PRETORIA

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POWER-SERIES EXPANSION OF MULTI-CHANNEL JOST MATRIX

Taylor-type power-series expansion
in scattering theory:

$$k^{2\ell+1}\cot\delta_\ell(k) = \sum_{n=0}^{\infty} c_{\ell n} k^{2n}$$

short-range potential

Effective-range expansion

ℓ = 0

$$k\cot\delta_0(k) = -\frac{1}{a} + \frac{1}{2}r_0 k^2 - P r_0^3 k^4 + Q r_0^5 k^6 + \cdots$$

Scattering length **Effective radius**

Limitations :

- valid near ***k=0*** (low energies)
- single-channel problem

Present work generalization →

- **Expansion near any complex *E***
- ***N*-channel problem**

Multi-channel Schrödinger equation

$$\left[\frac{\hbar^2}{2\mu_n}\Delta_{\vec r} + (E - E_n)\right]\psi_n(E,\vec r) = \sum_{n'=1}^{N} \mathcal{U}_{nn'}(\vec r)\psi_{n'}(E,\vec r)\,.$$

$$\Psi(E,\vec r) = \begin{pmatrix} \psi_1(E,\vec r) \\ \psi_2(E,\vec r) \\ \vdots \\ \psi_N(E,\vec r) \end{pmatrix}$$

$$\psi_n(E,\vec r) = \frac{u_n(E,r)}{r} Y_{\ell_n m_n}(\theta,\varphi)$$

$$\left[\partial_r^2 + k_n^2 - \frac{\ell_n(\ell_n+1)}{r^2}\right] u_n(E,r) = \sum_{n'=1}^{N} V_{nn'}(r) u_{n'}(E,r)$$

$$V_{nn'}(r) = \frac{2\mu_n}{\hbar^2}\int Y^*_{\ell_n m_n}(\theta,\varphi)\mathcal{U}_{nn'}(\vec r) Y_{\ell_{n'} m_{n'}}(\theta,\varphi)\, d\Omega_{\vec r}$$

$$k_n = \sqrt{\frac{2\mu_n}{\hbar^2}(E - E_n)}$$

$$V_{nn'}(r) \underset{r\to\infty}{\longrightarrow} 0 \qquad \text{exponentially}$$

channel momentum

$$\left[\partial_r^2 + k_n^2 - \frac{\ell_n(\ell_n+1)}{r^2}\right] u_n(E,r) = \sum_{n'=1}^{N} V_{nn'}(r) u_{n'}(E,r)$$

2N linearly independent solutions; ***N*** of them are regular at ***r = 0***

fundamental matrix of regular solutions (the basis)

$$\Phi(E,r) = \begin{pmatrix} \phi_{11}(E,r) & \phi_{12}(E,r) & \cdots & \phi_{1N}(E,r) \\ \phi_{21}(E,r) & \phi_{22}(E,r) & \cdots & \phi_{2N}(E,r) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_{N1}(E,r) & \phi_{N2}(E,r) & \cdots & \phi_{NN}(E,r) \end{pmatrix}$$

Physical solution

$$\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix} = C_1 \begin{pmatrix} \phi_{11} \\ \phi_{21} \\ \vdots \\ \phi_{N1} \end{pmatrix} + C_2 \begin{pmatrix} \phi_{12} \\ \phi_{22} \\ \vdots \\ \phi_{N2} \end{pmatrix} + \cdots + C_N \begin{pmatrix} \phi_{1N} \\ \phi_{2N} \\ \vdots \\ \phi_{NN} \end{pmatrix}$$

Regular at ***r = 0***

C_n are chosen to give certain asymptotics $r \longrightarrow \infty$ (bound, resonant, scattering)

Multi-channel Jost matrix

$$\left[\partial_r^2 + k_n^2 - \frac{\ell_n(\ell_n+1)}{r^2}\right] u_n(E,\vec{r}) \approx 0\,, \quad \text{when } r \to \infty$$

Equations decouple; their solutions are known:

$h^{(\pm)}_{\ell_n}(k_n r)$ **Riccati-Hankel** functions

2N linearly independent column-solutions can be grouped in two square matrices:

$$W^{(\mathrm{in})} = \begin{pmatrix} h^{(-)}_{\ell_1}(k_1 r) & 0 & \cdots & 0 \\ 0 & h^{(-)}_{\ell_2}(k_2 r) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & h^{(-)}_{\ell_N}(k_N r) \end{pmatrix}$$

in-coming and out-going spherical waves

$$W^{(\mathrm{out})} = \begin{pmatrix} h^{(+)}_{\ell_1}(k_1 r) & 0 & \cdots & 0 \\ 0 & h^{(+)}_{\ell_2}(k_2 r) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & h^{(+)}_{\ell_N}(k_N r) \end{pmatrix}$$

These ***2N*** columns form a basis in the space of solutions

Each column of $\Phi(E,r)$ at large distances becomes a linear combination of the basis columns

$$\Phi(E,r) \underset{r\to\infty}{\longrightarrow} W^{(\mathrm{in})}(E,r)F^{(\mathrm{in})}(E) + W^{(\mathrm{out})}(E,r)F^{(\mathrm{out})}(E)$$

Jost matrices

$$S(E) = F^{(\mathrm{out})}(E)\left[F^{(\mathrm{in})}(E)\right]^{-1}$$

spectral points: $E = \mathcal{E}_n$ (bound states and resonances)

$$\det F^{(\mathrm{in})}(\mathcal{E}_n) = 0$$

Transformation of the Schrödinger equation

$$\Phi(E,r) \xrightarrow[r\to\infty]{} W^{(\mathrm{in})}(E,r)F^{(\mathrm{in})}(E) + W^{(\mathrm{out})}(E,r)F^{(\mathrm{out})}(E)$$

$$\Phi(E,r) \equiv W^{(\mathrm{in})}(E,r)\mathcal{F}^{(\mathrm{in})}(E,r) + W^{(\mathrm{out})}(E,r)\mathcal{F}^{(\mathrm{out})}(E,r)$$

variation parameters method

$$W^{(\mathrm{in})}(E,r)\frac{\partial}{\partial r}\mathcal{F}^{(\mathrm{in})}(E,r) + W^{(\mathrm{out})}(E,r)\frac{\partial}{\partial r}\mathcal{F}^{(\mathrm{out})}(E,r) = 0$$

