3 November 2000

ELSEVIER

Chemical Physics Letters 330 (2000) 175–179

CHEMICAL
PHYSICS
LETTERS

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Three-electron integral evaluation in the transcorrelated method using a frozen Gaussian geminal

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Received 27 July 2000; in final form 12 September 2000

Abstract

Formulas are developed for evaluating the three-electron integrals, which appear in the transcorrelated method using a frozen Gaussian geminal. First, we derive expressions with intermediates, in which the angular momentum indices of the inter-electronic operators are temporarily increased. Following the inspection on the factorization property, we further derive more straightforward recurrence relations corresponding to the Obara–Saika one for electron repulsion integrals. It is shown that the relations can be applied outside the contraction loops over geminal primitives by introducing three-indexed auxiliary integrals. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

The quantum chemical methods are growing with extended varieties owing to the popularity of the Gaussian-type functions (GTFs), which facilitate a rapid and analytical evaluation of molecular integrals. For electron repulsion integrals over primitive GTFs, Dupuis–Rys–King [1], McMurchie–Davidson [2], and Obara–Saika [3,4] methods complete the basic strategies for efficient algorithms. After the invention of the Obara–Saika recurrence relation (the derivative expression of Schlegel [5] is a special case of this), the main research interest shifted to the development of algorithms for contracted electron repulsion integrals, i.e., those with early contractions [6–10] as the first attempt of People and Hehre [11]. Basically, they extract and preliminarily multiply primitive quantities, typically the Gaussian exponents, and the contracted transformation equations are applied outside the loops after accumulating the primitive integrals. Such approaches include esoteric tree-search problems more complicated than those in the original expressions. The development of a general algorithm for an arbitrary contraction degree still seems to be one of the important issues in the area.

In the previous work, we demonstrated that the convergence of reproducing the dynamic correlation effects is markedly accelerated using a transcorrelated Hamiltonian parameterized with a frozen Gaussian geminal [12]. This method reduces the scaling by localizing all of the extra part of the effective interactions. There are two possible ways for the evaluation of the necessary three-electron integrals. One is to employ the resolution of identity to the one-electron basis, which decomposes the integrals into vector products of two-electronic ones in a similar way used in the R12 approach [13]. The other is an explicit generation of the six-index integrals. The

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PII: S0009-2614(00)01067-8

latter will be useful for on-the-fly direct assemblies as those of Fock-type operators, and for accurate evaluations of a significant part of the integrals. In this Letter, we derive two different sets of formulas, which correspond to the McMurchie–Davidson and Obara–Saika expressions for electron repulsion integrals. Conclusions are given in Section 4.

2. McMurchie–Davidson-type formulas

In the transcorrelated method using a frozen Gaussian geminal [12], the three-electron integrals, $\langle pqr|\nabla_1 f(r_{12})\cdot\nabla_1 f(r_{13})|stu\rangle$ in the Dirac notation, appear, where the geminal, $f(r)$, is represented by a linear combination of s-type GTFs. In what follows, we derive the expressions of the integrals over Cartesian GTFs. We henceforward use the notations, κ for a Cartesian frame, i for indices of all three electrons, and j,k for the terminal electrons, 2 and 3. The integrals are written in the general form as

$$\begin{aligned}\Big[\mathbf{n}^{(1)}\bar{\mathbf{n}}^{(1)}\Big|\mathbf{n}^{(2)}\bar{\mathbf{n}}^{(2)}\Big|\mathbf{n}^{(3)}\bar{\mathbf{n}}^{(3)}\Big|\Big|\mathbf{m}^{(12)}\Big|\mathbf{m}^{(13)}\Big] &= \int \mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2\,\mathrm{d}\mathbf{r}_3\,\omega\Big(\mathbf{r}_1,\mathbf{n}^{(1)},\bar{\mathbf{n}}^{(1)}\Big)\\ &\quad\times\omega\Big(\mathbf{r}_2,\mathbf{n}^{(2)},\bar{\mathbf{n}}^{(2)}\Big)\omega\Big(\mathbf{r}_3,\mathbf{n}^{(3)},\bar{\mathbf{n}}^{(3)}\Big)\\ &\quad\times\Big[\nabla_{\mathbf{r}_1}^{\mathbf{m}^{(12)}}\phi(\mathbf{r}_1-\mathbf{r}_2;0,\zeta_{12})\Big]\\ &\quad\times\Big[\nabla_{\mathbf{r}_1}^{\mathbf{m}^{(13)}}\phi(\mathbf{r}_1-\mathbf{r}_3;0,\zeta_{13})\Big],\end{aligned} \tag{1}$$

