SpinDec

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Class Documentation

4.1 SpinDec::AdiabaticLabel Class Reference

Adiabatic eigenstates of a spin donor.

```
#include <AdiabaticLabel.h>
```

Public Member Functions

- **AdiabaticLabel** (const Sign &sign, const int quantum_number)
- const Sign & **get_sign** () const
- int **get_quantum_number** () const

Private Attributes

- Sign sign_

  Plus or minus.

- int quantum_number_

  $m = S + I$.

Friends

- std::ostream & operator<< (std::ostream &os, AdiabaticLabel const &label)

  Print.

4.1.1 Detailed Description

Adiabatic eigenstates of a spin donor. For a spin donor, the adiabatic energy eigenstates are labeled as follows:

$|\pm, m\rangle$, where $m = S + I$ is an integer, S and I are the electron and nuclear spin quantum numbers.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/AdiabaticLabel.h
- /home/sbalian/spindec/src/AdiabaticLabel.cpp

4.2 SpinDec::BoostEigen Class Reference

Static methods to extend Eigen functionality.

```
#include <BoostEigen.h>
```

Static Public Member Functions

- static double cosAngleBetween (const ThreeVector &a, const ThreeVector &b)

  Cosine of angle between real vectors.

- static double maxAbsCoeff (const ThreeVector &a)

  Maximum absolute coefficient.

- static ComplexVector exp (const ComplexVector &a)

  Element-wise exponentiation for complex vectors.

- static ComplexMatrix tensorProduct (const ComplexMatrix &A, const ComplexMatrix &B)

  Tensor product for complex matrices.

- static ComplexVector tensorProduct (const ComplexVector &a, const ComplexVector &b)

  Tensor product for complex vectors.

- static ComplexMatrix partialTrace (const ComplexMatrix &AB, const unsigned int dimension_B)

  Partial trace for complex matrices.

- static ComplexMatrix spectralDecomposition (const ComplexMatrix &eigenvectors, const ComplexVector &eigenvalues)

  Spectral decomposition of a complex matrix.

- static ComplexMatrix unitarySpectralDecomposition (const ComplexMatrix &eigenvectors, const ComplexVector &eigenvalues)

  Spectral decomposition of a unitary matrix.

- static bool isWithinDistance (const ThreeVector &r, const double distance)

  Is $|\mathbf{r}| \leq d$*?*

4.2.1 Detailed Description

Static methods to extend Eigen functionality. Note that the naming convention complies with that of Eigen, and is different from the rest of SpinDec. Eigen is for linear algebra and can be obtained for free: `http://eigen.tuxfamily.org/` .

4.2.2 Member Function Documentation

4.2.2.1 double SpinDec::BoostEigen::cosAngleBetween (const ThreeVector & *a*, const ThreeVector & *b*) `[static]`

Cosine of angle between real vectors. $\cos\theta = \frac{\mathbf{a}\cdot\mathbf{b}}{|\mathbf{a}||\mathbf{b}|}$.

4.2.2.2 double SpinDec::BoostEigen::maxAbsCoeff (const ThreeVector & *a*) `[static]`

Maximum absolute coefficient. Maximum of $[|a_1|, |a_2|, |a_3|]$ for real vector $\mathbf{a} = (a_1, a_2, a_3)$.

4.2.2.3 ComplexMatrix SpinDec::BoostEigen::partialTrace (const ComplexMatrix & *AB*, const unsigned int *dimension_B*) `[static]`

Partial trace for complex matrices. Given $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$, and the dimension of $\mathbf{B}$, this method outputs $\mathrm{Tr}_{\mathbf{B}} \mathbf{A}$.

4.2.2.4 ComplexMatrix SpinDec::BoostEigen::spectralDecomposition (const ComplexMatrix & *eigenvectors*, const ComplexVector & *eigenvalues*) `[static]`

Spectral decomposition of a complex matrix. This is $\mathbf{A} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1}$, where $\mathbf{D}$ is the diagonal of eigenvalues of $\mathbf{A}$ and $\mathbf{V}$ is the columnwise eigenvector matrix.

