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On some problems of the maximum entropy ansatz

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Abstract. Some problems associated with the use of the maximum entropy principle, namely, (i) possible divergence of the series that is exponentiated, (ii) input-dependent asymptotic behaviour of the density function resulting from the truncation of the said series, and (iii) non-vanishing of the density function at the boundaries of a finite domain are pointed out. Prescriptions for remedying the aforesaid problems are put forward. Pilot calculations involving the ground quantum eigenenergy states of the quartic oscillator, the particle-in-a-box model, and the classical Maxwellian speed and energy distributions lend credence to our approach.

Keywords. Maximum entropy ansatz; Padé-type approximants; boundary behaviour.

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1. Introduction

The estimation of the probability density (PD) function $\rho(x)$ from a knowledge of its moments constitutes what is known as the classical moment problem. In its usual form the problem is posed as follows: given as input information a set of moments $\mu_n (n \leq k)$ of a variable x in the range $[a, b]$, where

$$\mu_n = \langle x^n \rangle = \int_a^b x^n \rho(x) \mathrm{d}x, \quad n = 0, 1, 2, \cdots, k, \tag{1}$$

one has to find the positive function $\rho(x)$. The extent to which one can simulate the actual PD from a given set of moments has been widely discussed in the literature [1].

In recent years, there has been a number of efforts [2] based on the maximum entropy principle (MEP) [3] to confront the classical moment problem in a variety of situations. The MEP approach for finding $\rho(x)$ is to maximize the information entropy functional $I[\rho]$ given by

$$I[\rho] = -\int_a^b \rho(x) \ln[\rho(x)] \mathrm{d}x$$

subject to the constraints imposed by (1). By standard manipulations, one obtains an approximate density $\rho^{\mathrm{A}}(x)$, given by

$$\rho^{\mathrm{A}}(x) = \exp(-S^{\mathrm{A}}) = \exp\left(-\sum_{n=0}^{\infty}\lambda_n x^n\right), \tag{2}$$

where k in (1) has been assumed to extend to infinity corresponding to *maximum* possible input information. Here, the Lagrange parameters λ_n are introduced to take into account the knowledge of the moments μ_n. The parameter λ_0 is related to other λ_n's through the equation

$$\mathrm{e}^{\lambda_0} = \int_a^b \mathrm{d}x \exp\left(-\sum_{n=1}^{k}\lambda_n x^n\right). \tag{3}$$

The quantity on the right hand side of eq. (3) is called the partition function Z. If one introduces a potential F by

$$F = \ln Z + \sum_{n=1}^{k}\mu_n\lambda_n, \tag{4}$$

then the condition of stationarity of F with respect to λ_n, that is,

$$\frac{\partial F}{\partial \lambda_n} = 0, \quad n = 1, 2, \cdots, k, \tag{5}$$

generates k non-linear equations which, together with (3), can be solved to find the Lagrange multipliers.

The MEP *recipe*, outlined above, is said to provide the *least biased* estimate of the PD consistent with the available information. But, even at this stage, we realize that $\rho^{\mathrm{A}}(x)$ may *not* correspond to the exact PD, specifically in cases where the actual $\rho(x)$ does not admit well-defined (finite) values for all its moments, e.g. a Lorentzian. Further, in practice, it is impossible to incorporate an infinite set of input information. As a result, one invariably truncates the infinite series in (2) at some value n, say k, to obtain the distribution $\rho_k^{\mathrm{A}}(x)$:

$$\rho_k^{\mathrm{A}}(x) = \exp[-S_k^{\mathrm{A}}(x)], \tag{6}$$

where

$$S_k^{\mathrm{A}}(x) = \sum_{n=0}^{k}\lambda_n x^n. \tag{7}$$

The need for truncation arises primarily because one usually has information about only the first few moments. Even if one possesses the knowledge of a large number of moments, the numerical procedure (like Newton's algorithm or its variants) for the determination of the corresponding λ_n's becomes cumbersome and unreliable [4]. It is thus no wonder that general conclusions have been drawn only for a selected class of few-moment problems [5]. The numerical justification for the truncation of the series S rests on the assumption that, for large enough k, averages obtained by using $\rho(x)$ and $\rho_k^{\mathrm{A}}(x)$ agree with each other. This in turn requires that the series $S(x)$ is *convergent*. But whether this convergence is guaranteed *a priori* is the first point that we shall examine by considering some specific

