# Software Requirements Specification for Equation-of-motion methods: A set of tools for implementing and solving EOMs

Gabriela Sánchez Díaz

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# Contents

# Revision History

| Date | Version | Notes |
| --- | --- | --- |
| 08-10-2020 | 1.0 | Creation of SRS |
| 21-10-2020 | 1.1 | Address issues #5, #7 and #8 regarding package name abbreviation and Traceability matrices section. |

# 1 Reference Material

This section records information for easy reference.

## 1.1 Table of Units

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

| symbol | unit | SI |
|---|---|---|
| m | length | metre |
| J | energy | joule |

## 1.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units.

| symbol | unit | description |
|---|---|---|
| $n$ | unitless | number of spinorbitals in the basis set |
| $N$ | unitless | number of electrons in a system |
| $\phi_p$ | $m^{-3/2}$ | p-th spinorbital of the basis set, can also be represented as p |
| $\hat{a}_p$ | unitless | Second-quantization anihilation operator for spinorbital p |
| $\hat{a}_p^\dagger$ | unitless | Second-quantization creation operator for spinorbital p |
| $\delta_{ij}$ | unitless | Kronecker delta function (1 for i=j, 0 otherwise) |
| $\mathbf{I}$ | unitless | Identity matrix, its elements are $\delta_{ij}$ |
| $\Psi^N$ | $m^{-3/2}$ | N-electron stationary state wavefunction |
| $\lvert \Psi_0^{(N)} \rangle$ | $m^{-3/2}$ | N-electron ground state wavefunction (vector representation using Dirack's bra-ket notation) |
| $\lvert \Psi_n^{(N \pm K)} \rangle$ | $m^{-3/2}$ | (N $\pm$ K)-electron, n-th excited state wavefunction (vector representation using Dirack's bra-ket notation) |
| $\hat{H}$ | J | Hamiltonian operator |
| $\hat{Q}$ | unitless | Transition operator |
| $\hat{Q}^\dagger$ | unitless | Conjugate transpose of $\hat{Q}$ |
| $\hat{Q}_k^{\pm K}$ | unitless | $\hat{Q}$ of the (N$\pm$K)-stationary state $k$ (relative to the N-electron reference stationary state) |
| $\hat{h}$ | J | 1-electron Hamiltonian operator |
| $\mathbf{h}$ | J | 1-electron integral matrix |

| | | |
|---|---|---|
| $h_{pq}$ | J | p,q-th element of $\mathbf{h}$ |
| $\hat{v}$ | J | 2-electron Hamiltonian operator |
| $\mathbf{v}$ | J | 2-electron integral matrix |
| $v_{pqrs}$ | J | the p,q,r,s-th element of $\mathbf{v}$ |
| $E$ | J | energy |
| $\Delta E_k$ | J | energy difference between two stationary states ($k$ and the reference one) |
| $\boldsymbol{\gamma}$ | unitless | 1-electron reduced density matrix |
| $\gamma_{pq}$ | unitless | p,q-th element of $\boldsymbol{\gamma}$ |
| $\gamma_{pq}$ | unitless | p,q-th element of $\boldsymbol{\gamma}$ |
| $\Gamma_{pqrs}$ | unitless | p,q,r,s-th element of $\boldsymbol{\Gamma}$ |
| $\gamma_{m;0k}$ | unitless | m-th element of the transition density matrix between states $|\Psi_0^{(N)}\rangle$ and $|\Psi_k^{(N\pm K)}\rangle$ |
| $p, q, r, s$ | unitless | arbitrary spinorbital index |
| $\mathbf{r}$ | m | Electronic coordinates |
| $\mathbf{R}$ | m | Nuclear coordinates |

## 1.3   Notation

The symbols and notation used through this document are consistent with the quantum chemistry literature and with existing documentation for equation-of-motion methods (see, e.g., **?**, **?** and Chapters 1 nad 2 of **?**). Some examples of this notation are: the operator of an observable O is denoted by $\hat{O}$, Dirac's bra-ket notation ($\langle|\ |\rangle$) is used for the representation of a state's wave function and vector or matrix parameters are indicated with bold face (like the identity matrix in the table above).

## 1.4 Abbreviations and Acronyms

| symbol | description |
|--------|-------------|
| A | Assumption |
| BS | Basis set(s) |
| DD | Data Definition |
| EA | Electron affinity |
| EOMEE | Equation-of-motion for excited states |
| GD | General Definition |
| GS | Goal Statement |
| IM | Instance Model |
| IP | Ionization Potential |
| LC | Likely Change |
| MO | Molecular orbital |
| PS | Physical System Description |
| PC | Personal Computer |
| QC | Quantum chemistry |
| R | Requirement |
| SRS | Software Requirements Specification |
| RDM | Reduced density matrix |
| T | Theoretical Model |
| TDM | Transition density matrix |

# 2 Introduction

The spectroscopic characterization of atomic and molecular systems is one of the fundamental techniques in the fields related to Chemistry.

As part of the methods developed in computational quantum chemistry, Equation-of-motion (EOM) methods offer an alternative approach to the prediction of molecular properties such as excitation energies, ionization potentials or electron affinities by directly targeting the evaluation of these magnitudes.

The present document introduces the requirements description for the development of a set of tools for implementing and solving EOM equations (package name: Equation-of-motion for excited states, abbreviated as EOMEE). The formatting of this document will follow the SRS templates introduced by ? and ?.

## 2.1 Purpose of Document

This document intends to establish the parameters under which the quality of the program EOMEE can be assessed

## 2.2 Scope of Requirements

EOMEE will evaluate the energy variations in processes that involve up to two particle transitions. In a standard PC its applicability will be limited to molecular systems with about 60 molecular orbital (MO) basis due to the demands of memory resources.

## 2.3 Characteristics of Intended Reader

The reader of this document must have a Level-1 undergraduate knowledge of mathematics (specifically of linear algebra), and quantum chemistry or physics. Additionally, familiarity with the formalism of second-quantization and some programming skills are required.

## 2.4 Organization of Document

The outline of the document is as follows: In section 3 the context of the systems, its constraints and characteristics of the user are described. Section 4 deepens the description by providing information of the intended inputs and outputs, the mathematical models that characterize the physical problem and the assumptions being made. Section (4) lists the system's functional and nonfunctional requirements. The expected changes, and the invariable ones are stated in sections 5 and 6, respectively. Finally, section 7 shows the traceability matrices and graphs and section 8 lists the values of auxiliary constants.

