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General Pade Effective Potential for Coulomb Problems in Condensed and Soft Matters

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Abstract. Effective potentials for finding the ground states and physical configurations have essential meaning in many Coulomb problems of condensed and soft matters. The ordinary n-Pade approximation potentials define as the ratio of Pi(r)/Pi+1(r), where Pi(r) are the polynomials of i-th order of charge separation r, give quite good fit and agreement of calculation results and experimental data for Coulomb problems, where screening effects are not important or exchange photons still are massless. In this work we consider a general Pade effective potential by included a factor of exponential form, which could give more accurate results also for above mentioned cases. This general Pade effective potentials with analytical expressions were useful to perform analytical calculations, estimations and to reduce the amount of computational time for future investigations in condensed and soft matter topics. For example of soft matter problems, we study the case of MS2 virus, the general Pade potential gives much more correct results comparing with ordinary Pade approximation.

1. Introduction

In theoretical physics, one frequently encounters power series expansions whichs do not converge or converge very slowly, and there are many methods for accelerating the convergence of these sequences and the subsequent evaluation of the limit of an infinite sequence. Among them, the Pade approximation provides a practical method for performing numerically the analytic continuation of function. The Pade approximation is a very simple and powerful alternative to polynomial approximations for analytic functions. It is known that the "best" approximation of a function by a rational function of given order - under this technique, the approximant's power series agrees with the power series of the function it is approximating. The technique was developed around 1890 by Henri Pade, but goes back to Georg Frobenius who introduced the idea and investigated the features of rational approximations of power series [1].

The Pade approximation provides such a method, we define the [n,m] Pade approximant to f(z) as the ratio of Pn(z) and Qm(z) [2]:

$$f^{[n,m]}(z) \equiv \frac{P_n(z)}{Q_m(z)} = f(z) + 0.(z^{n+m+1}),$$

$P_n(z)$ and $Q_n(z)$ are polyminals of degree n and m respectively, which has the same n+m first derivatives as f(z) at z=0. e.g.

$$P_n(z) = b_1 + b_2 z + ... + b_N z^n.$$

The meaing of

$$\frac{P_n(z)}{Q_m(z)}$$

is that we can write:

$$f(z) = \underbrace{\frac{P_n(z)}{Q_m(z)} + d_{n+m+1}z^{n+m+1} + d_{n+m+z}z^{n+m+z} + ...,}_{0(z^{n+m+1})}$$

where the d's and also the coefficients of z the Pade approximate are functions of the coefficients in the Taylor series expansion.
From this point of view, the set of Pade approximants are a generalization of the Taylor series expansion - the [n, 0] approximants.
The Pade approximant often gives better approximation of the function than truncating its Taylor series, and it may still work where the Taylor series does not converge [15]. These techniques and concepts are found beside the benefit that is convergence acceleration (e.g. ϵ- algorithm), this method could be applicated to numerical solutions to partial differential equations ($\exp(At) \approx Q(At)^{-1}P(At)$), analytic continuation of power series (regions of convergence beyond a disk). It also includes study of orthogonal polys on interval (Pade denominators for Markov functions are orthogonal) and finding zeros/roots, poles/singularities (use zeros and poles of Pade approximants to predict - e.g. QD algorithm)[3].
All these interesting features, and the particular simplicity of the Pade approximation make it a very convenient tool for practical and physical applications. The range of applications to physical problems is very broad [16]. The first physical applications of the Pade approximation have been made in statistical mechanics[4]. Then there were many other application: in fluid [5], blasius problem [6]. In this work, we give particular emphasis to condensed and soft matter. We discuss various proofs of convergence, and show the approximation is particularly well suited for Coulomb problems. We finally review the various achievements of the approximation in the determination of Coulomb effective potential.
Very often, the equations describing a physical process are so complicated that the simplest way to obtain their solution, if not the only way, is to perform a power series expansion in some parameters. Furthermore, the physical values of the parameters may be such that this perturbation to the problem, i.e., it cannot be used quantitatively as such. However, the information is present in the coefficients of the perturbation series, and one may look for mathematical techniques that would be capable of treating this information in a convergent way. As above, we known that the Pade approximation use n+m+1 parameter, in this work, for simle, we just consider the case of m=n+1, so there are 2n+2 parameter here. There is a study about the modified pade approximation have been made, such as [7]. Now, we introduce a new modifies pade approximation, the general pade include a factor of exponential form, so there more one parameter in this extended part, it will make the convergence faster. The General Pade approximation is very well suited for as we shall see.

