Accurate evaluation of lattice constants using the multipoint-Padé-approximant technique

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The problem of accurate evaluation of lattice constants is overcome by having recourse to an extrapolation scheme. The scheme is applied to a sequence of gradually improved approximate estimates of such constants. The importance of the strategy used to generate the parent sequences, in the course of assessing the viability of the scheme, is emphasized. The good performance of the multipoint Padé approximants is demonstrated. Remarks on the effect of specific geometrical features on the convergence of the process, and hence the effective utilization of selective members of a given sequence in practical cases, are also made. Test calculations are performed for cubic and hexagonal lattices, for which fairly good-quality results are available.

I. INTRODUCTION

Investigation of various mechanical and thermal properties of solids at a molecular level, referring particularly to their relative stabilities, polymorphism, etc., is a very general problem in condensed matter physics.[1–4] Quantitative analysis, however, requires a reasonably accurate value for the energy of the system. For a simple atomic or molecular solid, the pairwise potential-energy function $\phi(r)$ is usually given by a Lennard-Jones-type expression

$$\phi_{m,n}(r)=\frac{\alpha}{r^m}-\frac{\beta}{r^n}\ , \tag{1}$$

where α and β are two empirical parameters. The zero-temperature potential energy[3] $E(0,R)$ will then assume the form

$$E(0,R)=\sum_j n_j\phi_{m,n}(r_j)=\frac{\alpha S_m}{R^m}-\frac{\beta S_n}{R^n}\ , \tag{2}$$

where R is the nearest-neighbor distance. In Eq. (2), S_m and S_n are the so-called lattice constants; m and n are taken as integers, generally with values ranging from 4 to 15. These are obtained from indirect experimental evidence.[4] If n_j is the number of jth neighbors at a distance r_j from the reference atom or molecule concerned ($r_j=p_jR$), the lattice constant S_m is obtained from[5]

$$S_m=\sum_{j=1}^{\infty} n_j/p_j^m\ . \tag{3}$$

We thus see that the problem of obtaining $E(0,R)$ with reasonable accuracy leads us directly to the intricacies associated with accurate estimates of S_m, involving an *infinite sum* as a primary step. It is apparent from (3) that this problem may be highly nontrivial in character owing to convergence difficulties. While the assumption of a finite lattice simplifies the calculations greatly, long-range interactions are neglected. On the other hand, if one proceeds to the infinite-lattice case, computational difficulties with (3) usually arise; in particular, it becomes difficult to speed up the very slow convergence in most situations. Thus, even for a very simple lattice, it turns out to be quite troublesome to obtain $E(0,R)$ with a good degree of precision. That is why the estimation of S_m has emerged as a significant aspect of the study of crystalline solids for many decades.[6–11] For the sake of simplification, one generally introduces first a finite-lattice approximation and then proceeds to improve upon it by assuming a uniform *continuum* thereafter. Such an approach was developed in Ref. 6 and subsequently modified by several authors;[7,10,11] textbook discussions also rely on these estimates.[2–4] The reason is probably that functional transformation procedures[2,8] are not quite as easy to implement in the general case, so there is no other suitable alternative. Further, one hopes that these quoted estimates would at least be appropriate for amorphous systems or liquids, which are essentially characterized by long-range *disorder.*