# 3   General System Description

This section provides general information about the system. It identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

## 3.1   System Context

Figure 1 describes EOMEE's context. External interactions are indicated by circles, the program by a rectangle area. Information pertinent to the input and output data are indicated at the left and right of the program.

The user will submit the programs arguments (1- and 2-electron integrals, 1- and 2- reduced density matrices (RDMs), and an EOM method); then EOMEE will process that information and return the resulting transition energies and density matrices (TDMs).
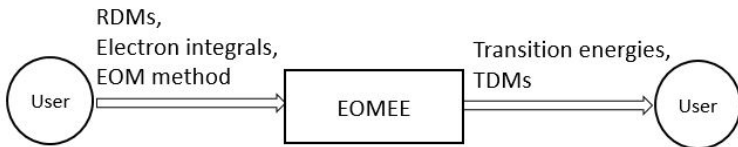
Figure 1: EOMEE Context

- User Responsibilities:

    - Provide the inputs for the atomic or molecular system of interest.
    - Guarantee that enough memory resources are available for the intended study system.
    - Verify that the output data has physical meaning for his intended system.

- EOMEE Responsibilities:

    - Detect data type mismatch, such as a string of characters instead of an array.
    - Detect data value mismatch, such as incorrect dimensions of input arrays.
    - Verify that the input matrices have the correct symmetries.
    - Transform the electron integrals and RDMs from the MO to the spinorbital representation.
    - Evaluate the transition energies and density matrices for the user selected EOM method.

## 3.2   User Characteristics

The user of EOMEE should have first-year undergraduate level of chemistry or physics so that she/he is familiar with the concepts of electronic excitation (or ionization) of an atomic or molecular system. To generate the program's input data, the user needs also experience in the field of computational an theoretical chemistry or physics.

## 3.3   System Constraints

Availability of general Python libraries is required for the development of EOMEE.

# 4   Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models.

## 4.1   Problem Description

The development of EOMEE is motivated by the need to create a common framework for the solution of EOM methods based on the RDMs. This will allow the comparison between different wavefunction based approaches from computational quantum chemistry and serve as an intermediate point for the development of future scientific work based in the TDMs.

### 4.1.1   Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- **reference stationary state**: State onto which the excitation operator acts. Is usually taken as the lowest energy N-electron stationary state (ground state).

- **excitation or transition operator**: Operator that transforms the reference N-electron stationary state into a different stationary state.

- **excited state**: an stationary state other than the ground one. Higher in energy and potentially with a different number of electrons.

- **electron density matrix**: matrix corresponding to the electron density distribution represented in the spinorbital basis set.

- **spinorbital**: orthonormal function of the space and spin coordinates of a single electron.

- **electron integrals**: energy contributions of the different interaction between the electrons and nuclei in the system.

- **quantum chemistry methods**: methods that deal with solving the Schrödinger equation.

### 4.1.2   Physical System Description

The EOMEE's physical system includes the following elements:

PS1: The N-electron reference stationary state $\Psi_0^{(N)}$, characterized by the 1- and 2-RDMs.

PS2: The $k$th excited state $\Psi_k^{(N\pm K)}$.

PS3: The excitation operator $\hat{Q}_k^{(N\pm K)}$ that transform $\Psi_0^{(N)}$ into $\Psi_k^{(N\pm K)}$.

PS4: The electronic Hamiltonian operator $\hat{H}$ which contains the information about the interactions between the particles in the system.

### 4.1.3   Goal Statements

Given the density matrices and the 1- and 2-electron integrals of a reference N-electron stationary state and an EOM method, the goal statements are:

GS1: Determine the transition energies.

GS2: Determine the transition density matrices.

## 4.2   Solution Characteristics Specification

The instance models that govern EOMEE are presented in Subsection 4.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

### 4.2.1   Assumptions

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square brackets refer to the theoretical model [T], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: The transition operator can be approximated by a finite expansion in second-quantization operators strings (BS). [ GD1]

A2: The EOM methods can be expressed in terms of the 1- and 2-reduced density matrices of the reference state and the 1- and 2-electron integrals. [IM1]-[IM5]

A3: The 1- and 2-electron integrals are in the MO basis representation. [DD2], [DD3]

A4: The input electron integrals and RDMs have the correct symmetries.[DD2], [DD3], [DD4], [DD5]

A5: The condition $\hat{Q}^\dagger |\Psi_0^N\rangle = 0$ ("killer condition") is fulfilled. [GD2]

A6: The EOM method is expressed as a determined system of equations by projecting onto the transition operator's BS. [GD2], [IM1]-[IM5]

### 4.2.2 Theoretical Models

This section focuses on the general equations and laws that EOMEE is based on.

| Number | T1 |
|---|---|
| Label | **Time-independent Schrödinger equation** |
| Equation | $\hat{H}\Psi^{(N)} = E\Psi^{(N)}$ |
| Description | The equation above represents the time-independent nonrelativistic Schrödinger equation. Where $\hat{H}$ is the Hamiltonian operator, $\Psi^{(N)}$, the N-electron stationary state wavefunction, and $(E)$ the corresponding total energy of the system. Finding the solutions to this equation is the main objective of quantum chemistry methods. |
| Source | **?** |
| Ref. By | GD2 |

A more explicit representation of this equation includes its dependence on the nuclear and electronic coordinates of the particles composing the system ($\mathbf{R}$ and $\mathbf{r}$ respectively):
$\hat{H}\Psi^{(N)}(\mathbf{r},\mathbf{R}) = E_{Tot}\Psi^{(N)}(\mathbf{r},\mathbf{R})$
where $\hat{H} = \hat{T}_{nuc} + \hat{T}_{el} + \hat{V}_{nuc-nuc} + \hat{V}_{el-el} + \hat{V}_{nuc-el}$ includes the kinetic ($\hat{T}$) and potential ($\hat{V}$) energies of the electrons ($el$) and nuclei ($nuc$).
Because quantum chemical methods are generally applied under the Born-Oppenheimer approximation (which allows to separates the nuclear and electronic motions) the actual expression used through this document is:
$\hat{H}_{el}\Psi_{el}^{(N)}(\mathbf{r},\mathbf{R}) = E_{el}(\mathbf{R})\Psi_{el}^{(N)}(\mathbf{r},\mathbf{R})$
in which the term $\hat{T}_{nuc}$ in not included in the Hamiltonian operator. The coulombic interactions between the atoms ($\hat{V}_{nuc-nuc}$) become a constant factor for a given set of $\mathbf{R}$ (molecular geometry), so that the electronic energy ($E_{el}(\mathbf{R})$) depends on these coordinates.
For notation simplicity we will drop the subscripts and use $\hat{H}\Psi^{(N)} = E\Psi^{(N)}$ as the electronic Schrödinger equation for an N-electron, M-atom system.

