Accurate calculation of Coulomb sums: Efficacy of Padé-like methods

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The adequacy of numerical sequence accelerative transforms in providing accurate estimates of Coulomb sums is considered, referring particularly to distorted lattices. Performance of diagonal Padé approximants (DPA) in this context is critically assessed. Failure in the case of lattice vacancies is also demonstrated. The method of multiple-point Padé approximants (MPA) has been introduced for slowly convergent sequences and is shown to work well for both regular and distorted lattices, the latter being due either to impurities or vacancies. Viability of the two methods is also compared. In divergent situations with distortions owing to vacancies, a strategy of obtaining reliable results by separate applications of both DPA and MPA at appropriate places is also sketched. Representative calculations involve two basic cubic-lattice sums, one slowly convergent and the other divergent, from which very good quality estimates of Madelung constants for a number of common lattices follow.

I. INTRODUCTION

Accurate calculation of Coulomb sums in ionic crystals is a problem that pertains to both solid-state physics[1] and chemistry.[2] These sums arise in the course of estimating the Coulomb potential at a lattice site due to all the surrounding ions, and they are commonly termed also as Madelung constants (μ). The stability of an ionic crystal depends primarily on μ. So, reliable estimates of μ are wanted in discussions on various mechanical and thermal properties of ionic solids from first principles.[3] The level of accuracy of calculated values for such lattice sums becomes more important in deciding relative stabilities of solids of competing structures in particular, for which the μ values turn out to be quite close. Apart from the relevance to crystal structures,[4] Madelung sums appear also in studies on phase transitions. It has been noted that the change in volume on melting is directly dependent on the change in μ upon going from the solid to the liquid phase, for ionic solids. Results of both Monte Carlo and molecular-dynamics calculations[5] on the melting of alkali halides[6] have revealed this feature. On the other hand, sums of similar nature show up in discussions on polymer chains[7] as well. Thus, the search for efficient strategies of computing accurate values of various types of lattice sums continues to be of interest.[1,2,8–14]

Coulomb sums may be evaluated in a number of ways (see, e.g., Ref. 2 for a fairly recent review). The major problem with the usual, straightforward calculations is concerned with rapidity of *convergence* of such approaches. Thus, perusal of the relevant literature reveals that emphasis is given primarily to the mathematical structure of such sums, especially in relation to applicability of various functional or algebraic transformation schemes,[2,7–9,12,13] summability, and convergence.[8] Moreover, these studies are mostly centered on *regular* two- and three-dimensional lattices[2,8,10–12] with special attention to the NaCl crystal.[9,12,13] The reason is clear. One obtains closed-form expressions for μ in terms of known functions *only* in these situations. Algebraic manipulations become convenient as well. Recently, however, it has been found that *numerical-* sequence accelerative transforms are also quite efficient[10,11,14] in handling such kinds of sums. An additional advantage of this latter approach is that these numerical schemes apply with equal facility to cases of lattice defects.[10] While Levin's u transform[15] (u-LT) was successfully implemented in Ref. 10, our preliminary investigation[11] showed the diagonal Padé approximants[16] (DPA) to work even better, at least for regular lattices. A thorough scrutiny in this context for *very* reliable estimates, however, is still lacking, the more so for lattice distortions. On the other hand, another efficient accelerative scheme for monotonic sequences, the method of multipoint Padé approximants[17] (MPA), has not been employed at all in such calculations, though the success of MPA in a related context, viz., calculation of lattice constants for covalent crystals,[18] is noteworthy, and Coulomb sums also generate, in some situations, sequences characterized by slow, monotonic convergence.

In view of the above remarks, the purpose of the present communication is threefold: (i) to demonstrate the usefulness of DPA in providing very accurate estimates of μ for regular lattices and lattices with isovalent impurities, and its failure in case of lattice vacancies; (ii) to show how efficiently MPA works in all the slowly convergent cases and how it compares with DPA; and (iii) to establish that, when DPA fails to perform satisfactorily and MPA does not apply, as is the situation with divergent lattice-sum sequences with vacant sites (see below), separate applications of *both* DPA and MPA may be very convenient. Remembering that lattice sums pose either the problem of slow convergence or divergence, we consider here both types of cases; in fact two *basic*[2] cubic lattice sums, one convergent and the other divergent, from which μ values for quite a few salts[2,14] follow.