4.2.2.5 ComplexVector SpinDec::BoostEigen::tensorProduct (const ComplexVector & *a*, const ComplexVector & *b*) `[static]`

Tensor product for complex vectors. Evaluates $\mathbf{c} = \mathbf{a} \otimes \mathbf{b}$. For example, for 2-vectors, this is

$$\mathbf{c} = \left(\begin{array}{c} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{array} \right)$$

4.2.2.6 ComplexMatrix SpinDec::BoostEigen::tensorProduct (const ComplexMatrix & *A*, const ComplexMatrix & *B*) `[static]`

Tensor product for complex matrices. Evaluates $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$. For example, for 2×2 matrices, this is

$$\mathbf{C} = \left(\begin{array}{cc} A_{11}\mathbf{B} & A_{12}\mathbf{B} \\ A_{21}\mathbf{B} & A_{22}\mathbf{B} \end{array} \right)$$

4.2.2.7 ComplexMatrix SpinDec::BoostEigen::unitarySpectralDecomposition (const ComplexMatrix & *eigenvectors*, const ComplexVector & *eigenvalues*) `[static]`

Spectral decomposition of a unitary matrix. For a unitary matrix, $\mathbf{A}^{-1} = \mathbf{V}^{\dagger}$

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/BoostEigen.h
- /home/sbalian/spindec/src/BoostEigen.cpp

4.3 SpinDec::CCE Class Reference

Solves for a CSD problem using the CCE.

```
#include <CCE.h>
```

Public Member Functions

- **CCE** (const UInt max_truncation_order, const auto_ptr< PulseExperiment > &pulse_experiment, const ClusterDatabase &cluster_database, const bool include_one_clusters)
- UInt **get_max_truncation_order** () const
- void calculate (const UInt order)

    Calculate the CCE.

- void **calculate** (const UInt order, const bool no_divisions)
- void calculate ()

    Calls CCE::calculate(const UInt order,false).

- TimeEvolution evolution (const UInt order) const

    Get the time evolution (has to be calculated with above method first).

- const ClusterDatabase & **get_database** () const

Private Member Functions

- void **check_order** (const UInt order) const
- TimeEvolution **reducible_correlation** (const Cluster &cluster)
- TimeEvolution **true_correlation** (const Cluster &cluster)

Private Attributes

- vector< TimeEvolution > **product_correlations_by_order_**
- UInt max_truncation_order_

    Maximum CCE truncation order.

- bool **include_one_clusters_**
- auto_ptr< PulseExperiment > **pulse_experiment_**
- ClusterDatabase **cluster_database_**

4.3.1 Detailed Description

Solves for a CSD problem using the CCE. The cluster correlation expansion (CCE) is used to solve for a central spin decoherence (CSD) problem. Relevant references are:

- Phys. Rev. B 74, 035322 (2006),
- Phys. Rev. B 78, 085315 (2008),
- Phys. Rev. B 78, 129901(E) (2008),
- Phys. Rev. B 79, 115320 (2009),
- Phys. Rev. B 86, 035452 (2012).

4.3.2 Member Function Documentation

4.3.2.1 void SpinDec::CCE::calculate (const UInt *order*)

Calculate the CCE. Input CCE truncation order to calculate. This input cannot exceed CCE::max_truncation_order_.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/CCE.h
- /home/sbalian/spindec/src/CCE.cpp

4.4 SpinDec::Cluster Class Reference

Contains labels for a cluster of spins.

```
#include <Cluster.h>
```

Public Member Functions

- **Cluster** (const UIntArray &labels)
- void **add** (const UInt label)
- bool **operator==** (const Cluster &rhs) const
- UInt num_spins () const

  Number of labels.

- UInt **get_label** (const UInt index) const
- const UIntArray & **get_labels** () const
- vector< Cluster > subsets () const

  Get all subsets (exludes the empty set).

- vector< Cluster > proper_subsets () const

  Get proper subsets (excludes the empty set).

