A Note on the Ground State Energy of an Assembly of Interacting Electrons

(electron gas/electron lattice/correlation energy/Padé approximants)

AKIRA ISIHARA* AND ELLIOTT W. MONTROLL

Institute for Fundamental Studies, Department of Physics and Astronomy, The University of Rochester, Rochester, New York 14627

Contributed by Elliott W. Montroll, October 14, 1971

ABSTRACT The ground state energy of an assembly of charged particles of density ρ imbedded in a continuum of charge of the other sign in an electrically neutral system is considered. Asymptotic formulae for the ground state energy of such systems are known in the high- and low-density regimes. An interpolation formula covering the entire density range is derived using the method of two-point Padé approximants. A phase transition from an electron lattice to an electron gas seems to occur at $r_s \simeq 14$, r_s being the radius of a sphere which, on the average, contains a single charge, in units of the Bohr radius of the electron in a hydrogen atom.

A perennial many-body problem common to the theories of metals and of the internal constitution of stars (especially the white dwarfs) is the determination of the ground state energy of an assembly of point-charged particles as a function of their number density. In a traditional model, the electrical neutrality of the assembly is maintained by imbedding the point charges, which we identify as electrons (in the theory of white dwarfs, the positively charged nuclei are considered to be the point charges), in a continuum of positive charge. In the ground state (0°K), the only parameters that appear in a nonrelativistic theory are Planck's constant h , the charged particle density ρ , mass m , and charge e . The basic dimensionless quantity produced from these parameters is $me^2/\hbar^2\rho^{1/2}$. An important variable proportional to this combination is $r_s = r_0/r_B$, where r_0 is related to the density ρ through the definition $(4/3)\pi r_0^3 \equiv \rho^{-1}$ and r_B is the Bohr radius, $\hbar^2/me^2$.

Since the energy of a perfect Fermi gas is, per particle,

$$E_f/N = (3/8)\hbar^2(3\rho/\pi)^{2/3}/5m \quad (1)$$

the introduction of the coulomb interactions changes the ground state energy by a factor that depends on r_s so that $E/E_f = \{1 + w(r_s)\}$. The central problem then becomes the determination of the functional form of $w(r_s)$. In metals $2 < r_s < 6$, while in stars its range is much broader.

The high- and low-density limit behavior of our assembly of interest is somewhat different from that observed in molecular systems. In their high-density regime, atoms and molecules become localized in a lattice structure whose zero point vibrations are quite small. For very light electrons, localization would, through the uncertainty principle, force the particles to have large momentum fluctuations which, in turn, correspond to a high kinetic energy. The total energy, kinetic plus potential, might then be higher than in the electron gas state in which the division of the two forms of energy might be better balanced. However, at low densities, lattice local-

ization need not be so severe, so that the kinetic and potential energies might take up more equal shares of the total. We have estimated that a phase transition from the low-density lattice state to the high-density gas state should occur at $r_s \simeq 14$.

Wigner [1] showed that among the cubic electron lattices, the body-centered one had the lowest lattice energy, its value being $U_{bcc} = -1.79186 r_s^{-1}$ Rydbergs. Since the lattice must suffer some small vibrations from its equilibrium state, a correction for the energy of zero point oscillations must be added to this value of the lattice energy in the estimation of the ground state energy of the electron lattice. The first estimate of the correction, made by Fuchs [2] in 1935, was improved by Caldwell-Horsefall and Maradudin [3], who found $E_H = 2.638 r_s^{-1/2}$ Rydbergs, while Carr [4] had independently reported a value of $2.66 r_s^{-1/2}$. Carr has also estimated the lowest-order anharmonic contribution which, when added to the above terms, yields the beginning of an asymptotic expansion for the ground state energy (in Rydbergs) in the low-density (large r_s) regime:

$$E_G = -1.79186 r_s^{-1} + 2.638 r_s^{-1/2} - 0.73 r_s^{-2} + \dots \quad (2)$$

At high densities, the limiting unperturbed state is that of the perfect Fermi gas. As the density decreases, exchange terms and electron correlations of various orders become important. These effects were investigated in a flurry of activities in the late 1950s and early 1960s. Gell-Mann and Brueckner [5] calculated the lowest-order correlation term, while Dubois [6] obtained the higher-order ones. The resulting small r_s expansion is

$$E_G \sim 2.21 r_s^{-2} - 0.916 r_s^{-1} + 0.0622 \ln r_s - 0.096 + r_s(0.0049 \ln r_s + C) + \dots \quad (3)$$

where $C \simeq -0.02$. Progress in series expansions essentially stopped when it seemed that the calculation of another term or two would require a tremendous effort which would probably not lead to a significant improvement in the understanding of the electron correlation phenomenon.

