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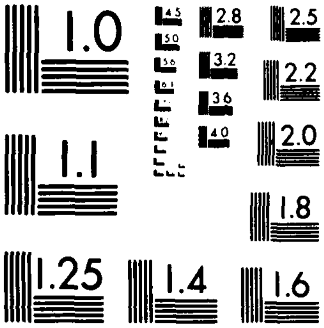

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EXPLOITING ROTATIONAL AND TRANSLATIONAL INVARIANCE OF THE ENERGY IN DERIVATIVE CALCULATIONS IN QUANTUM CHEMISTRY

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May 1986

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It is shown how the invariance of the Born-Oppenheimer potential energy to overall translations and rotations of a molecule can be used to reduce the computational labor required for derivative evaluations at various orders.

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I. INTRODUCTION

The impact of potential energy derivative studies within such areas as molecular structure determination, vibrational spectroscopy, molecular dynamics, and statistical rate theories is only beginning to be realized. Statistical and/or dynamical models[1-5] based upon ideas such as the Reaction Path Hamiltonian[2] require in the simplest application, second derivatives of the potential energy and in slightly more refined versions, they require some limited fourth derivative information.[5] The ultimate impact of these models depends to some extent on the availability of energy derivatives of various order for reliable ab-initio wavefunctions.

First derivatives of the Born-Oppenheimer potential energy for Hartree Fock wavefunctions have been available for quite some time now, and second derivatives have been available for a few years.[6 7] However, in order to investigate the broad regions of the potential energy surface implicit in some of the above applications, one needs a potential function which includes at least differentially, the effects of electron correlation. There has been a great deal of recent activity in potential energy derivative evaluation for correlated wavefunctions. There now exist codes which calculate analytically MCSCF second derivatives,[8-10] CI first derivatives based upon a Hartree Fock reference function[11 12] or on a multiconfigurational reference function[10] and CI second derivatives based upon a Hartree Fock reference function.[9] Third derivative equations have been published for various wavefunctions[13 14] and one can expect to see the implementation of some of these equations in the not too distant future.

We address here an issue pertinent to the efficient evaluation of any of these potential energy derivatives. The derivatives of the energy are most tractably evaluated in a basis of cartesian displacements of the atoms in a molecule. There are 3N such displacements where N is the number of atoms. Since the energy is invariant to overall translations and rotations of the molecule, the 3N elements of, for example, the cartesian gradient vector are not all independent. Given 3N-6 elements of the cartesian gradient vector, we show how one can generate the remaining six elements by consideration of the rotational and translational invariance of the energy.* We also show how the same ideas can be applied to the evaluation of second and third cartesian derivatives yielding even larger relative savings.

II. DEVELOPMENT

We denote the cartesian coordinates of a molecule by the vector x. If r_i is a coordinate representing an overall rotation or translation of the molecule (an "external" coordinate), then the change in cartesian coordinates accompanying a displacement along r_i can be expressed as

---

*For the sake of simplicity, the discussion in the text implicitly assumes a nonlinear configuration of the molecule. The arguments are fully applicable for a linear molecule for which one singles out five cartesian directions instead of six.

$$\underset{\sim}{x}(r_i) - \underset{\sim}{x}(r_i = 0) = \left(\frac{\partial \underset{\sim}{x}}{\partial r_i}\right)_0 r_i + \frac{1}{2}\left(\frac{\partial^2 \underset{\sim}{x}}{\partial r_i^2}\right)_0 r_i^2 + \mathrm{HOT}$$

$$= \underset{\sim}{L}_{r_i} r_i + \dots \qquad (1)$$

Here $\underset{\sim}{x}(r_i=0)$ are the cartesian coordinates of the reference geometry. If r_i represents a translation of the molecule, then the second and higher order terms are zero and Eq. (1) expresses a linear transformation. If r_i is a rotation, all terms contribute to the sum.