| Number | T2 |
| --- | --- |
| Label | **Excited State** |
| Equation | $\lvert \Psi_k^{(N \pm K)} \rangle = \hat{Q}_k^{(\pm k)} \lvert \Psi_0^{(N)} \rangle$ |
| Description | The wavefunction of the "excited" state ($\Psi_k^{(N \pm K)}$) is defined by the action of a transition operator $\hat{Q}_k^{(\pm K)}$ onto a reference N-electron stationary state (ground state $\Psi_0^{(N)}$). As a result of the transition, the number of electrons ($N$) in the initial reference system and the final one might differ ($N \pm K$). |
| Source | – |
| Ref. By | GD1, GD2, T4 |

| Number | T3 |
| --- | --- |
| Label | **Transition energy** |
| Equation | $\Delta E_k = E_k - E_0$ |
| Description | The above equation gives the energy difference between the initial ($E_0$) and final states ($E_k$) due to a transition process. The evaluation of this magnitude is the main goal of the present program. |
| Source | – |
| Ref. By | GD2 |

| Number | T4 |
| --- | --- |
| Label | **Transition Density Matrix** |
| Equation | $\gamma_{m;0k} = \langle \Psi_0^N \rvert \hat{q}_m \lvert \Psi_k^{N \pm k} \rangle$ |
| Description | Represents the probability of finding the state defined by $\hat{q}_m^{\dagger} \lvert \Psi_0^N \rangle$ in the "excited" state $\lvert \Psi_k^{N \pm K} \rangle$; where $\hat{q}_m$ is some string of second-quantization operators. |
| Source | ? |
| Ref. By | GD1, IM6 |

### 4.2.3 General Definitions

This section collects the laws and equations that will be used in building the instance models.

| Number | GD1 |
|---|---|
| Label | **Transition operator approximation** |
| SI Units | – |
| Equation | $\hat{Q}_k^{(\pm K)} = \sum_n c_{n;k} \hat{q}_n$ |
| Description | The equation above represents a general notation for the definition of the transition operator $(\hat{Q}_k^{(\pm K)})$ through a BS expansion $(\hat{q}_n)$. |
| | Some common transition operators for which only the 1- and 2-RDMs would be needed are: |
| | electron removal: $\hat{Q}_k^{-1} = \sum_n c_{n;k} a_n$ |
| | electron attachment: $\hat{Q}_k^{+1} = \sum_n c_{n;k} a_n^\dagger$ |
| | electron excitation: $\hat{Q}_k^0 = \sum_{pq} c_{pq;k} a_p^\dagger a_q$ |
| | double electron removal: $\hat{Q}_k^{-2} = \sum_{pq} c_{pq;k} a_p a_q$ |
| | double electron attachment: $\hat{Q}_k^{+2} = \sum_{pq} c_{pq;k} a_p^\dagger a_q^\dagger$ |
| Source | **??** |
| Ref. By | A1, A6, IM1-IM6 |

It is possible to define expression for $\hat{Q}_k^{(\pm K)}$ with more terms. For instance in the case of excitations, one could include higher than single excitation terms:

$$\hat{Q}_k^0 = \sum_{pq} c_{pq;k} a_p^\dagger a_q + \sum_{pqrs} c_{pqrs;k} a_p^\dagger a_q^\dagger a_s a_r + \sum_{pqrstu} c_{pqrstu;k} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s + ...$$

However the evaluation of the EOM equations would then required higher than the 1- and 2-RDMs, which is outside of the present program's scope.

| Number | GD2 |
|---|---|
| Label | **Eigenvalue Problem** |
| SI Units | – |
| Equation | $f(h_{pq}, v_{pqrs}, \gamma_{pq}, \Gamma_{pqrs})$: |
| | (1) $\langle \Psi_0^N | q_m^\dagger [\hat{H}, \hat{Q}] | \Psi_0^N \rangle = \Delta E_k \langle \Psi_0^N | q_m^\dagger \hat{Q} | \Psi_0^N \rangle$ |
| | (2) $\langle \Psi_0^N | [q_m^\dagger, [\hat{H}, \hat{Q}]]_\pm | \Psi_0^N \rangle = \Delta E_k \langle \Psi_0^N | [q_m^\dagger, \hat{Q}]_\pm | \Psi_0^N \rangle$ |
| Description | The equations above are the representation of the EOM methods as a generalized eigenvalue problem. By expanding the operator $\hat{Q}$ in some BS (see GD1 for specific expressions) and doing some algebraic manipulations of the resultant expressions, these equations can be reformulated in terms of the RDMs of the state $\Psi_0^N$ and the 1- and 2-electron integrals. |
| Source | **?** |
| Ref. By | A2, A5, A6, T1, T2, T3, IM1-IM5 |

**Derivation of the eigenvalue problems**

The Schrödinger equation (T1) for the excited state $\Psi_k^{(N\pm K)}$ (T2) is:

$$\hat{H} | \Psi_k^{(N\pm K)} \rangle = E_k | \Psi_k^{(N\pm K)} \rangle \tag{1}$$
$$\hat{H} \hat{Q}_k^{(\pm K)} | \Psi_0^{(N)} \rangle = E_k \hat{Q}_k^{(\pm k)} | \Psi_0^{(N)} \rangle$$

To directly determine the energy change due to the excitation process we apply the transition operator $\hat{Q}_k^{(\pm K)}$ to the Schrödinger equation for $\Psi_0^{(N)}$, subtracting it from Eq. (1):

$$\hat{Q}_k^{(\pm K)} \hat{H} | \Psi_0^{(N)} \rangle = E_0 \hat{Q}_k^{(\pm k)} | \Psi_0^{(N)} \rangle \tag{2}$$

$$(\hat{H} \hat{Q}_k^{(\pm K)} - \hat{Q}_k^{(\pm K)} \hat{H}) | \Psi_0^{(N)} \rangle = (E_k - E_0) \hat{Q}_k^{(\pm K)} | \Psi_0^{(N)} \rangle \tag{3}$$
$$[\hat{H}, \hat{Q}_k^{(\pm K)}] | \Psi_0^{(N)} \rangle = \Delta E_k \hat{Q}_k^{(\pm K)} | \Psi_0^{(N)} \rangle$$

