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Modified Mathieu functions for radial Schrödinger equation with polarization potential: reliable numerical algorithms

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Abstract. The new numerical approach to calculation of modified Mathieu functions is proposed. These functions play an important role in theories of electron scattering from (highly) polarizable atoms, like alkali. The algorithms we developed show very high accuracy in a wide range of energy and polarizability, which are the two principal parameters of the problem. The numerical scheme does not lose the accuracy in the so-called 'unstable' regions, where the characteristic exponent of Mathieu functions becomes complex. This stability makes possible the analytical continuation of these methods in the complex plane of parameters.

1. Introduction

There are many physical situations when a neutral atom interacts with a charged particle and the resultant polarization of the atom plays an important role in transition or scattering processes [1–4]. Accurately taking into account the polarization effects is essential for the realistic theoretical description of such processes. In this paper we will consider only the charge-induced dipole part of the polarization potential. The aim of this article being the development of a new computational approach, we will not discuss the applicability of the dipole approximation, although such a discussion can be found in [1] and references therein.

We attempt to build algorithms that will be stable in a wide range of parameters for quasianalytical solutions to the following radial Schrödinger equation (atomic units throughout):

$$\left(\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2} + \frac{\alpha}{r^4} + 2E\right)\psi_l(r, E, \alpha) = 0. \tag{1}$$

Only the case $E > 0$ will be considered in this paper, therefore (1) describes the scattering of l-wave electrons with the energy E from neutral atoms with static polarizability α. An excellent theoretical treatment of this problem in terms of modified Mathieu functions was given by Holzwarth [1], but we found that the numerical algorithms proposed in that paper become very inaccurate in the so-called 'unstable' region, where the characteristic exponent is complex (see section 2 below).

Very illustrative is the application of Mathieu function solutions of (1) to modified effective range theory (ERT) proposed by Fabrikant [2, 3]. In ERT the scattering phase shifts are given by

$$\tan\delta_l = -\frac{Mc+d}{Ma+b}. \tag{2}$$

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The quantity M is irrelevant to our study, and the coefficients a, b, c, d match solutions with prescribed asymptotic behaviour at $r \to \infty$ and $r \to 0$:

$$F(r, E) \sim \cos(\sqrt{\alpha}/r - \pi l/2) \qquad \text{when } r \to 0 \tag{3}$$

$$G(r, E) \sim \sin(\sqrt{\alpha}/r - \pi l/2) \qquad \text{when } r \to 0 \tag{4}$$

$$\varphi(r, E) \sim \frac{1}{r}\sin(kr - \pi l/2) \qquad \text{when } r \to \infty \tag{5}$$

$$\psi(r, E) \sim \frac{1}{r}\cos(kr - \pi l/2) \qquad \text{when } r \to \infty \tag{6}$$

$$\psi(r, E) = F(r, E)a(E) + G(r, E)b(E) \tag{7}$$

$$\varphi(r, E) = F(r, E)c(E) + G(r, E)d(E) \tag{8}$$

where we have introduced $k = \sqrt{2E}$.

The ERT phase shifts can be easily found by direct numerical integration of (1) with the initial conditions (3)–(6), and then one satisfies the matching conditions (7) and (8) (together with their derivatives) at some point r_0, but this approach is only effective when E is real. On the other hand, if one is interested in the analytical structure of S-matrix in the complex plane of E, then the direct numerical integration becomes dramatically inaccurate because of growing exponents in the boundary conditions at $r \to \infty$. In this case the quasi-analytical solutions in terms of modified Mathieu functions can be used very effectively.

2. Some formulae from Mathieu function theory

Although there are many papers and books that deal with Mathieu functions (e.g. see [5]), in this section we will follow the article by Holzwarth [1], because it relates these functions very closely to the scattering problems. First we introduce a new parameter $f = \sqrt{\alpha}$ and change the function and variable:

$$P_l(r) = \sqrt{r}\psi_l(r, k, f) \tag{9}$$

$$x = \sqrt{k/f}r \tag{10}$$

and (1) transforms into the form that proves to be the most useful†:

$$\left[x^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x\frac{\mathrm{d}}{\mathrm{d}x} - \left(l + \frac{1}{2}\right)^2 + kf\left(\frac{1}{x^2} + x^2\right)\right]P_l(x) = 0. \tag{11}$$

