Coefficients for some splitting methods to be used with the imaginary time propagation technique

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The methods are described in the paper *Solving the Schrödinger eigenvalue problem by the imaginary time propagation technique using splitting methods with complex coefficients*, by the same authors

1 Introduction

These are methods designed for solving the Schrödinger equation in imaginary time

$$-\frac{\partial}{\partial \tau}\psi(x,\tau) = H\psi(x,\tau), \qquad \psi(x,0) = \psi_0(x), \tag{1}$$

with Hamiltonian

$$H = T + V(x) = -\frac{1}{2}\Delta + V(x). \tag{2}$$

Symmetric methods are considered and, since T and V have qualitatively different properties, both TVT- and VTV-type compositions are analyzed. These are defined as

$$\text{TVT:} \qquad \Psi_h^{[p]} = \mathrm{e}^{-a_1hT}\mathrm{e}^{-b_1hV}\mathrm{e}^{-a_2hT}\cdots\mathrm{e}^{-a_2hT}\mathrm{e}^{-b_1hV}\mathrm{e}^{-a_1hT}, \tag{3}$$

$$\text{VTV:} \qquad \Psi_h^{[p]} = \mathrm{e}^{-b_1hV}\mathrm{e}^{-a_1hT}\mathrm{e}^{-b_2hV}\cdots\mathrm{e}^{-b_2hV}\mathrm{e}^{-a_1hT}\mathrm{e}^{-b_1hV} \tag{4}$$

respectively.

2 Methods without modified potentials

To simplify notation, we denote compositions (3) and (4) as

$$\mathrm{T}n_m = a_1\, b_1\, a_2\, \cdots\, a_2\, b_1\, a_1 \qquad \text{and} \qquad \mathrm{V}n_m = b_1\, a_1\, b_2\, \cdots\, b_2\, a_1\, b_1$$

respectively. Here n indicates the order (or generalized order) of the method and m corresponds to the number of stages, i.e. the number of b_i coefficients in the TVT composition or the number of a_i coefficients in the VTV composition. The coefficients of the selected TVT methods are collected in Table 1, whereas those corresponding to the TVT methods are displayed in Table 2.

Table 1: Compositions TVT without modified potentials.

$\mathrm{T4}_5 = a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1$
$a_1 = 0.0871770401947680041317965 + 0.0692594337596574537637064i$
$b_1 = 0.1743540803895360082635929 + 0.1385188675193149075274128i$
$a_2 = 0.2083976635333157695734475 + 0.0524786469564098021205086i$
$b_2 = 0.2424412466770955308833020 - 0.0335615736064953032863956i$
$a_3 = 0.2044252962719162262947561 - 0.1217380807160672558842150i$
$b_3 = 0.1664093458667369217062101 - 0.2099145878256392084820343i$

$\mathrm{T6}_7 = a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_4\, b_4\, a_4\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1$
$a_1 = 0.0600114472433222558387391 + 0.0200406904988006851922750i$
$b_1 = 0.1156502131648962851083019 + 0.04480265967098350686763387i$
$a_2 = 0.1139255281780226726075734 - 0.03778105183520674993878067i$
$b_2 = 0.1287287053011587838332214 - 0.1234667129878517723617557i$
$a_3 = 0.1661602375643228985178319 - 0.0652648069736542106228585i$
$b_3 = 0.1868922874386694136745153 + 0.0011531052408406993673548i$
$a_4 = 0.1599027870143321730358555 + 0.0830051683100602753693642i$
$b_4 = 0.137457588190551034767923 + 0.155021896152055132253534i$

$\mathrm{T84}_5 = a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1$
$a_1 = 0.0714011315400446981476365 + 0.01015543101988678959874893i$
$b_1 = 0.1786968542646319789859369 + 0.0281975063132180212573754i$
$a_2 = 0.2363838051900747368708890 + 0.0704270071395345229504498i$
$b_2 = 0.1984534747081546498530198 + 0.0829623147338549632623515i$
$a_3 = 0.1922150632698805649814746 - 0.0805824381594213125491987i$
$b_3 = 0.2456993420544267423220865 - 0.2223196420941459690394537i$