where ω denotes a product of Cartesian GTFs,

$$\begin{aligned}\omega\Big(\mathbf{r}_i,\mathbf{n}^{(i)},\bar{\mathbf{n}}^{(i)}\Big) &= \phi\Big(\mathbf{r}_i-\mathbf{R}_i,\zeta_i,\mathbf{n}^{(i)}\Big)\\ &\quad\times\phi\Big(\mathbf{r}_i-\bar{\mathbf{R}}_i,\bar{\zeta}_i,\bar{\mathbf{n}}^{(i)}\Big),\end{aligned} \tag{2}$$

$$\begin{aligned}\phi(\mathbf{r}-\mathbf{R};\mathbf{n},\zeta) &= \exp\Big[-\zeta(\mathbf{r}-\mathbf{R})^2\Big]\\ &\quad\times\prod_{\kappa=x,y,z}(r_\kappa-R_\kappa)^{n_\kappa},\end{aligned} \tag{3}$$

and we used the abbreviation of the differential operators, $\nabla_{\mathbf{r}}^{\mathbf{m}} \equiv \prod_{\kappa=x,y,z}(\partial/\partial r_\kappa)^{m_\kappa}$. The derivative of a product of GTFs is written in the form

$$\begin{aligned}\frac{1}{2Z_i}\frac{\partial}{\partial r_{i\kappa}}\omega\Big(\mathbf{r}_i,\mathbf{n}^{(i)},\bar{\mathbf{n}}^{(i)}\Big) &= -\omega\Big(\mathbf{r}_i,\mathbf{n}^{(i)}+1_\kappa,\bar{\mathbf{n}}^{(i)}\Big)\\ &\quad+(\mathbf{P}_i-\mathbf{R}_i)_\kappa\omega\Big(\mathbf{r}_i,\mathbf{n}^{(i)},\bar{\mathbf{n}}^{(i)}\Big)\\ &\quad+\frac{1}{2Z_i}\Big[n_\kappa^{(i)}\omega\Big(\mathbf{n}^{(i)}-1_\kappa,\bar{\mathbf{n}}^{(i)}\Big)\\ &\quad+\bar{n}_\kappa^{(i)}\omega\Big(\mathbf{n}^{(i)},\bar{\mathbf{n}}^{(i)}-1_\kappa\Big)\Big],\end{aligned} \tag{4}$$

where we used the relation and parameters,

$$\mathbf{r}_i-\bar{\mathbf{R}}_i = (\mathbf{r}_i-\mathbf{R}_i)+(\mathbf{R}_i-\bar{\mathbf{R}}_i), \tag{5}$$

$$Z_i = \zeta_i+\bar{\zeta}_i, \tag{6}$$

$$\mathbf{P}_i = \frac{\mathbf{R}_i\zeta_i+\bar{\mathbf{R}}_i\bar{\zeta}_i}{Z_i}. \tag{7}$$

The notation, $\mathbf{n}\pm 1_\kappa$, means that the Cartesian component is increased or decreased by 1 in the vector, $\mathbf{n}$. As in the case of electron repulsion integrals [3,4], the key property for expressions is that the integral involving a differential operator with respect to an integration coordinate is identically zero, $\int \mathrm{d}\mathbf{r}\ (\partial/\partial r_\kappa)\varphi(\mathbf{r}) = 0$, if the integrand converges to zero at infinitely large separations, $\lim_{|r_\kappa|\to\infty}\varphi(\mathbf{r}) = 0$. The application of the property to the three-electron integrals leads to the relations, which increase $n_\kappa^{(i)}$ expending on $m_\kappa^{(1j)}$,