The two linearly independent solutions to (11) can be written as

$$\mathcal{M}_{\pm\tau}(x) = \sum_{n=-\infty}^{\infty} C_n(\tau)x^{\pm(\tau+2n)}. \tag{12}$$

Substituting (12) into (11) one obtains the recurrence relations for coefficients $C_n(\tau)$:

$$C_n(\tau) + \frac{kf}{(\tau + 2n)^2 - \left(l + \frac{1}{2}\right)^2}(C_{n+1}(\tau) + C_{n-1}(\tau)) = 0 \tag{13}$$

† Changing variable $x = e^{\mu}$ one can obtain the classic form of modified Mathieu equation, but we do not need it in this paper.

which is an infinite homogeneous system of linear algebraic equations and the determinant of it must be zero in order to have a non-trivial solution for the constants $C_n(\tau)$. This condition determines a unique value of the 'characteristic exponent' τ.

Although representation (12) really solves the radial Schrödinger equation (1), it is not very convenient in computations and it does not explicitly show the asymptotic properties of the solution at $r \to 0$ and $r \to \infty$, which are usually needed in the scattering theory. Therefore, the Bessel product series representations are most widely used, of which we will cite only this one:

$$\mathcal{JJ}_{\pm\tau}(r) = \sum_{n=-\infty}^{\infty} (-1)^n C_n(\tau) J_{\pm(\tau+n)}(a) J_{\pm n}(b) \tag{14}$$

where $a = \max(kr, f/r)$ and $b = \min(kr, f/r)$. Bessel functions of these arguments ensure rapid convergence of the series for all values of r.

The two representations (12) and (14) are related in the following way:

$$\mathcal{M}_{\pm\tau}(x) = K^{\pm}\mathcal{JJ}_{\pm\tau}(r) \qquad \text{when } x \geqslant 1 \tag{15}$$

$$\mathcal{M}_{\pm\tau}(x) = K^{\mp}\mathcal{JJ}_{\mp\tau}(r) \qquad \text{when } x \leqslant 1\,. \tag{16}$$

Noting that $\mathcal{M}_{+\tau}(x=1) = \mathcal{M}_{-\tau}(x=1)$, the ratio of constants K^-/K^+ can be determined from the Bessel product representation (14):

$$\frac{K^-}{K^+} = \frac{\mathcal{JJ}_{+\tau}(r=\sqrt{f/k})}{\mathcal{JJ}_{-\tau}(r=\sqrt{f/k})}\,. \tag{17}$$

We can use the asymptotic form of Bessel functions (see e.g. [6]) and the normalization condition $C_0(\tau) = 1$ to get the asymptotic forms of $\mathcal{M}_{\pm\tau}(x)$

$$\mathcal{M}_{\pm\tau}(x) \sim K^{\pm}\sqrt{2/\pi kr}\cos(kr \mp \pi\tau/2 - \pi/4) \qquad \text{when } r \to \infty \tag{18}$$

$$\mathcal{M}_{\pm\tau}(x) \sim K^{\mp}\sqrt{2r/\pi f}\cos(f/r \pm \pi\tau/2 - \pi/4) \qquad \text{when } r \to 0\,. \tag{19}$$

To finish up the review of modified Mathieu functions a few remarks on 'characteristic exponent' τ are in order. It can be shown (see e.g. [5]) that the expression for τ can be written as

$$\sin^2 \pi\tau/2 = \tfrac{1}{2}\Delta^l(\tau = 0) \tag{20}$$

and to make the solution unique one requires

$$\tau \to l + \tfrac{1}{2} \qquad \text{when } kf \to 0 \tag{21}$$

where Δ^l is the determinant of linear system (13) (called 'Hill determinant'). It is evident from (20) that τ is real, if $0 \leqslant \Delta^l(\tau = 0) \leqslant 2$, but when $\Delta^l(\tau = 0) < 0$ or $\Delta^l(\tau = 0) > 2$ the characteristic exponent τ becomes a complex number†. The very remarkable feature of a complex τ is that its real part is always an integer number.

† The region where τ is complex is often called 'unstable'.