The state of affairs is reminiscent of that which existed in the investigation of the 3D Ising model in the 1950s. By counting the number of ways appropriate graphs could be constructed on lattices, a number of terms in a power series expansion in reciprocal temperature could be obtained for the thermodynamic properties of the Ising ferromagnet. The stage was reached at which the determination of a new term required tremendous effort. Until Domb [7] and his collaborators and G. Baker [8] showed how to extract in-

* Permanent address: State University of New York at Buffalo.

FIG. 1. Variation of ground state energy of electron plasma with r_s (which is proportional to the inverse cube-root of the density).

formation from the coefficients, it was hardly worth expending any more effort to obtain more coefficients.

The Baker technique is to systematically express a power series $f(x) = c_0 + c_1x + c_2x^2 + \dots$ as the ratio of two polynomials

$$f_n(x) = (a_0 + a_1x + \dots + a_mx^m)/(1 + b_1x + \dots + b_nx^n) \quad (4)$$

by using the method of Padé approximants [7, 8]. The a 's and b 's are determined from the c 's. The nature of singularities in $f(x)$ are found as well as their location. With 10–20 terms, one obtains results of considerable precision.

Our individual electron assembly expansions have fewer terms but, together, the large and small r_s expansions do have a considerable number of terms. We assume that they are two asymptotic forms of the same expression and attempt to use the Padé expansion to lead us to an approximation of that expression. One of the difficulties in doing so is that our small r_s expansion includes logarithmic terms and the small and large r_s expansions are not of the same type. This fact makes a simple application of the Padé approximant method impossible. However, one can circumvent this difficulty by differentiating E_G twice with respect to r_s and expressing the results in terms of a new variable $x = r_s^{1/2}$. Then, one finds

$$r_s^4 d^2 E_G / dr_s^2 =$$

$$\begin{cases} 13.258 - 1.832x^2 - 0.0622x^4 + 0.018x^6 + \dots & \text{if } x \ll 1 \quad (5) \\ -3.584x^2 + 9.8925x - 4.38 - tx^{-1} + \dots & \text{if } x \gg 1 \quad (6) \end{cases}$$

where Eq. (5) corresponds to Eq. (3) and Eq. (6) to Eq. (2). In Eq. (6) an additional term, tx^{-1} , has been introduced with an unknown coefficient t .

Note that Eqs. (5) and (6) are counterparts of each other for the two limiting domains of x . Since the right-hand sides are simple power series in x or x^{-1} , it is now possible to apply the Padé approximants to

$$f_n(x) = r_s^4 (d^2 E_G / dr_s^2). \quad (7)$$

In the low-density regime as $x \rightarrow \infty$ in Eq. (6), the first term dominates for very large x . Therefore, in Eq. (4), $m = n + 2$.

In the traditional applications of Padé approximants, one considers the expansion of a function about one point, while here we wish to take advantage of the fact that we have independent information concerning the behavior of E_G at two points, $x = 0$ and $x = \infty$. A similar situation has arisen in the polaron problem. Sheng and Dow [9] have applied two-point Padé approximants to that problem.

The systematic procedure for the determination of the a_i 's and b_i 's in (4) from asymptotic formulae such as (5) and (6) is discussed in Appendix 1. The values of these constants for the case $n = 2$ and $m = 4$ are

$$a_0 = 13.2594, \quad a_1 = 2.6600, \quad a_2 = -1.3617, \quad a_3 = -0.3676$$

$$a_4 = -0.12729, \quad b_1 = 0.2006, \quad b_2 = 0.03552$$

while those for the case $n = 3$ and $m = 5$ are

$$a_0 = 13.2594, \quad a_1 = 11.848, \quad a_2 = 1.0146$$

$$a_3 = -1.2165, \quad a_4 = -0.4557, \quad a_5 = -0.1137$$

$$b_1 = 0.8954, \quad b_2 = 0.21474, \quad b_3 = 0.03173$$

The expression for $f(x)$ given by (4) with these constants must be integrated twice in order to obtain a formula for the ground state energy of an electron gas, E_G . A systematic discussion of this integration and the resulting equations are presented in Appendix 2. The computed curves for E_G as a function of r_s based on Eqs. (7) and (6) of Appendix 2, for $n = 2$ and 3, are plotted as (i) and (ii) in Fig. 1. The zeros of the denominator of $f(x)$ of Eq. (4) for the $n = 2$ and $n = 3$ cases have no positive poles. Hence, these approximations to E_G have no singularities in the r_s range $0 < r_s < \infty$.