II. THE SCHEME

We first generate a sequence of values $(s_1,s_2,\ldots,s_n)$ approximating the Madelung sum under consideration. This identifies the μ value with the limit point S_0 of $\{s_j\}$. Larger n corresponds to taking effects of more distant neighbors into account during calculations of potentials at a particular lattice site. Next, we transform $\{s_j\}$ to obtain a new sequence ($\{t_j\}$ or $\{t_j'\}$) that converges to S_0 at a much faster rate. Choice of the method to be employed for this purpose depends on the nature of the parent $\{s_j\}$. If, symbolically, we denote by X a method for accelerating monotonic sequences while Y refers to one that applies to sawtooth sequences, then, in general, we shall see that the following alternative strategies (1A to 3B) might be quite conveniently employed for the various emergent situations.

Case 1. The sequence converges monotonically. Here, alternatives are (i) 1A: employ X on $\{s_j\}$ directly, or (ii) 1B: employ X on the *subsequences,* e.g., $s_1,s_3,\ldots$ or $s_2,s_4,\ldots$ or $s_1,s_4,\ldots$, etc.

Case 2. The sequence converges in a sawtooth manner. This means, any two successive members s_j and s_{j+1} bracket S_0 from above and below and that such a bracketting becomes tighter as j increases. Here one may adopt (i) 2A: Y on $\{s_j\}$, or (ii) 2B: 1A or 1B, after separating the monotonic *subsequences* $s_1,s_3,s_5,\ldots$ and $s_2,s_4,\ldots$, with a subsequent averaging of the final results, if necessary.

Case 3. The sequence diverges. Again, s_j and s_{j+1} bracket S_0 from above and below, but the bracketting worsens with increasing j. Here, possibilities are (i) 3A: follow Y straightforwardly, or (ii) 3B: look first for a known divergent sequence $r_1,r_2,\ldots$ that leads to an accurate estimate R_0 by Y; consider the *new* sequence $(s_1-r_1),(s_2-r_2),\ldots$ ($\equiv p_1,p_2,\ldots$) to check if it corresponds to Case 1; employ 1A or 1B subsequently. If 3B works, and we find P_0 as the limit point of $\{p_j\}$, we infer then that $S_0=P_0+R_0$ on the basis of one of Hardy's axioms.[14,19]

In the present work, however, only Padé-like methods will be considered. So, we restrict ourselves to MPA corresponding to method X and DPA to Y. For the sake of completeness, now, a very brief outline of the procedures of constructing the transformed sequences follows:

(i) DPA. In the method of DPA, one associates a power-series with the given parent sequence, $s_1,s_2,\ldots,s_n$ by defining

$$F(x)=\sum_{i=0}^{\infty} f_i x^i,\quad f_0=s_1\ ,$$
$$f_j=s_{j+1}-s_j=\Delta s_j,\quad j\le n-1\ , \tag{1}$$

so that the identity $S_0=F(1)$ follows. Then, one constructs an approximant $t_r(x)=P_r(x)/Q_r(x)$ to $F(x)$, with $P_r(x)=p_0+p_1x+\cdots+p_rx^r$ and $Q_r(x)=1+q_1x+\cdots+q_rx^r$ such that

$$P_r(x)/Q_r(x)=F(x)+O(x^{2r+1}) \tag{2}$$

follows, for $n=2r+1$. Coefficients $p_0,p_1,\ldots$ and $q_1,q_2,\ldots$ are calculated accordingly. The value of $t_r(x)$ at $x=1$ is the required approximation to S_0. In practice, however, these approximants may be very conveniently and directly obtained via the ε algorithm.[16] Let us also note, for a given total number n of terms of $\{s_j\}$, the transformed sequence $\{t_j\}$ will contain a total of $(n-1)/2$ terms. Invariance properties of DPA and its relation to some other approximants are well known (see, e.g., Refs. 11 and 16) and these justify its employment, if not the results to follow.