In view of the above remarks, our intention has been to seek a *direct* method that is able to offer sufficiently accurate values for S_m. To this end, we choose to treat the problem as a problem of *sequence acceleration.* In the present day, various efficient sequence-acceleration techniques are also available,[12–14] and have been employed successfully in a variety of contexts.[14] So, we think, it will be worthwhile to explore whether such techniques may profitably be invoked in the present discipline to estimate S_m with a good degree of precision. Indeed, in this case, we have found one such modern technique, the method of multipoint Padé approximants[12] (MPA), which works very successfully. Thus, we here report values for S_m that are more accurate than the standard values[3] quoted in the literature. We like to adopt a direct *numerical* method also because it permits one to go on evaluating S_m even for lattices with *defects,* unlike the prevalent functional transformation schemes. Moreover, the present technique has a few additional merits. First, the problem at hand serves as a testing ground for assessing the suitability of the MPA, as we shall see in what follows. Keeping in mind the wide-ranging numerical studies on other extrapolation schemes like the Levin transformation, ε algorithm, etc.,[13,14] our calculations in favor of the MPA deserve closer attention. Second, we realize rather directly the importance that the strategy behind a sequence generation has on the success of some sequence-accelerating transform that will be applied subsequently. This is an aspect that usually goes unnoticed. Finally, one finds here also an occasion to explain the advantage of employing *selective* members of a given sequence in MPA. This selectivity owes its origin to *geometrical* features of the system concerned. Some insight may be gained into this unexplored area as well.

II. THE METHOD

Let us consider the problem of calculation of S_m as follows. We start out counting the nearest-neighbor interactions first and go on gradually improving the results by taking contributions of the more-distant neighbors into consideration. Thus, basically we always remain within a finite-lattice approximation and obtain a *set* of increasingly improved estimates of the quantity concerned. This sequential approximation method possesses a convergence rate characteristic of its own. But, the point is, such a set may be suitably transformed to find a *new* set with a much better rate of convergence, so that the chosen last few values of this derived set do not change to within a certain degree of desired accuracy that is greater than that of the previous set.

The method of MPA proceeds in the following manner. Suppose, we have a set of data, denoted by $S(1), S(2), \ldots, S(n)$, approximating some physical quantity S. The exact value is $S(0)$. If the set is monotonic, it is found that often the MPA works quite efficiently.[12] One assumes here that $S(n)$ can be written as a power series in $1/n$. We thus write

$$S(j)=s_1+s_2/j+s_3/j^2+\cdots \quad . \tag{4}$$

Defining a different variable $w=1/j$, Eq. (4) may also be written as

$$\bar{S}(w)=s_1+s_2w+s_3w^2+\cdots \quad , \tag{5}$$

where $S(j)\equiv\bar{S}(w)$. Evidently, from a knowledge of $S(j)$ for $j=1$ to $j=n$, one obtains the coefficients $\{s_j\}$ up to $j=n$. Thus, (5) is in principle known to $O(w^{n-1})$. Now, one proceeds to construct Padé approximants[12] (PA) to the power-series representation (5). One hopes that such approximants would offer better estimates of $\bar{S}(w)$ than the straightforward parent series expansions, to a given order. So, we write

$$\begin{aligned}\bar{S}(w)&=\frac{P_r(w)}{Q_t(w)}+O(w^{r+t+1}), \quad r+t=n-1\\ &=[r/t]\bar{S}(w)+O(w^{r+t+1}) \ ,\end{aligned} \tag{6}$$

where $P_r(w)$ is a polynomial of degree r, $Q_t(w)$ is one of degree t. In MPA, two *particular* choices of the PA are considered: (i) $r=t+1$, $t=k$, when $n=2k+2$ and (ii) $r=t=k$ for $n=2k+1$. This means, in the first case one has an *even* number of input data to fit while in the second case, where *diagonal* PA are employed, an *odd* number of $S(j)$ is taken as input. The approximants are so constructed that in choice (i), we find