Private Member Functions

- vector< UIntArray > **subsets** (const UIntArray &v, const UInt size) const
- vector< UIntArray > **subsets** (const UIntArray &v) const

Private Attributes

- UIntArray **labels_**

Friends

- std::ostream & operator<< (std::ostream &os, Cluster const &cluster)

  Print.

4.4.1 Detailed Description

Contains labels for a cluster of spins. Labels are always sorted in increasing order.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Cluster.h
- /home/sbalian/spindec/src/Cluster.cpp

4.5 SpinDec::ClusterDatabase Class Reference

Stores clusters and associated complex time evolutions.

```
#include <ClusterDatabase.h>
```

Public Member Functions

- ClusterDatabase (const SpinBath &spin_bath, const UInt max_order, const double cluster_cutoff, const string &build_method)

  Build method is "global" or "local".

- const ClusterDatabaseEntry & **get_entry** (const UInt order, const UInt index) const
- const Cluster & **get_cluster** (const UInt order, const UInt index) const
- void **set_time_evolution** (const Cluster &cluster, const TimeEvolution &time_evolution)
- bool **is_solved** (const Cluster &cluster) const
- UInt **get_max_order** () const
- UInt **num_clusters** (const UInt order) const
- const TimeEvolution & **get_time_evolution** (const Cluster &cluster) const
- void **print** () const

Private Member Functions

- void build_pairs ()

  Build 2-clusters.

- void build_ones ()

  Build 1-clusters.

- void build_with_local_cutoff ()

  Higher order clusters with local cutoff.

- void build_with_global_cutoff ()

  Higher order clusters with global cutoff.

- UInt **get_index** (const Cluster &cluster) const
- void add_unsolved_entry (const Cluster &cluster)

  Add cluster if it does not exist.

- bool **is_order_built** (const UInt order) const
- bool **cluster_exists** (const Cluster &cluster) const

Private Attributes

- UInt max_order_

  Maximum build order.

- SpinBath **spin_bath_**
- database_map database_

Cluster size (order), vector of database entries. All unique clusters.

- double cluster_cutoff_

  In Å.

4.5.1 Detailed Description

Stores clusters and associated complex time evolutions. For use with SpinDec::CCE (cluster correlation expansion). Has two build methods, one with a local cluster cutoff where the maximum separation between any pair of spins in any cluster is cluster_cutoff. The other (global) method builds pairs with cluster_cutoff maximum separation, then adds spins which are at a maximum of cluster_cutoff from any of the two spins to form 3-clusters, and so on for 4-clusters etc.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/ClusterDatabase.h
- /home/sbalian/spindec/src/ClusterDatabase.cpp

4.6 SpinDec::ClusterDatabaseEntry Class Reference

Entry for ClusterDatabase.

```
#include <ClusterDatabaseEntry.h>
```

Public Member Functions

- ClusterDatabaseEntry (const Cluster &cluster)

  is_solved_ = false.
- const Cluster & **get_cluster** () const
- bool **is_solved** () const
- const TimeEvolution & **get_time_evolution** () const
- void **set_time_evolution** (const TimeEvolution &time_evolution)

Private Attributes

- Cluster **cluster_**
- TimeEvolution **time_evolution_**
- bool **is_solved_**

4.6.1 Detailed Description

Entry for ClusterDatabase.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/ClusterDatabaseEntry.h
- /home/sbalian/spindec/src/ClusterDatabaseEntry.cpp

4.7 SpinDec::Constants Class Reference

Mathematical and physical constants.

```
#include <Constants.h>
```

Static Public Attributes

- static const double kPi = 3.141592653589793

  Pi.

- static const double kReducedPlanck = 1.054571726e-34

  Reduced Planck constant (J s).

- static const double kPlanck = 6.62606957e-34

  Plank constant (J s).

- static const double kElectronGyromagneticRatio = 1.760859708e5

  Electronic gyromagnetic ratio (M rad s^{-1} T^{-1}).

4.7.1 Detailed Description

Mathematical and physical constants.

4.7.2 Member Data Documentation

4.7.2.1 const double SpinDec::Constants::kElectronGyromagneticRatio = 1.760859708e5 `[static]`

Electronic gyromagnetic ratio (M rad s^{-1} T^{-1}). From CODATA 22/10/2013.