(ii) MPA. The method of MPA, on the other hand, proceeds quite differently. Here, one first assumes that the parent members $\{s_j\}$ admit a power-series representation of the form

$$s_j=\alpha_0+\alpha_1/j+\alpha_2/j^2+\cdots,\quad 1\le j\le n\ , \tag{3}$$

where $\alpha_0\equiv S_0$, so that the limiting condition ($s_j=S_0$ as $j\to\infty$) is satisfied. Then, instead of solving directly for $(n-1)$ coefficients α_j from (3), one relies on the Padé representation of the right-hand side of (3) for an even better fitting. Thus, we are led either to the association

$$s_j=\frac{P_r(1/j)}{Q_r(1/j)},\quad 1\le j\le 2r+1=n\ , \tag{4}$$

for odd n, or to

$$s_j=\frac{P_{r+1}(1/j)}{Q_r(1/j)},\quad 1\le j\le 2r+2=n\ , \tag{5}$$

for even n. The polynomials P and Q are of the same form as in the previous case [Eq. (2)], except that the variable $1/j$ has now appeared. Solving for the unknown coefficients $\{p_j\}$ and $\{q_j\}$, one finally identifies $S_0\equiv p_0$, the value of the rhs of (4) or (5) in the limit $j\to\infty$. Computations to this end may be conveniently done by having recourse to Thiele's reciprocal difference method,[17] a discussion on which is avoided here for brevity. In MPA, from a given number n of terms of the parent sequence, the transformed sequence will emerge with $(n-1)$ members; to distinguish from the DPA-assisted transforms, we designate these by $\{t_j'\}$ in what follows.

III. RESULTS AND DISCUSSION

We first consider the generation of sequences. For NaCl, it is given by

$$S(1,0)=\lim_{j\to\infty} s_j(1,0)=\lim_{j\to\infty}\sum_{M,N,P=-j}^{j}(-1)^Z/R\ , \tag{6}$$

where $Z=M+N+P$ and $R^2=M^2+N^2+P^2$, with $R>0$. Calculation of the Madelung constant for CsCl also follows from (6) with the additional restriction that here the set (M,N,P) would take only *all-even* and *all-odd* integral values. In the presence of defects, however, ions suffer displacements from the original position. Owing to the distortion in geometry, the Coulomb sum at the defect site would involve a change[20] in the value of R in (6). Point defects are the simplest ones and these will concern us here. In case of an isovalent impurity, thus, one finds[10,20] a sum like

TABLE I. Convergence behavior of DPA-assisted transforms ($\{t_j\}$) for various NaCl and CsCl lattice sums [Eqs. (6), (7), and (8)] including lattice defects ($k=0.05$).

n	$t_{(n-1)/2}(1,0)$		$t_{(n-1)/2}(1,1)$		$t_{(n-1)/2}(1,2)$	
	NaCl	CsCl	NaCl	CsCl	NaCl	CsCl
3	−1.76	−0.8	−1.58	−0.76	−2.4	−0.9
7	−1.747 57	−1.017 689	−1.566 5	−0.995 52	−2.5	−1.13
11	−1.747 564 6	−1.017 680 76	−1.566 497 84	−0.995 532 999	−2.56	−1.14
15	−1.747 564 594 63	−1.017 680 754 73	−1.566 497 832 08	−0.995 532 996 95	−2.57	−1.141

$$S(1,1)=\lim_{j\to\infty} s_j(1,1)$$
$$=\lim_{j\to\infty}\sum_{M,N,P=-j}^{j}(-1)^Z/(R+k/R^2)\,, \qquad (7)$$

replacing (6), where k is a measure of the amount of distortion, related to the elastic constants of the medium. For convenience, we shall call it a defect of *type 1*. On the other hand, if a vacancy is present, an electric displacement occurs[10,20] in addition, the amount being dependent on the dielectric constant of the medium. Then, the form of the lattice-sum correspondingly changes to

$$S(1,2)=\lim_{j\to\infty} s_j(1,2)$$
$$=\lim_{j\to\infty}\sum_{M,N,P=-j}^{j}(-1)^Z/[R+(-1)^Z k/R^2]\,, \qquad (8)$$

where the strength parameter k plays a similar role as in (7). This will be termed a defect of *type 2*. Again, for the CsCl case, restriction on the set (M,N,P) remains same in (7) or (8), viz., all-even and all-odd integers. Such expressions as (7) and (8) naturally reduce to form (6) in the limit $k\to 0$. Notably, however, these k dependent sums for distorted lattices seldom appear in the relevant literature as they are not readily amenable to functional transformation techniques for accurate evaluation. So, u-LT was employed in Ref. 10 for k values ranging from 0.01 to 0.05 in (7) and (8). It is apparent that $k=0.05$ corresponds to a reasonably *strong* perturbation to the regular sums and that the convergence problem becomes gradually different as k increases. Hence, we choose here $k=0.05$. Another important point is, while the partial sums s_j for $j=1,2,\ldots$ in (6), (7), or (8) form a sawtooth sequence which gradually converges for NaCl (Case 2), all sequences for the CsCl lattice are divergent (Case 3).