$$\begin{aligned}\Big[\mathbf{n}^{(1)}+1_\kappa :\Big] &= \langle : \rangle_{1\kappa}+\frac{1}{2Z_1}\Big(\Big[\mathbf{m}^{(12)}+1_\kappa :\Big]\\ &\quad+\Big[\mathbf{m}^{(13)}+1_\kappa :\Big]\Big),\end{aligned} \tag{8}$$

$$\Big[\mathbf{n}^{(j)}+1_\kappa :\Big] = \langle : \rangle_{j\kappa}-\frac{1}{2Z_j}\Big[\mathbf{m}^{(1j)}+1_\kappa :\Big], \tag{9}$$

$$\begin{aligned}\langle : \rangle_{i\kappa} &= (\mathbf{P}_i-\mathbf{R}_i)_\kappa[:]+\frac{1}{2Z_i}\Big(n_\kappa^{(i)}\Big[\mathbf{n}^{(i)}-1_\kappa :\Big]\\ &\quad+\bar{n}_\kappa^{(i)}\Big[\bar{\mathbf{n}}^{(i)}-1_\kappa :\Big]\Big),\end{aligned} \tag{10}$$

where we used an implicit abbreviation for unchanged indices. These are reminiscences to the McMurchie–Davidson expression for electron repulsion integrals [2], which uses intermediates with additional three-dimensional indices depending on the Cartesian axis.

We proceed with deriving a formula for the integrals, $[\cdot||\mathbf{m}^{(12)}|\mathbf{m}^{(13)}]$. The dot in the integral denotes a set of zero angular momentum indices. The product of s-type GTFs is

$$\omega(\mathbf{r}_i,\mathbf{0};\mathbf{0}) = \phi(\mathbf{R}_i - \bar{\mathbf{R}}_i;\mathbf{0},\xi_i)\phi(\mathbf{r}_i - \mathbf{P}_i;\mathbf{0},Z_i), \tag{11}$$

$$\xi_i = \frac{\zeta_i\bar{\zeta}_i}{Z_i}. \tag{12}$$

Thus the differential operator, $\partial/\partial r_j$, can be replaced by the one with respect to the product center as

$$\frac{\partial}{\partial r_{i\kappa}}\omega(\mathbf{r}_i;\mathbf{0},\mathbf{0}) = -\phi(\mathbf{R}_i - \bar{\mathbf{R}}_i;\mathbf{0},\xi_i) \times \frac{\partial}{\partial P_{i\kappa}}\phi(\mathbf{r}_i - \mathbf{P}_i;\mathbf{0},Z_i). \tag{13}$$

We combine Eqs. (4), (9) and (13) to yield

$$\left[\cdot\,||\mathbf{m}^{(12)}|\mathbf{m}^{(13)}\right] = \nabla_{\mathbf{P}_2}^{\mathbf{m}^{(12)}}\nabla_{\mathbf{P}_3}^{\mathbf{m}^{(13)}}[\cdot], \tag{14}$$

$$\begin{aligned}[\cdot] = {} & \pi^{9/2}[(\zeta_{12}+Z_2)(\zeta_{13}+Z_3)(Z_1+\eta_2+\eta_3)]^{-3/2} \\ & \times \prod_{i=1}^{3}\phi(\mathbf{R}_i - \bar{\mathbf{R}}_i;\mathbf{0},\xi_i)\exp\Big[-\Xi_2(\mathbf{P}_1-\mathbf{P}_2)^2 \\ & - \Xi_3(\mathbf{P}_1-\mathbf{P}_3)^2 - \Omega(\mathbf{P}_2-\mathbf{P}_3)^2\Big],\end{aligned} \tag{15}$$

where the parameters are defined by

$$\frac{1}{\eta_j} = \frac{1}{\zeta_{1j}} + \frac{1}{Z_j}, \tag{16}$$

$$\Xi_j = \frac{Z_1\eta_j}{Z_1+\eta_2+\eta_3}, \tag{17}$$

$$\Omega = \frac{\eta_2\eta_3}{Z_1+\eta_2+\eta_3} \tag{18}$$

and we used the expression of the N-center overlap integrals for the initial integral, $[\cdot]$,