Lagrange condition

$$\partial_r\mathcal{F}^{(\mathrm{in})} = -\frac{1}{2i}K^{-1}W^{(\mathrm{out})}V\left[W^{(\mathrm{in})}\mathcal{F}^{(\mathrm{in})} + W^{(\mathrm{out})}\mathcal{F}^{(\mathrm{out})}\right]$$

$$\partial_r\mathcal{F}^{(\mathrm{out})} = \frac{1}{2i}K^{-1}W^{(\mathrm{in})}V\left[W^{(\mathrm{in})}\mathcal{F}^{(\mathrm{in})} + W^{(\mathrm{out})}\mathcal{F}^{(\mathrm{out})}\right]$$

$$K = \begin{pmatrix} k_1 & 0 & \cdots & 0 \\ 0 & k_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & k_N \end{pmatrix}$$

$$h_\ell^{(+)}(z) + h_\ell^{(-)}(z) \equiv 2j_\ell(z)$$

boundary conditions

$$\mathcal{F}^{(\mathrm{in})}(E,0) = \mathcal{F}^{(\mathrm{out})}(E,0) = \frac{1}{2}I$$

$$\mathcal{F}^{(\mathrm{in/out})}(E,r) \xrightarrow[r\to\infty]{} F^{(\mathrm{in/out})}(E)$$

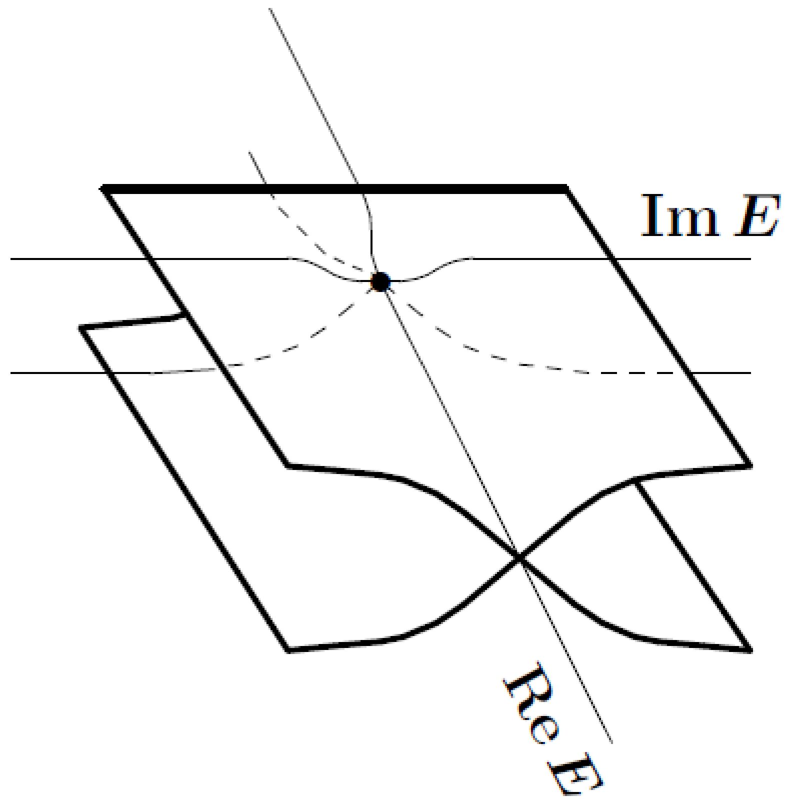
Riemann surface

channel momenta →

$$k_n = \pm\sqrt{\frac{2\mu_n}{\hbar^2}(E - E_n)}\,, \qquad n = 1, 2, \ldots, N$$

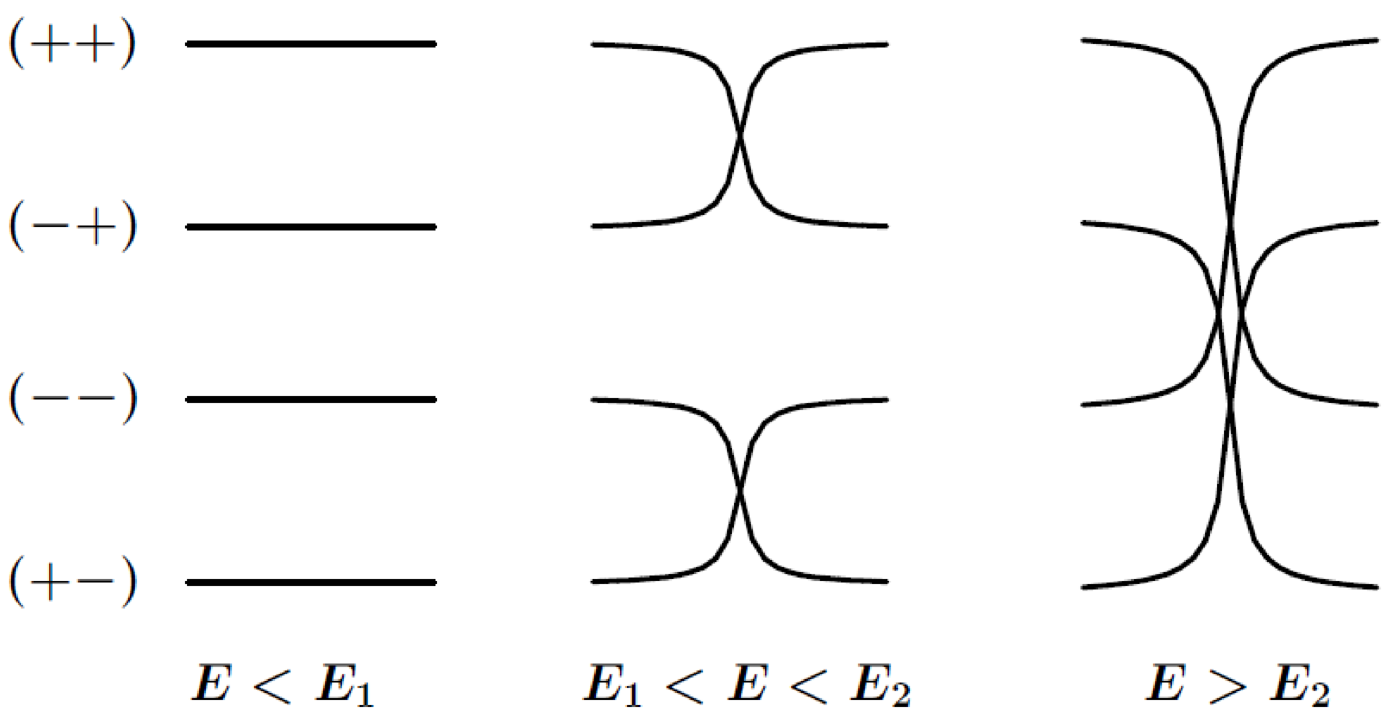
matrices $\boldsymbol{F}^{(\text{in/out})}(\boldsymbol{E})$ have $\mathbf{2}^{\boldsymbol{N}}$ different values