cases. Secondly, the use of $\rho_k^{\mathrm{A}}(x)$ as given by (6) implies that the asymptotic behaviour of the density should go as exp $(-\lambda_k x^k)$. The *large-x* behaviour of $\rho^{\mathrm{A}}(x)$ is thus curiously *dictated* by the number of moments employed to *construct* it! But, for a given problem, the corresponding density should have a unique asymptotic growth or decay. Thirdly, there are many instances where the density function is known, purely on physical grounds, to vanish at one or both boundaries. But the MEP ansatz ignores extra information of this sort. The form (6) does not ensure that the density function would vanish at the boundaries when (i) $x \in [-\infty, +\infty]$, (ii) $x \in [0, \infty]$, and (iii) $x \in [a, b]$. Only in case (i) we can enforce the required behaviour in (6) by additionally restricting k to be an even integer and $\lambda_k > 0$ in (7). In others, one can never achieve the same by sticking to the primitive ansatz. We suggest a simple scheme whereby the correct boundary behaviour can be built into the MEP form of the PD.

Having discussed the complications, the purpose of the present communication is threefold: (i) to circumvent the problem of divergence, if any, of the series $S(x)$; (ii) to show how crucial it is to incorporate the correct asymptotic behaviour of $\rho(x)$ in the approximate PD; (iii) to highlight the performance of MEP-inspired $\rho^{\mathrm{A}}(x)$ in $[0, \infty]$ and finite intervals by employing a suitable prefactor.

Our work is organized as follows. First, in §2, we consider the problem of constructing the PD corresponding to the ground eigenenergy state of the quartic oscillator via the traditional approach. We demonstrate that by employing a power Padé form for $S(x)$ one can bypass the problem of divergence of $S(x)$ while at the same time satisfy the required asymptotic decay of the PD. Section 3 is devoted to studies on problems in $[0, \infty]$. Here we treat the classical Maxwell speed and energy distributions to bring into focus the need of a prefactor in the conventional MEP ansatz. In §4, problems in finite domain will be considered. We investigate energy eigenstates of a particle-in-a-box (PB) and again point out the need of incorporating a proper prefactor in the MEP form of the density function. The above examples, both from classical and quantum domains, will hopefully bring into focus some difficulties of a general nature inherent in the MEP ansatz. The present endeavour aims at removing these difficulties and thus making the MEP *recipe* applicable to a wider variety of situations.

2. The problem of divergence

The posssibility that the series $S(x)$ in (7) can be divergent in some cases does not seem to have been recognized before. We examine this point with reference to the quantum mechanical PD of the quartic oscillator governed by the Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^4.$$

By virtue of the symmetry of the potential, the odd moments of x vanish. Assuming that the values of a few even moments are given, Plastino *et al* [6] followed the MEP route and employed the form (6) with $S_k^{\mathrm{A}}(x)$ given naturally by

$$S_k^{\mathrm{A}}(x) = \sum_{n=1}^{k} \lambda_{2n} x^{2n}. \tag{8}$$

Normalizability requires $\lambda_{2k} > 0$, and also fixes λ_0 in (7). The approximate PD of the ground state is generally expected to approach the exact one with increasing k.

We take the quantity defined by

$$\Delta = \frac{1}{N}\sum_{n=1}^{N}\left(1 - \frac{\tilde{\mu}_{2n}}{\mu_{2n}}\right)^2, \quad N \geq k \tag{9}$$

to test the degree of accuracy of $\rho^{\mathrm{A}}(x)$. Here μ_n and $\tilde{\mu}_n$ refer, respectively, to the true nth moment and the moment calculated by using $\rho^{\mathrm{A}}(x)$. The minimization of Δ yields the optimum set of λ_n's. Conventionally, one obtains these by solving the system of non-linear equations given by (5).

In table 1, we present some results to show how the quality of the sought-for density gradually improves with the number of terms k in (8). The improvement can be assessed by noting, apart from the minimum value of Δ $(\Delta_{\min})$, the values of global properties like (i) the average ground state energy E_0, (ii) the virial ratio R defined by $R = \langle \mathrm{kinetic\ energy} \rangle / 2 \langle \mathrm{potential\ energy} \rangle$, and (iii) the information entropy I_0. For convenience, exact or near exact results [7] are shown in parentheses in the same table.