This last expression can be solved by projecting onto a suitable set of states. Because we are interested in using the 1- and 2-RDMs, it is convenient to use the same basis set in which $Q_k^{(\hat{\pm} K)}$ is expanded [GD1] to build this set:

$$\langle \Psi_0^{(N)} | q_m^\dagger [\hat{H}, \hat{Q}_k^{(\pm K)}] | \Psi_0^{(N)} \rangle = \Delta E_k \langle \Psi_0^{(N)} | q_m^\dagger \hat{Q}_k^{(\pm K)} | \Psi_0^{(N)} \rangle \tag{4}$$

This last equation is suitable for the electron attachment and removal operators defined in [GD1], with which the final expressions only need the 1- and 2-RMDs.

Alternative expressions, more suitable for the cases of the excitation, double electron removal or attachment operators, can be derived by invoking the "killer condition" [A5]. This allows to add/subtract zero from (4) so that:

$$\langle \Psi_0^{(N)}| \, q_m^\dagger [\hat{H}, \hat{Q}_k^{(\pm K)}] \pm [\hat{H}, \hat{Q}_k^{(\pm K)}] q_m^\dagger \, |\Psi_0^{(N)}\rangle = \Delta E_k \, \langle \Psi_0^{(N)}| \, q_m^\dagger \hat{Q}_k^{(\pm k)} \pm \hat{Q}_k^{(\pm k)} q_m^\dagger \, |\Psi_0^{(N)}\rangle \quad (5)$$

$$\langle \Psi_0^N| \, [q_m^\dagger, [\hat{H}, \hat{Q}_k^{(\pm k)}]]_\pm \, |\Psi_0^N\rangle = \Delta E_k \, \langle \Psi_0^N| \, [q_m^\dagger, \hat{Q}_k^{(\pm k)}]_\pm \, |\Psi_0^N\rangle$$

Expressions (4) and (5) constitute determined systems of linear equations. The equations defined by (5) can be used with any of the transition operators in [GD1]. As mentioned before they are more appropriate then (4) for the operators involving two particle transitions, because the commutation or anti-commutation relations can produce final operators with lower number of particles, so that only the 1 and 2-RDMs are required.

### 4.2.4 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.

| Number | DD1 |
|---|---|
| Label | **Electronic Hamiltonian operator** |
| Symbol | $\hat{H}$ |
| SI Units | J |
| Equation | $\hat{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$ |
| Description | Second-quantization notation for the electronic Hamiltonian operator under the Born-Oppenheimer approximation. |
| | $h_{pq}$ and $v_{pqrs}$ are the one and two electron integrals in the spinorbital basis. |
| Sources | ? |
| Ref. By | T1, DD2, DD3 |

| Number | DD2 |
|---|---|
| Label | **1-electron integrals** |
| Symbol | $h_{pq}$ |
| SI Units | J |
| Equation | $h_{pq} = \int \phi_p^*(\mathbf{x})[\hat{t} + \hat{v}_{ext}]\phi_q(\mathbf{x})$ |
| Description | Where: |
| | $\hat{t}$ and $\hat{v}_{ext}$ are the kinetic and external potential operators respectively. |
| | $\phi_i$ are the orthonormal spinorbitals and $\mathbf{x}$ represents the spatial and spin coordinates. |
| | The symmetry of this matrix is: $(h_{pq})^T = h_{qp}$ |
| Sources | **?** |
| Ref. By | DD1, IM1-IM5 |

| Number | DD3 |
|---|---|
| Label | **2-electron integrals** |
| Symbol | $v_{pqrs}$ |
| SI Units | J |
| Equation | $< pq|rs > = \int \int \phi_p^*(\mathbf{x})\phi_q^*(\mathbf{x})r_{12}^{-1}\phi_r(\mathbf{x})\phi_s(\mathbf{x})d\mathbf{x}_1 d\mathbf{x}_2$ |
| Description | These are the 2-electron integrals in the physicist notation. Where: |
| | $r_{12}$ is the distance between 2 electrons, |
| | $\phi_i$ the orthonormal spinorbitals and $\mathbf{x}$ the spatial and spin coordinates. |
| Sources | **?** |
| Ref. By | DD1, IM1-IM5 |

For real spinorbitlas the permutational symmetries of the $v_{pqrs}$ matrix are:

$$< pq|rs > = < qp|sr > = < rs|pq > = < sr|qp >$$
$$< rq|ps > = < qr|sp > = < ps|rq > = < sp|qr > \tag{6}$$

The antysymmetrized 2-electron integrlas are defined as:

$$< pq||rs > = < pq|rs > - < pq|sr > \tag{7}$$

With the following permutational symmetries:

$$< pq|rs > = < qp|sr > = < rs|pq > = < sr|qp >$$
$$- < pq|sr > = - < qp|rs > = - < sr|pq > = - < rs|qp >$$

(8)

| Number | DD4 |
|---|---|
| Label | **1-electron reduced density matrix** |
| Symbol | $\gamma_{pq}$ |
| SI Units | $-$ |
| Equation | $\gamma_{pq} = \langle \Psi_0 | a_p^\dagger a_q | \Psi_0 \rangle$ |
| Description | Where: |
| | $\Psi_0$ is an stationary state wavefunction, and $a_p^\dagger / a_q$ the creation/annihilation operator. |
| | The symmetry of this matrix is: $(\gamma_{pq})^* = \gamma_{qp}$ |
| Sources | **?** |
| Ref. By | IM1-IM6 |

| Number | DD5 |
|---|---|
| Label | **2-electron reduced density matrix** |
| Symbol | $\Gamma_{pqrs}$ |
| SI Units | $-$ |
| Equation | $\Gamma_{pqrs} = \langle \Psi_0 | a_p^\dagger a_q^\dagger a_s a_r | \Psi_0 \rangle$ |
| Description | Where: |
| | $\Psi_0$ is an stationary state wavefunction, and $a_p^\dagger / a_q$ the creation/annihilation operator. |
| | The Permutational symmetries of this matrix are: |
| | $\Gamma_{pqrs} = \Gamma_{qpsr} = \Gamma_{rspq} = -\Gamma_{qprs} = -\Gamma_{pqsr}$ |
| Sources | **?** |
| Ref. By | IM1-IM6 |

