

# Ab initio quantum chemistry DMRG and TNS

Sebastian Wouters

*Ab initio* quantum chemistry DMRG/TNS papers.<sup>1–88</sup> Not yet published:  
<http://arxiv.org/abs/1502.06157>, <http://arxiv.org/abs/1502.07731>.

- 
- <sup>1</sup> S. R. White and R. L. Martin, *J. Chem. Phys.* **110**, 4127 (1999).
  - <sup>2</sup> S. Daul, I. Ciofini, C. Daul, and S. R. White, *Int. J. Quantum Chem.* **79**, 331 (2000).
  - <sup>3</sup> A. O. Mitrushenkov, G. Fano, F. Ortolani, R. Linguerri, and P. Palmieri, *J. Chem. Phys.* **115**, 6815 (2001).
  - <sup>4</sup> G. K.-L. Chan and M. Head-Gordon, *J. Chem. Phys.* **116**, 4462 (2002).
  - <sup>5</sup> O. Legeza, J. Röder, and B. A. Hess, *Phys. Rev. B* **67**, 125114 (2003).
  - <sup>6</sup> G. K.-L. Chan and M. Head-Gordon, *J. Chem. Phys.* **118**, 8551 (2003).
  - <sup>7</sup> O. Legeza, J. Röder, and B. A. Hess, *Mol. Phys.* **101**, 2019 (2003).
  - <sup>8</sup> A. O. Mitrushenkov, R. Linguerri, P. Palmieri, and G. Fano, *J. Chem. Phys.* **119**, 4148 (2003).
  - <sup>9</sup> O. Legeza and J. Sólyom, *Phys. Rev. B* **68**, 195116 (2003).
  - <sup>10</sup> G. K.-L. Chan, *J. Chem. Phys.* **120**, 3172 (2004).
  - <sup>11</sup> G. K.-L. Chan, M. Kállay, and J. Gauss, *J. Chem. Phys.* **121**, 6110 (2004).
  - <sup>12</sup> O. Legeza and J. Sólyom, *Phys. Rev. B* **70**, 205118 (2004).
  - <sup>13</sup> G. Moritz, B. A. Hess, and M. Reiher, *J. Chem. Phys.* **122**, 024107 (2005).
  - <sup>14</sup> G. K.-L. Chan and T. V. Voorhis, *J. Chem. Phys.* **122**, 204101 (2005).
  - <sup>15</sup> G. Moritz, A. Wolf, and M. Reiher, *J. Chem. Phys.* **123**, 184105 (2005).
  - <sup>16</sup> G. Moritz and M. Reiher, *J. Chem. Phys.* **124**, 034103 (2006).
  - <sup>17</sup> J. Hachmann, W. Cardoen, and G. K.-L. Chan, *J. Chem. Phys.* **125**, 144101 (2006).
  - <sup>18</sup> J. Rissler, R. M. Noack, and S. R. White, *Chem. Phys.* **323**, 519 (2006).
  - <sup>19</sup> G. Moritz and M. Reiher, *J. Chem. Phys.* **126**, 244109 (2007).
  - <sup>20</sup> J. J. Dorando, J. Hachmann, and G. K.-L. Chan, *J. Chem. Phys.* **127**, 084109 (2007).
  - <sup>21</sup> J. Hachmann, J. J. Dorando, M. Avilés, and G. K.-L. Chan, *J. Chem. Phys.* **127**, 134309 (2007).
  - <sup>22</sup> K. H. Marti, I. M. Ondík, G. Moritz, and M. Reiher, *J. Chem. Phys.* **128**, 014104 (2008).
  - <sup>23</sup> D. Zgid and M. Nooijen, *J. Chem. Phys.* **128**, 014107 (2008).
  - <sup>24</sup> D. Zgid and M. Nooijen, *J. Chem. Phys.* **128**, 144115 (2008).
  - <sup>25</sup> D. Zgid and M. Nooijen, *J. Chem. Phys.* **128**, 144116 (2008).
  - <sup>26</sup> D. Ghosh, J. Hachmann, T. Yanai, and G. K.-L. Chan, *J. Chem. Phys.* **128**, 144117 (2008).
  - <sup>27</sup> G. K.-L. Chan, *Phys. Chem. Chem. Phys.* **10**, 3454 (2008).