Riemann surface of the energy for a single-channel problem →



$$k_n = \pm\sqrt{\frac{2\mu_n}{\hbar^2}(E - E_n)}\ , \qquad n = 1, 2$$

Schematically shown interconnections of the layers of the Riemann surface for a two-channel problem at three different energy intervals. The layers correspond to different combinations of the signs (indicated in brackets) of $\mathrm{Im}\,k_1$ and $\mathrm{Im}\,k_2$



In the present work, we construct the Jost matrices in such a way that in their matrix elements the dependences on odd powers of all channel momenta are factorized analytically

$$h_\ell^{(\pm)}(z) = j_\ell(z) \pm i y_\ell(z)$$

$$\boldsymbol{J} = \frac{1}{2}\left[\boldsymbol{W}^{(\mathrm{in})} + \boldsymbol{W}^{(\mathrm{out})}\right] = \begin{pmatrix} j_{\ell_1}(k_1 r) & 0 & \cdots & 0 \\ 0 & j_{\ell_2}(k_2 r) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & j_{\ell_N}(k_N r) \end{pmatrix}$$

$$\boldsymbol{Y} = \frac{i}{2}\left[\boldsymbol{W}^{(\mathrm{in})} - \boldsymbol{W}^{(\mathrm{out})}\right] = \begin{pmatrix} y_{\ell_1}(k_1 r) & 0 & \cdots & 0 \\ 0 & y_{\ell_2}(k_2 r) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & y_{\ell_N}(k_N r) \end{pmatrix}$$

$$\begin{aligned} \boldsymbol{\mathcal{A}}(E,r) &= \boldsymbol{\mathcal{F}}^{(\mathrm{in})}(E,r) + \boldsymbol{\mathcal{F}}^{(\mathrm{out})}(E,r)\ , \\ \boldsymbol{\mathcal{B}}(E,r) &= i\left[\boldsymbol{\mathcal{F}}^{(\mathrm{in})}(E,r) - \boldsymbol{\mathcal{F}}^{(\mathrm{out})}(E,r)\right] \end{aligned}$$

$$\Phi(E,r) \equiv W^{(\mathrm{in})}(E,r)\mathcal{F}^{(\mathrm{in})}(E,r) + W^{(\mathrm{out})}(E,r)\mathcal{F}^{(\mathrm{out})}(E,r)$$

$$\Phi(E,r) = J(E,r)\mathcal{A}(E,r) - Y(E,r)\mathcal{B}(E,r)$$

$$\partial_r \mathcal{A} = -K^{-1} Y V \left(J\mathcal{A} - Y\mathcal{B}\right)$$

$$\partial_r \mathcal{B} = -K^{-1} J V \left(J\mathcal{A} - Y\mathcal{B}\right)$$

Boundary conditions

$$\mathcal{A}(E,0) = I$$

$$\mathcal{B}(E,0) = 0$$

$$\mathcal{A}(E,r) \underset{r\to\infty}{\longrightarrow} A(E) \,, \qquad \mathcal{B}(E,r) \underset{r\to\infty}{\longrightarrow} B(E)$$

$$F^{(\mathrm{in})}(E) = \frac{1}{2}\left[A(E) - iB(E)\right] \,, \qquad F^{(\mathrm{out})}(E) = \frac{1}{2}\left[A(E) + iB(E)\right]$$

Factorization

$$j_\ell(kr) = \left(\frac{kr}{2}\right)^{\ell+1} \sum_{n=0}^{\infty} \frac{(-1)^n \sqrt{\pi}}{\Gamma(\ell+3/2+n)n!} \left(\frac{kr}{2}\right)^{2n} = k^{\ell+1} \tilde{j}_\ell(E,r)$$

$$y_\ell(kr) = \left(\frac{2}{kr}\right)^{\ell} \sum_{n=0}^{\infty} \frac{(-1)^{n+\ell+1}}{\Gamma(-\ell+1/2+n)n!} \left(\frac{kr}{2}\right)^{2n} = k^{-\ell} \tilde{y}_\ell(E,r)$$

$$J = \begin{pmatrix} k_1^{\ell_1+1} & 0 & \cdots & 0 \\ 0 & k_2^{\ell_2+1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & k_N^{\ell_N+1} \end{pmatrix} \tilde{J}\,, \qquad Y = \begin{pmatrix} k_1^{-\ell_1} & 0 & \cdots & 0 \\ 0 & k_2^{-\ell_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \vdots & k_N^{-\ell_N} \end{pmatrix} \tilde{Y}$$

