. In particular, the $\rho_l$'s have asymptotic values for $\alpha_2 \to \pm\infty$ or $\beta_2 \to \pm\infty$, which are equal to the Millar value and deviate only by a small amount (~25% for $\rho_2$) from the mean value, whereas the deviations of $\kappa_l$ are rather large, not to mention $\kappa$, which may become arbitrarily small if large contributions come from higher Fourier coefficients.

It is the purpose of these considerations to find a quantity which for general corrugation functions does not vary too strongly; $\rho_1$ and $\rho_2$ have this property—at least for profiles which are given only by the lowest few Fourier terms, which are the cases of physical interest. In order to test also its limiting behaviour for $N \to \infty$, a few non-analytic profiles are considered in § 6.

## 6. Convergence parameters for piecewise linear surface profiles

The one-dimensional surface is defined by figure 4. It coincides with the rectangular profile for $q = 0$ and the triangular for $q = 1$ whose convergence factor has been discussed in van den Berg and Fokkema (1979). The Fourier series for general $q$ $(0 \leq q \leq 1)$ is

$$d(x) = \sum_{l=0}^{\infty} (-)^l \frac{4}{\pi^2 q} \frac{\sin \frac{1}{2}\pi q(2l+1)}{(2l+1)^2} \cos (2l+1) \frac{2\pi x}{a}. \tag{6.1}$$

In order to apply the saddle-point method, we take analytic approximations which are identical to the partial sums $d_N(x)$ with $N = 2l_{\max} + 2$.

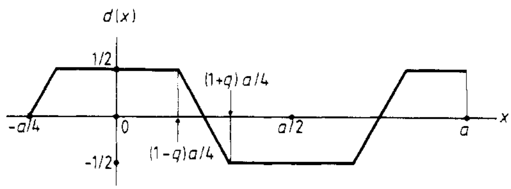


**Figure 4.** A piecewise linear corrugation with $q \in (0, 1)$ becoming rectangular for $q = 0$ and triangular for $q = 1$.

The convergence parameters can be found with an iterative procedure, since the saddle points practically do not change for large $N$-values. It was possible to determine the asymptotical behaviour of $h$ for $q = 0$ and $q = 1$, i.e. for the rectangular and the triangular corrugations.

For $q = 0$, the results could numerically be shown to behave like

$$h \sim \text{constant}\ \rho \sim a_1/N + a_2/N^3 + a_3/N^5 + \ldots, \tag{6.2}$$

whereas for the triangular profile, the prevailing term for large $N$ was

$$h \sim \text{constant}\, \rho \sim N^{-1}(a_1 \ln N + b_1), \tag{6.3}$$

where the next order leads to a numerical estimate of $N^{-5/3}$. Any $q$ in between (e.g. $\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$) leads to an oscillation of $h$ or their lowest-order differences, indicating that the asymptotes contain oscillating terms like the Fourier series (6.1) and do not obey a simple asymptotic formula.

It is very intuitive to relate the non-analyticity to the smallest radius of the curvature $k$, and to look for a connection between $k$ and $h$. The smaller $k$, the smaller $h$ will be, since $k$ and $h$ decrease with increasing $N$. Because of the non-uniform convergence for $q = 0$, the well known Gibbs phenomenon occurs for large $N$, and the point with largest curvature will be in an overshooting peak close to the discontinuity (Sommerfeld 1947) and as such not representative for the curvature in the (continuous) edges.

Such an edge is in the triangular profile for $x = 0$, which for all partial sums exhibits a maximum. By symmetry, it is plausible that in this point, the curvature has a maximum, giving $d''(0) = \text{constant}\ N$. Therefore the radius of curvature $k = \text{constant}\ N$, and we get the relations

$$h \sim \text{constant}\, \rho \sim \text{constant}\, (\ln N)/N, \tag{6.4}$$

$$h \sim \text{constant}\, \rho \sim \text{constant}\, k \ln(1/k), \tag{6.5}$$

for large $N$ or $k$ going to zero. This shows that there is no linear relation between the smallest curvature of the corrugation and the convergence parameters $h$ or $\rho$.

This relation can be used to distinguish an NCP, which is nearly invariant also in the limit $N \to \infty$. Since for the triangular profile $\alpha_N = 4/\pi^2 N^2$ for all odd and $\alpha_N = 0$ for even Fourier terms, the partial sums (5.3) become asymptotically $\sigma_0 \sim \text{constant}$, $\sigma_1 \sim \text{constant} \ln N$, and $\sigma_2 \sim \text{constant}\ N$. Therefore the NCP $\rho_1 \sim \text{constant}\, (\ln N)^2/N$ tends to zero, whereas $\rho_2 \sim \text{constant}$ for $N \to \infty$. The second NCP $\rho_2$ has the property of a pseudoinvariant for all $N$, i.e. it is also nearly invariant, as found by analysing the results of the profile (6.1) for $q = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ and 1. The same seems to be true for profiles with continuous slope but discontinuous second derivative (sectors with constant and parabolic $d(x)$).