The energy is invariant to external displacements.

$$E(r_i) = \text{constant}. \qquad (2)$$

Differentiating Eq. (2) with respect to r_i and evaluating the result at $r_i=0$ yields directly a relationship among the components of the cartesian gradient vector.

$$\left[\frac{dE(r_i)}{dr_i}\right]_{r_i=o} \quad \sum_{j=1}^{3N} \frac{dE}{dx_j}\frac{dx_j}{dr_i} = \underset{\sim}{L}^+_{r_i}\, \underset{\sim}{g} = 0 \qquad (3)$$

where $\underset{\sim}{g}$ is the gradient vector in cartesian coordinates. There are six such equations corresponding to the six external directions r_i, i = 1,6. Taken together, they constitute a linear system of equations of order six for which the unknowns are six components of the cartesian gradient vector.

$$\sum_{j=i}^{6} L_{j,r_i}\, g_j = -b_i \qquad i=1,6 \qquad (4)$$

where

$$b_i = \sum_{j=7}^{3n} L_{j,r_i} g_j \quad . \qquad (5)$$

Equation (4) is the working equation for gradient calculations. Care must be taken such that the six cartesian directions separated out in Eq. (4) are linearly independent, otherwise the matrix of coefficients is singular and the solution undefined.*

A useful relationship similar to Eq. (4) can be obtained for each row or column of the cartesian second derivative matrix by differentiating Eq. (3) with respect to a cartesian displacement.

---

*A similar situation is encountered when one exploits the inter-relationships among the two electron integrals under a rotation. See L.R. Kahn, "Relationships Among Derivatives of the Integrals in the Calculation of the Gradient of the Electronic Energy with Respect to the Nuclear Coordinates," J. Chem. Phys., Vol. 75, p. 3962, 1981.

$$0 = \frac{}{x_k} \; L^{+}_{r_i} g \; = L^{+}_{r_i} \; F_k + T^{k^{+}}_{r_i} \; g . \qquad (6)$$

In this equation, F_k is the k^{th} row or column of the cartesian second derivative matrix and

$$\underset{\sim}{T}^{k}_{r_i} = \frac{\partial}{\partial x_k} (\underset{\sim}{L}_{r_i}) \quad . \qquad (7)$$

There are six of these equations just as in the gradient case. Casting this equation in the same working form as Eq. (4), the vector $\underset{\sim}{F}_k$ takes the place of $\underset{\sim}{g}$ and the right hand side now has added to it the second (gradient dependent) term.

$$\sum_{j=1}^{6} L_{j,r_i} \; F_{j,k} = - \; b^{k}_{i} \qquad i = 1,6 \qquad (8)$$

with

$$b^{k}_{i} = \sum_{j=7}^{3n} L_{j,r_i} \; F_{j,k} + \sum_{j=1}^{3n} T^{k}_{j,r_i} g_j \; . \qquad (9)$$

It is interesting to note that $\underset{\sim}{L}_{r_i}$ is an eigenvector of $\underset{\sim}{F}$, with eigenvalue zero only if the second term in Eq. (6) is zero. This is always true for translations since in this case $\underset{\sim}{T}^{k}_{r_i} = \underset{\sim}{0}$. For rotations, this is the case if the gradient is zero, i.e., at a stationary point.

The extension to third derivatives is straightforward. Eq. (3) is differentiated with respect to two cartesian components x_k, x_l to obtain relationships among the elements of the vector $\underset{\sim}{G}_{kl}$

where

$$\underset{\sim}{G}_{kl} = \frac{\partial}{\partial \underset{\sim}{x}} (F_{kl}) \cdot \qquad (10)$$

One obtains

$$\underset{\sim}{L}^{+}_{r_i} \; \underset{\sim}{G}_{kl} + \underset{\sim}{T}^{l^{+}}_{r_i} \; \underset{\sim}{F}_{k} + \underset{\sim}{T}^{k^{+}}_{r_i} \; \underset{\sim}{F}_{l} + \underset{\sim}{T}^{k,l}_{r_i} \; \underset{\sim}{g} = 0 \qquad (11)$$

or

$$\sum_{j=1}^{6} L_{j,r_i} \; G_{jkl} = - \; b^{kl}_{i} \qquad i = 1,6 \qquad (12)$$

with

$$b_i^{kl} = \sum_{j=7}^{3n} L_{j,r_i} G_{jkl} + \sum_{j=i}^{3n} (T^l_{j,r_i} F_{jk} + T^k_{j,r_i} F_{jl} + T^{k,l}_{j,r_i} g_j) \qquad (13)$$

and

$$T^{k,l}_{\underset{\sim}{r}_i} = \frac{\partial^2}{\partial x_k \partial x_l} (L_{\underset{\sim}{r}_i}) \quad . \qquad (14)$$

The linear equations, Eq. (12) can then be solved for each k, l pair.