$\mathrm{T864}_7 = a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_4\, b_4\, a_4\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1$
$a_1 = 0.05570582111086423655901360 + 0.01867038456508504999344773i$
$b_1 = 0.11577944962699042229896023 + 0.04613135617338284727635611i$
$a_2 = 0.11884328216349256412844908 - 0.02415180532279663475808490i$
$b_2 = 0.12912892080402645015486162 - 0.11903941330377420934338268i$
$a_3 = 0.15859151557519557833132885 - 0.07630255189357959984394132i$
$b_3 = 0.18464346415443894469736863 - 0.00305376144537618259996293i$
$a_4 = 0.16685938115044762098120845 + 0.08178397265129118460857849i$
$b_4 = 0.14089633082908836569761899 + 0.15192363715153508933397902i$

$\mathrm{T86}_9 = a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_4\, b_4\, a_5\, b_5\, a_5\, b_4\, a_4\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1$
$a_1 = 0.042257897299860339794 - 0.014215780224181831787i$
$b_1 = 0.094894869367770736829 - 0.037963806472588094119i$
$a_2 = 0.095260398471830494971 + 0.004518725891475591900i$
$b_2 = 0.097374660381711248404 + 0.088518877931710497170i$
$a_3 = 0.099960578944766657818 + 0.090271995071312563389i$
$b_3 = 0.118584793520055816930 + 0.038356250608401259291i$
$a_4 = 0.14869553040260848774 + 0.01143811718761408929i$
$b_4 = 0.136865119760326031197 - 0.023587404969570006861i$
$a_5 = 0.11382559488093401968 - 0.09201305792622041279i$
$b_5 = 0.10456111394027233328 - 0.13064783419590731096i$

Table 2: Compositions VTV without modified potentials.

$\mathrm{V}4_5 = b_1\, a_1\, b_2\, a_2\, b_3\, a_3\, b_3\, a_2\, b_2\, a_1\, b_1$
$b_1 = 0.0871770401947680041317946 - 0.0692594337596574537637056i$

$\mathrm{V}4_5 = b_1\, a_1\, b_2\, a_2\, b_3\, a_3\, b_3\, a_2\, b_2\, a_1\, b_1$

$$b_1 = 0.0871770401947680041317946 - 0.0692594337596574537637056i$$
$$a_1 = 0.1743540803895360082635894 - 0.1385188675193149075274114i$$
$$b_2 = 0.208397663533315769573446 - 0.052478646956409802120508i$$
$$a_2 = 0.2424412466770955308833031 + 0.0335615736064953032863950i$$
$$b_3 = 0.2044252962719162262947590 + 0.1217380807160672558842140i$$
$$a_3 = 0.166409345866736921706215 + 0.209914587825639208482033i$$

$\mathrm{V}6_7 = b_1\, a_1\, b_2\, a_2\, b_3\, a_3\, b_4\, a_4\, b_4\, a_3\, b_3\, a_2\, b_2\, a_1\, b_1$

$$b_1 = 0.0584500187773306421946528 + 0.0217141273080301708808834i$$
$$a_1 = 0.1169000375546612843893053 + 0.04342825461606034176176669i$$
$$b_2 = 0.1232295694183747735677120 - 0.04028067878601612576815832i$$
$$a_2 = 0.1295591012820882627461195 - 0.1239896121880925932980834i$$
$$b_3 = 0.1580457970471110402715959 - 0.0604410907390099589784613i$$
$$a_3 = 0.1865324928121338177970721 + 0.0031074307100726753411608i$$
$$b_4 = 0.1602746147571835439660394 + 0.0790076422169959138657363i$$
$$a_4 = 0.134016736702233270135006 + 0.154907853723919152390312i$$

$\mathrm{V}84_5 = b_1\, a_1\, b_2\, a_2\, b_3\, a_3\, b_3\, a_2\, b_2\, a_1\, b_1$

$$b_1 = 0.0524725255161290266494054 - 0.0109589408424581389146811i$$
$$a_1 = 0.1759621406567323625019241 - 0.0544830562281605577870538i$$
$$b_2 = 0.2460235633327538803174761 - 0.1252285479248343520185923i$$
$$a_2 = 0.181259898687454283502367 - 0.034864508232090522462078i$$
$$b_3 = 0.2015039111511170930331185 + 0.1361874887672924909332734i$$
$$a_3 = 0.2855559213116267079914180 + 0.1786951289205021604982633i$$