3. The new numerical algorithms for Mathieu functions

It was shown in the previous section that one can find the solution to (11) by the following consecutive steps.

- Find the 'characteristic exponent' τ.
- Solve the system of equations (13) for coefficients $C_n(\tau)$.
- Use series representation (14) or (12) to calculate Mathieu function.

The usual way to proceed (see e.g. [1]) is to calculate τ using (20) and then find $C_n(\tau)$ by solving the continuous fractions associated with recurrence relation (13). In this approach one uses different matrices to satisfy the self-consistency condition of the system of linear equations and to solve this system; moreover, the different methods are used for this very closely connected tasks. This eventually leads to the loss of accuracy as parameter kf increases, especially in the 'unstable' region.

To remove this drawback we propose to use the same matrix to find τ and to calculate C_n, and to solve both problems using the same method. Our instrument in implementing this program will be the LU-decomposition, whose definition and some useful (though not very well known) properties are described in appendix.

First of all, we notice that the contribution of the non-diagonal elements in (13) falls off as $1/n^2$, so we can find the maximum number from the condition that the absolute values of the non-diagonal elements are equal to small quantity ε:

$$n_{\max} \approx \tfrac{1}{2}\sqrt{\left|\left(l+\tfrac{1}{2}\right)^2 + kf/\varepsilon\right| + |\tau|}\,. \tag{22}$$

This condition ensures that omitted non-diagonal elements are less than ε, and by changing this parameter one can check the convergence of the calculations. Now we can calculate the determinant of the set of equations (13) taking into account rows which are between $-n_{\max}$ and $+n_{\max}$. Because of the tridiagonal character of the associated matrix the LU-decomposition gives a very simple recursion formula for the determinant

$$D_{n_{\max}}(\tau) = \prod_{i=-n_{\max}+1}^{n_{\max}} d_i \tag{23}$$

where

$$d_{i+1} = 1 - \frac{(kf)^2/d_i}{((2i+\tau)^2 - (l+\tfrac{1}{2})^2)((2(i+1)+\tau)^2 - (l+\tfrac{1}{2})^2)} \qquad d_{-n_{\max}} = 1\,. \tag{24}$$

Using (22), (23) and (24) and the fact that $\lim_{n\to\pm\infty} d_n = 1$, it is easy to show that the relative error of $D_{n_{\max}}(\tau)$ calculation can be estimated as

$$\delta_D = \frac{|D_{n_{\max}}(\tau) - D_{n_{\max}+1}(\tau)|}{|D_{n_{\max}}(\tau)|} = \lambda\varepsilon^2 \qquad \text{where } \lambda \approx 1\,.$$

The 'characteristic exponent' is equal to the zero of $D_{n_{\max}}(\tau)$, which can be easily found numerically with the solution of (20) serving as a convenient initial approximation†. The

† Although (20) is exact, the *numerical solution* for τ loses accuracy in the 'unstable' region. While being close to the correct value, this numerical solution can not be made accurate enough to ensure the self-sufficiency of the system of the linear algebraic equations for the coefficients $C_n(\tau)$, but it is quite satisfactory as an initial approximation.

accuracy of the τ calculation is chosen to be equal to ε, which means that the iterations go on until

$$\frac{D_{n_{\max}}(\tau)}{D'_{n_{\max}}(\tau)} = \varepsilon \,.$$

The additional *absolute* error due to the imprecise calculation of $D_{n_{\max}}(\tau)$ can be estimated as follows:

$$\Delta_\tau = \frac{\lambda\varepsilon^2 D_{n_{\max}}(\tau)}{D'_{n_{\max}}(\tau)} = \lambda\varepsilon^3 \ll \varepsilon$$

which shows that the calculations are expected to be stable and with the accuracy of the order of magnitude of ε.