First, let us examine how strategy 2A or 3A works. Table I shows the convergence behavior of $\{t_j\}$ for all the NaCl and CsCl sums. The regular case[11] (6) has been included chiefly for the sake of comparison. We find, while DPA works very desirably and comparably for sums (6) and (7), the case with (8), i.e., lattice vacancies, is *quite* unsatisfactory.

Noticing that all the NaCl sequences correspond to Case 2, it is tempting to adopt strategy 2B at this point, especially in view of the failure of DPA for (8). Table II displays such a study first for the regular lattice, Eq. (6). For a given maximum number of terms n, the last two estimates thus obtained from the two subsequences shown may be averaged to quote the final MPA estimate. Admittedly, a smooth convergence of the MPA-assisted transforms ($\{t'_j\}$) is obtained.

It is now natural to extend the analysis to cases of defects and compare efficiencies of 2A and 2B. This is precisely what is displayed in Table III. Here the DPA results are obtained directly. The estimates quoted for MPA, on the other hand, are the averaged results of the even and odd terms, taken separately. It is surprising that, while DPA performs a shade better than MPA both for (6) and (7), the latter works very efficiently, and in a balanced manner, for *all* the sums. Thus, in MPA, converged results up to 16 decimal places have been obtained for $n=31$. The method of DPA, with similar input, though it offers stability of up to 20 places for (6) and (7), performs poorly on (8). Thus, we conclude, in order to

TABLE II. Acceleration of convergence by MPA for μ(NaCl)/2, given by (6).

j	$s_{2j+1}(1,0)$	$t'_j(1,0)$ (odd)	$s_{2j}(1,0)$	$t'_{j-1}(1,0)$ (even)
0	−2.13			
1	−1.91	−1.69	−1.52	
2	−1.85	−1.748	−1.62	−1.72
3	−1.82	−1.747 4	−1.66	−1.747 56
4	−1.81	−1.747 565	−1.68	−1.747 57
5	−1.80	−1.747 564 9	−1.69	−1.747 566
10	−1.774	−1.747 564 594 60	−1.719	−1.747 564 594 6
12	−1.770	−1.747 564 594 633 3	−1.724	−1.747 564 594 633 2
15	−1.766	−1.747 564 594 633 182 2	−1.729	−1.747 564 594 633 182 0

TABLE III. A comparative study of the performance level of DPA and MPA for various NaCl lattice sums ($k=0.05$).

r	n	$t(1,r)$	$t'(1,r)$
0	5	−1.747 9	−1.73
	9	−1.747 564 9	−1.747 57
	13	−1.747 564 594 7	−1.747 564
	21	−1.747 564 594 633 183	−1.747 564 594 6
	31	−1.747 564 594 633 182 190 64	−1.747 564 594 633 182 1
1	5	−1.566 8	−1.55
	9	−1.566 498	−1.566 497 2
	13	−1.566 497 832 1	−1.566 497 4
	21	−1.566 497 832 088 653	−1.566 497 832
	31	−1.566 497 832 088 652 644 85	−1.566 497 832 088 652 6
2	5	−2.65	−2.56
	9	−2.90	−2.587 8
	13	−2.53	−2.587 789
	21	−2.58	−2.587 785 928 8
	31	−2.584	−2.587 785 928 805 015 1

treat slowly-convergent sums of the form (8), MPA is definitely recommendable.

At this point, we may also draw attention to the *unbalanced* performance of u-LT (Ref. 10) that closely resembles the performance of DPA transforms. Thus, while $S(1,1)$ is reported correctly to 6 decimal places in Ref. 10 for NaCl at $k=0.05$, the datum for $S(1,2)$ is correct *only* up to 2 decimal places for similar input. Again, one is led to a similar conclusion as above.