Since the electron lattice is the stable form of an assembly in the low-density regime, while the electron gas is the stable state in the high-density regime, one expects a phase transition, the lattice melting, to occur at some intermediate r_s value. Various estimates, which range from $r_s = 5$ to $r_s = 2000$, have been made for the critical r_s value. Our two approximations to E_G discussed above seem to be unsatisfactory because they give no indication of the existence of such a critical value.

If we try to make the next ($n = 4$) approximation to E_G we are faced with the difficulty that we need to know the value of the coefficient t of x^{-1} in Eq. (6). This corresponds to the second-order anharmonicity contribution of the electron lattice to $r_s^4 d^2 E_G / dr_s^2$. This has not yet been calculated, but we can investigate its influence by assuming that it falls in the interval $-2 < t < 7$ and considering E_G as a function of r_s for several values of t in this range. The striking new feature of the $n = 4, m = 6$ approximation to $f(x)$ is that it yields a pole in $d^2 E_G / dr_s^2$ at $r_s \simeq 14$.

The denominator of the left-hand side of (7) in our present approximation is a fourth-degree polynomial with one positive, one negative, and two complex roots. It is the positive root that leads to the singularity at $r_s \simeq 14$. Eq. (7) can be rewritten as

$$d^2 E_G / dr_s^2 = (a_0 + \sum_{i=1}^6 a_i x^i) / b_4 x^5 P_4(x) \quad (8)$$

with

$$P_4(x) \equiv (x - a)(x + b)(x^2 - 2ax + c^2) \quad (9)$$

$$c^2 = \alpha^2 + \beta^2. \quad (10)$$

TABLE 1. Coefficients and roots of the fourth-order Padé approximant

t	7	3	2	0	-2
a_0	13.2594	"	"	"	"
a_1	1.0315	0.9720	0.9571	0.9274	0.8976
$-a_2$	1.6864	1.6887	1.6893	1.6905	1.6917
$-a_3$	0.2701	0.2629	0.2611	0.2575	0.2539
$-a_4$	0.1406	0.1399	0.1398	0.1397	0.1395
$-a_5$	0.008609	0.008360	0.008297	0.008173	0.008049
a_6	0.1561	0.01562	0.01562	0.01562	0.01563
b_0	1.0	"	"	"	"
b_1	0.07780	0.07331	0.07219	0.06994	0.06770
b_2	0.01103	0.01086	0.01081	0.01072	0.01063
$-b_3$	0.009674	0.009694	0.009714	0.009752	0.009791
$-b_4$	0.00435	0.004357	0.004358	0.004359	0.004361
a	3.8158	3.7957	3.7907	3.7807	3.7706
b	4.4629	4.4814	4.4919	4.5035	4.5150
$-\alpha$	0.7807	0.7672	0.7638	0.7571	0.7503
$(\pm i)\beta$	3.5882	3.5901	3.5906	3.5916	3.5926
K_1	2.2099	"	"	"	"
K_2	-0.91633	"	"	"	"
K_3	0.0622	"	"	"	"
K_4	0.08558	0.08627	0.08644	0.08678	0.08712
K_5	0.00977	0.00988	0.00987	0.00982	0.00977
K_6	0.000753	0.000773	0.000778	0.000789	0.000799
$-K_7$	0.002441	0.002396	0.002385	0.002363	0.002341
$-K_8$	0.008289	0.008264	0.008258	0.008245	0.008231
$-K_9$	0.001158	0.001543	0.001679	0.001830	0.002020
K_{10}	0.000645	0.000860	0.000913	0.001019	0.0011250
K_{11}	0.100797	0.101628	0.101834	0.102241	0.102644
K_{12}	0.062200	"	"	"	"