$$\int \mathrm{d}\mathbf{r}\prod_{i=1}^{N}\exp\left[-\zeta_i(\mathbf{r}-\mathbf{R}_i)^2\right] = \pi^{3/2}Z_N^{-3/2}\prod_{i>j}^{N}\exp\left[-\frac{\zeta_i\zeta_j}{Z_N}(\mathbf{R}_i-\mathbf{R}_j)^2\right] \tag{19}$$

$$Z_N = \sum_{i=1}^{N}\zeta_i. \tag{20}$$

One notes that the differential operators to the product centers are commutative. Eqs. (14) and (15) lead to the recurrence relation, which increases $\mathbf{m}^{(1j)}$,

$$\begin{aligned}\left[\cdot\,||\mathbf{m}^{(1j)}+1_\kappa :\right] & = 2\nabla_{\mathbf{P}_2}^{\mathbf{m}^{(12)}}\nabla_{\mathbf{P}_3}^{\mathbf{m}^{(13)}}\Big[\Xi_j\big(\mathbf{P}_1-\mathbf{P}_j\big)_\kappa - \Omega\big(\mathbf{P}_j-\mathbf{P}_k\big)_\kappa\Big][\cdot] \\ & = 2\Big[\Xi_j\big(\mathbf{P}_1-\mathbf{P}_j\big)_\kappa - \Omega\big(\mathbf{P}_j-\mathbf{P}_k\big)_\kappa\Big][\cdot||\,:] \\ & \quad - 2\big(\Xi_j+\Omega\big)m_\kappa^{(1j)}\left[\cdot\,||\mathbf{m}^{(1j)}-1_\kappa :\right] \\ & \quad + 2\Omega m_\kappa^{(1k)}\left[\cdot\,||\mathbf{m}^{(1k)}-1_\kappa :\right]\end{aligned} \tag{21}$$

The above results mean that the three-electron integrals are expressed by factorizing $[\cdot]$ with polynomials of $n_\kappa^{(i)}$, $\bar{n}_\kappa^{(i)}$, $1/(2Z_i)$, $(\mathbf{P}_i-\mathbf{R}_i)_\kappa$, $(\mathbf{P}_i-\bar{\mathbf{R}}_i)_\kappa$, $m_\kappa^{(1j)}$, $2\Xi_j$, 2Ω, and $(\mathbf{P}_i-\mathbf{P}_j)_\kappa$. This fact implies the existence of more straightforward expressions without the temporal increments of $\mathbf{m}^{(1j)}$ involving the multiplications of the vector quantities, $(\mathbf{P}_i-\mathbf{P}_j)_\kappa$.

3. Obara–Saika-type formulas

Following the factorization property described in the last section, we derive another set of expressions, which are closely related to the Obara–Saika recurrence relation [3,4]. One can see that the relation of the Hermite GTFs [2],

$$\left[(\mathbf{r}_1-\mathbf{r}_j)_\kappa\nabla_{\mathbf{r}_1}^{\mathbf{m}^{(1j)}} + \frac{1}{2\zeta_{1j}}\nabla_{\mathbf{r}_1}^{\mathbf{m}^{(1j)}+1_\kappa} + m_\kappa^{(1j)}\nabla_{\mathbf{r}_1}^{\mathbf{m}^{(1j)}-1_\kappa}\right] \times \phi\big(r_1-r_j,0,\zeta_{1j}\big) = 0, \tag{22}$$

transfers the increment, $\mathbf{n}^{(j)}+1_\kappa$, in Eq. (9) to $\mathbf{n}^{(1)}+1_\kappa$ as

$$\left[\mathbf{n}^{(1)}+1_\kappa :\right] = [[:]]_{j\kappa} + (\mathbf{P}_1-\mathbf{R}_1)_\kappa[:] - \frac{1}{2\eta_j}\left[\mathbf{m}^{(1j)}+1_\kappa :\right], \tag{23}$$

$$[[:]]_{j\kappa} = \big(\mathbf{P}_j-\mathbf{P}_1\big)_\kappa[:] - m_\kappa^{(1j)}\left[\mathbf{m}^{(1j)}-1_\kappa :\right] + \frac{1}{2Z_j}\left(n_\kappa^{(j)}\left[\mathbf{n}^{(j)}-1_\kappa :\right] + \bar{n}_\kappa^{(j)}\left[\bar{\mathbf{n}}^{(j)}.-1_\kappa :\right]\right), \tag{24}$$

where we used the relation

$$\mathbf{r}_j-\mathbf{R}_j = (\mathbf{r}_1-\mathbf{R}_1) - (\mathbf{r}_1-\mathbf{r}_j) + (\mathbf{R}_1-\mathbf{R}_j). \tag{25}$$