4.7.2.2 const double SpinDec::Constants::kPi = 3.141592653589793 `[static]`

Pi. From Wikipedia 06/12/2012.

4.7.2.3 const double SpinDec::Constants::kPlanck = 6.62606957e-34 `[static]`

Plank constant (J s). From CODATA 06/12/2012.

4.7.2.4 const double SpinDec::Constants::kReducedPlanck = 1.054571726e-34 `[static]`

Reduced Planck constant (J s). From CODATA 06/12/2012.

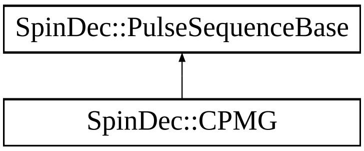
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Constants.h
- /home/sbalian/spindec/src/Constants.cpp

4.8 SpinDec::CPMG Class Reference

Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence.

`#include <CPMG.h>`Inheritance diagram for SpinDec::CPMG::



Public Member Functions

- **CPMG** (const UInt order, const EvolutionOperator &evolution_operator, const Pulse &pi_pulse)
- void **set_time** (const double time_value)
- virtual auto_ptr< PulseSequenceBase > **clone** () const

Private Attributes

- UInt **order_**
- EvolutionOperator **evolution_operator_**
- vector< bool > **is_unitary_**

4.8.1 Detailed Description

Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence.

- Order $N = 0$ (FID): evolve for duration t.
- $N = 1$ (Hahn): evolve for $t/2$, π-pulse, evolve for $t/2$.
- $N > 1$: [evolve for $t/(2N)$, π-pulse, evolve for $t/(2N)]^N$.

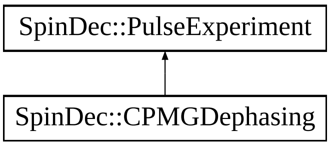
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/CPMG.h
- /home/sbalian/spindec/src/CPMG.cpp

4.9 SpinDec::CPMGDephasing Class Reference

CPMG pulse sequence.

`#include <CPMGDephasing.h>`Inheritance diagram for SpinDec::CPMGDephasing::



Public Member Functions

- **CPMGDephasing** (const CSDProblem &csd_problem, const TimeArray &time_array, const UInt cpmg_order, const CDouble &c0, const UInt level_label0, const CDouble &c1, const UInt level_label1)
- virtual TimeEvolution **time_evolution** (const UIntArray bath_indices)
- virtual auto_ptr< PulseExperiment > **clone** () const

Private Attributes

- UInt **cpmg_order_**
- TwoStateSuperposition **initial_system_state_**
- PiPulse **system_pi_pulse_**
- vector< pair< UInt, Pulse > > **pulses_**

4.9.1 Detailed Description

CPMG pulse sequence.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/CPMGDephasing.h
- /home/sbalian/spindec/src/CPMGDephasing.cpp

4.10 SpinDec::CrystalBasis Class Reference

Basis vectors for crystal structures in 3D.

```
#include <CrystalBasis.h>
```

Public Member Functions

- void **add_basis_vector** (const ThreeVector &basis_vector)
- const std::vector< ThreeVector > & **get_basis_vectors** () const
- const ThreeVector & **get_basis_vector** (const UInt index) const
- UInt **num_basis_vectors** () const

Protected Attributes

- std::vector< ThreeVector > **basis_vectors_**

4.10.1 Detailed Description

Basis vectors for crystal structures in 3D. Length units are Å. They are in the basis of lattice vectors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, NOT (x, y, z)!

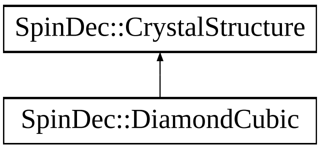
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/CrystalBasis.h
- /home/sbalian/spindec/src/CrystalBasis.cpp

4.11 SpinDec::CrystalStructure Class Reference

$i\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3 + \sum_n \mathbf{b}_n$.