The integration of (8) is discussed in Appendix 2. The result is

$$\begin{aligned}
 E_G \sim & K_1 r_s^{-2} + K_2 r_s^{-1} - (K_3 - K_5 r_s) \ln r_s - K_4 r_s^{1/2} \\
 & + K_6 \{ (r_s - a^2) \ln (r_s^{1/2} - a)^2 - 2ar_s^{1/2} \} + K_7 \{ (r_s - b^2) \\
 & \times \ln (r_s^{1/2} + b)^2 + 2br_s^{1/2} \} + K_8 \{ [r_s + (\beta^2 - \alpha^2)] \\
 & \times \ln [(r_s^{1/2} - \alpha)^2 + \beta^2] - 2\alpha r_s^{1/2} \} + K_9 \{ 4r_s^{1/2} + 2\alpha \\
 & \times \ln [(r_s^{1/2} - \alpha)^2 + \beta^2] \} + K_{10} r_s \{ \tan^{-1} [(r_s^{1/2} - \alpha)/|\beta|] \\
 & - 1/2\pi + |\beta| r_s^{-1/2} \} + K_{11} \tan^{-1} [(r_s^{1/2} - \alpha)/|\beta|] \\
 & - 1/2\pi \} + K_{12} \quad (11)
 \end{aligned}$$

The various coefficients and roots are given in Table 1 for various values of t . The parameters a_0 , b_0 , K_1 , K_2 , K_3 , and K_{12} are completely independent of t , while K_9 and K_{10} have the strongest t dependence. The sensitivity is greatest for those terms that are large for large r_s . However, through certain basic cancellations, E_G itself is very small for large r_s and it is insensitive to t in that range. In the smaller- r_s regime, E_G is essentially independent of t .

Our estimate of the ground state energy is plotted in Fig. 1. The most striking feature of the curve is the anomaly at $r_s \simeq 14.4$. The location of the singularity depends slightly on t . That dependence on t , as well as that of the energy at the minimum and r_s value at the minimum of E_G is exhibited in Table 2. Curve (iii) corresponds to $t = 7$.

Note that while the location of the singular point depends only weakly on t , the dependence is roughly linear. At the singular r_s , the second derivative, $d^2 E_G / dr_s^2$, diverges, but E_G itself is continuous. In the immediate neighborhood of the singularity, the curve shows a van der Waals-type loop. By using an argument similar to that due to Maxwell for the interpretation of the van der Waals loop, the Maxwell equal area construction implies that a first-order phase transition occurs at the singular r_s . For large values of r_s , the curve is close to that reported by Carr, Caldwell-Horsefall, and Maradudin⁴ [3, 4]. The minimum in E_G for all t values investigated in the fourth-order Padé approximant lies somewhat deeper than in the third-order case. The rising part of the curve in the range $3.8 < r_s < 14$ might be attrib-

TABLE 2. Certain E_G characteristics as a function of t

t	7	3	2	0	-2
E_G minimum	-0.16342	-0.16311	-0.16303	-0.16287	-0.16271
r_s at minimum	3.77	3.76	3.76	3.76	3.76
Location of singularities	14.56	14.41	14.37	14.29	14.22

uted to local ordering, which persists at densities higher than the melting point.

The melting of an electron lattice may be treated in accordance with Lindemann's criterion. For a body centered cubic lattice it is $r_s = 0.4054\delta^{-1/2}$, where δ is the ratio of the amplitude of lattice vibration to the interlattice spacing. Using the value $r_s = 14.37$, we found that δ is approximately 0.4. A similar value of δ has been found by Shavin and Kovetz from a thermodynamic discussion [10].

APPENDIX 1

Two-Point Padé Approximants. Let us examine a situation in which two asymptotic forms are known for a function $f(x)$

$$f(x) \sim \begin{cases} A_0 + A_1x + A_2x^2 + \dots & \text{as } x \rightarrow 0 \\ B_0x^2 + B_1x + B_2 + \dots & \text{as } x \rightarrow \infty. \end{cases} \quad (1a) \quad (1b)$$

We discuss a systematic manner of approximating $f(x)$ by a ratio of two polynomials

$$f_n(x) \equiv [n+2, n] = \frac{a_0 + a_1x + \dots + a_{n+2}x^{n+2}}{1 + b_1x + \dots + b_nx^n}. \quad (2)$$

Consider first the small x expansion of this ratio. By elementary division, if the ratio is to be consistent with (1a)

$$\begin{aligned} a_0 &= A_0, & a_1 &= A_0b_1 + A_1 \\ a_2 &= A_0b_2 + A_1b_1 + A_2 \\ a_3 &= A_0b_3 + A_1b_2 + A_2b_1 + A_3 \quad \text{etc.} \end{aligned} \quad (3)$$