2. Method

2.1. Potential in one layer on the screening effect of a nearby ground-plane

As an example of how the approximation can be used, it is of interest to study briefly what can be considered as a commonly used Pade approximant in physics: the screening effect of a ground-plane on a two-dimensional system.
In a two-dimensional electron system (2DES), strong Coulomb interactions between electrons can lead to exotic phenomena such as the Wigner crystal state, the fractional quantum Hall

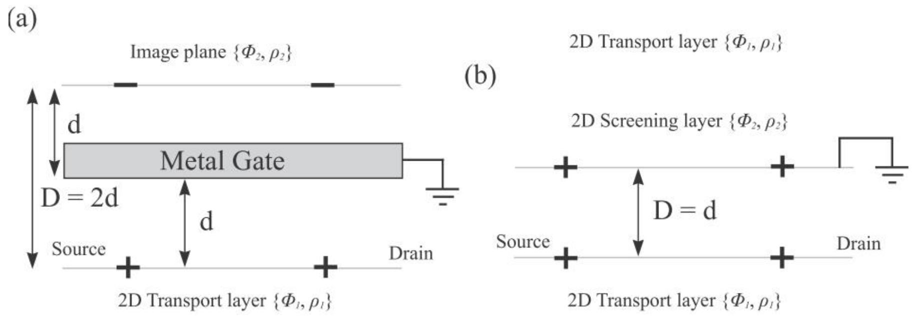

Figure 1. Schematics showing the two systems considered in this paper. The transport layer is screened by (a) a metal surface gate and (b) a second 2D system. In both cases the screening layer is separated by a distance d from the transport layer, and the transport (1) and screening (2) layers have independent potentials ϕ and charge densities ρ.

effect, and the anomalous 2D metallic state. So, the role of studying Coulomb interactions is very important.
We now begin considering the screening effect of a nearby ground-plane on a 2D system (transport layer) for two different coniïňĄgurations. In the ïňĄrst, the ground-plane (i.e., screening layer) is a metal surface gate (see Fig. 2(a)) and in the second, the ground-plane is another 2D system (see Fig. 2(b)). In both cases the transport and screening layers are separated by a distance d. If we consider some positive external test charge ρ_{ext1} added to the transport layer, this leads to induced charge in both the transport layer ρ_{ind1} and in the screening layer ρ_{ind2}. Charge in one layer leads to a potential in the other via the interlayer Coulomb interaction[9]:

$$U(q) = \frac{1}{4\pi\varepsilon\sqrt{r^2 + D^2}}.$$

First, we considered some ordinary Pade approximations, $U(q)^{[1,2]}$, $U(q)^{[2,3]}$, $U(q)^{[3,4]}$ and also consider the Taylor series of (1). We see that the ordinary Pade approximation just accurate in a small range of r (Fig.2). Beside, we also consider the Taylor series of Eq.(*), it's the dashing black line, it's worse than ordinary Pade approximation.
Now, we will look for an analytical expression that can fits the wider range of r-values. Therefore, we have approximated the full effective potential by general Pade approximant. It's form is: $F = \frac{a_0}{r}e^{-b_0 r}$, where a_0, b_0 is determined after fitting the data to expression in Eq.(*), we found $a_0 = 0.0774905, b_0 = 15.8339.10^{-6}$.
The ordinary Pade approximant is known better than Taylor series, for this function we also use general Pade approximant, contained a factor of exponential, formed then compared with the cases above (Fig. 2). We see that the new Pade approximation is fitter for a larger range of r than other ordinary Pade approximations and ofcourse's Taylor series.

2.2. Two soft particles interaction
In another case in soft matter, we now consider consider the electrostatic interaction between two dissimilar spherical soft spheres 1 and 2 (figure 4). We denote by dl and d2 the thicknesses of the surface charge layers of spheres 1 and 2, respectively. Let the radius of the core of soft sphere 1 be and that for sphere 2 be a2 . We imagine that each surface layer is uniformly charged. Let Z1 and N1 , respectively, be the valence and density of the fixed charge layer of sphere 1 and Z2 and N2 be those for sphere 2.
For the special case of two similar soft spheres carrying Z1=Z2=Z, N1= N2= N, d1= d2= d so that $\rho_{fix1} = \rho_{fix2} = \rho_{fix}$. The interaction energy Vsp(H) between two similar soft spheres 1