### 4.2.5   Instance Models

This section transforms the problem defined in Section 4.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 4.2.4 to replace the abstract symbols in the models identified in Sections 4.2.2 and 4.2.3.
The goals GS1 and GS2 are solved by IM1 to IM6.

| Number | IM1 |
|---|---|
| Label | **Electron removal** |
| Input | $h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$ and IP_EOM($h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$) |
| Output | $\Delta E_k$ and $c_{n;k}$ |
| Description | $h_{pq}$ and $v_{pqrs}$ are the 1- and 2-electron integrals in the spinorbital base |
| | $\gamma_{pq}$ and $\Gamma_{pqrs}$ are the RDMs for the reference N-electron state. |
| | IP_EOM() is the EOM method corresponding to the electron removal transition operator. |
| | $\Delta E_k$ and $c_{n;k}$ are the ionization potentials and coefficients from the BS expansion respectively. |
| Sources | – |
| Ref. By | GD1,GD2, DD2,DD3, DD4, DD5 |

**Derivation of the Electron removal EOM**

Taking the transition operator $(\hat{Q}_k^{-1})$ from GD1 and Eq. (1) from GD2 we get:

$$\langle \Psi_0^{(N)} | a_m^\dagger [\hat{H}, \hat{Q}_k^{(-1)}] | \Psi_0^{(N)} \rangle = \Delta E_k \langle \Psi_0^{(N)} | a_m^\dagger \hat{Q}_k^{(-1)} | \Psi_0^{(N)} \rangle \tag{9}$$

$$\sum_n c_{n;k} \langle \Psi_0^{(N)} | a_m^\dagger [\hat{H}, a_n] | \Psi_0^{(N)} \rangle = \Delta E_k \sum_n c_{n;k} \langle \Psi_0^{(N)} | a_m^\dagger a_n | \Psi_0^{(N)} \rangle$$

From the above equation, after some algebraic manipulations of the operators it is possible to deduct the following expression in terms of the RDMs and Hamiltonian integrals:

$$-\sum_{nq} h_{nq} \gamma_{mq} c_{n;k} + \frac{1}{2} \sum_{nqrs} v_{qnrs} \Gamma_{mqrs} c_{n;k} = \Delta E_k \sum_n \gamma_{mn} c_{n;k} \tag{10}$$

| Number | IM2 |
|---|---|
| Label | **Electron attachment** |
| Input | $h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$ and EA_EOM($h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$) |
| Output | $\Delta E_k$ and $c_{n;k}$ |
| Description | $h_{pq}$ and $v_{pqrs}$ are the 1- and 2-electron integrals in the spinorbital base |
| | $\gamma_{pq}$ and $\Gamma_{pqrs}$ are the RDMs for the reference N-electron state. |
| | EA_EOM() is the EOM method corresponding to the electron attachment transition operator. |
| | $\Delta E_k$ and $c_{n;k}$ are the electron affinities and coefficients from the BS expansion respectively. |
| Sources | – |
| Ref. By | GD1,GD2, DD2,DD3, DD4, DD5 |

**Derivation of the Electron attachment EOM**

We start with Eq. (1) from GD2 and take the transition operator $(\hat{Q}_k^{+1})$ from GD1:

$$\langle \Psi_0^{(N)} | a_m [\hat{H}, \hat{Q}_k^{(+1)}] | \Psi_0^{(N)} \rangle = \Delta E_k \langle \Psi_0^{(N)} | a_m \hat{Q}_k^{(+1)} | \Psi_0^{(N)} \rangle \tag{11}$$

$$\sum_n c_{n;k} \langle \Psi_0^{(N)} | a_m [\hat{H}, a_n^\dagger] | \Psi_0^{(N)} \rangle = \Delta E_k \sum_n c_{n;k} \langle \Psi_0^{(N)} | a_m a_n^\dagger | \Psi_0^{(N)} \rangle$$

From above's equation, after some algebraic manipulations of the operators it is possible to get the following expression in terms of the RDMs and electron integrals:

$$\left( \begin{array}{c} \sum_n h_{mn} c_{n;k} - \sum_{np} h_{pn} \gamma_{pm} c_{n;k} \\ + \sum_{nps} v_{mpns} \gamma_{ps} c_{n;k} + \frac{1}{2} \sum_{npqs} v_{pqns} \Gamma_{pqsm} c_{n;k} \end{array} \right) = \Delta E_k \sum_n (\delta_{mn} - \gamma_{nm}) c_{n;k}$$

| Number | IM3 |
|---|---|
| Label | **Electron excitation** |
| Input | $h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$ and Exc_EOM($h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$) |
| Output | $\Delta E_k$ and $c_{ij;k}$ |
| Description | $h_{pq}$ and $v_{pqrs}$ are the 1- and 2-electron integrals in the spinorbital base |
| | $\gamma_{pq}$ and $\Gamma_{pqrs}$ are the RDMs for the reference N-electron state. |
| | Exc_EOM() is the EOM method corresponding to the electron excitation transition operator. |
| | $\Delta E_k$ and $c_{ij;k}$ are the excitation energies and coefficients from the BS expansion respectively. |
| Sources | – |
| Ref. By | GD1,GD2, DD2,DD3, DD4, DD5 |

**Derivation of the Electron excitation EOM**

Taking the transition operator $(\hat{Q}_k^0)$ from GD1 and Eq. (2) from GD2 we get:

$$\langle \Psi_0^{(N)} | [a_k^\dagger a_l, [\hat{H}, \hat{Q}_k^{(0)}]] | \Psi_0^{(N)} \rangle = \Delta E_k \langle \Psi_0^{(N)} | a_k^\dagger a_l \hat{Q}_k^{(0)} | \Psi_0^{(N)} \rangle \tag{12}$$

$$\sum_{ij} c_{ij;k} \left\langle \Psi_0^{(N)} \left| \left[ a_k^\dagger a_l, \left[ \hat{H}, a_i^\dagger a_j \right] \right] \right| \Psi_0^{(N)} \right\rangle = \Delta E_k \sum_n c_{ij;k} \left\langle \Psi_0^{(N)} \left| a_k^\dagger a_l a_i^\dagger a_j \right| \Psi_0^{(N)} \right\rangle$$