We note that, for a fixed N, there is a gradual improvement as k increases. It should, however, be pointed out that if we fix k and go on increasing N results first improve and then worsen after a certain stage. Obviously, a handful of variables cannot be expected to shape $\rho(x)$ so as to satisfy a large number of constraint relations. Table 2, where we display the optimized sets of parameters λ_{2n}, reveals a disturbing feature. We find that in some cases λ_{2k} assumes negative values defying the normalization requirement. Here,

Table 1. $\Delta_{\min}$, E_0, R and I_0 corresponding to the quartic oscillator obtained by using the MEP ansatz (6).

k	N	$\Delta_{\min}$	E_0	R	I_0
2	6	0.94113321E-05	1.06055239	1.00343025	0.42638758
	7	0.17528804E-04	1.06060730	1.00650854	0.42477246
	8	0.29539315E-04	1.06067222	1.01011694	0.42302022
3	6	0.11266142E-05	1.06041507	1.00040237	0.42894234
	7	0.23798140E-05	1.06042972	1.00166371	0.42816542
	8	0.43121077E-05	1.06044708	1.00323848	0.42731520
4	6	0.36426119E-10	1.06036221	0.99998675	0.43034952
	7	0.13446238E-09	1.06036227	0.99997578	0.43034422
	8	0.37330872E-09	1.06036234	0.99996546	0.43033484
5	6	0.30983152E-11	1.060362168	0.99999606	0.43035172
	7	0.20091253E-10	1.060362181	0.99998937	0.43035018
	8	0.75667825E-10	1.060362217	0.99998022	0.43034606
6	7	0.39681399E-15	1.06036209087	0.99999998	0.43035232
	8	0.15132401E-13	1.06036209088	1.00000016	0.43034606
			(1.06036209048)[a]	(1)	(0.4303523166)

[a] See ref. [7]

Table 2. Optimized values of the parameters in the MEP form of ρ, with $N = 8$, for the ground state of quartic oscillator.

k	λ_2	λ_4	λ_6	λ_8	λ_{10}	λ_{12}
2	1.133032	0.132744	0	0	0	0
3	1.101244	0.151341	−0.002524	0	0	0
4	1.063508	0.181284	−0.009339	0.000406	0	0
5	1.062616	0.182606	−0.009966	0.000518	−0.000006	0
6	1.060473	0.186920	−0.012960	0.001390	−0.000113	0.000004

such cases are managed through a cut-off in the upper limit of integration. In addition to the above difficulty, we also note that with increasing k, λ_{2k} becomes *intractably small*. In the light of results displayed in tables 1 and 2, one can legitimately ask: can we gradually reach exactness by routinely increasing k in (8)? The answer to this question appears to be in the negative. Apart from the numerical troubles mentioned above, a more cogent justification comes from a different angle. For the x^4 problem, the Schrödinger equation tells us that the PD of the ground state should decay as exp $(-b|x^3|)$ with $b > 0$. This feature alone is a strong indication of the inefficiency of $S(x)$-series appearing in the MEP prescription, because a series like (8) consisting solely of even powers of x *cannot* show an odd power-law decay unless it is summed to infinity. So, it is difficult to improve the quality of the PD by routinely increasing the number of parameters in the manner sketched above. It is also noteworthy that such a procedure will lead to a systematic worsening of the asymptotic behaviour of the PD.

Having ascertained that a routine increase in the number of terms in $S(x)$ does not lead to improved accuracy we look for an alternative strategy. We regard $S^{\mathrm{A}}(x)$ as a function that goes as $b|x^3|$ at large x as also admits of a series representation of the form (2). We thus replace $S^{\mathrm{A}}(x)$ by a Padé-type approximant

$$S^{\mathrm{A}}(x) = \frac{[p_m^{\mathrm{A}}(x)]^s}{[q_n^{\mathrm{A}}(x)]^t} \equiv [m, s/n, t], \tag{10}$$

where p_r^{A} and q_r^{A} are polynomials of degree $2r$ with constant terms zero and unity, respectively. The parameters m, s, n, t are chosen to satisfy the asymptotic behaviour for the specific potential problem. We set $s = 1$ so that the density goes as exp $(-cx^2), c > 0$ when $x \to 0$ which is also a desirable requirement. Note that a plain Padé form for $S^{\mathrm{A}}(x)$ would not suit our purpose. So, a power-Padé form has been chosen here.