  - <sup>28</sup> G. K.-L. Chan, J. J. Dorando, D. Ghosh, J. Hachmann, E. Neuscamman, H. Wang, and T. Yanai, in *Frontiers in Quantum Systems in Chemistry and Physics*, Progress in Theoretical Chemistry and Physics, Vol. 18, edited by S. Wilson, P. J. Grout, J. Maruani, G. Delgado-Barrio, and P. Piecuch (Springer, 2008) pp. 49–65.
  - <sup>29</sup> T. Yanai, Y. Kurashige, D. Ghosh, and G. K.-L. Chan, *Int. J. Quantum Chem.* **109**, 2178 (2009).
  - <sup>30</sup> J. J. Dorando, J. Hachmann, and G. K.-L. Chan, *J. Chem. Phys.* **130**, 184111 (2009).
  - <sup>31</sup> Y. Kurashige and T. Yanai, *J. Chem. Phys.* **130**, 234114 (2009).
  - <sup>32</sup> G. K.-L. Chan and D. Zgid, in *The Density Matrix Renormalization Group in Quantum Chemistry*, Annual Reports in Computational Chemistry, Vol. 5, edited by R. A. Wheeler (Elsevier, 2009) pp. 149–162.
  - <sup>33</sup> T. Yanai, Y. Kurashige, E. Neuscamman, and G. K.-L. Chan, *J. Chem. Phys.* **132**, 024105 (2010).
  - <sup>34</sup> E. Neuscamman, T. Yanai, and G. K.-L. Chan, *J. Chem. Phys.* **132**, 024106 (2010).
  - <sup>35</sup> K. H. Marti and M. Reiher, *Mol. Phys.* **108**, 501 (2010).
  - <sup>36</sup> K. H. Marti and M. Reiher, *Z. Phys. Chem.* **224**, 583 (2010).
  - <sup>37</sup> H.-G. Luo, M.-P. Qin, and T. Xiang, *Phys. Rev. B* **81**, 235129 (2010).
  - <sup>38</sup> W. Mizukami, Y. Kurashige, and T. Yanai, *J. Chem. Phys.* **133**, 091101 (2010).
  - <sup>39</sup> K. H. Marti, B. Bauer, M. Reiher, M. Troyer, and F. Verstraete, *New J. Phys.* **12**, 103008 (2010).
  - <sup>40</sup> V. Murg, F. Verstraete, O. Legeza, and R. M. Noack, *Phys. Rev. B* **82**, 205105 (2010).
  - <sup>41</sup> G. K.-L. Chan and S. Sharma, *Annu. Rev. Phys. Chem.* **62**, 465 (2011).
  - <sup>42</sup> K. H. Marti and M. Reiher, *Phys. Chem. Chem. Phys.* **13**, 6750 (2011).
  - <sup>43</sup> G. Barcza, O. Legeza, K. H. Marti, and M. Reiher, *Phys. Rev. A* **83**, 012508 (2011).
  - <sup>44</sup> K. Boguslawski, K. H. Marti, and M. Reiher, *J. Chem. Phys.* **134**, 224101 (2011).
  - <sup>45</sup> Y. Kurashige and T. Yanai, *J. Chem. Phys.* **135**, 094104 (2011).
  - <sup>46</sup> A. O. Mitrushchenkov, G. Fano, R. Linguerri, and P. Palmieri, *Int. J. Quantum Chem.* **112**, 1606 (2012).
  - <sup>47</sup> S. Sharma and G. K.-L. Chan, *J. Chem. Phys.* **136**, 124121 (2012).
  - <sup>48</sup> S. Wouters, P. A. Limacher, D. Van Neck, and P. W. Ayers, *J. Chem. Phys.* **136**, 134110 (2012).
  - <sup>49</sup> K. Boguslawski, K. H. Marti, O. Legeza, and M. Reiher, *J. Chem. Theory Comput.* **8**, 1970 (2012).
  - <sup>50</sup> T. Yanai, Y. Kurashige, E. Neuscamman, and G. K.-L. Chan, *Phys. Chem. Chem. Phys.* **14**, 7809 (2012).
  - <sup>51</sup> K. Boguslawski, P. Tecmer, O. Legeza, and M. Reiher, *J.*