$$[k+1/k]\bar{S}(w)=S(j) \ , \quad j=1,2,\ldots,(2k+2), \ w=1/j \ , \tag{7}$$

holds for all $k=0,1,2,\ldots$. Similarly, in choice (ii) we obtain

$$[k/k]\bar{S}(w)=S(j) \ , \quad j=1,2,\ldots,(2k+1), \ w=1/j \ , \tag{8}$$

which is true for all $k=1,2,\ldots$. It is easy to see from (7) that one obtains the $[k+1/k]$ PA by requiring that it would reproduce all the $(2k+2)$ values for members of the basic sequence; similarly, (8) shows that the corresponding PA fits exactly with the values for all the $(2k+1)$ members of the parent sequence. In fact, coefficients of the PA involved in (6) are determined by such requirements only. This is precisely why the method is termed a multipoint PA or the method of n-point PA.[12] The limit point refers to the choice $j=\infty$, and a sequence of approximations for it is obtainable from the above-mentioned approximants (7) and (8) for a given set of data up to $j=n$. These approximants will be denoted by $T(j)$, $j=1,2,\ldots,n-1$. One also finds that the approach of $S(1),S(2),\ldots,$ to the true limit point $S(0)$ is usually much slower in practice than the same of the quantities $[k+1/k]\bar{S}(w=0)$, $k=0,1,2,\ldots,$ and $[k/k]\bar{S}(w=0)$, $k=1,2,\ldots,$ to $S(0)$. In other words, convergence of a given sequence to some limit point is generally accelerated by adopting the MPA.

In practice, however, the construction of the MPA expressions, the left-hand side of (7) and (8), is considerably simplified if one goes on implementing the so-called Thiele's reciprocal difference method.[12] The essence of this strategy is, the aforementioned PA may equally well be represented by continued fractions. So, instead of going for the coefficients of PA, one may choose to evaluate coefficients of the corresponding continued-fraction representation, which are simpler. In view of a thorough discussion on this point in Ref. 12, we refrain from making any detailed description here on this technical aspect of the problem. It may only be remarked here that MPA is very conveniently supplemented by the Thiele scheme.

III. RESULTS AND DISCUSSION

We have already mentioned that, in the present context of lattice-constant evaluation, work has chiefly been done on cubic and hexagonal lattices. For example, works in Refs. 8 and 11 have concentrated on simple-cubic (sc), face-centered-cubic (fcc), body-centered-cubic (bcc), and hexagonal-close-packed (hcp) lattices; Ref. 9 has paid attention to bcc, sc, and diamond lattices; in Ref. 10, fcc and hcp lattices have again been considered. In fact, these are the very popular structures for which various approaches have emerged and values are quoted in the literature.[2–4] One also finds for these cases a collection of data[3,9,10] for n_j and p_j, referred to in Eq. (3), for computing S_m in a stepwise manner.

To choose the most straightforward way, we first proceed through Eq. (3) for computing S_m. Let us then define the sequence $S_m(1), S_m(2), \ldots$, where the members satisfy

$$S_m(j) = \sum_{k=1}^{j} n_k / p_k^m . \tag{9}$$

Now, one may readily check that the rate of convergence of this type of sequence is exceedingly poor. Sample results for the fcc lattice case ($m=4$) are displayed in Table I, for convenience. It is quite apparent that one has to proceed a long way in order to achieve convergence to any reasonable degree. An immediate suggestion could be the adoption of some sequence acceleration scheme on $\{S_m(j)\}$. Surprisingly, however, one finds that even the method of MPA, for example, does not turn out to be quite profitable here. Table I also demonstrates this undesirable feature. To follow the table, it may be useful to note that, from a knowledge of the parent sequence up to $j=n$, one can construct the transformed sequence $\{T(j)\}$ up to $j=n-1$. The poor and irregular performance of the MPA-accelerated transformed sequence is rather evident, though rather unexpected. This may be due either to the inefficiency of the method chosen for the transformation or to the lack of a sufficient *systematization* of the basic sequence $\{S_m(j)\}$, defined by (9), that is necessary for a successful implementation of any sequence-accelerating extrapolation scheme to obtain the limit point $S_m(0) \equiv S_m$. But, we have mentioned earlier (see also below) that the MPA is a very powerful tool.[12] So, one is inclined to think that the above *way* of generating the parent sequence along a *radial* distance is not helpful in so far as extrapolation to the limit is concerned. However, we shall soon see that if such a sequence is constructed by choosing a three-dimensional network, the MPA acceleration scheme performs well. This behavior is not surprising, though. In the course of studying Madelung constants of ionic crystals, it has also been pointed out[15] that convergence of the electrostatic-potential calculations depends crucially on how one proceeds to obtain the sequence. In this respect, the emphasis on the *natural* (three-dimensional) development of the crystal lattice has already been laid. Here, we find a similar situation.