$\mathrm{V}864_7 = b_1\, a_1\, b_2\, a_2\, b_3\, a_3\, b_4\, a_4\, b_4\, a_3\, b_3\, a_2\, b_2\, a_1\, b_1$

$$b_1 = 0.0600177707525289267514820 - 0.0096961507469077379948181i$$
$$a_1 = 0.108904710931114447239804 - 0.075700232434276860567484i$$
$$b_2 = 0.0670179873168538175697634 + 0.00392756774282254286438477i$$
$$a_2 = 0.1065941143001561823363895 + 0.1396519036449407611712411i$$
$$b_3 = 0.1893008723880054768245063 + 0.0910551038795303855896332i$$
$$a_3 = 0.2048970164144161053612591 + 0.0097190579551431122987707i$$
$$b_4 = 0.1836633695426117788542482 - 0.0852865208754451904591999i$$
$$a_4 = 0.1592083167086265301250951 - 0.1473414583316140258050559i$$

$\mathrm{V}86_9 = b_1\, a_1\, b_2\, a_2\, b_3\, a_3\, b_4\, a_4\, b_5\, a_5\, b_5\, a_4\, b_4\, a_3\, b_3\, a_2\, b_2\, a_1\, b_1$

$$b_1 = 0.032497706037458608212 + 0.010641310380458924639i$$
$$a_1 = 0.087895680441261752856 + 0.036052576182866484630i$$
$$b_2 = 0.094180923422602148008 + 0.023866875362648754426i$$
$$a_2 = 0.095351855399045611562 - 0.065128376035135147692i$$
$$b_3 = 0.10113295309723118071 - 0.11220175733704484150i$$
$$a_3 = 0.121865575594908413709 - 0.054974002471495827538i$$
$$b_4 = 0.16094138211943489217 - 0.01612764389695289113i$$
$$a_4 = 0.14150688271846209764 + 0.02460722904652402687i$$
$$b_5 = 0.11124703532327317090 + 0.09382121549089005356i$$
$$a_5 = 0.10676001169264424847 + 0.11888514655448092746i$$

3 Methods with modified potentials

New methods of generalized order (6,4) and (8,4) with positive coefficients are constructed, as well as 6th-order schemes with complex coefficients. In all cases, compositions TVT and VTV compositions with up to 5 stages are considered. They are denoted as

$$\begin{aligned} \mathrm{T}n\mathrm{M}_m &= a_1\,(b_1\,c_1)\,a_2\,\cdots\,a_2\,(b_1\,c_1)\,a_1, \\ \mathrm{V}n\mathrm{M}_m &= (b_1\,c_1)\,a_1\,(b_2\,c_2)\,\cdots\,(b_2\,c_2)\,a_1\,(b_1\,c_1) \end{aligned}$$

Here the parenthesis is used to help counting of the number of exponentials, and the letter M indicates that the methods use modified potentials. Notice that the number of free parameters can differ for the TVT and VTV sequences with the same number of exponentials because the exponent of a modified potential contains two parameters. The coefficients of the selected methods are collected in Table 3 and Table 4 for the TVT and VTV compositions, respectively.

Table 3: Compositions TVT with modified potentials.

$\mathrm{T64M}_4 = a_1\,(b_1\,c_1)\,a_2\,(b_2\,c_2)\,a_3\,(b_2\,c_2)\,a_2\,(b_1\,c_1)\,a_1$

$a_1 = (1-3a_3)/2$
$b_1 = (8+\sqrt{55})/72$
$c_1 = \frac{1}{207360}\left(-144(20+\sqrt{55})+\sqrt{9936975+863970\sqrt{55}}\right)$
$a_2 = a_3$
$c_2 = \frac{1}{207360}\left(144(80+\sqrt{55})-\sqrt{15(8042345+294958\sqrt{55})}\right)$
$b_2 = (1-2b_1)/2$
$a_3 = \frac{1}{3}\sqrt{\frac{1}{15}(25-2\sqrt{55})}$

$\mathrm{T84M}_5 = a_1\,(b_1\,c_1)\,a_2\,(b_2\,c_2)\,a_3\,(b_3\,c_3)\,a_3\,(b_2\,c_2)\,a_2\,(b_1\,c_1)\,a_1$

$a_1 = 0.0585209633596948659027541$
$b_1 = 0.145381537601615725642498 9$
$c_1 = 0.0002459065492612288193531$
$a_2 = 0.2079030474428717711417244$
$b_2 = 0.2443514086966383279189334$
$c_2 = 0.0002591785614191258651533$
$a_3 = 0.2335759891974333629555214$
$b_3 = 0.2205341074034918928771353$
$c_3 = 0.0009381057017111535364871$

$\mathrm{T86M}_5 = a_1\,(b_1\,c_1)\,a_2\,(b_2\,c_2)\,a_3\,(b_3\,c_3)\,a_3\,(b_2\,c_2)\,a_2\,(b_1\,c_1)\,a_1$