We have to find $C_n(\tau)$ now, and for this purpose we choose $C_0(\tau) = 1$ and remove the equation number 0 from the system (13). We are left with two independent inhomogeneous systems of linear algebraic equations

$$A^- \cdot C^- = b^- \tag{25}$$

$$A^+ \cdot C^+ = b^+ \tag{26}$$

where

$$C_i^- = C_{-n_{\max}+i-1}(\tau) \tag{27}$$

$$b_i^- = b^- \delta_{i,n_{\max}} \tag{28}$$

$$C_i^+ = C_{n_{\max}+i-1}(\tau) \tag{29}$$

$$b_i^+ = b^+ \delta_{i,n_{\max}} \,. \tag{30}$$

The equations have been rearranged so that in the vectors $b^\pm$ only the last element is not equal to zero. It is done in order to make the equations with lower triangular matrix easy to solve analytically.

Now the LU-algorithm for coefficients $C_n(\tau)$ can be written as an explicit series of arithmetic operations. First we perform the LU-decomposition of matrices $A^\pm$

$$u_1^\pm = \frac{kf}{(2n_{\max} \pm \tau)^2 - \left(l + \frac{1}{2}\right)^2} \tag{31}$$

$$s_i^\pm = \frac{kf}{(2(n_{\max} - i + 1) \pm \tau)^2 - \left(l + \frac{1}{2}\right)^2} \tag{32}$$

$$d_i^\pm = 1 - u_{i-1}^\pm s_i^\pm \tag{33}$$

$$u_i^\pm = s_i^\pm / d_i^\pm \tag{34}$$

and now we solve the equations

$$C_{\pm 1} = -\frac{s_{n_{\max}}^\pm}{d_{n_{\max}}^\pm} \tag{35}$$

$$C_{\pm i} = -C_{\pm i-1} u_{n_{\max}-i+1} \,. \tag{36}$$

In all these formulae i changes from 2 to $n_{\max}$. After the coefficients $C_n(\tau)$ have been found we can verify the consistency of our calculations by checking that the eliminated equation number 0 really holds, that is

$$1 + \frac{kf}{\tau^2 - \left(l + \frac{1}{2}\right)^2}(C_1(\tau) + C_{-1}(\tau)) = 0 \,. \tag{37}$$

The above condition is not trivial because $C_1(\tau)$ and $C_{-1}(\tau)$ are the solutions of the two absolutely independent systems of equations, and (37) can be satisfied only for the specially chosen quantity τ.

4. Application to effective range theory

By comparing the asymptotic forms (3)–(6) with the asymptotics of Mathieu functions (18) and (19), we can write explicit formulae† for coefficients a, b, c and d:

$$a = (1/\zeta - \zeta)\cos(\pi\tau) \tag{38}$$

$$b = (1/\zeta + \zeta)\sin(\pi\tau) + (-1)^l(1/\zeta - \zeta) \tag{39}$$

$$c = (1/\zeta + \zeta)\sin(\pi\tau) - (-1)^l(1/\zeta - \zeta) \tag{40}$$

$$d = -a \tag{41}$$

where ζ stands for the ratio K^-/K^+ which is given by (17). The quantity ζ becomes complex in the 'unstable region' and, for the tangent of the phase shift in (2) to stay real, ζ must have the absolute value equal to unity:

$$\frac{K^-}{K^+} = \exp(i\varphi) \qquad \text{in the 'unstable region'} \tag{42}$$

where φ is a real number. This property can be proved using the Bessel product representation (14), the translational properties of the coefficients $C_n(\tau)$ (that follow from (13)) and the fact that the real part of τ in the 'unstable region' is an integer number.

Being of crucial importance for meaningful description of the scattering in the framework of ERT, (42) is very sensitive to the quality of numerical algorithms used in computations‡ and therefore serves as a good test of accuracy. In table 1 we give the representative values of the parameter φ in the 'unstable region'. We present the results of calculations to 12 decimal places, which far exceeds the accuracy of reasonable physical assumptions in realistic applications, but demonstrates the convergence of this technique and can be useful for the purposes of testing the algorithm.

The analytic continuation§ in the complex plane of parameters can be used to calculate the energies and widths of ^{3}P resonances in alkali atoms in the framework of ERT. To do this we find poles of the S-matrix in the complex plane of k solving the following equation:

$$\tan\delta_l = -i \tag{43}$$

where the tangent of phase shift is given by (2). The width and energies for Rb, Cs‖ and K are presented in table 2 and can be compared with the results obtained by Fabrikant in [2] and [3] by the Breit–Wigner parameterization of phase shifts dependence on energy.