TABLE I. Behavior of the parent radial sequence, generated by Eq. (9) for the fcc lattice constant at $m=4$ and its MPA transform.

j	$S(j)$	$T(j-1)$
1	12.0	
2	13.5	15.0
3	16.2	6.6
4	16.9	18.9
5	17.9	30.2
⋮		
10	19.86	22.0
⋮		
20	21.53	39.25
⋮		
40	22.59	26.46
⋮		
50	22.91	24.29
⋮		
55	23.04	24.33
56	23.05	24.35
57	23.08	24.51
58	23.120	24.34
59	23.123	24.55
60	23.140	24.36

With the above remarks in mind, we now generate the sequences in the following manner:

$$\text{sc:}\quad S_m(j) = \sum_{i=1}^{j} \sum_{M,N,P=-i}^{i} (M^2+N^2+P^2)^{-m/2} , \tag{10a}$$

$$\text{bcc:}\quad S_m(j) = \sum_{i=1}^{j} \left[3^{m/2} \sum_{M,N,P=-i}^{i} [(2M+1)^2+(2N+1)^2+(2P+1)^2]^{-m/2} + (\sqrt{3}/2)^{m/2} \sum_{M,N,P=-i}^{i} (M^2+N^2+P^2)^{-m/2} \right] , \tag{10b}$$

$$\text{fcc:}\quad S_m(j) = \sum_{i=1}^{j} \left[\sum_{M,N,P=-i}^{i} 3(2M^2+N^2+P^2)^{-m/2} - 2(1-m/2)(M^2+N^2+P^2)^{-m/2} \right] , \tag{10c}$$

$$\text{hcp:}\quad S_m(j) = \sum_{i=1}^{j} \sum_{M,N,P=-i}^{i} (X^2+Y^2+Z^2)^{-m/2} ,$$

$$X = M/2,\ Y = (\sqrt{3}/2)[(1-(-1)^P)/6+N],\ Z = \sqrt{(2/3)}P,\ X+Y-Z = 2k,\ k = 0, \pm 1, \pm 2, \ldots . \tag{10d}$$

It will be seen that *these* parent sequences are accelerated quite readily by the method of MPA. Thus, the importance of the strategy behind a sequence generation becomes very apparent in the course of estimating the limit points.

Table II shows the results of applying the MPA acceleration scheme. Estimates of S_m ($m=4,5,6$) for sc, bcc, and fcc lattices are presented here. The convergence

TABLE II. Comparative convergence behavior of the parent and MPA-transformed sequences for some cubic lattice constants. Available values (Ref. 3) are quoted within parentheses.