$$\mathcal{A}_{ij} = \frac{k_j^{\ell_j+1}}{k_i^{\ell_i+1}} \tilde{\mathcal{A}}_{ij}$$

$$\mathcal{B}_{ij} = k_i^{\ell_i} k_j^{\ell_j+1} \tilde{\mathcal{B}}_{ij}$$

$$\partial_r \tilde{\mathcal{A}} = -\tilde{Y} V \left(\tilde{J}\tilde{\mathcal{A}} - \tilde{Y}\tilde{\mathcal{B}}\right)$$

$$\partial_r \tilde{\mathcal{B}} = -\tilde{J} V \left(\tilde{J}\tilde{\mathcal{A}} - \tilde{Y}\tilde{\mathcal{B}}\right)$$

Symmetry of the Jost matrices

$$F^{(\mathrm{in})}_{mn} = \frac{k_n^{\ell_n+1}}{2k_m^{\ell_m+1}}\tilde{A}_{mn} - \frac{ik_m^{\ell_m}k_n^{\ell_n+1}}{2}\tilde{B}_{mn}$$

$$F^{(\mathrm{out})}_{mn} = \frac{k_n^{\ell_n+1}}{2k_m^{\ell_m+1}}\tilde{A}_{mn} + \frac{ik_m^{\ell_m}k_n^{\ell_n+1}}{2}\tilde{B}_{mn}$$

$$F^{(\mathrm{in})}_{mn}(-k_1,-k_2,\dots,-k_N) = (-1)^{\ell_m+\ell_n}F^{(\mathrm{out})}_{mn}(k_1,k_2,\dots,k_N)$$

$$S_{mn} = (-1)^{\ell_m+\ell_n}F^{(\mathrm{in})}_{mn}(-k_1,-k_2,\dots,-k_N)\left[F^{(\mathrm{in})}_{mn}(k_1,k_2,\dots,k_N)\right]^{-1}$$

Power-series expansion

$$\partial_r \tilde{\mathcal{A}} = -\tilde{Y} V \left(\tilde{J} \tilde{\mathcal{A}} - \tilde{Y} \tilde{\mathcal{B}} \right)$$

$$\partial_r \tilde{\mathcal{B}} = -\tilde{J} V \left(\tilde{J} \tilde{\mathcal{A}} - \tilde{Y} \tilde{\mathcal{B}} \right)$$

$$\tilde{J}(E,r) = \sum_{n=0}^{\infty} (E - E_0)^n \gamma_n(E_0, r)$$

$$\tilde{Y}(E,r) = \sum_{n=0}^{\infty} (E - E_0)^n \eta_n(E_0, r)$$

$$\tilde{\mathcal{A}}(E,r) = \sum_{n=0}^{\infty} (E - E_0)^n \alpha_n(E_0, r)$$

$$\tilde{\mathcal{B}}(E,r) = \sum_{n=0}^{\infty} (E - E_0)^n \beta_n(E_0, r)$$

$$\partial_r \alpha_n = - \sum_{i+j+k=n} \eta_i V \left(\gamma_j \alpha_k - \eta_j \beta_k \right)$$

$$\partial_r \beta_n = - \sum_{i+j+k=n} \gamma_i V \left(\gamma_j \alpha_k - \eta_j \beta_k \right)$$

Boundary conditions

$$\alpha_n(E_0, 0) = \delta_{n0} I$$

$$\beta_n(E_0, 0) = 0$$

$\alpha_n(E_0, r) \underset{r \to \infty}{\longrightarrow} a_n(E_0)$, and $\beta_n(E_0, r) \underset{r \to \infty}{\longrightarrow} b_n(E_0)$

$$\partial_r \alpha_n = - \sum_{i+j+k=n} \eta_i V (\gamma_j \alpha_k - \eta_j \beta_k)$$

$$\partial_r \beta_n = - \sum_{i+j+k=n} \gamma_i V (\gamma_j \alpha_k - \eta_j \beta_k)$$