Substituting the terms including $[\mathbf{m}^{(1j)} + 1_\kappa :]$ into Eq. (8), we obtain the recurrence relation, which increases $\mathbf{n}^{(1)}$,

$$\begin{aligned}\left[\mathbf{n}^{(1)} + 1_\kappa : \right] = \langle : \rangle_{1\kappa} + \sum_j \frac{\Xi_j}{Z_1}[[:]]_{j\kappa} \\ - \frac{\Xi_2 + \Xi_3}{2Z_1^2}\Big(n_\kappa^{(1)}\left[\mathbf{n}^{(1)} - 1_\kappa :\right] \\ + \bar{n}_\kappa^{(1)}\left[\bar{\mathbf{n}}^{(1)} - 1_\kappa : \right]\Big).\end{aligned} \tag{26}$$

For the increments of $\mathbf{m}^{(1j)}$, we equate $[\mathbf{n}^{(1)} + 1_\kappa :]$ in Eqs. (23) and (26),

$$\begin{aligned}\left[\mathbf{m}^{(1j)} + 1_\kappa : \right] = 2(\Xi_j + \Omega)[[:]]_{j\kappa}. - 2\Omega[[:]]_{k\kappa} \\ - \frac{\Xi_j}{Z_1}\Big(n_\kappa^{(1)}\left[\mathbf{n}^{(1)} - 1_\kappa : \right] \\ + \bar{n}_\kappa^{(1)}\left[\bar{\mathbf{n}}^{(1)} - 1_\kappa : \right]\Big).\end{aligned} \tag{27}$$

It is easy to check that Eq. (21) is a special case of the above expression taking the orbitals to be s-type. Finally, we obtain the recurrence relation for the angular momentum indices of the terminal electrons by substituting Eq. (27) into Eq. (9) as

$$\begin{aligned}\left[\mathbf{n}^{(j)} + 1_\kappa : \right] = \langle : \rangle_{j\kappa} - \frac{\Xi_j + \Omega}{Z_j}[[:]]_{j\kappa} + \frac{\Omega}{Z_j}[[:]]_{k\kappa} \\ + \frac{\Xi_j}{2Z_1Z_j}\Big(n_\kappa^{(1)}\left[\mathbf{n}^{(1)} - 1_\kappa : \right] \\ + \bar{n}_\kappa^{(1)}\left[\bar{\mathbf{n}}^{(1)} - 1_\kappa : \right]\Big).\end{aligned} \tag{28}$$

The Eqs. (26)–(28), are the recurrence relations for the three-electron integrals. The naive use of the relations in the transcorrelated method is however very costly, because the integrals are quadratic to the geminals, which are represented by linear combinations of GTFs.

We can proceed using the fact that only the parameters, $2\Xi_j$ and 2Ω, include the exponents of the inter-electronic operators in the equations. We multiply the parameters and take summations over the primitives for the geminals [12] to introduce auxiliary integrals scaled by the parameters

$$[:]^{(\mathbf{L})} = \sum_G^{N_G}\sum_{G'}^{N_G} c_G c_{G'}(2\Omega)^{L_{12}}(2\Xi_2)^{L_2}(2\Xi_3)^{L_3}[:], \tag{29}$$

and the corresponding quantities $\langle : \rangle_{j\kappa}^{(\mathbf{L})}$ and $[[:]]_{j\kappa}^{(\mathbf{L})}$. The target integrals are the auxiliary ones with the integration indices, $\mathbf{L} = 0$. Replacing the integrals by the auxiliary ones, we can rewrite the recurrence relations, such that they work outside the double loop over geminal primitives,