The numerical approach presented in this paper was successfully applied to the calculation of alkali metal Rydberg state broadening cross sections in the ambient alkali vapours; the comparison with the experiment and the existing theoretical results is given in [4].

† Up to a common multiplicative factor, which eventually cancels in (2).

‡ For example, we could not satisfy (42), when we tried to apply algorithms proposed in [1].

§ The analytic continuation is possible because the algorithm converges well, contains only analytical functions and does not use such 'non-analytic' operations as the complex conjugation or calculation of the modulus.

‖ Whether there is a ^{3}P resonance in Cs is an open question but for our purposes we consider only those parameters that allow such a resonance to exist.

Table 1. Representative values of the parameters φ and τ in the 'unstable region'. The values obtained by Holzwarth [1] in the points on the margin of the 'unstable region' are marked by asterisks and can be compared with our solutions.

kf	l	τ	φ
0.6945	0	0.988 769 003 448	—
0.6945*	0	0.998 5*	—
0.7	0	$1-0.055\,237\,398\,934\,3\,i$	−0.064 487 717 737 0
0.8	0	$1-0.248\,815\,099\,392\,i$	−0.286 449 838 196
0.9	0	$1-0.349\,538\,893\,100\,i$	−0.400 254 582 634
1.0	0	$1-0.427\,882\,018\,280\,i$	−0.490 281 612 366
1.5	0	$1-0.693\,815\,926\,261\,i$	−0.832 547 780 933
2.0	0	$1-0.866\,578\,516\,158\,i$	−1.112 777 627 295
3.0	0	$1-1.086\,034\,496\,318\,i$	−1.596 813 426 531
5.0	0	$1-1.249\,458\,897\,491\,i$	−2.395 441 337 495
1.671	1	1.011 991 263 560	—
1.671*	1	1.012 4*	—
1.7	1	$1+0.075\,379\,914\,012\,7\,i$	3.013 405 406 503
1.8	1	$1+0.159\,521\,698\,724\,i$	2.886 811 739 097
1.9	1	$1+0.211\,207\,756\,511\,i$	2.824 433 107 077
2.0	1	$1+0.251\,080\,789\,166\,i$	2.786 805 309 406
2.5	1	$1+0.374\,487\,532\,841\,i$	2.748 963 407 582
3.0	1	$1+0.426\,688\,824\,887\,7\,i$	2.812 429 335 695
4.0	1	$1+0.270\,319\,381\,615\,4\,i$	3.046 867 675 656
5.0	1	$2-0.431\,581\,205\,073\,8\,i$	3.033 318 259 483
3.245	2	2.012 824 202 518	—
3.245*	2	2.013 1*	—
3.3	2	$2+0.095\,376\,513\,656\,1\,i$	−0.279 532 182 697
3.5	2	$2+0.209\,931\,024\,180\,i$	−0.575 711 765 195
4.0	2	$2+0.373\,578\,754\,269\,i$	−0.874 731 639 043
5.0	2	$2+0.596\,433\,605\,534\,i$	−1.046 757 659 204

Table 2. The energies and widths of ^{3}P resonances in alkali atoms as poles of the S-matrix. The results of the Breit–Wigner parameterization obtained by Fabrikant are marked by asterisks (data for K are taken from [2], Rb and Cs from [3]).

Atom	α	M	E_r(eV)	Γ(eV)
Rb	328	$(-0.150\,7+0.1562E(\text{eV}))^{-1}$	0.0232	0.023 6
Rb*	328	$(-0.150\,7+0.1562E(\text{eV}))^{-1}$	0.023	0.025
Cs	402	$(-0.092\,27+0.4021E(\text{eV}))^{-1}$	0.0124	0.008 92
Cs*	402	$(-0.092\,27+0.4021E(\text{eV}))^{-1}$	0.0126	0.009 1
K	303	$(-0.106\,5+0.1877E(\text{eV}))^{-1}$	0.0189	0.015 3
K*	303	$(-0.107\,8+0.1957E(\text{eV}))^{-1}$	0.019	0.016

5. Conclusion

We have demonstrated the improved algorithmic approach to the calculation of various physical parameters using the modified Mathieu functions. The method is fully compatible with the previous results for small values of kf. For instance, we were able to reproduce table 1 in [1] apart from one obvious misprint and discrepancies at the margins of the 'unstable region', where the previous algorithm begins to break down.