Lattice	j	$m=4$ $S(2j+1)$	$m=4$ $T(2j)$	$m=5$ $S(2j+1)$	$m=5$ $T(2j)$	$m=6$ $S(2j+1)$	$m=6$ $T(2j)$
sc	1	13.6	16.6	10.0	10.6	8.3	8.5
	2	14.6	16.532	10.2	10.376	8.39	8.40
	3	15.1	16.532 31	10.3	10.377 53	8.40	8.401 926
	5	15.6	16.532 315 96	10.34	10.377 524 83	8.400	8.401 923 9
	7	15.9	16.532 315 96	10.36	10.377 524 83	8.401	8.401 923 97
	10	16.0	16.532 315 96	10.37	10.377 524 83	8.401 7	8.401 923 98
	15	16.2	16.532 315 96	10.373	10.377 524 83	8.401 8	8.401 923 97
			(16.532 3)		(10.377 5)		(8.401 92)
bcc	1	19.3	22.6	14.4	15.0	12.2	12.3
	2	20.5	22.64	14.6	14.76	12.24	12.25
	3	21.1	22.638 7	14.7	14.758 5	12.25	12.253 7
	5	21.6	22.638 721 64	14.73	14.758 509 36	12.252	12.253 667 85
	7	21.9	22.638 721 64	14.74	14.758 509 37	12.253	12.253 667 86
	10	22.1	22.638 721 64	14.75	14.758 509 37	12.253 5	12.253 667 87
	15	22.3	22.638 721 64	14.754	14.758 509 37	12.253 6	12.253 667 87
			(22.638 72)		(14.758 5)		(12.253 3)
fcc	1	21.1	25.4	16.5	17.3	14.4	14.6
	2	22.6	25.33	16.8	16.96	14.43	14.44
	3	23.3	25.338 3	16.9	16.967 51	14.445	14.453 9
	5	24.0	25.338 304 3	16.92	16.967 518 7	14.451	14.453 921
	7	24.4	25.338 304 31	16.94	16.967 518 46	14.453	14.453 921 05
	10	24.6	25.338 304 31	16.95	16.967 518 45	14.453 6	14.453 921 04
	15	24.9	25.338 304 31	16.961	16.967 518 46	14.453 8	14.453 921 04
			(25.338 30)		(16.967 5)		(14.453 92)

of the parent sequences $\{S(j)\}$, constructed through (10), for various values of m are displayed to allow us to develop a feel for the efficiency of the transformation. The transformed sequences $\{T(j)\}$ are also tabulated. One may appreciate the advantage of the present endeavor quite readily by noting that, whereas the parent sequences do not show any stability up to the first or second decimal place even after $j=30$, the transformed sequences converge very rapidly with the aid of the first 10–15 terms of the parent sequence only, and here stability up to eight decimal places is assured. While in Table II we show explicitly the nature of convergence for $m=4$

TABLE III. Irregular and slow convergence of MPA-accelerated sequences for straightforward application on the hcp lattice case.

j	$m=4$ $S(j)$	$m=4$ $T(j-1)$	$m=5$ $S(j)$	$m=5$ $T(j-1)$	$m=6$ $S(j)$	$m=6$ $T(j-1)$
1	10.5		10.4		10.3	
2	16.5	22.5	14.7	19.0	13.6	17.0
3	19.0	24.8	15.8	17.6	14.1	14.8
4	20.4	26.0	16.2	17.3	14.3	14.5
5	21.3	25.31	16.5	18.4	14.37	14.2
6	21.9	25.40	16.6	16.97	14.40	14.42
7	22.3	25.338	16.7	16.93	14.42	14.43
8	22.7	25.356	16.76	16.962	14.431	14.23
9	23.0	25.341	16.80	16.962	14.438	14.451
10	23.2	25.345 7	16.83	16.962	14.442	14.458
11	23.4	25.341 5	16.85	16.966	14.445	14.454
12	23.5	25.342 3	16.87	16.955	14.447 5	14.456
13	23.7	25.341 5	16.89	16.967 6	14.449 0	14.454 4
14	23.8	25.340 8	16.90	16.972 9	14.450 2	14.455 1
15	23.9	25.341 6	16.91	16.968 0	14.451 0	14.454 7
⋮						
30	24.60	25.339 2	16.952	16.968 45	14.454 39	14.454 899
31	24.63	25.338 9	16.953	16.968 43	14.454 44	14.454 896

to $m=6$, final converged results are displayed for other m values in Table V. Obviously, for larger m values, convergence is achieved more readily. Comparing with the standard literature values,[3] quoted within parentheses in the tables concerned, we note also that the estimates reported here are better.

It is of more interest to notice that the case with the hcp lattice is radically different. Table III summarizes our findings when applying a similar strategy, the MPA, as considered in Table II. Here, one discovers a poor performance of the MPA. Results are good *only* to the extent that stability up to the second or third decimal place has been achieved. If compared with the corresponding performance for sc, bcc, or fcc lattices, we must doubt that probably something more subtle somehow becomes important. Indeed this is so. A geometrical consideration[4] reveals that, in this hcp case, *alternate* $S(j)$ are to be paid more attention since they refer to *similar environmental effects* and thus are likely to afford a tolerable degree of systematization that is necessary for a smooth convergence of MPA, or for that matter any such transformation scheme. This is also apparent from (10d) if we care to look at the variable Y, which shows that the contribution has an *alternating* character.