`#include <CrystalStructure.h>`Inheritance diagram for SpinDec::CrystalStructure::



Public Member Functions

- CrystalStructure (const LatticeVectors &lattice_vectors, const CrystalBasis &basis, const int min_i, const int max_i, const int min_j, const int max_j, const int min_k, const int max_k, const double min_x, const double max_x, const double min_y, const double max_y, const double min_z, const double max_z, const double fractional_abundance)

  Calls fill_site_vectors.

- CrystalStructure (const string &file_name)

  Reads from file. Three columns: x, y, z.

- **CrystalStructure** (const vector< ThreeVector > &site_vectors)
- const std::vector< ThreeVector > & **get_site_vectors** () const
- const ThreeVector & **get_site_vector** (const UInt index) const
- UInt **num_site_vectors** () const
- double **max_site_vector_length** () const
- double max_abs_component () const

  $\max[\max(|x_1|, |y_1|, |z_1|), \ldots, \max(|x_n|, |y_n|, |z_n|)]$, *for n site vectors.*

- double **average_site_vector_separation** () const
- void **write_site_vectors** (const string &file_name) const

Protected Member Functions

- void fill_site_vectors (const LatticeVectors &lattice_vectors, const CrystalBasis &basis, const int min_i, const int max_i, const int min_j, const int max_j, const int min_k, const int max_k, const double min_x, const double max_x, const double min_y, const double max_y, const double min_z, const double max_z, const double fractional_abundance)

  Fills site vectors.

- void **add_site_vector** (const ThreeVector &site_vector)
- void **scale_site_vectors** (const double scale_factor)
- std::vector< ThreeVector > cartesian_basis_vectors (const LatticeVectors &lattice_vectors, const CrystalBasis &basis) const

  Get the basis vectors in Cartesian coordinates.

Protected Attributes

- std::vector< ThreeVector > **site_vectors_**

Private Member Functions

- void **read_site_vectors** (const string &file_name)

Friends

- std::ostream & operator<< (std::ostream &os, CrystalStructure const &crystal_structure)

  Print with cout (x, y, z).

4.11.1 Detailed Description

$i\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3 + \sum_n \mathbf{b}_n$. The above = crystal structure, where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are linearly independent lattice vectors, the $\mathbf{b}_n$ are n basis vectors and i, j, k are integers.

The length units are Å. Using Cartesian coordinates.

4.11.2 Member Function Documentation

4.11.2.1 void SpinDec::CrystalStructure::fill_site_vectors (const LatticeVectors & *lattice_vectors*, const CrystalBasis & *basis*, const int *min_i*, const int *max_i*, const int *min_j*, const int *max_j*, const int *min_k*, const int *max_k*, const double *min_x*, const double *max_x*, const double *min_y*, const double *max_y*, const double *min_z*, const double *max_z*, const double *fractional_abundance*) `[protected]`

Fills site vectors. Here, the integer arguments are the i, j, k. The double arguments define the spatial ranges for all the x, y, z components for shaping the final crystal structure. The fractional abundance (converted to parts per million) is the fraction of site vectors added using a uniform distribution (using cstdlib rand(); see RandomNumberGenerator.h). If the fractional abundance is 1.0, then all site vectors are included.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/CrystalStructure.h
- /home/sbalian/spindec/src/CrystalStructure.cpp

4.12 SpinDec::CSDProblem Class Reference

Central spin decoherence problem.

```
#include <CSDProblem.h>
```

Public Member Functions

- **CSDProblem** (const CSDProblem &csd_problem)
- CSDProblem & **operator=** (const CSDProblem &csd_problem)
- **CSDProblem** (const auto_ptr< SpinSystemBase > &central_spin_system_base, const SpinBath &spin_bath, const vector< SpinInteractionEdge > &system_bath_edges, const UniformMagneticField &field)
- **CSDProblem** (const auto_ptr< SpinSystemBase > &central_spin_system_base, const SpinBath &spin_bath, const SpinInteractionEdge &system_bath_edge, const UniformMagneticField &field)

- void **set_central_spin_state** (const SpinState &spin_state) const
- SpinSystem **get_reduced_problem** (const UIntArray bath_indices)
- const SpinBath & **get_spin_bath** () const
- auto_ptr< SpinSystemBase > **get_central_spin_system** () const