As an example, let $n = 2$ in (2). Then $b_3 = b_4 = \dots = 0$ and

$$\begin{aligned} a_0 &= A_0, & a_1 &= A_0b_1 + A_1 \\ a_2 &= A_0b_2 + A_1b_1 + A_2 \\ a_3 &= A_1b_2 + A_2b_1 + A_3 \\ a_4 &= A_2b_2 + A_3b_1 + A_4. \end{aligned} \quad (4)$$

Similar equations can be constructed for $n = 3$, etc. The connection between the a 's, b 's, and B 's is obtained by writing (with $y = x^{-1}$).

$$\begin{aligned} [n+2, n] &= (x^2a_{n+2}/b_n) \\ &\times \left\{ \frac{1 + (a_{n+1}/a_{n+2})y + \dots + (a_0/a_{n+2})y^{n+2}}{1 + (b_{n-1}/b_n)y + \dots + (1/b_n)y^n} \right\}. \end{aligned} \quad (5)$$

When $n = 2$, the first two terms in the expansion imply

$$a_4 = B_0b_2, \quad a_3 = B_0b_1 + B_1b_2. \quad (6)$$

When $n = 3$, the first three terms imply

$$a_5 = B_0b_3, \quad a_4 = B_0b_2 + B_1b_3, \quad a_3 = B_0b_1 + B_1b_2 + B_2b_3 \quad (7)$$

and, when $n = 4$, the first four terms imply

$$\begin{aligned} a_6 &= B_0b_4, & a_5 &= B_0b_3 + B_1b_4 + B_2b_3 + B_3b_4 \\ a_4 &= B_0b_2 + B_1b_3 + B_2b_2 + B_3b_1 + B_4b_2. \end{aligned} \quad (8)$$

The pattern is obvious for larger values of n .

We are now in a position to discuss the evaluation of the $\{a_j\}$ and $\{b_j\}$ when $(n+3) A$'s and $n B$'s are given. This is sufficient input data to find the $(2n+3)$ constants required for the $[n+2, n]$ approximation.

When $n = 2$, the given data values would be $B_0, B_1, A_0 - A_4$. The basic equations would be the sets (6) and (4). The values of b_1 and b_2 would be determined by equating both expressions for a_4 and a_3

$$\begin{aligned} a_4 &= B_0b_2 = A_2b_2 + A_3b_1 + A_4 \\ a_3 &= B_0b_1 + B_1b_2 = A_1b_2 + A_2b_1 + A_3. \end{aligned} \quad (9)$$

Then b_1 and b_2 are expressible as the ratio of the two (2×2) determinants. The quantity $1 + b_1x + b_2x^2$, which appears in the denominator of (2), can then be written as the ratio of a (3×3) and a (2×2) determinant.

$$1 + b_1x + b_2x^2 = \frac{\begin{vmatrix} 1 & A_3 & A_4 \\ -x & B_0 - A_2 & 0 - A_3 \\ -x^2 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}{\begin{vmatrix} B_0 - A_2 & 0 - A_3 \\ B_1 - A_1 & B_0 - A_2 \end{vmatrix}} \quad (10)$$

as the reader can easily verify. Clearly the combination $\alpha_1 + \alpha_2b_1 + \alpha_3b_2$ has the corresponding determinant representation

$$\alpha_1 + \alpha_2b_1 + \alpha_3b_2 = \frac{\begin{vmatrix} \alpha_1 & A_3 & A_4 \\ -\alpha_2 & B_0 - A_2 & 0 - A_3 \\ -\alpha_3 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}{\begin{vmatrix} B_0 - A_2 & 0 - A_3 \\ B_1 - A_1 & B_0 - A_2 \end{vmatrix}}. \quad (11)$$

The numerator of (2) has the form (using 4)

$$\begin{aligned} a_0 + x a_1 + x^2 a_2 + x^3 a_3 + x^4 a_4 \\ = (A_0 + x A_1 + x^2 A_2 + x^3 A_3 + x^4 A_4) \\ + b_1(x A_0 + x^2 A_1 + x^3 A_2 + x^4 A_3) \\ + b_2(x^2 A_0 + x^3 A_1 + x^4 A_2). \end{aligned}$$