From the above equation, after some algebraic manipulations of the operators it is possible to derive the following expression in terms of the RDMs and Hamiltonian integrals:

$$\left( \begin{array}{c} \sum_{ij} \left[ h_{li}\gamma_{kj} + h_{jk}\gamma_{il} - \sum_q (h_{jq}\delta_{li}\gamma_{kq} + h_{qi}\delta_{jk}\gamma_{ql}) \right] c_{ij;k} \\ + \sum_{ij} \left[ \sum_{qs} (v_{lqis}\Gamma_{kqjs} + v_{jqks}\Gamma_{iqls}) \right] c_{ij;k} \\ + \frac{1}{2} \sum_{ij} \left[ \sum_{rs} (v_{jlrs}\Gamma_{kirs} + \sum_q v_{qjrs}\delta_{li}\Gamma_{kqrs}) \right] c_{ij;k} \\ + \frac{1}{2} \sum_{ij} \left[ \sum_{pq} (v_{pqik}\Gamma_{pqlj} + \sum_s v_{pqsi}\delta_{jk}\Gamma_{pqls}) \right] c_{ij;k} \end{array} \right) = \Delta E_k \sum_{ij} (\delta_{li}\gamma_{kj} - \Gamma_{kijl}) c_{ij;k}$$

$$\tag{13}$$

| Number | IM4 |
|---|---|
| Label | **Double IP** |
| Input | $h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$ and DIP_EOM($h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$) |
| Output | $\Delta E_k$ and $c_{ij;k}$ |
| Description | $h_{pq}$ and $v_{pqrs}$ are the 1- and 2-electron integrals in the spinorbital base |
| | $\gamma_{pq}$ and $\Gamma_{pqrs}$ are the RDMs for the reference N-electron state. |
| | DIP_EOM() is the EOM method corresponding to the double electron removal transition operator. |
| | $\Delta E_k$ and $c_{ij;k}$ are the double ionization energies and coefficients from the BS expansion respectively. |
| Sources | – |
| Ref. By | GD1,GD2, DD2,DD3, DD4, DD5 |

**Derivation of the Double IP EOM**

Taking the transition operator $(\hat{Q}_k^{-2})$ from GD1 and Eq. (2) from GD2 we get:

$$\langle\Psi_0^{(N)}|\,[a_k^\dagger a_l^\dagger,[\hat{H},\hat{Q}_k^{(-2)}]]\,|\Psi_0^{(N)}\rangle = \Delta E_k \langle\Psi_0^{(N)}|\,[a_k^\dagger a_l^\dagger,\hat{Q}_k^{(-2)}]\,|\Psi_0^{(N)}\rangle \tag{14}$$

$$\sum_{ij} c_{ij;k}\left\langle\Psi_0^{(N)}\left|\left[a_k^\dagger a_l^\dagger,\left[\hat{H},a_i a_j\right]\right]\right|\Psi_0^{(N)}\right\rangle = \Delta E_k \sum_{ij}\left\langle\Psi_0^{(N)}\left|\left[a_k^\dagger a_l^\dagger, a_i a_j\right]\right|\Psi_0^{(N)}\right\rangle c_{ij;k}$$

From the above equation, after some algebraic manipulations of the operators it is possible to derive the following expression in terms of the RDMs and Hamiltonian integrals:

$$\begin{pmatrix} 2\sum_{ij}(-h_{jl}\delta_{ik}+h_{jk}\delta_{il})c_{ij;k} \\ +2\sum_{ij}(h_{ik}\gamma_{lj}-h_{il}\gamma_{kj})c_{ij;k} \\ +2\sum_{ij,q}h_{jq}(\delta_{ik}\gamma_{lq}-\delta_{il}\gamma_{kq})c_{ij;k} \\ +\sum_{ij}\nu_{jikl}c_{ij;k}+2\sum_{ijq}\nu_{qjkl}\gamma_{qi}c_{ij;k} \\ +\sum_{ijr}(\nu_{jilr}\gamma_{kr}-\nu_{jikr}\gamma_{lr})c_{ij;k} \\ +2\sum_{ij,qr}(\nu_{iqrk}\delta_{lj}+\nu_{iqlr}\delta_{kj})\gamma_{qr}c_{ij;k} \\ +2\sum_{ij,qr}(\nu_{jqrk}\Gamma_{qlri}+\nu_{jqlr}\Gamma_{qkri})c_{ij;k} \\ +\sum_{ij,qrs}\nu_{qjrs}(\delta_{ki}\Gamma_{qlrs}-\delta_{li}\Gamma_{qkrs})c_{ij;k} \end{pmatrix} = \Delta E_k \sum_{ij}\begin{pmatrix} 2\delta_{jk}\gamma_{li}+2\delta_{il}\gamma_{kj} \\ -2\delta_{jk}\delta_{il} \end{pmatrix}c_{ij;k} \tag{15}$$

| Number | IM5 |
|---|---|
| Label | **Double EA** |
| Input | $h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$ and DEA_EOM($h_{pq}$, $v_{pqrs}$, $\gamma_{pq}$, $\Gamma_{pqrs}$) |
| Output | $\Delta E_k$ and $c_{ij;k}$ |
| Description | $h_{pq}$ and $v_{pqrs}$ are the 1- and 2-electron integrals in the spinorbital base |
| | $\gamma_{pq}$ and $\Gamma_{pqrs}$ are the RDMs for the reference N-electron state. |
| | DEA_EOM() is the EOM method corresponding to the double electron attachment transition operator. |
| | $\Delta E_k$ and $c_{ij;k}$ are the double electron attachment energies and coefficients from the BS expansion respectively. |
| Sources | – |
| Ref. By | GD1,GD2, DD2,DD3, DD4, DD5 |

**Derivation of the Double EA EOM**

We start with Eq. (2) from GD2 and take the transition operator $(\hat{Q}_k^{+2})$ from GD1:

$$\langle \Psi_0^{(N)} | [a_k a_l, [\hat{H}, \hat{Q}_k^{(+2)}]] | \Psi_0^{(N)} \rangle = \Delta E_k \langle \Psi_0^{(N)} | [a_k a_l, \hat{Q}_k^{(+2)}] | \Psi_0^{(N)} \rangle \tag{16}$$

$$\sum_{ij} c_{ij;k} \left\langle \Psi_0^{(N)} \left| \left[ a_k a_l, \left[ \hat{H}, a_i^\dagger a_j^\dagger \right] \right] \right| \Psi_0^{(N)} \right\rangle = \Delta E_k \sum_{ij} \left\langle \Psi_0^{(N)} \left| \left[ a_k a_l, a_i^\dagger a_j^\dagger \right] \right| \Psi_0^{(N)} \right\rangle c_{ij;k}$$