Boudary conditions

$$\alpha_n(E_0, 0) = \delta_{n0} I$$

$$\beta_n(E_0, 0) = 0$$

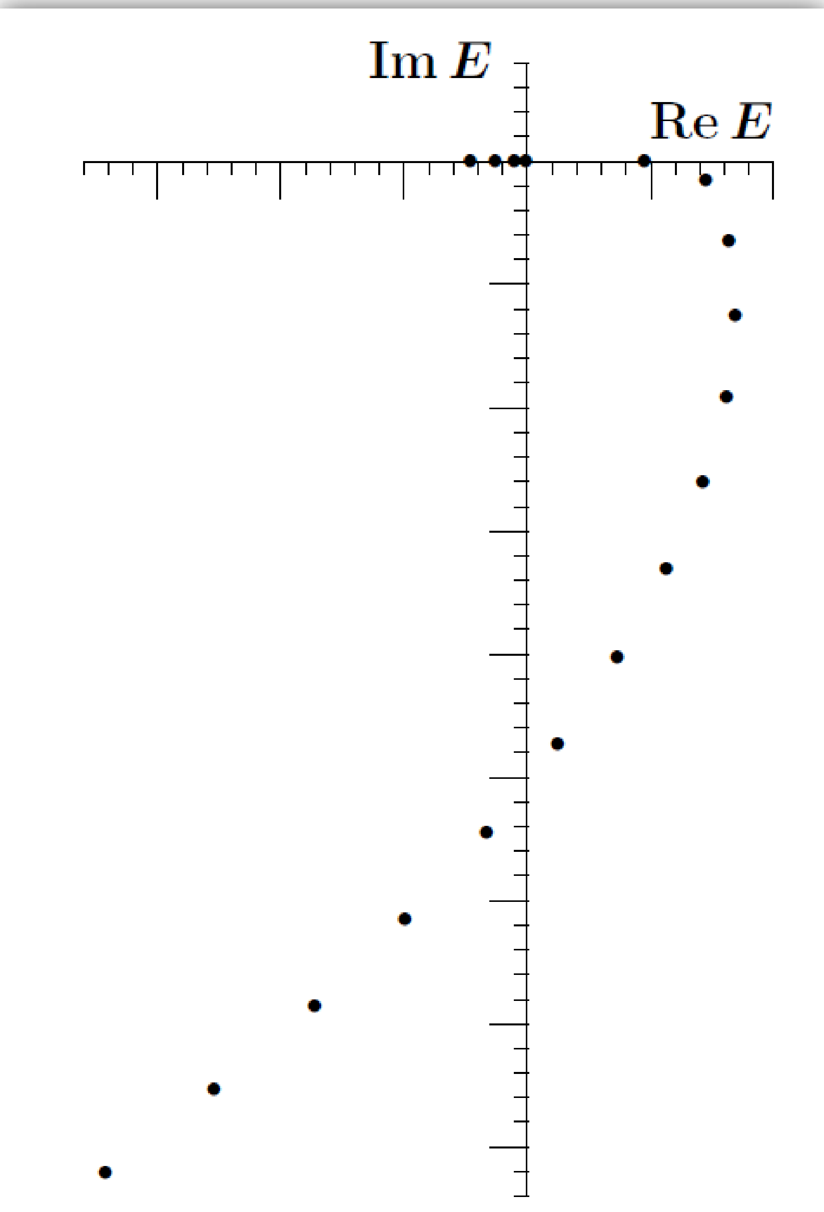
$$\alpha_n(E_0, r) \underset{r\to\infty}{\longrightarrow} a_n(E_0) \ , \qquad \text{and} \qquad \beta_n(E_0, r) \underset{r\to\infty}{\longrightarrow} b_n(E_0)$$

$$F^{(\mathrm{in})}_{mn} = \sum_{j=0}^{M} (E - E_0)^j \left[\frac{k_n^{\ell_n+1}}{2k_m^{\ell_m+1}} (a_j)_{mn} - \frac{i k_m^{\ell_m} k_n^{\ell_n+1}}{2} (b_j)_{mn} \right]$$

$$F^{(\mathrm{out})}_{mn} = \sum_{j=0}^{M} (E - E_0)^j \left[\frac{k_n^{\ell_n+1}}{2k_m^{\ell_m+1}} (a_j)_{mn} + \frac{i k_m^{\ell_m} k_n^{\ell_n+1}}{2} (b_j)_{mn} \right]$$

Example

Two-channel model



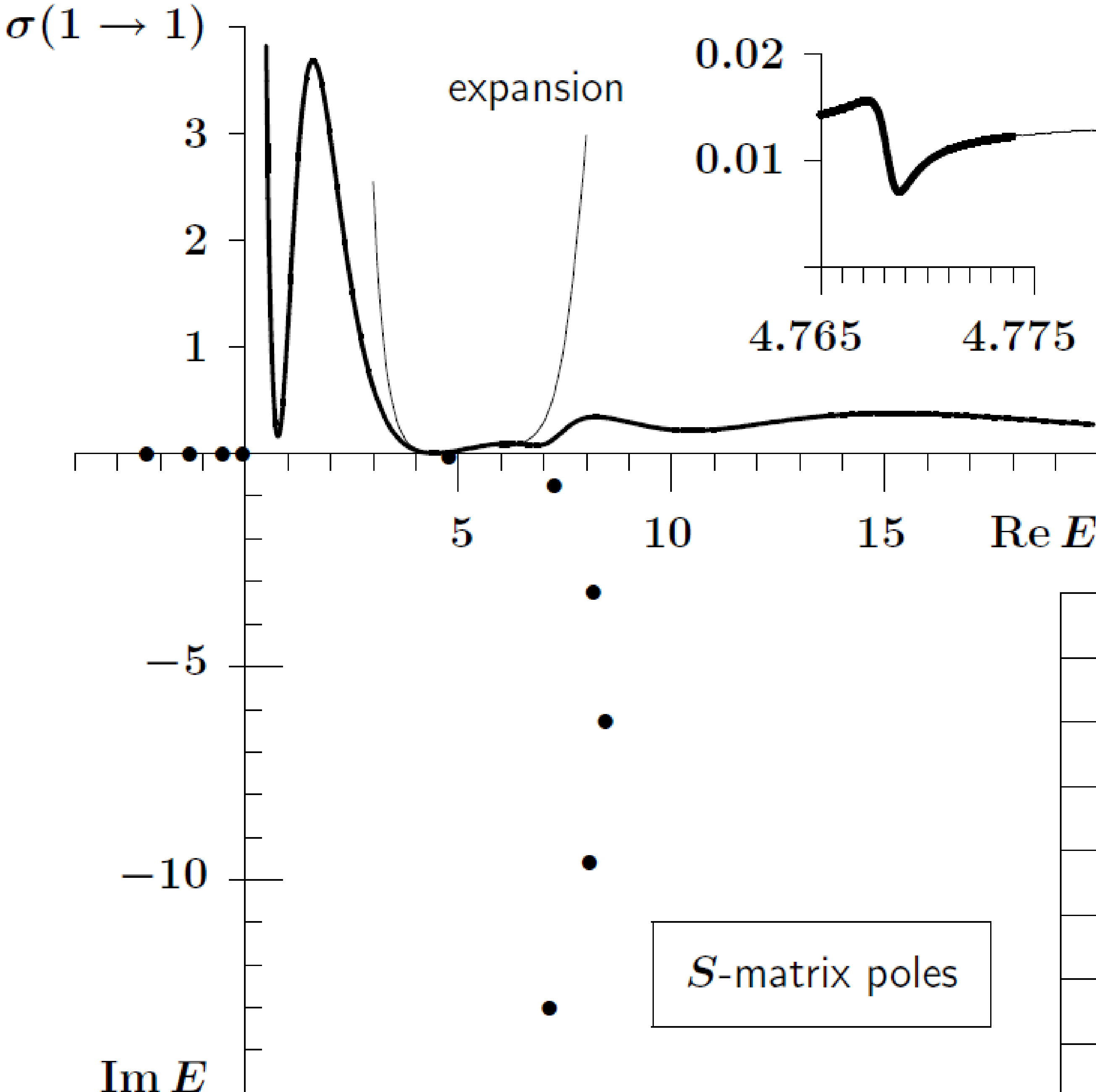
$$V(r) = \begin{pmatrix} -1.0 & -7.5 \\ -7.5 & 7.5 \end{pmatrix} r^2 e^{-r}$$