Hence,

$$F_2(x) \equiv [4, 2] = \frac{\begin{vmatrix} \Sigma_0^4 A_j x^j & A_3 & A_4 \\ -x \Sigma_0^3 A_j x^j & B_0 - A_2 & 0 - A_3 \\ -x^2 \Sigma_0^2 A_j x^j & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}{\begin{vmatrix} 1 & A_3 & A_4 \\ -x & B_0 - A_2 & 0 - A_3 \\ -x^2 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}. \quad (12)$$

When $n = 3$, the basic equation for the determination of the b 's as a ratio of two determinants follow from (3) with $b_4 = b_5 \dots = 0$. And (7):

$$a_5 = A_2b_3 + A_3b_2 + A_4b_1 + A_5 = B_0b_3 \quad (13a)$$

$$a_4 = A_1b_3 + A_2b_2 + A_3b_1 + A_4 = B_0b_2 + B_1b_3 \quad (13b)$$

$$a_3 = A_0b_3 + A_1b_2 + A_2b_1 + A_3 = B_0b_1 + B_1b_2 + B_2b_3. \quad (13c)$$

Once the b 's are written as a ratio of determinants, the same can be done for the denominator of (2) when $n = 3$. Finally, $F_3(x)$ is easily shown to have the form

$$F_3(x) = [5, 3] = \frac{(S_5, -xS_4, -x^2S_3, -x^3S_2)}{(1, -x, -x^2, -x^3)} \quad (14a)$$

where we define $S_n = \Sigma_0^n A_j x^j$ and

$$(\alpha_1, \alpha_2, \alpha_3, \alpha_4) \equiv \frac{\begin{vmatrix} \alpha_1 & A_3 & A_4 & A_5 \\ \alpha_2 & B_0 - A_2 & 0 - A_3 & 0 - A_4 \\ \alpha_3 & B_1 - A_1 & B_0 - A_2 & 0 - A_3 \\ \alpha_4 & B_2 - A_2 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}{\begin{vmatrix} B_0 - A_2 & 0 - A_3 & 0 - A_4 \\ B_1 - A_1 & B_0 - A_2 & 0 - A_3 \\ B_2 - A_2 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}. \quad (14b)$$

Also,

$$F_4(x) = [6, 4] \equiv \frac{(S_6, -xS_5, -x^2S_4, -x^3S_3, -x^4S_2)}{(1, -x, -x^2, -x^3, -x^4)} \quad (15a)$$

$(\alpha_1, \dots, \alpha_5)$

$$\equiv \frac{\begin{vmatrix} \alpha_1 & A_3 & A_4 & A_5 & A_6 \\ \alpha_2 & B_0 - A_2 & 0 - A_3 & 0 - A_4 & 0 - A_5 \\ \alpha_3 & B_1 - A_1 & B_0 - A_2 & 0 - A_3 & 0 - A_4 \\ \alpha_4 & B_2 - A_0 & B_1 - A_1 & B_0 - A_2 & 0 - A_3 \\ \alpha_5 & B_3 - 0 & B_2 - A_0 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}{\begin{vmatrix} B_0 - A_2 & 0 - A_3 & 0 - A_4 & 0 - A_5 \\ B_1 - A_1 & B_0 - A_2 & 0 - A_3 & 0 - A_4 \\ B_2 - A_0 & B_1 - A_1 & B_0 - A_2 & 0 - A_3 \\ B_3 - 0 & B_2 - A_0 & B_1 - A_1 & B_0 - A_2 \end{vmatrix}}. \quad (15b)$$

The generalization to any $F_n(x)$ is obvious. Similar expressions exist for two-point Padé approximants for $[n + \mu, n]$.

APPENDIX 2

Integration of d^2E_G/dr^2 . In this appendix, we are concerned with the integration of expressions (with $x = r_s^{1/2}$ and $b_0 = 1$) such as

$$d^2E_G^{(n)}/dr^2 = x^{-2} \left(\sum_0^{n+2} a_j x^j \right) / \left(\sum_0^n b_j x^j \right) \quad (1)$$

