
Algorithm 3 CHEBYCHEVCOEFFICIENTS for $f(\pm \hat{A} dt) = e^{\pm i \hat{A} dt}$.

Input: spectral radius Δ of \hat{A} ; minimum eigenvalue E_{\min} of \hat{A} ; time step dt

Output: Array of Chebychev coefficients $[a_0 \dots a_n]$ allowing to approximate $f(\hat{A} dt)$ to pre-defined precision.

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1: procedure EXPCHEBYCOEFFS( $\Delta$ ,  $E_{\min}$ ,  $dt$ )
2:    $\alpha = \frac{1}{2} \Delta dt$ 
3:    $a_0 = J_0(\alpha)$  ▷ 0'th order Bessel-function of first kind
4:   for  $i = 1 : n_{\max} \approx 4 \lfloor \alpha \rfloor$  do
5:      $a_i = 2J_i(\alpha)$  ▷  $i$ 'th order Bessel-function of first kind
6:     if  $|a_i| < \text{limit}$  then exit loop with  $n = i$ 
7:   end for
8:   return  $[a_0, \dots a_n]$ 
9: end procedure
```