Private Member Functions

- void **init** (const auto_ptr< SpinSystemBase > &central_spin_system_base, const SpinBath &spin_bath, const vector< SpinInteractionEdge > &system_bath_edges, const UniformMagneticField &field)
- vector< SpinInteractionEdge > **make_system_bath_edges** (const UInt order, const SpinInteractionEdge &edge) const
- vector< SpinInteractionEdge > **make_system_bath_edges** (const UInt order) const
- SpinSystem **construct_reduced_problem** (const UInt order) const
- UIntArray **get_bath_vertex_labels** (const UInt order) const

Private Attributes

- auto_ptr< SpinSystemBase > **central_spin_system_**
- SpinBath **spin_bath_**
- UniformMagneticField **field_**
- vector< SpinInteractionEdge > system_bath_edges_
- vector< pair< UInt, SpinSystem > > **reduced_problems_**

4.12.1 Detailed Description

Central spin decoherence problem. Currently supports a single spin bath.

4.12.2 Member Data Documentation

4.12.2.1 vector<SpinInteractionEdge> SpinDec::CSDProblem::system_bath_edges_ [private]

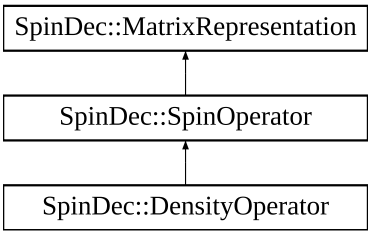
Edges should comply as in the join methods for SpinInteractionGraph, with the first graph being the central spin graph and the second being the graph for a single bath system.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/CSDProblem.h
- /home/sbalian/spindec/src/CSDProblem.cpp

4.13 SpinDec::DensityOperator Class Reference

`#include <DensityOperator.h>`Inheritance diagram for SpinDec::DensityOperator::



Public Member Functions

- DensityOperator (const SpinState &state, const SpinState &state0, const SpinState &state1)

  State is the combined (tensor product) qubit-other system state.

- DensityOperator reduced () const

  Return the qubit reduced density matrix.

- CDouble off_diagonal_reduced () const

  Off-diagonal of reduced density matrix.

Private Member Functions

- **DensityOperator** (const ComplexMatrix &matrix, const SpinBasis &basis, const SpinState &state0, const SpinState &state1)

Private Attributes

- SpinState **state0_**
- SpinState **state1_**

4.13.1 Detailed Description

In general, composite density operator for spins in the Zeeman basis. $\rho_{\mathrm{qubit}} \otimes \rho_{\mathrm{other}}$, qubit states $|0\rangle$ and $|1\rangle$.

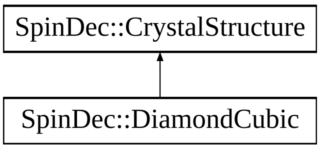
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/DensityOperator.h
- /home/sbalian/spindec/src/DensityOperator.cpp

4.14 SpinDec::DiamondCubic Class Reference

Diamond cubic crystal structure.

`#include <DiamondCubic.h>`Inheritance diagram for SpinDec::DiamondCubic::



Public Member Functions

- DiamondCubic (const double lattice_constant, const double side_length)

  Cubic lattice constant and side length of superlattice cube in Å.

- **DiamondCubic** (const double lattice_constant, const double side_length, const double fractional_abundance)
- void **make_sphere** (const double radius)
- void **make_shell** (const double min_radius, const double max_radius)

Private Member Functions

- SimpleCubicLatticeVectors construct_lattice_vectors (const double lattice_constant) const

  Set up and return the lattice vectors.

- CrystalBasis construct_basis_vectors () const

  Set up and return the basis vectors.

- int int_range_centred_cube (const double side_length, const double lattice_constant) const

4.14.1 Detailed Description

Diamond cubic crystal structure. This is implemented as a simple cubic lattice with 8 basis vectors. Source: `http://en.wikipedia.org/wiki/Diamond_cubic.`

4.14.2 Member Function Documentation

4.14.2.1 int SpinDec::DiamondCubic::int_range_centred_cube (const double *side_length*, const double *lattice_constant*) const `[private]`

Get integer range (for constructing crystal structure) in a centred cube given the side length.