$$\mu_1 = \mu_2 = \hbar c = 1$$

$$E_1 = 0 \text{ and } E_2 = 0.1$$

$$\ell_1 = \ell_2 = 0.$$

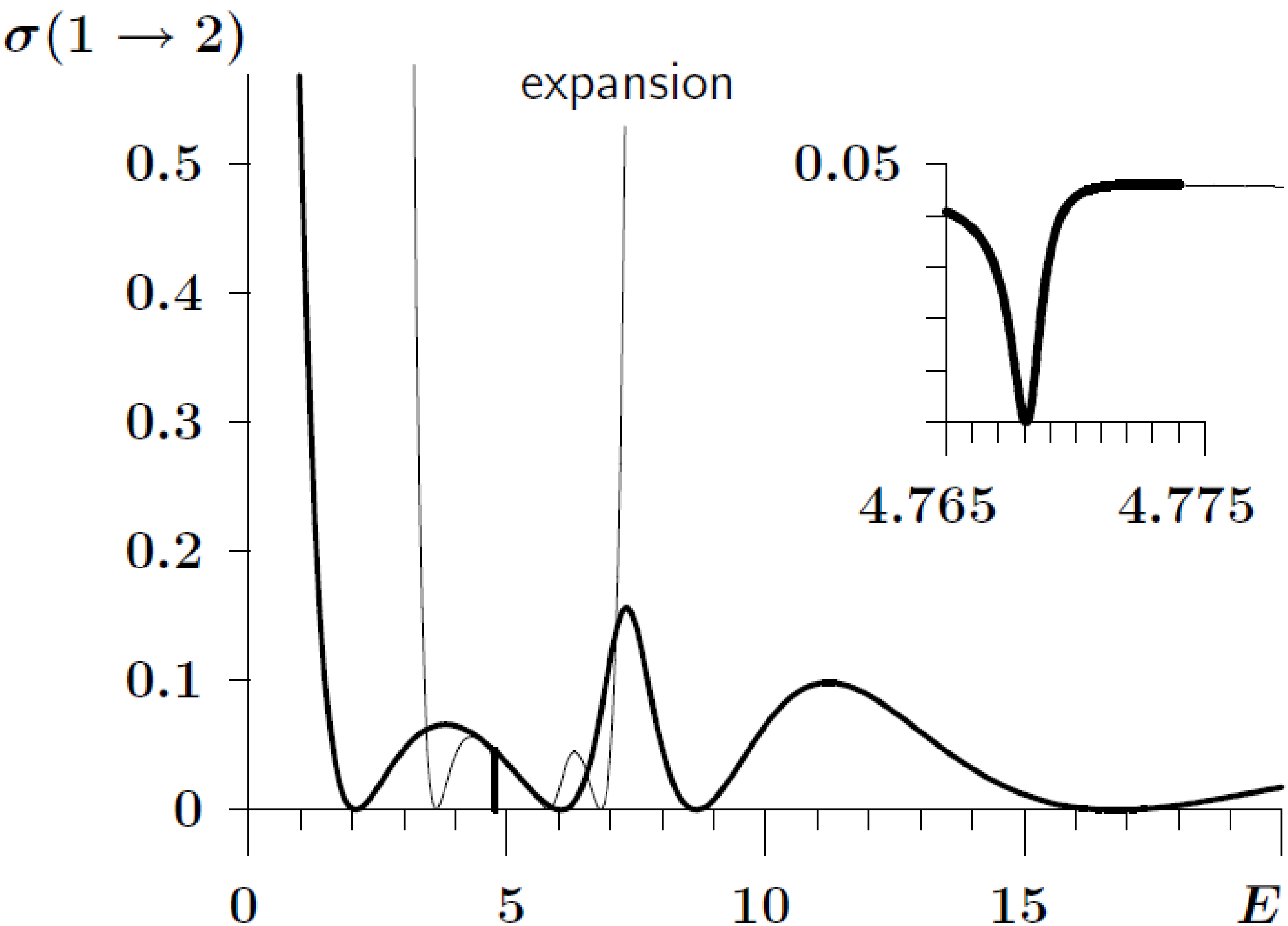
E_r	Γ
-2.314391	0
-1.310208	0
-0.537428	0
-0.065258	0
4.768197	0.001420
7.241200	1.511912
8.171217	6.508332



$E_0 = 5 + i0$

$M = 5$

E_r	Γ
-2.314391	0
-1.310208	0
-0.537428	0
-0.065258	0
4.768197	0.001420
7.241200	1.511912
8.171217	6.508332