$$\begin{aligned}\left[\mathbf{n}^{(1)} + 1_\kappa : \right]^{(\mathbf{L})} = \langle : \rangle_{1\kappa}^{(\mathbf{L})} + \sum_j \frac{1}{2Z_1}[[:]]_{j\kappa}^{(\mathbf{L}+1_j)} \\ - \frac{1}{(2Z_1)^2}\Big(n_\kappa^{(1)}[\mathbf{n}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_2)} \\ + \bar{n}_\kappa^{(1)}[\bar{\mathbf{n}}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_2)}\Big) \\ - \frac{1}{(2Z_1)^2}\Big(n_\kappa^{(1)}[\mathbf{n}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_3)} \\ + \bar{n}_\kappa^{(1)}[\bar{\mathbf{n}}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_3)}\Big),\end{aligned} \tag{30}$$

$$\begin{aligned}[\mathbf{m}^{(1j)} + 1_\kappa :]^{(\mathbf{L})} = [[:]]_{j\kappa}^{(\mathbf{L}+1_{12})} + [[:]]_{j\kappa}^{(\mathbf{L}+1_j)} - [[:]]_{k\kappa}^{(\mathbf{L}+1_{12})} \\ - \frac{1}{2Z_1}\Big(n_\kappa^{(1)}[\mathbf{n}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_j)} \\ + \bar{n}_\kappa^{(1)}[\bar{\mathbf{n}}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_j)}\Big),\end{aligned} \tag{31}$$

$$\begin{aligned}[\mathbf{n}^{(j)} + 1_\kappa :]^{(\mathbf{L})} = \langle : \rangle_{j\kappa}^{(\mathbf{L})} \\ - \frac{1}{2Z_j}\Big([[:]]_{j\kappa}^{(\mathbf{L}+1_{12})} + [[:]]_{j\kappa}^{(\mathbf{L}+1_j)}\Big) \\ + \frac{1}{2Z_j}[[:]]_{k\kappa}^{(\mathbf{L}+1_{12})} + \frac{1}{4Z_1Z_j} \\ \times \Big(n_\kappa^{(1)}[\mathbf{n}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_j)} \\ + \bar{n}_\kappa^{(1)}[\bar{\mathbf{n}}^{(1)} - 1_\kappa :]^{(\mathbf{L}+1_j)}\Big).\end{aligned} \tag{32}$$

With the relations, the operation for the transformation does not increase with the contraction degree of the geminal. Similar expressions for two-electron integrals are used implicitly in the previous implementation of our transcorrelated method [12].

The present formulas will also be effective in other methods using correlation factors. For instance, the three-electron integrals, $\langle pqr|r_{12}r_{13}^{-1}|stu\rangle$, appear in the R12 method of Klopper and Kutzelnigg [13]. If the linear term to the inter-electron distance is approximately represented by a linear combination of s-type GTFs as in the method of Persson and Taylor [14], the Laplace transform of the Coulomb operator [3,4],

$$r_{13}^{-1} = \frac{2}{\pi^{1/2}} \int_0^\infty \exp(-r_{13}^2 u^2)\, \mathrm{d}u, \tag{33}$$

reduces the integrals to those treated in this Letter. This process involves the one-dimensional numerical integration in place of the contraction over geminal primitives. For a code with maximum efficiency based on the present formulas, it will be necessary to solve a tree-search problem to determine the optimal ordering of the application of the recurrence relations. This algorithmic aspect is out of scope in this particular work.

4. Conclusion

We have derived two different sets of formulas for the three-electron integrals. The first set, which includes temporal increments in the angular momentum of inter-electronic operators, is a reminiscent of the McMurchie–Dvidson expression for electron repulsion integrals. Following the factorization property of the expressions, we further derived more straightforward Obara–Saika-type recurrence relations, which bypass the temporal increments of the angular momentum. Among the factors to be multiplied in increasing the angular momentum of orbitals, the three parameters, $2\Xi_j (j = 2, 3)$ and 2Ω, includes the exponent of the geminal. This fact enables us to apply the transformation equations to three-indexed auxiliary integrals outside the loops for the contraction of the geminal primitives, without increasing the operations irrespective to the contraction degree.

Acknowledgements

The present work is partly supported by the Grant-in-Aids for priority areas (A2) (No. 12042233) from the Ministry of Education, Science, Sports and Culture in Japan.

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