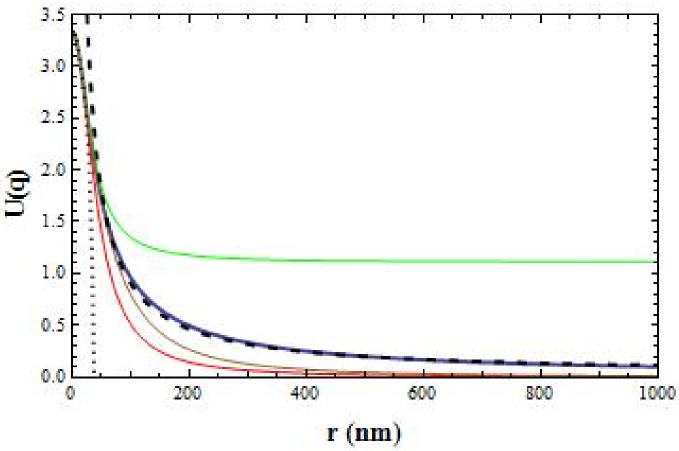

Figure 2. The potential in one layer is caused by the charge in the other layer, the blue, thick line is of Original function; the black, dashing, thick is of General Pade approximation, red: Pade [1,2]; green: Pade [2,3]; brown: Pade [3,4] and the black, dotted's one is for Taylor series.

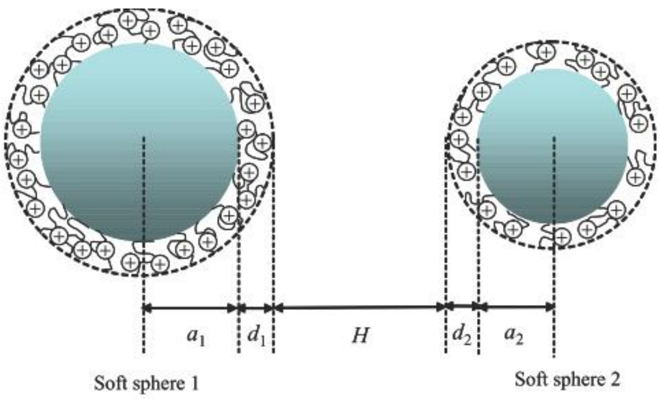

Figure 3. Interaction between two soft spheres.

and 2, separated by a ρ_{fix}, and a1= a2= a, equation (79) reduces to distance H between their surfaces is[3,4]:

$$V_{sp}(H) = \frac{2\pi a \rho_{fix}^2 \sinh^2(\kappa d)}{\varepsilon_r \varepsilon_0 \kappa^4} \ln\left(\frac{1}{1 - e^{-\kappa(H+2d)}}\right).$$

With a more complicated function, the approximants give much different. The Taylor series is worst of them (Fig. 4a), and the ordinay Pade approximants have more error than general Pade approximant (Fig. 4b). So in this case, the General Pade is more exactly than any others.

3. Conclusion

The ordinary Pade approximation is known that better than Taylor series, this work shown that the general Pade approximation by included a factor of exponential form give more accurate results than the ordinary Pade approximation, it fitted with a larger range, especialy in the complicated function. This new Pade approximation giving a simple approximant function formed of $F = \frac{a_0}{r} e^{-b_0 r}$, is useful to perform analytical calculations, estimations and to reduce the amount of computational time for future investigations in condensed and soft matter topics.

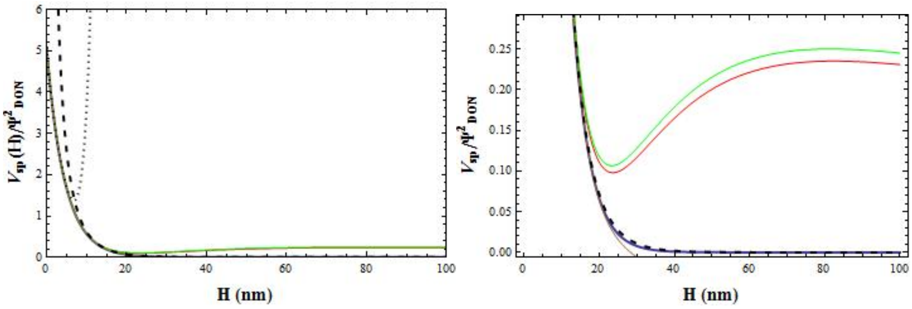

Figure 4. The interaction energy between two similar soft spheres, the blue, thick line is of Origin function; the black, dashing, thick is of General Pade approximation, red: Pade [1,2]; green: Pade [2,3]; brown: Pade [3,4] and the black, dotted's one is for Taylor series.

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