The basic integrals required are

$$I_m(1) = \int x^{-m} dx / (1 + x).$$

Note that

$$I_0(1) = \log(1 + x); \quad I_1(1) = \log[x/(1 + x)]$$

$$I_2(1) = -x^{-1} - \log[x/(1 + x)]$$

while,

$$I_m + I_{m-1} = \int (x^{-m} + x^{-m+1})dx/(1+x) = x^{-(m-1)}/(m-1),$$

$$I_m = (I_m + I_{m-1}) - (I_{m-1} + I_{m-2}) + \dots$$

$$+ (-1)^m(I_2 + I_1) - (-1)^m I_1$$

$$= \sum_{s=1}^{m-1} (-1)^{m+s} x^{-s} - (-1)^m \log [x/(1+x)].$$

Furthermore,

$$I_m(y) \equiv \int x^{-m} dx/(x+y)$$

$$= y^{-m} \left\{ (-1)^{m+1} \log [x/(y+x)] \right.$$

$$\left. + \sum_{s=1}^{m-1} (-1)^{m+s} (y/x)^s \right\}. \quad (2)$$

The quantities $[g_n(x)]^{-1} \equiv (1 + b_1 x + \dots + b_n x^n)^{-1}$ in Eq. (1) have the following partial fraction representations for $n = 2, 3, 4$ respectively:

$$b_2^{-1} \{ [(x - \alpha_1)\Delta_{12}]^{-1} + [(x - \alpha_2)\Delta_{21}]^{-1} \}; \quad \Delta_{1j} \equiv \alpha_1 - \alpha_j \quad (3a)$$

$$b_3^{-1} \{ [(x - \alpha_1)\Delta_{12}\Delta_{13}]^{-1} + [(x - \alpha_2)\Delta_{21}\Delta_{23}]^{-1} \}$$

$$+ [(x - \alpha_3)\Delta_{31}\Delta_{32}]^{-1} \} \quad (3b)$$

$$b_4^{-1} \{ [(x - \alpha_1)\Delta_{12}\Delta_{13}\Delta_{14}]^{-1} + \dots$$

$$+ [(x - \alpha_4)\Delta_{41}\Delta_{42}\Delta_{43}]^{-1} \}. \quad (3c)$$

The $\{\alpha_j\}$ for a given n are the roots of $g_n(\alpha) = 0$.

Since $dE_G/dr_s \rightarrow 0$ as $r_s \rightarrow \infty$, the integration of (1) from r to ∞ yields, by the use of (2) and (3),

$$dE_G^{(n)}/dr = (2/b_n) \sum_{m=0}^{n+2} a_m \left\{ \frac{J_{7-m}(r, -\alpha_1)}{\Delta_{12}\Delta_{13} \dots \Delta_{1n}} + \frac{J_{7-m}(r, -\alpha_2)}{\Delta_{21}\Delta_{23} \dots \Delta_{2n}} \right.$$

$$\left. + \dots + \frac{J_{7-m}(r, -\alpha_n)}{\Delta_{n1}\Delta_{n2} \dots \Delta_{n,n-1}} \right\} \quad (4)$$

if $n > 4$, where

$$J_k(r, -\alpha) = -\alpha^{-k} \log [r^{1/2}/(r^{1/2} - \alpha)]$$

$$+ \sum_{p=1}^{k-1} p^{-1} \alpha^{p-k} r^{-p/2}. \quad (5)$$

This function is easily integrated and the constant of integration can be chosen so that the integral vanishes as $r \rightarrow \infty$ as is required by our problem. If α is real and positive, and $r^{1/2} < 0$, the term $(r^{1/2} - \alpha)$ should be written as $|r^{1/2} - \alpha|$. The form of the integral when $k > 4$ is

$$F_k(r, -\alpha) = 2 \sum_{p=3}^{k-1} \frac{\alpha^{p-k} r^{1-p/2}}{p(2-p)} + r^{1/2} \alpha^{1-k}$$

$$+ (1/2) \alpha^{2-k} + \alpha^{-k} (r - \alpha^2) \log [(r^{1/2} - \alpha)/r^{1/2}]. \quad (6a)$$

When $k = 2$ and 3 , the term expressed as a sum over p is omitted, and when $k = 1$,

$$F_1(r, -\alpha) = \alpha^{-1} \{ \alpha r^{1/2} - \alpha^2 \log r^{1/2}$$

$$+ (r - \alpha^2) \log [(r^{1/2} - \alpha)/r^{1/2}] \}. \quad (6b)$$

Again, when α is real and positive and $r^{1/2} < \alpha$, the terms $(r^{1/2} - \alpha)$ in (6a) and (6b) should be replaced by $|r^{1/2} - \alpha|$.