The problem that still remains is how one would estimate $S(1,2)$ for the CsCl lattice, i.e., Case 3. MPA cannot be employed because here the parent sequence $\{s_j\}$ is divergent. So, we seek an alternative strategy, applicable to a number of situations, and not just for CsCl. From the work of Ref. 2, it follows that Coulomb sums for various cubic lattices may be expressed as linear combinations of a few *basic* lattice sums. For a number of salts including CsCl, one observes that while $S(1,0)$, given by (6), presents itself as one of the components, another basic sum reads as

$$S(2,0)=\lim_{j\to\infty} s_j(2,0)=\lim_{j\to\infty}\sum_{M,N,P=-j}^{j}(-1)^M/R \qquad (9)$$

with $R>0$. The corresponding expressions for lattice defects of types 1 and 2 mentioned earlier would then become, accordingly,

$$S(2,1)=\lim_{j\to\infty} s_j(2,1)$$
$$=\lim_{j\to\infty}\sum_{M,N,P=-j}^{j}(-1)^M/(R+k/R^2)\,, \qquad (10)$$

and

$$S(2,2)=\lim_{j\to\infty} s_j(2,2)$$
$$=\lim_{j\to\infty}\sum_{M,N,P=-j}^{j}(-1)^M/(R+(-1)^M k/R^2)\,. \qquad (11)$$

So, instead of focusing attention on the CsCl lattice sum directly, we concentrate on sums (9), (10), and (11) along with the three [(6)–(8)] studied above. In terms of such basic sums, the μ values may be expressed. In case of the regular CsCl lattice, for example, one would find that $\mu(\text{CsCl})=S(1,0)/2+3S(2,0)/2$. For NaCl, similarly, one observes[2] $\mu(\text{NaCl})=2S(1,0)$. The sums (9), (10), and (11) are however divergent (Case 3).

Table IV now displays results for sums (9) to (11), ob-

TABLE IV. Efficiency of DPA in estimating $S(2,0)$, $S(2,1)$, and $S(2,2)$ at $k=0.05$.

j	$s_j(2,0)$	$t_{(j-1)/2}(2,0)$	$s_j(2,1)$	$t_{(j-1)/2}(2,1)$	$s_j(2,2)$	$t_{(j-1)/2}(2,2)$
1	−5.45		−5.45		−5.34	
2	7.08		7.04		7.19	
3	−11.83	−0.45	−11.85	−0.48	−11.72	−0.34
4	13.46		13.43		13.58	
5	−18.19	−0.776	−18.22	−0.806	−18.22	−0.665
11	−37.25	−0.774 386 12	−37.28	−0.805 211 36	−37.14	−0.662 412
21	−68.99	−0.774 386 141 424 003	−69.02	−0.805 211 385 235 300 2	−68.88	−0.662 412 7
31	−100.73	−0.774 386 141 424 002 815 212 8	−100.76	−0.805 211 385 235 300 739 526 3	−100.62	−0.662 412 2

TABLE V. Fast convergence of the MPA-accelerated sequences for indirect estimation of $S(2,2)$ at $k=0.05$.

j	$s_j(2,2)-s_j(2,0)$	$t'_{(j-1)/2}$	j	$s_j(2,2)-s_j(2,0)$	$t'_{j/2-1}$
1	0.109 5		2	0.110 8	
3	0.111 55	0.114	4	0.111 77	0.113
5	0.111 86	0.112 3	6	0.111 91	0.112 1
11	0.111 96	0.111 97	10	0.111 96	0.111 97
15	0.111 97	0.111 973 95	14	0.111 97	0.111 973 7
21	0.111 972	0.111 973 923 59	20	0.111 972	0.111 973 923 4
31	0.111 973 3	0.111 973 923 556 80	30	0.111 973 2	0.111 973 923 556 81

tained by 3A. It performs nicely for sequences (9) and (10). With an input similar to the NaCl case ($n=31$), stability of the estimate up to the 22nd decimal place is achieved. On the other hand, the method does not work so well for $S(2,2)$. In this case, the estimate is correct only up to the seventh place, somewhat better than the NaCl case with defect of type 2 (see, e.g., the DPA estimate in Table III), but still far from an accuracy level which is comparable with the corresponding estimates in other situations.