## 7. Conclusion

The convergence-limit equations of Hill and Celli (1978) are shown to follow from the eikonal approximation of the scattering problem; it gives the correct asymptotics of the scattering amplitudes for $G \to \infty$, though it was originally introduced as an approximation within the Ewald circle.

The asymptotic evaluation of the scattering amplitudes leads to many saddle points, the one giving the main contribution to $A_G$ being the dominant saddle point, which can be characterised by having the smallest convergence factor $H$. Since $H$ strongly depends on the normalised profile function $d$, or its Fourier coefficients, the relative corrugation amplitude $\rho$ and its normalised forms $\rho_1$ and $\rho_2$ have been introduced. Though $\rho$ depends on the lattice constant, $\rho_1$ and $\rho_2$ do not. In particular $\rho_2$ (in contrast to $\rho_1$) is also independent of the number of terms used for an analytic approximation by truncated Fourier series of trapezoidal profiles. The convergence parameter $\rho_2$ is a pseudoinvariant for a wide range of corrugation functions. It can therefore be used to estimate the convergence factor $H$ roughly by the Fourier coefficients of its corrugation functions. Of all cases considered here, case (a) gives the widest range of possible $\rho_2$ values, varying roughly from 0.12 to 0.20; this range is also valid for a three-term cosine corrugation with $\alpha_1 = 1$, $\alpha_2 \in (-1, 1)$ and $\alpha_3 \in (-1, 1)$, but it cannot be excluded that, especially for larger $N$, this range has to be extended.

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**Appendix**

To simplify formulae, $z = 2\pi x/a$ is introduced; for the finite Fourier series, we then have

$$d(z) = \sum_{n=1}^{N} d_n(z) = \sum_{n=1}^{N} \alpha_n \cos nz + \beta_n \sin nz, \tag{A1}$$

with $z = x + \mathrm{i}y$ (do not confound with $x$ above),

$$F(x, y) = \sum_{n=1}^{N} d'_n(x) \cosh ny = 0, \tag{A2}$$

$$G(x, y) = -y \sum_{n=1}^{N} n d_n(x) \sinh ny + \sum_{n=1}^{N} d_n(x) \cosh ny - d_{\min} = 0, \tag{A3}$$

both even functions in $y$. Since $F(x_e, 0) = d'(x_e) = 0$ for all extrema $x_e$ ($e = 1, 2, \ldots, E \leqslant 2N$), an expansion for small $y$ is

$$F(x, y) = \sum_{n=1}^{N} d'_n(x) + \frac{y^2}{2} \sum_{n=1}^{N} n^2 d'_n(x) = 0, \tag{A4}$$

giving

$$y \approx (2d'(x)/d'''(x))^{1/2} = [(2d''(x_e)/d'''(x_e))(x - x_e)]^{1/2}. \tag{A5}$$

For the absolute minimum $x = x_{\min}$ and $y = 0$, $F = G = 0$, and for small $y$,

$$G(x, y) = d(x) - d_{\min} + \tfrac{1}{2} y^2 d''(x), \tag{A6}$$

and for $x \approx x_{\min}$

$$G(x, y) = \tfrac{1}{2} d''(x_{\min})[(x - x_{\min})^2 + y^2], \tag{A7}$$

i.e. $(x_{\min}, 0)$ is an isolated zero of $G = 0$.

The behaviour for large $y$ is determined by the last few terms in the Fourier series, e.g.

$$F(x, y) \sim \sum_{n=1}^{N} d'_n(x)\, \mathrm{e}^{ny}/2 = 0, \tag{A8}$$

giving

$$\mathrm{e}^{y} \sim -d'_{N-1}(x)/d'_N(x), \tag{A9}$$

with the $F$-asymptote $x_F$ following from

$$d'_N(x_F) = 0, \tag{A10}$$

i.e.

$$x_F = \pi n/N + \tan^{-1}(\beta_N/\alpha_N), \qquad n = 0, 1, \ldots, 2N-1. \tag{A11}$$

In analogy,

$$G(x, y) \sim -y \sum_{n=1}^{N} n d_n(x)\, \mathrm{e}^{ny}/2 + \sum_{n=1}^{N} d_n(x)\, \mathrm{e}^{ny}/2 = 0, \tag{A12}$$

giving

$$y\, \mathrm{e}^{y} \sim -[(N-1)/N] d_{N-1}(x)/d_N(x), \tag{A13}$$

with the $G$-asymptote $x_G$ following from

$$d_N(x_G) = 0, \tag{A14}$$

i.e.

$$x_G = \pi(n + \tfrac{1}{2})/N + \tan^{-1}(\beta_N/\alpha_N), \qquad n = 0, 1, \ldots, 2N-1. \tag{A15}$$

The asymptotes of $G$ lie in between the asymptotes of $F$ (see figure 1).

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