The final expression for $E_G^{(n)}(r_s)$ is

$$E_G^{(n)}(r_s) = (2/b_n) \sum_{m=0}^{n+2} a_m D_{7-m}^{(n)}(r_s) \quad (7a)$$

$$D_k^{(n)}(r) \equiv \frac{F_k(r, -\alpha_1)}{\Delta_{12} \dots \Delta_{1n}} + \frac{F_k(r, -\alpha_2)}{\Delta_{21}\Delta_{23} \dots \Delta_{2n}} + \dots + \frac{F_k(r, -\alpha_n)}{\Delta_{n1} \dots \Delta_{n,n-1}}. \quad (7b)$$

Several technical points are to be observed in the application of these formulas. First, various symmetrical functions of the roots α_j of $g_n(\alpha) = 0$ occur naturally. For example,

$$\alpha_1 + \alpha_2 + \dots + \alpha_n = -b_1/b_n;$$

$$\alpha_1 \alpha_2 \dots \alpha_n = (-1)^n/b_n, \text{ etc.} \quad (8)$$

A recurrence formula exists for the combination

$$\delta_{-j}^{(n)} \equiv \frac{\alpha_1^{-j}}{\Delta_{12} \dots \Delta_{1n}} + \dots + \frac{\alpha_n^{-j}}{\Delta_{n1} \dots \Delta_{n,n-1}}, \quad (9a)$$

$$\delta_{-j}^{(n)} = -b_1 \delta_{-j+1}^{(n)} - b_2 \delta_{-j+2}^{(n)} \dots - b_n \delta_{-j+n}^{(n)}. \quad (9b)$$

This is easily deduced from the relation

$$\alpha^{-j} = -b_1 \alpha^{-j+1} - b_2 \alpha^{-j+2} \dots - b_n \alpha^{-j+n}. \quad (10)$$

When $n = 2, 3, 4$, the initial values to be used with (9b) are respectively,

$$\delta_0^{(2)} = 0, \quad \delta_{-1}^{(2)} = -b_2 \quad (11a)$$

$$\delta_1^{(3)} = \delta_0^{(3)} = 0, \quad \delta_{-1}^{(3)} = -b_3 \quad (11b)$$

$$\delta_2^{(4)} = \delta_1^{(4)} = \delta_0^{(4)} = 0, \quad \delta_{-1}^{(4)} = -b_4 \quad (11c)$$

In the case in which one pair of roots, say $\alpha_1 = -a + ib$ and $\alpha_2 = -a - ib$ are complex, one notes that

$$\log (r^{1/2} + a - ib) = 1/2 \log [(a + r^{1/2})^2 + b^2]$$

$$- i \tan^{-1} [b/(a + r^{1/2})]. \quad (12)$$

Through the appropriate combinations of α_1 and α_2 that appear in our problem, no imaginary terms appear in final formulae for $E_G^{(n)}$. Finally, some care has to be taken in the integration, which yields logarithms when a given α_1 is real and positive. However, the singularity at α_1 leads to no difficulty in performing the required integrations. As was stated earlier in this case, the logarithm terms in (6) are to be replaced by $\log [|r^{1/2} - \alpha|/r^{1/2}]$.

This study was partly conducted under the auspices of the ARPA MRC with the University of Michigan (DAHC-15-67-0062, No. P-004). It was also partly sponsored by ARPA and monitored by ONR (N00014-17-C-0308).

1. Wigner, E., *Trans. Faraday Soc.*, **34**, 678 (1938).
2. Fuchs, K., *Proc. Roy. Soc., London*, **151**, 585 (1935).
3. Coldwell-Horsfall, R. A., and A. A. Maradudin, *Phys. Rev.*, **1**, 395 (1960).
4. Carr, W. J., Jr., *Phys. Rev.*, **122**, 1437 (1961); Carr, W. J., Jr., R. A. Coldwell-Horsfall, and E. A. Fein, *Phys. Rev.*, **124**, 747 (1961).
5. Gell-Mann, M., and K. Brueckner, *Phys. Rev.*, **106**, 364 (1957).
6. DuBois, D. F., *Ann. Phys. (New York)*, **7**, 174 (1959).
7. Domb, C., *Phil. Mag. Suppl.*, **9**, 149 (1960).
8. Baker, G., Jr., *Phys. Rev.*, **124**, 768 (1961).
9. Sheng, P., and J. D. Dow, *Phys. Rev.*, **B4**, 1343 (1971).
10. Shavin, G., and A. Kovetz, *Astrophys. J.*, in press.