The unknown parameters appearing in $\rho^{\mathrm{A}}(x)$ are once again found by minimizing Δ given by (9). In table 3, we display the results following from the procedure just outlined above corresponding to the case discussed in table 1. Comparing these results with the earlier ones, it is quite clear that if the trial density conforms to the correct asymptotic behaviour, there is a significant improvement in the various global properties, and hence in the quality of the PD. The expansion of the modified form of $S^{\mathrm{A}}(x)$ employed in (10) as a power series in x^2 justifies our assertion that the primitive MEP form of the PD for the x^4 potential as given by (2) involves a *divergent series*. A similar conclusion holds for any potential of the form x^{4M}, where M is a positive integer. For reasons of brevity, we do not display further results here, e.g. for the octic oscillator.

Table 3. $\Delta_{\min}$, E_0, R and I_0 for the ground state of the quartic oscillator with power-Padé form of $S(x)$.

Form of $p^{\mathrm{A}}(x)$	Form of $q^{\mathrm{A}}(x)$	t	N	$\Delta_{\min}$	E_0	R	I_0
$a_1x^2+a_2x^4$	$(1+a_3x^2)$	$\frac{1}{2}$	6	0.32097E-09	1.060362095	0.99997710	0.43036972
			7	0.93398E-09	1.060362097	0.99995286	0.43038314
			8	0.21882E-08	1.060362101	0.99991930	0.43040034
$a_1x^2+a_2x^4$	$(1+a_3x^2+a_4x^4)$	$\frac{1}{4}$	6	0.16197E-10	1.060362095	0.99999453	0.43034862
			7	0.40352E-10	1.060362097	0.99999481	0.43034534
			8	0.85066E-10	1.060362100	0.99999704	0.43034092
$a_1x^2+a_2x^4$	$(1+a_3x^2+a_4x^4$ $+a_5x^6+a_6x^8)$	$\frac{1}{8}$	6	0.89868E-16	1.06036209051	0.99999999	0.430352316
			7	0.68271E-15	1.06036209054	0.99999996	0.430352314
			8	0.29058E-14	1.06036209057	0.99999989	0.430352308

3. Problems in [0, ∞]

Let us consider the well-known classical Maxwell's speed (c) and energy (E) distributions whose moments are assumed known. We wish to see how far the standard MEP prescription is able to reproduce these functions solely on the basis of the information regarding a few moments. Here, for convenience, we have chosen reduced units, viz. $k_{\mathrm{B}}T = 1$ and $m = 2$. The results are presented in the upper half of table 4. From a glance at the data, it may appear that a gradual increase in the number of moments along with the Lagrangian parameters will lead us towards exactness. But this is illusory. The physics of the problem imposes a boundary constraint, namely, $\rho(c) = 0$ at $c = 0$ and $\rho(E) = 0$ at $E = 0$. But, the MEP formalism does not allow us to incorporate such constraints in a suitable way. As a result, the density functions constructed via MEP are liable to deviate considerably in form compared to the exact ones leading to poor pointwise convergence. The simplest way to ensure the correct boundary behaviour is to modulate the MEP forms of PD with the help of suitable prefactors as follows:

$$\tilde{\rho}(c) = c^{\alpha}\rho_{\mathrm{MEP}}(c), \tag{11}$$

$$\tilde{\rho}(E) = E^{\beta}\rho_{\mathrm{MEP}}(E), \tag{12}$$

where α and β are adjustable parameters chosen so as to minimize Δ.

The advantage of the modification suggested above is immediately seen in the lower half of table 4. The reduction in $\Delta_{\min}$ is quite remarkable. Employing just a few moments, we find that the optimized values of the parameters α and β turn out to be very close to the exact values 2 and $1/2$, respectively. In table 5, we list the values of the optimized parameters. We find that in the modified form of ρ, the coefficients of the terms in $S(x)$ are all virtually zero barring the one that is present in the actual distribution. On the other hand, ρ_{MEP} tries to satisfy the moment constraints by invoking spurious terms in the power series.

Figures 1 and 2 quite clearly show the improvement resulting from the use of the forms (11) and (12). Here the exact distributions and the distributions $\tilde{\rho}(c)$ and $\tilde{\rho}(E)$ practically

Table 4. Maxwell's speed and energy distributions approximated by MEP and modified MEP ansatz.

Scheme	Number of parameters	Number of moments employed	$\Delta_{\min}$ values corresponding to distribution of	
			speed	energy
Conventional MEP (ρ given by eq. (6))	3	4	1.19580141E-06	1.46372131E-05
		5	5.15468284E-06	2.61242056E-05
		6	1.39004932E-05	3.31882625E-05
	4	5	2.12994526E-08	4.14893306E-06
		6	1.20830464E-07	3.29566917E-05
Modified MEP (ρ given by eq. (11) or (12))	3	4	5.26454520E-19	1.59817250E-12
		5	1.42584824E-17	4.70544395E-12
		6	2.06393832E-16	8.79984041E-12
	4	5	5.64870536E-19	3.29602484E-13
		6	1.5468839E-17	1.16956610E-12

Table 5. Optimized parameters for the Maxwellian speed and energy distributions.