From the above equation, after some algebraic manipulations of the operators it is possible to derive the following expression in terms of the RDMs and Hamiltonian integrals:

$$\begin{pmatrix} 2\sum_{ij}(h_{li}\delta_{kj} - h_{ki}\delta_{lj})c_{ij;k} \\ +2\sum_{ij}(h_{ki}\gamma_{jl} - h_{li}\gamma_{jk})c_{ij;k} \\ +2\sum_{ijp}(h_{pi}\delta_{lj}\gamma_{pk} + h_{pj}\delta_{ki}\gamma_{pl})c_{ij;k} \\ +\sum_{ij}\nu_{lkij}c_{ij;k} + 2\sum_{ijr}\nu_{lkjr}\gamma_{ir}c_{ij;k} \\ +\sum_{ijq}(\nu_{qlij}\gamma_{qk} - \nu_{qkij}\gamma_{ql})c_{ij;k} \\ +2\sum_{ij,qr}(\nu_{qljr}\delta_{ki} - \nu_{qkjr}\delta_{li})\gamma_{qr}c_{ij;k} \\ +2\sum_{ij,qr}(\nu_{qlir}\Gamma_{qjrk} - \nu_{qkir}\Gamma_{qjrl})c_{ij;k} \\ +\sum_{ij,pqr}\nu_{pqjr}(\delta_{li}\Gamma_{pqrk} - \delta_{ki}\Gamma_{pqrl})c_{ij;k} \end{pmatrix} = \Delta E_k \sum_{ij} \begin{pmatrix} 2\delta_{li}\delta_{kj} - 2\delta_{li}\gamma_{jk} \\ -2\delta_{kj}\gamma_{il} \end{pmatrix} c_{ij;k} \tag{17}$$

| Number | IM6 |
|---|---|
| Label | **Transition Density Matrix** |
| Input | $\gamma_{pq}$, $\Gamma_{pqrs}$ and $c_{n;k}$ |
| Output | $\gamma_{n;0k}$ |
| Description | $\gamma_{pq}$ and $\Gamma_{pqrs}$ are the RDMs for the reference N-electron state. |
| | $c_{n;k}$ are the amplitudes of the BS expansion of the transition operator. |
| Sources | – |
| Ref. By | T4, GD1, DD4, DD5 |

## Derivation of the Transition Density Matrices

Starting from the definitions given in T2, T4 and GD1 for the TDM, excited state and transition operator the following expresions can be derived:

$\hat{Q}_k^{(-1)}$ :

$$\gamma_{m;0k} = \sum_n c_{n;k} \langle \Psi_0^{(N)} | a_m^\dagger a_n | \Psi_0^{(N)} \rangle = \sum_n \gamma_{mn} c_{n;k} \tag{18}$$

$\hat{Q}_k^{(+1)}$ :

$$\gamma_{m;0k} = \sum_n c_{n;k} \langle \Psi_0^{(N)} | a_m a_n^\dagger | \Psi_0^{(N)} \rangle = \sum_n (\delta_{mn} - \gamma_{mn}) c_{n;k} \tag{19}$$

$\hat{Q}_k^{(0)}$ :

$$\gamma_{kl;0k} = \sum_{ij} c_{ij;k} \langle \Psi_0^{(N)} | a_k^\dagger a_l a_i^\dagger a_j | \Psi_0^{(N)} \rangle = \sum_{ij} (\delta_{li} \gamma_{kj} - \Gamma_{kijl}) c_{ij;k} \tag{20}$$

$\hat{Q}_k^{(-2)}$ :

$$\gamma_{kl;0k} = \sum_{ij} c_{ij;k} \langle \Psi_0^{(N)} | a_k^\dagger a_l^\dagger a_i a_j | \Psi_0^{(N)} \rangle = \sum_{ij} \Gamma_{klji} c_{ij;k} \tag{21}$$

$\hat{Q}_k^{(+2)}$ :

$$\gamma_{kl;0k} = \sum_{ij} c_{ij;k} \langle \Psi_0^{(N)} | a_k a_l a_i^\dagger a_j^\dagger | \Psi_0^{(N)} \rangle = \sum_{ij} (2\delta_{li}\delta_{kj} + 2\delta_{lj}\gamma_{ik} + 2\delta_{ki}\gamma_{jl} + \Gamma_{ijlk}) c_{ij;k} \tag{22}$$

### 4.2.6 Input Data Constraints

Table 1 shows the data constraints on the input output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The column for software constraints restricts the range of inputs to reasonable values. The software constraints will be helpful in the design stage for picking suitable

algorithms. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise.

The specification parameters in Table 1 are listed in Table 2.

Table 1: Input Variables

| Var | Physical Constraints | Software Constraints | Typical Value | Uncertainty |
|---|---|---|---|---|
| $\gamma_{pq}$ | $Tr(\gamma_{pq}) = N$ | $\gamma_{pq} \geq \epsilon$ | 0 or 1 | – |
| $\Gamma_{pqrs}$ | $Tr(\Gamma_{pq}) = 0.5 * N(N-1)$ | $\Gamma_{pq} \geq \epsilon$ | 0 or 1 | – |
| $h_{pq}$ | $h_{pq} \geq 0$ | $h_{pq} \geq \epsilon$ | 0.5 | – |
| $v_{pqrs}$ | $v_{pqrs} \geq 0$ | $v_{pqrs} \geq \epsilon$ | 0.5 | – |

(*) The value of $\epsilon$ is to prevent numerical instabilities during the solution of the EOM equations (IM1-IM5)

Table 2: Specification Parameter Values

| Var | Value |
|---|---|
| $N$ | Number of electrons |
| $\epsilon$ | $10^{-10}$ |

### 4.2.7 Properties of a Correct Solution

EOMEE will provide and estimate of the single excitation, ionization potentials or electron affinity energies for an atomic or molecular system as selected by the user. These are expected to be positive energy values. For the transition density matrices the values should be between 0 and 1 for the calculation to be correct. These constraints are summarized in Table 3

## 5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

Table 3: Output Variables

| Var | Physical Constraints |
| --- | --- |
| $\Delta E_k$ | $\Delta E_k > 0$ |
| $\gamma_{n;0k}$ | $0 \leq \gamma_{n;0k} \leq 1$ |

## 5.1 Functional Requirements

R1: Input the 1- and 2-electron integrals in the MO basis representation, the 1- and 2-RDMs, and a selection of the EOM method to solve.