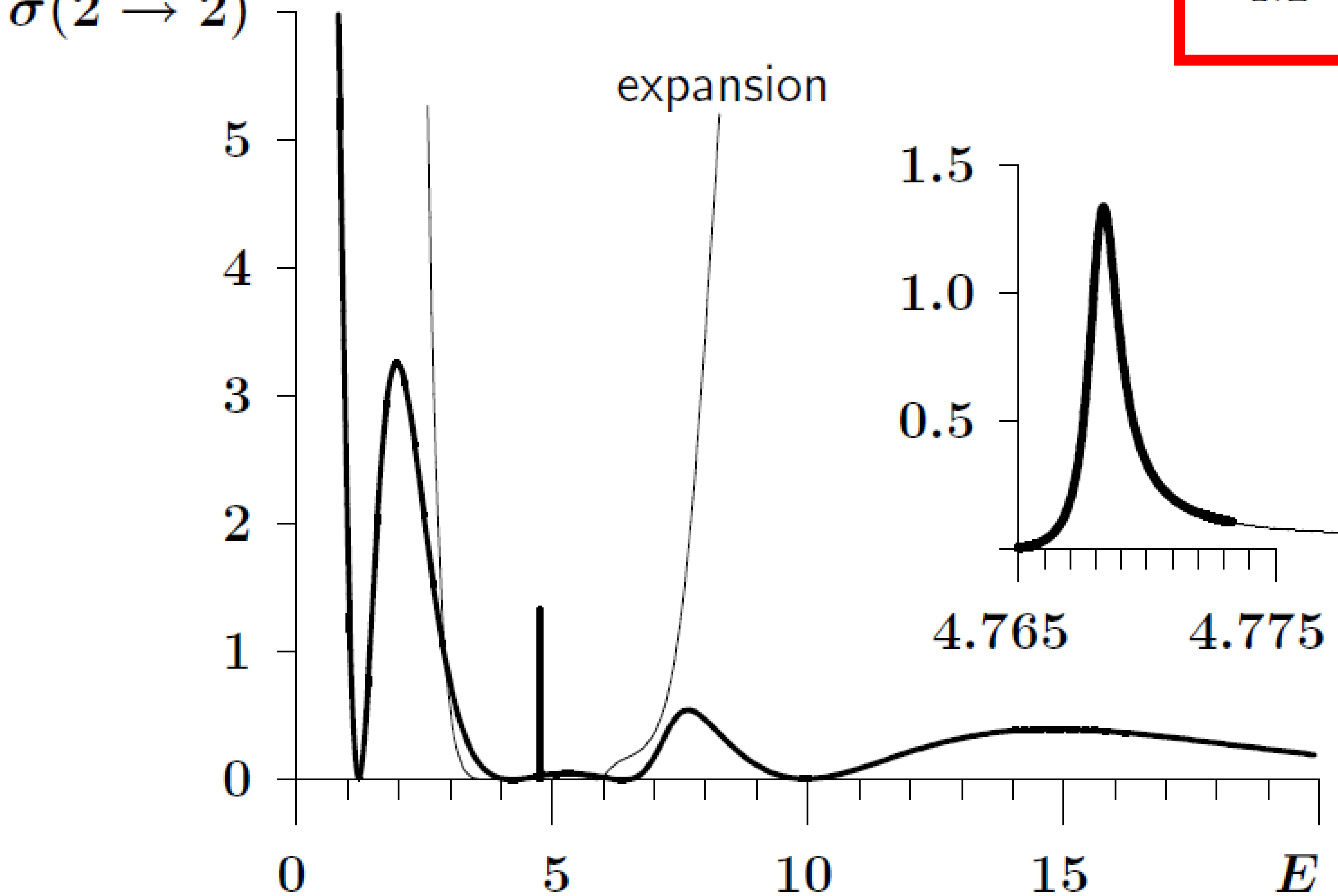


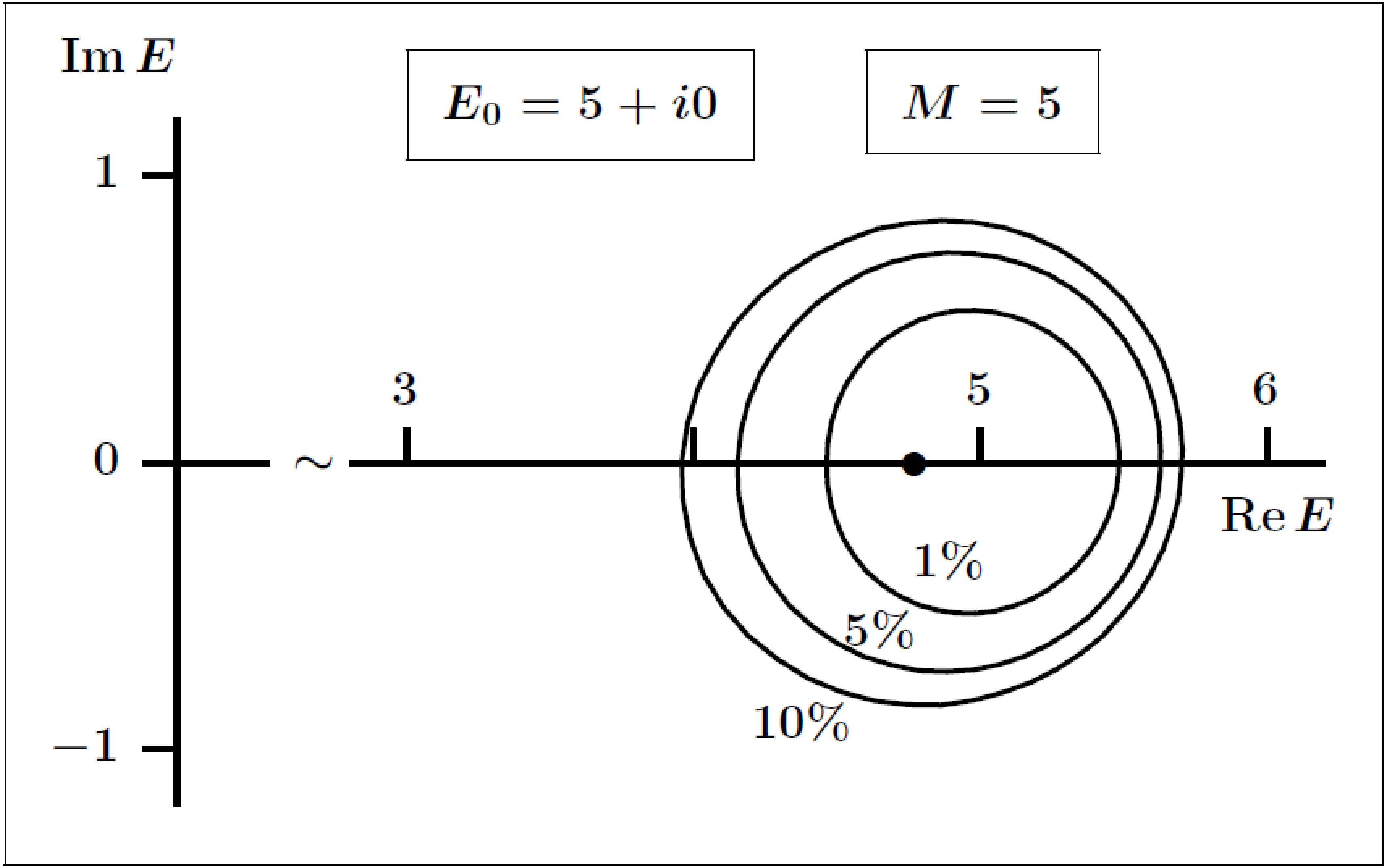
$E_0 = 5 + i0$

$M = 5$

$$E_0 = 5 + i0$$

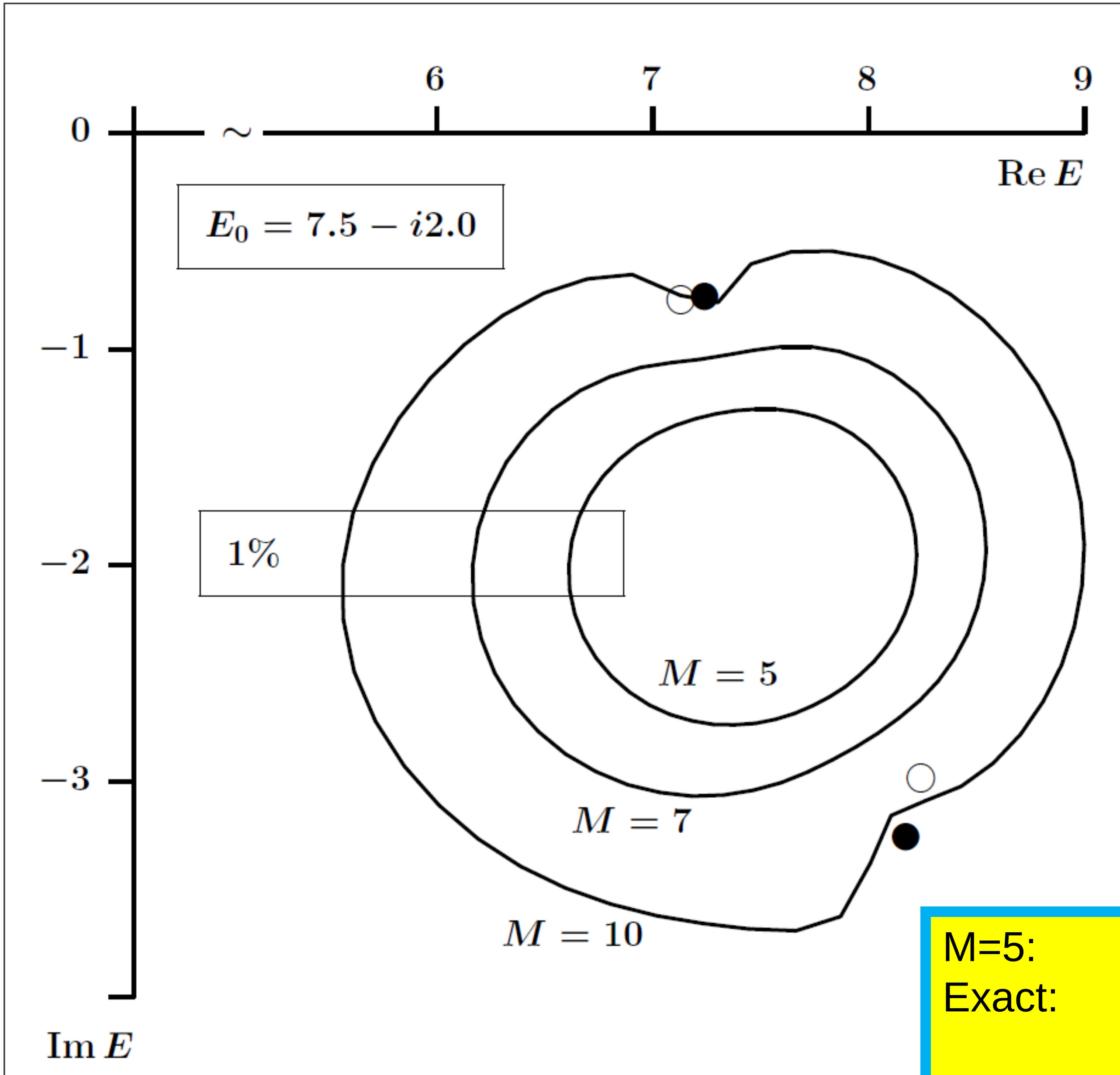
$$M = 5$$





First resonance →

Expansion (M=5): E = **4.768178−*i*0.000686**
Exact value: E = **4.768197−*i*0.000710**



Two resonances

M=5: E = **7.241200 −i0.755956**
Exact: E = **7.131204− i0.768670**

M=5: E **= 8.241795 − i2.982867**
Exact: E = **8.171217 − i3.254166**

SUMMARY

- odd powers of the channel momenta in the Jost matrices are factorized
- for the remaining energy dependent factors, a system of differential equations is obtained
- these energy dependent functions are expanded in power series
- the expansion coefficients are determined by a system of differential equations