Scheme	No. of parameters	No. of moments used	Optimized parameters for					
			speed distribution function			energy distribution function		
MEP			λ_1	λ_2	λ_3	λ_1	λ_2	λ_3
	3	4	−6.26850	3.64222	−0.42352	−0.07335	0.23073	−0.01614
		5	−5.97288	3.42137	−0.37595	−0.03824	0.21834	−0.01510
		6	−5.71611	3.23212	−0.33554	−0.05397	0.22361	−0.01552
Modified MEP			λ_1	λ_2	α	λ_1	λ_2	β
	3	4	1.29355E-06	0.9999997	2.000006	1.00008	−4.77097E-06	0.50011
		5	2.75592E-06	0.9999994	2.000001	1.00006	−3.10291E-06	0.50009
		6	5.65483E-06	0.9999988	2.000003	1.00004	−2.17330E-06	0.50008

coincide everywhere within the domain while ρ_{MEP} in both cases show considerable deviation. The role of the prefactor in such problems is thus quite transparent.

4. Problems in $[-1, 1]$

It is curious to note that while the MEP has been successfully employed [6] to construct the ground state PD of a number of quantum mechanical systems, its applicability to the simple textbook problem of the PB has not been tested, to the best of our knowledge. The reason possibly is that the MEP ansatz for the PD fails to satisfy the boundary behaviour. In this section, we examine how the form (6) for density can be modulated to simulate the ground state PD of a very simple system. We consider the PB potential, where

$$V(x) = 0, \quad -1 \leq x \leq 1$$
$$= \infty, \quad |x| > 1.$$

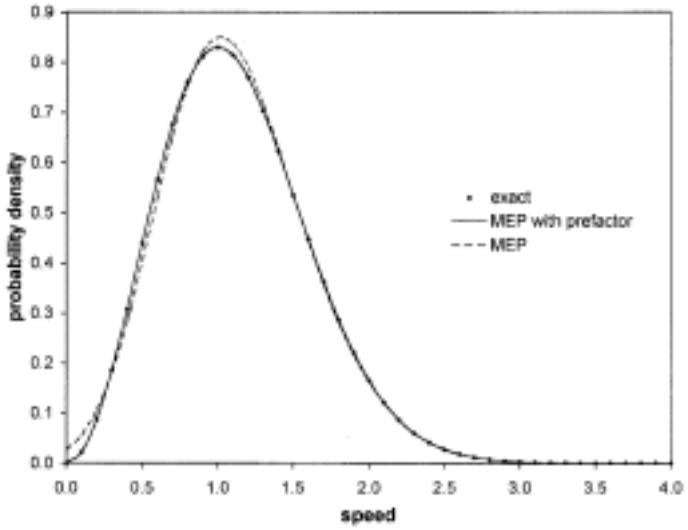

Figure 1. Plot of Maxwell's speed distribution along with those approximated by MEP and modified MEP ansatz.

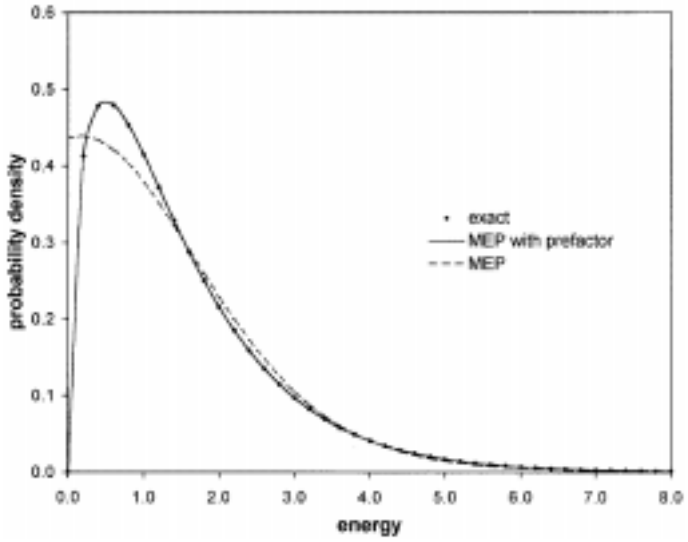

Figure 2. Comparison of Maxwell's exact energy distribution function with MEP and modified MEP distributions.