- Phys. Chem. Lett. **3**, 3129 (2012).
- <sup>52</sup> G. K.-L. Chan, WIREs Comput. Mol. Sci. **2**, 907 (2012).
- <sup>53</sup> W. Mizukami, Y. Kurashige, and T. Yanai, J. Chem. Theory Comput. **9**, 401 (2013).
- <sup>54</sup> N. Nakatani and G. K.-L. Chan, J. Chem. Phys. **138**, 134113 (2013).
- <sup>55</sup> K. Boguslawski, P. Tecmer, G. Barcza, O. Legeza, and M. Reiher, J. Chem. Theory Comput. **9**, 2959 (2013).
- <sup>56</sup> Y. Kurashige, G. K.-L. Chan, and T. Yanai, Nat. Chem. **5**, 660 (2013).
- <sup>57</sup> Y. Ma and H. Ma, J. Chem. Phys. **138**, 224105 (2013).
- <sup>58</sup> M. Saitow, Y. Kurashige, and T. Yanai, J. Chem. Phys. **139**, 044118 (2013).
- <sup>59</sup> F. Liu, Y. Kurashige, T. Yanai, and K. Morokuma, J. Chem. Theory Comput. **9**, 4462 (2013).
- <sup>60</sup> P. Tecmer, K. Boguslawski, O. Legeza, and M. Reiher, Phys. Chem. Chem. Phys. **16**, 719 (2014).
- <sup>61</sup> N. Nakatani, S. Wouters, D. Van Neck, and G. K.-L. Chan, J. Chem. Phys. **140**, 024108 (2014).
- <sup>62</sup> S. Knecht, O. Legeza, and M. Reiher, J. Chem. Phys. **140**, 041101 (2014).
- <sup>63</sup> T. V. Harris, Y. Kurashige, T. Yanai, and K. Morokuma, J. Chem. Phys. **140**, 054303 (2014).
- <sup>64</sup> S. Sharma, T. Yanai, G. H. Booth, C. J. Umrigar, and G. K.-L. Chan, J. Chem. Phys. **140**, 104112 (2014).
- <sup>65</sup> M. Mottet, P. Tecmer, K. Boguslawski, O. Legeza, and M. Reiher, Phys. Chem. Chem. Phys. **16**, 8872 (2014).
- <sup>66</sup> S. Wouters, W. Poelmans, P. W. Ayers, and D. Van Neck, Comput. Phys. Commun. **185**, 1501 (2014).
- <sup>67</sup> S. F. Keller and M. Reiher, Chimia **68**, 200 (2014).
- <sup>68</sup> Y. Kurashige, Mol. Phys. **112**, 1485 (2014).
- <sup>69</sup> T. N. Lan, Y. Kurashige, and T. Yanai, J. Chem. Theory Comput. **10**, 1953 (2014).
- <sup>70</sup> Y. Kurashige, M. Saitow, J. Chalupsky, and T. Yanai, Phys. Chem. Chem. Phys. **16**, 11988 (2014).
- <sup>71</sup> S. Wouters, T. Bogaerts, P. Van Der Voort, V. Van Speybroeck, and D. Van Neck, J. Chem. Phys. **140**, 241103 (2014).
- <sup>72</sup> S. Sharma and G. K.-L. Chan, J. Chem. Phys. **141**, 111101 (2014).
- <sup>73</sup> S. Wouters and D. Van Neck, Eur. Phys. J. D **68**, 272 (2014).
- <sup>74</sup> S. Sharma, K. Sivalingam, F. Neese, and G. K.-L. Chan, Nat. Chem. **6**, 927 (2014).
- <sup>75</sup> J. Yang, W. Hu, D. Usvyat, D. Matthews, M. Schütz, and G. K.-L. Chan, Science **345**, 640 (2014).
- <sup>76</sup> Y. Kurashige, J. Chalupsky, T. N. Lan, and T. Yanai, J. Chem. Phys. **141**, 174111 (2014).
- <sup>77</sup> E. Fertitta, B. Paulus, G. Barcza, and O. Legeza, Phys. Rev. B **90**, 245129 (2014).
- <sup>78</sup> J. Chalupsky, T. A. Rokob, Y. Kurashige, T. Yanai, E. I. Solomon, L. Rulisek, and M. Srnec, J. Am. Chem. Soc. **136**, 15977 (2014).
- <sup>79</sup> S. M. Parker and T. Shiozaki, J. Chem. Phys. **141**, 211102 (2014).
- <sup>80</sup> Y. Kurashige and T. Yanai, Bull. Chem. Soc. Jpn. **87**, 1071 (2014).
- <sup>81</sup> S. Sharma, J. Chem. Phys. **142**, 024107 (2015).
- <sup>82</sup> T. Yanai, Y. Kurashige, W. Mizukami, J. Chalupský, T. N. Lan, and M. Saitow, Int. J. Quantum Chem. **115**, 283 (2015).
- <sup>83</sup> C. Duperrouzel, P. Tecmer, K. Boguslawski, G. Barcza, O. Legeza, and P. W. Ayers, Chem. Phys. Lett. **621**, 160 (2015).
- <sup>84</sup> R. Olivares-Amaya, W. Hu, N. Nakatani, S. Sharma, J. Yang, and G. K.-L. Chan, J. Chem. Phys. **142**, 034102 (2015).
- <sup>85</sup> T. Nguyen Lan, Y. Kurashige, and T. Yanai, J. Chem. Theory Comput. **11**, 73 (2015).
- <sup>86</sup> T. Dresselhaus, J. Neugebauer, S. Knecht, S. Keller, Y. Ma, and M. Reiher, J. Chem. Phys. **142**, 044111 (2015).
- <sup>87</sup> H. Goossens, J. M. Winne, S. Wouters, L. Hermosilla, P. J. De Clercq, M. Waroquier, V. Van Speybroeck, and S. Catak, J. Org. Chem. **80**, 2609 (2015).
- <sup>88</sup> V. Murg, F. Verstraete, R. Schneider, P. R. Nagy, and O. Legeza, J. Chem. Theory Comput. **11**, 1027 (2015).