III. IMPLEMENTATION

As previously mentioned, the six cartesian directions which are separated out must not be linearly dependent. To insure this, we choose them as all three components of one atom, two components of a second atom and one component of a third atom which is not collinear with the first two atoms.

The three vectors $L_{\underset{\sim}{r}_i}$ corresponding to translations can be chosen as normalized translational vectors in the three cartesian directions. The other three vectors can be chosen as rotational vectors about any three linearly independent axes. For convenience, we choose these to be the cartesian axes. Thus to first order, a rotation about the z axis for example is a cartesian vector for which the y component on each atom is proportional to the x coordinate of that atom and the x component is proportional to the negative of the y coordinate. Three such vectors are formed and subsequently Schmidt orthogonalized to the translations. The result is three first order rotations in the cartesian planes. Infinitesimal displacements along the direction of these vectors correspond to infinitesimal rotations of the molecule.

The $T^k_{\underset{\sim}{r}_i}$ is the derivative of the external vector $L_{\underset{\sim}{r}_i}$ with respect to a cartesian displacement and can be readily generated by a finite difference procedure.

$$T^k_{\underset{\sim}{r}_i} = \frac{1}{2\delta} (L_{r_i} (x_k + \delta) - L_{r_i} (X_k - \delta)). \qquad (15)$$

The $T^{k,l}_{\underset{\sim}{r}_i}$ can be generated similarly.

IV. DISCUSSION

Using the procedures outlined above, one can ignore six of the cartesian directions in derivative evaluations. These components are calculated from the others by a simple procedure at the end of the calculation. It is worthwhile to examine, for a few specific cases, just what computation is by passed by using this technique.

The most straight forward derivatives to evaluate are those based upon wavefunctions which are determined variationally. Recognizing the stationary condition with respect to the variational parameters, one can avoid the derivatives of variational parameters with respect to nuclear coordinates. The difficult step in SCF and MCSCF first derivative calculations arises through the dependence of the energy on the positions of the basis functions; the evaluation of the derivatives of the two electron integrals with respect to nuclear coordinates. Using the technique presented here, one can select six directions for which derivatives of the integrals need not be calculated. Since the translational invariance of the integrals themselves is exploited in most derivative integral computer programs,[15] the actual savings one can expect comes from the neglect of three cartesian directions.* One can choose these components to be on the atoms having the largest number of basis functions and therefore affect the largest number of integrals.

Gradients for CI wavefunctions based upon SCF or MCSCF orbitals and second or third derivative for SCF or MCSCF wavefunctions require the first order response of the SCF or MCSCF variational parameters to nuclear displacements. This leads, for each cartesian displacement, to the evaluation of a linear system of equations the order of which is the number of variational parameters. Solving these coupled perturbed Hartree-Fock or MCSCF equations can become a time consuming step in these calculations. Six of these linear systems can be avoided.

CI second derivatives and MCSCF or SCF fourth derivatives require the second order changes in the SCF or MCSCF variational parameters. This leads to a linear system of equations for each pair of cartesian coordinates. One need solve only 1/2 (3N-6) (3N-5) instead of 1/2 (3N) (3N+1) sets of linear equations. CI second derivatives have the additional time consuming step of solving the coupled perturbed - CI equations. This requires an integral transformation and solving a linear set of equations, the order of which is the number of CI coefficients. Thus, the solution of the coupled perturbed -CI equations for each cartesian coordinate is approximately equivalent to the evaluation of the original CI wavefunction. For relatively small systems, avoiding six of these coordinates yields a significant reduction in computer time.

The emphasis in this discussion has been on the application of the described technique to analytical derivative evaluations. This is because there is a great deal of current activity in this area. One can also apply this scheme to derivatives calculated by finite difference procedures.

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*Rotational relationships among the two electron integrals can also be used in integral first derivative evaluation. However, considering the complexity of the implementation in conjunction with the number of operations required to solve the equations versus solving the integrals themselves, this is not generally done.

In summary, we have presented equations expressing the interrelationships among the cartesian derivatives of the Born-Oppenheimer potential energy. These relationships are derived from the invariance of the energy to overall rotations and translations of a molecule. We show how the energy invariance can be used to reduce the computational effort for various derivative calculations. Finally it is emphasized that these equations are both simple to implement and themselves require negligible computational labor.

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