The primitive MEP ansatz with any finite set of λ's *cannot* ensure the vanishing of $\rho^{\mathrm{A}}(x)$ at $x = \pm 1$. We enforce this behaviour through a *prefactor* of the form $(1 - x^2)^p$. For the ground state, we thus choose

$$\rho_0^{\mathrm{A}}(x) = (1 - x^2)^p \exp[-S^{\mathrm{A}}(x)], \tag{13}$$

where

Table 6. Testing the probability density for the ground state of PB built via MEP and its modified form.

Scheme	Number of parameters	Number of moments used	$\Delta_{\min}$	E_0	I_0
MEP	3	4	0.23023E-06	2.24932	0.38633
		5	0.11919E-05	2.26804	0.38601
		6	0.36429E-05	2.28595	0.38554
Modified MEP	3	4	0.58151E-14	2.4674068	0.3862943
		5	0.24354E-13	2.4674062	0.3862944
		6	0.61460E-13	2.4674057	0.3862944
				(2.4674011)	(0.3862944)

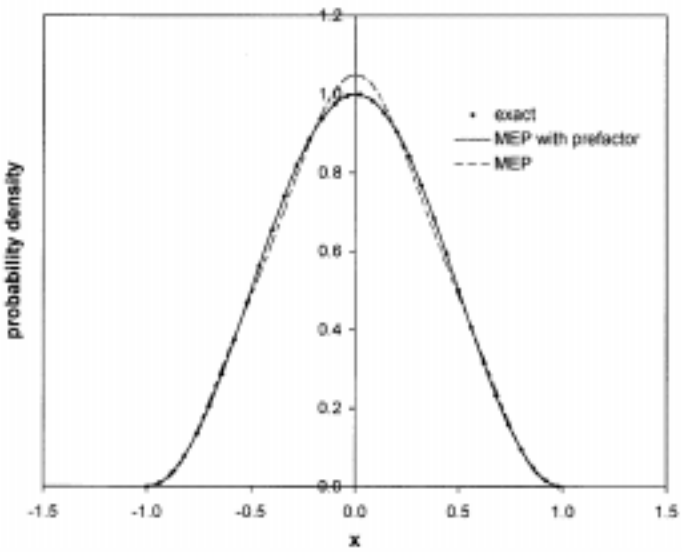

Figure 3. Plot of the exact probability density for the ground state of PB along with the traditional and modified MEP densities.

$$S^{\mathrm{A}}(x) = \sum_{n=1}^{N} \lambda_n x^{2n}. \tag{14}$$

Let us note that here, unlike the x^4 potential case, the large-x behaviour poses no problem, and hence only a few terms of the series representation for $S^{\mathrm{A}}(x)$ will suffice. The coefficients λ_n and the exponent p in (13) are determined by minimizing Δ given by (9). In table 6, we show the results of our computation with just three parameters in $S^{\mathrm{A}}(x)$ of which one is the exponent p. The optimized value of p turns out to be 2.0003, remarkably close to the exact one: $p = 2$. Unlike the cases considered earlier, the PB problem is exactly solvable. So it will be of interest to compare the exact values of E_0 and I_0 with those calculated by using the optimized density. Relevant data in table 6 show clearly that our prescription works much better. Additionally, figure 3 shows that the optimized density given by (13) converges to the analytical result almost everywhere in the domain of

the variable x. On the other hand, plain MEP fails to perform nicely on this count. This clearly justifies the suggested modification.

5. Conclusion

To summarize, our motivation has primarily been to explore how one should modify the standard MEP form of the PD to gain advantage. It has been found that the knowledge of the asymptotic behaviour of the true density is crucial on two counts: first, to demonstrate that the possibility of reaching exactness by routinely increasing the number of parameters in the traditional form of MEP density function may be illusory; secondly, to provide a definite clue as regards the divergence of the series that is exponentiated in the primitive MEP ansatz. Both these points are amply substantiated in the present study. For problems in semi-infinite or finite intervals, MEP ansatz does not ensure vanishing of the PD at the boundaries even when the physics of the problem demands so. In such cases, we have found that a suitable prefactor can handle the situation quite commendably. In fine, we may assert that, to make the MEP ansatz applicable to a wider variety of problems it may have to be modified by (i) incorporating a suitable prefactor, (ii) using a functional form in place of the series representation of $S(x)$.

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