Having understood the basic problem, we thought that it would be worthwhile to consider the *even* and *odd* members of the parent sequence *separately* in the hcp case, for some chosen value of m, and then to apply the transformation. The adequacy of such a choice of alternate members, i.e., a *selective* choice from among a given set, is evident *a posteriori*. Table IV demonstrates the suitability of our choice in a very transparent manner. The parent members are already shown in Table III; so here only the transformed sequences are displayed. What we obtain from a consideration of only the *odd* members, viz., $S(1), S(3), \ldots$, etc., are listed as $T(o,j)$ and results of applying the MPA on the *even* ones, viz., $S(2), S(4), \ldots$, etc., are denoted by $T(e,j)$. It is remarkable that both these transformed sequences converge to the same final result, and quite quickly too. In case of any difference in final estimates, results should naturally be averaged, but such a situation does not arise here. A comparison with the results (Table III) of applying the strategy flatly, ignoring the prescription for generation of the parent sequence, clearly reveals the importance of selectively choosing the parent members.

One may be curious to determine whether or not a selective choice from among a given set $\{S(j)\}$, $j=1,\ldots,n$, would affect a transformation adversely. This is because a *reduction* of information is involved, and consequently the transformation scheme might not shape itself properly to the rhythm of the sequence, leading finally to a poor showing. Usually, it is so. Thus, the extent of correctness of data presented in Table IV is inferior to those given in Table II, for some chosen upper limit of j value. In Table IV, we note that stability up to eight decimal places is achieved by considering 14–16 terms of the parent even or odd sequences, which actually amounts to considering 30–31 original terms. The situation with Table II is better. Admittedly, however, in the present case, there is a tradeoff; whenever successive terms of a sequence do *not* systematically incorporate or neglect certain contributions, a selective choice becomes mandatory, even at the cost of a reduction of information. This is precisely why Table IV exhibits a much improved performance relative to what we observe in Table III. In a widely different context, the evaluation of critical parameters from series expansions, a situation of somewhat similar nature prevails. Thus, in the course of studying the high-temperature-susceptibility series of mixed-spin Ising models on the bcc lattice, it has been found[16] that the critical temperature may be determined either by considering the even-order terms *or* the odd-order ones; of course, the results are virtually the same, as expected. However, selectivity is generally not advantageous in extrapolation problems. For example, if we choose to proceed for the MPA $T(j)$ sequences by taking either the even or the odd terms in sc, bcc, or fcc cases, one would find a *slower* convergence than what have been

TABLE IV. Fast convergence of MPA-accelerated sequences obtained separately from the odd and even members of the parent sequences for the hcp lattice. Known results (Ref. 3) are given within parentheses.

	$m=4$		$m=5$		$m=6$	
j	$T(o,j-1)$	$T(e,j-1)$	$T(o,j-1)$	$T(e,j-1)$	$T(o,j-1)$	$T(e,j-1)$
2	27.4	24.2	21.2	17.8	18.0	15.0
3	25.3	25.38	17.4	17.2	14.6	14.5
4	25.37	25.338	16.98	16.9	14.4	14.43
5	25.34	25.339 8	16.96	16.969 9	14.44	14.45
6	25.339	25.339 3	16.967	16.968 3	14.456	14.454 4
7	25.339 1	25.339 04	16.968 5	16.968 42	14.454 9	14.454 9
8	25.339 084	25.339 086	16.968 42	16.968 45	14.454 87	14.454 9
9	25.339 079	25.339 083	16.968 435	16.968 436 8	14.454 89	14.454 895
10	25.339 081	25.339 082	16.968 437	16.968 436 2	14.454 897 7	14.454 897 1
11	25.339 082 4	25.339 082 3	16.968 436 4	16.968 436 35	14.454 897 2	14.454 897 3
12	25.339 082 31	25.339 082 33	16.968 436 33	16.968 436 35	14.454 897 27	14.454 897 27
13	25.339 082 34	25.339 082 30	16.968 436 35	16.968 436 35	14.454 897 29	14.454 897 28
14	25.339 082 33	25.339 082 34	16.968 436 35	16.968 436 35	14.454 897 27	14.454 897 28
15	25.339 082 34	25.339 082 34	16.968 436 35	16.968 436 35	14.454 897 28	14.454 897 28
					(14.454 89)	