Moreover, the new method serves as a reliable instrument for calculations in the 'unstable region' where it was shown to satisfy the fundamental condition (42), which sets an important

checking point for any calculation that is supposed to have any physical sense at all.

The simplicity and essentially arithmetic character of the proposed algorithm make it very easy to continue analytically into the complex plane of parameters. This property makes it very useful when investigating numerically the analytical properties of the S-matrix in the complex plane of energy and in applications where the calculations in the complex plane are necessary, for instance in the adiabatic collisions with participation of highly polarizable atoms. The results of calculations of the S-matrix poles given in table 2 show very good agreement with the conventional methods of computation.

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Appendix. LU-decomposition

Although the LU-decomposition can be found in any linear algebra textbook or manual of computational methods, for example [7], we think the short review of this method will greatly facilitate understanding and application of the algorithms expounded in section 3.

Suppose we are to solve the matrix equation

$$\boldsymbol{A}\cdot\boldsymbol{x}=\boldsymbol{b} \tag{A1}$$

where $\boldsymbol{A}$ is an $n\times n$ matrix, $\boldsymbol{x}$ is a vector of unknown quantities, and $\boldsymbol{b}$ is some prescribed vector. The basic idea is to represent the initial matrix $\boldsymbol{A}$ as a product of two matrices

$$\boldsymbol{A}=\boldsymbol{L}\cdot\boldsymbol{U}$$

where $\boldsymbol{L}$ and $\boldsymbol{U}$ are $n\times n$ matrices, such that

$$L_{ij}=0 \quad \text{if} \quad i<j \qquad U_{ij}=0 \quad \text{if} \quad i>j \qquad U_{ii}=1\,. \tag{A2}$$

The matrices $\boldsymbol{L}$ and $\boldsymbol{U}$ are lower and upper triangular respectively. The condition (A2) is equivalent to $\det(\boldsymbol{U})=1$ or $\det(\boldsymbol{A})=\det(\boldsymbol{L})$ and makes such a decomposition of $\boldsymbol{A}$ unique.

The LU-decomposition is performed as a step-by-step transformation of the matrix $\boldsymbol{A}$. On the lth step only columns from $l+1$ to n and rows from l to n are being changed by the following algorithm:

$$A_{lj}^{(l)}=A_{lj}^{(l-1)}/A_{ll}^{(l-1)} \qquad \text{for} \quad l+1\leqslant j\leqslant n \tag{A3}$$

$$A_{ij}^{(l)}=A_{ij}^{(l-1)}-A_{il}^{(l-1)}A_{lj}^{(l)} \qquad \text{for} \quad l+1\leqslant (i,j)\leqslant n \tag{A4}$$

where $\boldsymbol{A}^{(l)}$ represents the matrix $\boldsymbol{A}=\boldsymbol{A}^{(0)}$ after the lth transformation. After $n-1$ transformations have been performed, the diagonal elements of the matrix $\boldsymbol{A}^{(n-1)}$ and all the elements below diagonal form the matrix $\boldsymbol{L}$, and all the elements above diagonal of $\boldsymbol{A}^{(n-1)}$ give the non-diagonal part of the matrix $\boldsymbol{U}$, and the diagonal part of $\boldsymbol{U}$ is given by (A2).

Once the LU-decomposition is established, the solution of (A1) is easy to find subsequently, solving two equations with triangular matrices

$$L \cdot y = b \qquad U \cdot x = y .$$

As a by-product one can easily calculate the determinant of the matrix A as a product of diagonal elements of L:

$$\det(A) = \prod_{i=1}^{n} L_{ii} .$$

Another very important property of the LU-algorithm lies in the fact that it preserves the band structure of the matrix A. This means that if A has non-zero main diagonal elements, p non-zero diagonals above the main diagonal and q non-zero diagonals below the main one, the matrix L will have non-zero elements only on the main diagonal and q subdiagonals and U will have non-zero elements only on the main diagonal and p diagonals above it. This property makes the LU-decomposition very useful when working with narrow-band matrices (e.g. tridiagonal as in this paper).

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