$a_1 = 0.0635560519974931022645619 + 0.0106068903966809206507259 2i$
$b_1 = 0.1569395253472245630106418 + 0.0279313062004158194793769i$
$c_1 = 0.0001337391817461255683508 10 + 0.0000855401532202136613691 17i$
$a_2 = 0.2089988172317563224881429 + 0.0402402038265233958276438i$
$b_2 = 0.2223831366759822135906966 + 0.0260332620900359385933254i$
$c_2 = 0.000484323504408882233530820 + 0.000241671051573332429722116i$
$c_3 = 0.000179180363327321745275990 - 0.000858304413034511261183627i$

Table 4: Compositions VTV with modified potentials.

$\text{V6M}_4 = (b_1\, c_1)\, a_1\, (b_2\, c_2)\, a_2\, (b_3\, c_3)\, a_2\, (b_2\, c_2)\, a_1\, (b_1\, c_1)$

$b_1 = 0.070024595602928186257168 12 + 0.015533573983094094415277 49i$
$c_1 = 0$
$a_1 = 0.21007378680878455877150 43 + 0.04660072194928228324583 24i$
$b_2 = 0.28019069698466035507188 98 + 0.04503590282244056019518 67i$
$c_2 = 0.00090623822323053129475 11475 + 0.00061463185081971803708 14421i$
$a_2 = 0.28992621319121544122849 56 - 0.04660072194928228324583 24i$
$b_3 = 0.29956941482482291734188 40 - 0.12113895361106930922092 84i$
$c_3 = 0.00052629246895059078789 7511 - 0.00156639755769975713361 6464i$

$\text{V64M}_4 = (b_1\, c_1)\, a_1\, (b_2\, c_2)\, a_2\, (b_3\, c_3)\, a_2\, (b_2\, c_2)\, a_1\, (b_1\, c_1)$

$b_1 = 0.0643421003811126714295577$
$c_1 = 0.000217958066128410213612 9$
$a_1 = 0.2048397108622296193229738$
$b_2 = 0.2936324622996246405816496$
$c_2 = 0.0006018722059398803357006$
$a_2 = 0.2951602891377703806770261$
$b_3 = 0.2840508746385253759775853$
$c_3 = 0.0015255449479001958853354$

$\text{V84M}_5 = (b_1\, c_1)\, a_1\, (b_2\, c_2)\, a_2\, (b_3\, c_3)\, a_3 (b_3\, c_3)\, a_2\, (b_2\, c_2)\, a_1\, (b_1\, c_1)$

$b_1 = 0.0423084512431273651368 9035$
$c_1 = 0.0002329662695654982088 9656$
$a_1 = 0.1429393242677161848000 8504$
$b_2 = 0.2193035687533871103788 9577$
$c_2 = 5.566771202311302086267 8 \cdot 10^{-7}$
$a_2 = 0.2424745082345314934671 6436$
$b_3 = 0.2383879800034855244842 1386$
$c_3 = 0.0007944907774794317840 4625$
$a_3 = 0.2291723349955046434655 0119$

$\text{V84M}_4^{LR} = (b_1\, c_1)\, a_1\, (b_2\, c_2)\, a_2\, (b_3\, c_3)\, a_2\, (b_2\, c_2)\, a_1\, (b_1\, c_1)$

$b_1 = 1/20, \qquad c_1 = \dfrac{3861 - 791\sqrt{21}}{129600}, \qquad a_1 = 1/2 - \sqrt{3/28}$
$b_2 = 49/180, \qquad c_2 = 0, \qquad c_3 = 0$

$\text{V86M}_5 = (b_1\, c_1)\, a_1\, (b_2\, c_2)\, a_2\, (b_3\, c_3)\, a_3 (b_3\, c_3)\, a_2\, (b_2\, c_2)\, a_1\, (b_1\, c_1)$

$b_1 = 0.04621362583815209550434 11 - 0.00782452935598310834449 82i$
$c_1 = 0.00003583046133952045231 70031 + 0.00007437085768542116256 6151i$
$a_1 = 0.15265095010479981741639 37 - 0.03027996716369906570197 69i$
$b_2 = 0.22425805267885638445435 16 - 0.05087928240276177294945 76i$
$c_2 = 0.00033805343504138213506 4241 - 0.00049050891327937236789 2220i$
$a_2 = 0.22636427518603976262255 8 - 0.01653724961993651565995 2i$
$c_3 = 0.00040831164487400362000 6800 + 0.00048437196743368313844 3166i$