Analytical formula for large-order coefficients

It is supposed that the function $E(z)$ has imaginary part for real z when $z < z_{\rm c}$, and has no singularities in the complex plane outside an interval $(-\infty, z_{\rm c})$. Then according to Cauchy theorem

$$E_n = \frac{1}{2\pi i} \oint z^{-n-1} E(z) dz, \tag{1}$$

where integration is done in positive direction along small circle embracing the origin. After

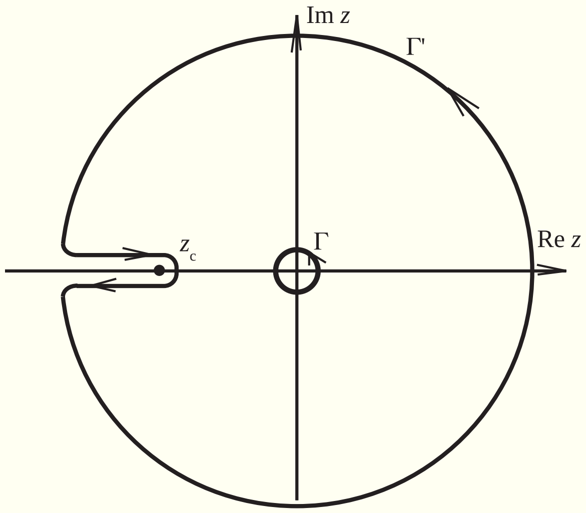

FIG. 1. Original contour of integration in the complex z-plane Γ and the transformed contour Γ'.

transforming the contour of integration as shown in Fig. 1, equation (1) is re-written as an integral over a real interval,

$$E_n = \frac{1}{\pi} \int_{-\infty}^{z_{\rm c}} z^{-n-1} {\rm Im}\, E(z) dz \tag{2}$$

It is supposed here that $z_{\rm c} < 0$ and in the vicinity of $z_{\rm c}$ the function behaves as

$$E(z) \sim \sum_{n=0}^{\infty} \epsilon_n (z - z_{\rm c})^n \tag{3}$$

with coefficients ϵ_n growing factorially as $n \to \infty$,

$$\epsilon_n \sim c\, n^{\beta}\, n!. \tag{4}$$

Divergence of the series according equation (4) is typical for tunnelling-instability systems like quartic anharmonic oscillator or Stark effect in a hydrogen atom, although a more general behavior $\sim \Gamma(bn)$ with $b \neq 1$ is in principle possible. It is well-known that factorial divergence of coefficients in the asymptotic expansion of the function, equation (4), implies that the function has a branch cut starting from the branch point $z_{\rm c}$ with appearance of an imaginary part when z is real and exceeds $z_{\rm c}$,

$$\operatorname{Im} E(z) \sim C(z_{\rm c} - z)^{\alpha} \exp\left(-\frac{\beta}{z_{\rm c} - z}\right). \tag{5}$$

By substitution of equation (5) into equation (2) and scaling $z = z_{\rm c} x$ it is found that

$$E_n = \frac{C}{\pi} z_{\rm c}^{-n+\alpha} I_n, \tag{6}$$

where

$$I_n = \int_1^{\infty} (x-1)^a x^{-n-1} \exp\left(-\frac{b}{x-1}\right) dx, \tag{7}$$

$a = \alpha$ and $b = \beta / z_{\rm c}$. I_n is estimated by rewriting equation (7) as

$$I_n = \int_1^{\infty} \exp(-F(x)) dx, \tag{8}$$

where

$$F(x) = \frac{b}{x-1} + (n+1)\ln x - a\ln(x-1), \tag{9}$$

and expanding the function $F(x)$ around its maximum x_0,

$$F(x) \sim F(x_0) + \tfrac{1}{2} F''(x_0)(x - x_0)^2. \tag{10}$$

I_n is estimated then as the Gaussian integral

$$I_n \sim \left(\frac{2\pi}{F''(x_0)}\right)^{1/2} \exp(F(x_0)). \tag{11}$$

It is found that

$$\begin{aligned}
x_0 &= 1 + b^{1/2} n^{-1/2} + \frac{a+b}{2} n^{-1} + O\left(n^{-1}\right), && (12)\\
F(x_0) &= 2b^{1/2} n^{1/2} - \frac{a}{2}\ln n - \tfrac{1}{2}(b + a\ln b) + O(n^{-1/2}), && (13)\\
\tfrac{1}{2} F''(x_0) &= b^{-1/2} n^{-3/2} - (2 + a/b) n^{-1} + O(n^{-1/2}), && (14)
\end{aligned}$$

and

$$\ln I_n \sim -2b^{1/2} n^{1/2} - \tfrac{1}{4}(2a+3)\ln n + C_0 + C_1 n^{-1/2} + O(n^{-1}), \tag{15}$$

where

$$C_0 = \tfrac{1}{4} + \tfrac{1}{2} a \ln b + \tfrac{1}{2} b + \tfrac{1}{2} \ln \pi, \tag{16}$$

$$C_1 = \frac{3a^2 + b(24 - b) + 6a(1 + b)}{12 b^{1/2}}. \tag{17}$$

Finally,

$$\ln |E_n| \sim -n \ln |z_c| - 2b^{1/2} n^{1/2} - \tfrac{1}{4}(2\alpha + 3) \ln n + (\tfrac{1}{4} + \tfrac{1}{2}\alpha \ln b + \tfrac{1}{2} b + \ln C + \alpha ln|z_c|) + O(n^{-1/2}). \tag{18}$$

I. COEFFICIENTS OF EXPANSION OF THE MODEL FUNCTION

The model function

$$E_B(z) = P_B(z) B(z - z_B), \tag{19}$$

where $P_B(z)$ is a polynomial, $z_B < 0$ and

$$B(z') = \int_0^\infty (1 + z't)^{3/2} e^{-t} dt \tag{20}$$

could model reasonably well a "type-B" singularity of the Møller - Plesset perturbation series [?]. The function $B(z')$ has a cut along negative real axis. The discontinuity of the function is estimated by evaluation of the function at real $x < 0$:

$$B(x \pm i0) = \int_0^{-1/x} (1 + xt)^{3/2} e^{-t} dt \pm i \int_{-1/x}^{\infty} (-1 - xt)^{3/2} e^{-t} dt, \tag{21}$$

where the imaginary part is

$$\operatorname{Im} B(x) = \pm \int_{-1/x}^{\infty} (-1 - xt)^{3/2} e^{-t} dt = \tfrac{3}{4}\sqrt{\pi}(-x)^{3/2} e^{1/x}. \tag{22}$$

Behavior of the imaginary part of the function $E_B(z)$ is described by equation (5) with constants

$$C = \tfrac{3}{4}\sqrt{\pi} P_B(z_B), \quad \alpha = \tfrac{3}{2}, \quad \beta = 1. \tag{23}$$

Correspondingly, as follows from equation (18),

$$\ln |E_{Bn}| \sim -n \ln |z_B| - 2 z_B^{-1/2} n^{1/2} + \tfrac{3}{2} \ln n + \left(\tfrac{1}{4} + \frac{1}{2 z_B} + \ln\left(\tfrac{3}{4}\sqrt{\pi} P_B(z_B)\right) + \tfrac{3}{4} \ln |z_B| \right). \tag{24}$$