TABLE V. Accurate estimates of S_m ($m = 7-15$) by the MPA-acceleration of parent sequences. Data within parentheses refer to standard literature values (Ref. 3).

m	sc	bcc	fcc	hcp
7	7.467 057 78 (7.467 0)	11.054 243 48 (11.054 24)	13.359 387 70 (13.359 39)	13.360 346 78 (13.360 35)
8	6.945 807 93 (6.945 80)	10.355 197 91 (10.355)	12.801 937 23 (12.801 94)	12.802 821 85 (12.802 82)
9	6.628 859 20 (6.628 8)	9.894 589 66 (9.894 5)	12.492 546 70 (12.492 55)	12.493 321 73 (12.493 32)
10	6.426 119 10 (6.426 1)	9.564 400 62 (9.564)	12.311 245 67 (12.311 25)	12.311 896 23 (12.311 90)
11	6.292 294 50 (6.292 29)	9.313 262 54 (9.313 26)	12.200 920 35 (12.200 9)	12.201 447 10
12	6.202 149 05 (6.202 1)	9.114 183 27 (9.114 18)	12.131 880 20 (12.131 88)	12.132 293 77 (12.132 29)
13	6.140 599 58 (6.140)	8.951 807 32 (8.951 80)	12.087 726 32 (12.087 72)	12.088 042 55
14	6.098 184 13 (6.098 18)	8.816 770 23 (8.816 7)	12.058 991 94 (12.058 99)	12.059 228 26 (12.059 23)
15	6.068 764 30 (6.068 76)	8.702 984 56 (8.702 98)	12.040 024 06 (12.040 02)	12.040 197 14

recorded in Table II. This we have checked. The reason for this is the halving of information.

Results of S_m for other m values of the hcp lattice, obtained by adopting a similar scheme, are finally placed in Table V along with the estimates for cubic lattices. Comparing with the accepted estimates,[3] we note that a remarkable improvement has been achieved through the method of MPA. For example, now we have estimates of S_4, S_5, S_{11}, S_{13}, and S_{15} for the hcp lattice. For the sc and bcc lattices, the previous estimates were, in cases, correct only up to three or four decimal places. But here, the MPA acceleration strategy permits one to evaluate all the lattice constants correct up to eight decimal places. These refined estimates, we hope, may be useful as good-quality standard benchmark values with which to compare the need for and reliability of any other scheme.[11]

IV. CONCLUSION

To summarize, our purpose has primarily been to obtain accurate estimates of lattice constants S_m for various lattices. We have demonstrated how adoption of the MPA successfully accomplishes this purpose. This observation, in turn, provides a context in which the MPA can be effectively applied. In the course of our exploration, the problem of whether the use of a judiciously selected subsequence would be worthwhile has also surfaced. As we have seen, this problem is related to specific geometrical arrangements, and is important only for the hcp lattice case. The merit of bypassing the straightforward application of any sequence acceleration scheme to a given sequence, and the need of a closer look at the strategy of generating a sequence—with due consideration given for a systematic counting of environmental effects—have also been emphasized in this paper. This is an additional instructive feature of the present work. We hope future work along similar lines may shed more light on such an interesting aspect as sequence acceleration whereby properties of the infinite lattice may be obtained from the properties of the finite-lattice by extrapolation.

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