To obtain an accurate estimate of $S(2,2)$, we now employ strategy 3B. We know already that $S(2,0)$ is DPA summable sufficiently accurately. Also, the fact that the sum $S(2,2)$ corresponds to a *perturbed* lattice, the regular one being referred to by $S(2,0)$, is obvious. So, it seems quite likely, especially in view of the success of MPA in estimating $S(1,2)$, that the *perturbation part* in $S(2,2)$ may be evaluated efficiently by employing the MPA. Accordingly, we choose the derived sequence $\{p_j\}$ $[p_j=s_j(2,2)-s_j(2,0),\ j=1,2,3,\ldots]$. This sequence has really turned out to correspond to Case 1. So, MPA should now be a fitting tool. This is nicely demonstrated in Table V. For improved convergence, here we have found strategy 1B more apt. A smooth convergence has thus followed to 14 places. Had we followed 1A, stability up to only sixth place would have resulted. This has been checked by us, but, for brevity, the detailed demonstrative computations have not been presented. We note, however, that such an interesting observation resembles closely an earlier case pointed out by us[18] in a somewhat different context. Anyway, from the result of Table V, coupled with the DPA estimate of $S(2,0)$ given in Table IV, we finally obtain the value $S(2,2)=-0.662\,412\,217\,867\,198$.

From the known relationships (given in Table II of Ref. 2) between μ values and basic sums such as $S(1,0)$ and $S(2,0)$, which may be extended to cases of lattice defects as well, we are now in a position to estimate the Madelung constants of several salts, including the CsCl case with vacancies. Table VI shows a few representative cases. Notably, the values reported here are sufficiently accurate compared to other available estimates (shown in the table) for distorted lattices. The work of Ref. 10 is also not at all reliable in case of type-2 defects, as may be easily seen from the table.

IV. CONCLUSION

To summarize, we have demonstrated how high-precision calculations of μ could be successfully performed by employing Padé-like sequence accelerative transforms. In the course of our study, we observe the

TABLE VI. Estimated values of Madelung constants for a few salts in regular and distorted ($k=0.05$) lattices: A defect of type 1 refers to substitution by an isovalent impurity while a vacancy corresponds to a defect of type 2. Literature values for regular (Ref. 2) and distorted (Ref. 10) lattices, wherever available, are shown within parentheses.

	Lattice specification		
Salt	Regular	Type-1 defect	Type-2 defect
NaCl	$-3.495\,129\,189\,266\,364\,381\,28$ ($-3.495\,129\,189$[a])	$-3.132\,995\,664\,177\,305\,289\,70$ ($-3.132\,994$[b])	$-5.175\,571\,857\,610\,030\,2$ ($-5.176\,806$[b])
CsCl	$-2.035\,361\,509\,452\,595\,318\,14$ ($-2.035\,361\,510$[a])	$-1.991\,065\,993\,897\,277\,431\,70$ ($-1.991\,064$[b])	$-2.287\,511\,291\,203\,304\,6$ ($-2.280\,324$[b])
ZnS	$-3.782\,926\,104\,085\,777\,508\,78$ ($-3.782\,926\,104$[a])	$-3.557\,563\,825\,985\,930\,076\,56$	$-4.875\,297\,220\,008\,319\,7$
NbO	$-3.008\,539\,962\,661\,774\,693\,57$ ($-3.008\,539\,964$[a])	$-2.752\,352\,440\,750\,629\,337\,04$	$-4.212\,885\,002\,141\,121\,7$

[a]Reference 2.
[b]Reference 10.

following: (i) DPA works nicely for both regular and impurity-perturbed lattices where the parent sequences are sawtooth in nature; (ii) for distorted lattices owing to vacant sites, however, the performance of DPA, very similar to performance of u-LT,[10] is not at all satisfactory, whether $\{s_j\}$ is convergent or divergent; (iii) MPA accelerates effectively and in a balanced manner for all types of lattices whenever problems of slow convergence arise; (iv) more complicated situations of divergence with distortions due to lattice-vacancies may be handled efficiently by separate applications of both DPA and MPA at appropriate places.

The present endeavor also provides sufficiently accurate results of μ for distorted lattices in particular. Such good-quality estimates are not available in the literature and may be useful in testing the viability of any other transformation technique. Variation of the level of accuracy of these values has also been shown as a function of the input (n) information. This would serve as an indicator of the efficiency of the schemes employed and guide how far the input n would be considered in achieving still higher, preassigned accuracy level of μ. This latter part is now, of course, a routine procedure; the strategy will remain unaltered.

Throughout the work, we have followed a strategy (1A to 3B), depicted in Sec. II. This appears to be quite general in character in view of its great success for all the sequences that have emerged. Further, one may also consider other transforms as X and Y, though here we have concentrated only on Padé-like schemes. So, finally, we hope that reliable results for distorted lattices with even more complex types of defects may as well be obtained by having recourse to the same strategy.

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