R2: Verify that the input RDMs satisfy the physical constraints listes in Table 1.

R3: Verify that the input electron integrals satisfy the symmetry properties in DD3.

R4: Calculate the energies and TDMs using the instance models corresponding to the method selected by the user (IM1 - IM6)

R5: Output $\Delta E_0$ (from IM1 - IM5 as applicable) and $\gamma_{n;0k}$ (from IM6).

R6: The user should have the knowledge to assess whether the returned parameters have physical meaning for their system of interest.

## 5.2 Nonfunctional Requirements

- Reusable: The code should be modular so that future improvements (like the implementation of new EOMs) don't imply major feature changes.

- Portable: The software should run in multiple platforms.

- Usable: The software should be well documented so that an intermediate user doesn't need more than a day to understand the code's purpose and not more than three hours to prepare and run a calculation.

- Correct: It should follow the inputs and outputs requirements. It can be tested using as reference available literature data for atomic IP and electronic excitation energies.

# 6 Likely Changes

LC1: Alternative expressions for the evaluation of IP, EA or excitation energies can be derived based on the application of the "killer condition" (A5)

LC2: A different projection space than the one generated by the transition operator's BS could be used (A6), in which case TDMs might be required as inputs instead of the RDMs

# 7 Unlikely Changes

LC3: The matrix representation of the EOM equations.

# 8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an "X" may have to be modified as well. Table 6 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 5 shows the dependencies of instance models, requirements, and data constraints on each other. Table 4 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

# 9 Values of Auxiliary Constants

There are not auxiliary constants defined.

|      | A1 | A2 | A3 | A4 | A5 | A6 |
| ---- | -- | -- | -- | -- | -- | -- |
| T1   |    |    |    |    |    |    |
| T2   |    |    |    |    |    |    |
| T3   |    |    |    |    |    |    |
| T4   |    |    |    |    |    |    |
| GD1  | X  |    |    |    |    |    |
| GD2  |    |    |    |    | X  | X  |
| DD1  |    |    |    |    |    |    |
| DD2  |    |    | X  | X  |    |    |
| DD3  |    |    | X  | X  |    |    |
| DD4  |    |    |    | X  |    |    |
| DD5  |    |    |    | X  |    |    |
| IM1  |    | X  |    |    |    | X  |
| IM2  |    | X  |    |    |    | X  |
| IM3  |    | X  |    |    |    | X  |
| IM4  |    | X  |    |    |    | X  |
| IM5  |    | X  |    |    |    | X  |
| IM6  |    |    |    |    |    |    |

Table 4: Traceability Matrix Showing the Connections Between Assumptions and Other Items

|      | IM1 | IM2 | IM3 | IM4 | IM5 | IM6 | R1 | R2 | R3 | R4 | R5 | R6 |
|------|-----|-----|-----|-----|-----|-----|----|----|----|----|----|----|
| IM1  |     |     |     |     |     |     |    |    |    | X  | X  |    |
| IM2  |     |     |     |     |     |     |    |    |    | X  | X  |    |
| IM3  |     |     |     |     |     |     |    |    |    | X  | X  |    |
| IM4  |     |     |     |     |     |     |    |    |    | X  | X  |    |
| IM5  |     |     |     |     |     |     |    |    |    | X  | X  |    |
| IM6  |     |     |     |     |     |     |    |    |    | X  | X  |    |
| R1   |     |     |     |     |     |     |    |    |    |    |    |    |
| R2   |     |     |     |     |     |     |    |    |    |    |    |    |
| R3   |     |     |     |     |     |     |    |    |    |    |    |    |
| R4   |     |     |     |     |     |     |    |    |    |    |    |    |
| R5   |     |     |     |     |     |     |    |    |    |    |    |    |
| R6   |     |     |     |     |     |     |    |    |    |    |    |    |

Table 5: Traceability Matrix Showing the Connections Between Requirements and Instance Models

|  | T1 | T2 | T3 | T4 | GD1 | GD2 | DD1 | DD2 | DD3 | DD4 | DD5 | IM1 | IM2 | IM3 | IM4 | IM5 | IM6 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T1 |  |  |  |  |  | X | X |  |  |  |  |  |  |  |  |  |  |
| T2 |  |  |  | X | X | X |  |  |  |  |  |  |  |  |  |  |  |
| T3 |  |  |  |  |  | X |  |  |  |  |  |  |  |  |  |  |  |
| T4 |  | X |  |  | X |  |  |  |  |  |  |  |  |  |  |  |  |
| GD1 |  | X |  | X |  |  |  |  |  |  |  | X | X | X | X | X | X |
| GD2 | X | X | X |  |  |  |  |  |  |  |  | X | X | X | X | X |  |
| DD1 | X |  |  |  |  |  |  | X | X |  |  |  |  |  |  |  |  |
| DD2 |  |  |  |  |  |  | X |  |  |  |  | X | X | X | X | X |  |
| DD3 |  |  |  |  |  |  | X |  |  |  |  | X | X | X | X | X |  |
| DD4 |  |  |  |  |  |  |  |  |  |  |  | X | X | X | X | X | X |
| DD5 |  |  |  |  |  |  |  |  |  |  |  | X | X | X | X | X | X |
| IM1 |  |  |  |  | X | X |  | X | X | X | X |  |  |  |  |  |  |
| IM2 |  |  |  |  | X | X |  | X | X | X | X |  |  |  |  |  |  |
| IM3 |  |  |  |  | X | X |  | X | X | X | X |  |  |  |  |  |  |
| IM4 |  |  |  |  | X | X |  | X | X | X | X |  |  |  |  |  |  |
| IM5 |  |  |  |  | X | X |  | X | X | X | X |  |  |  |  |  |  |
| IM6 |  |  |  |  | X |  |  |  |  | X | X |  |  |  |  |  |  |

Table 6: Traceability Matrix Showing the Connections Between Items of Different Sections