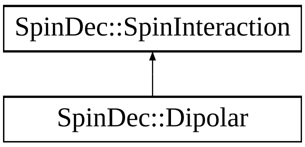
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/DiamondCubic.h
- /home/sbalian/spindec/src/DiamondCubic.cpp

4.15 SpinDec::Dipolar Class Reference

Secular dipolar interaction strength between a pair of spins.

`#include <Dipolar.h>`Inheritance diagram for SpinDec::Dipolar::



Public Member Functions

- Dipolar ()

  If you wish to calculate.

- Dipolar (const double strength)

  If you don't wish to calculate.

- virtual void **calculate** (const SpinParameters &spin_parameters1, const SpinParameters &spin_parameters2, const ThreeVector &position1, const ThreeVector &position2, const UniformMagneticField &field)
- virtual void **fill** (ComplexMatrix ∗hamiltonian, const SpinParametersVector &spin_parameters_vector, const SpinBasis &basis, const UInt spin_label1, const UInt spin_label2) const
- virtual auto_ptr< SpinInteraction > **clone** () const
- virtual string **get_type** () const

4.15.1 Detailed Description

Secular dipolar interaction strength between a pair of spins. For two spins, $\hat{\mathbf{S}}_1, \hat{\mathbf{S}}_2$,

$$\hat{H}_D = D\hat{S}_1^z\hat{S}_2^z - \frac{D}{4}[\hat{S}_1^+\hat{S}_2^- + \hat{S}_1^-\hat{S}_2^+]$$

This class calculates

$$D = \frac{D_0\gamma_1\gamma_2(1-3\cos^2[\theta])}{(10^{-10}r)^3}$$

and fills the Hamiltonian matrix elements for the Hamiltonian $\hat{H}_D$ above. The energy units are M rad s^{-1}.

The parameters are:

- γ_1, γ_2 [M rad s^{-1}T^{-1}]: gyromagnetic ratios of the two interacting spins.
- θ [rad]: angle between the magnetic field direction and the vector parallel to the line connecting the two spins.
- r [Å]: distance between the two spins.
- $D_0 = 10^6(\mu_0/(4\pi))\hbar$ [M rad s^{-1} m^3].
- $\hbar$ [J s]: reduced Plank constant.

- $\mu_0/(4\pi) = 10^{-7}$ NA^{-2} (μ_0 is the vacuum permeability).

From: arXiv:cond-mat/0211567 (Phys. Rev. B 68, 115322 (2003)).

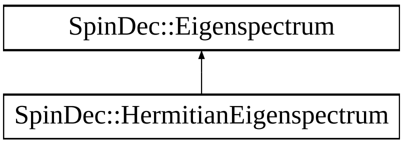
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Dipolar.h
- /home/sbalian/spindec/src/Dipolar.cpp

4.16 SpinDec::Eigenspectrum Class Reference

Holds the eigenvectors and eigenvalues of a matrix.

`#include <Eigenspectrum.h>`Inheritance diagram for SpinDec::Eigenspectrum::



Public Member Functions

- **Eigenspectrum** (const ComplexMatrix &matrix)
- const ComplexVector & **get_eigenvalues** () const
- const ComplexMatrix & **get_eigenvectors** () const
- CDouble **get_eigenvalue** (const UInt index) const
- ComplexVector **get_eigenvector** (const UInt index) const
- virtual ComplexMatrix spectralDecomposition () const

  Note the Eigen naming convention here.

- void set_spectrum (const ComplexMatrix &eigenvectors, const ComplexVector &eigenvalues)

  NOTE: use with care.

Protected Member Functions

- virtual void **diagonalize** (const ComplexMatrix &matrix)

Protected Attributes

- ComplexMatrix **eigenvectors_**
- ComplexVector **eigenvalues_**

4.16.1 Detailed Description

Holds the eigenvectors and eigenvalues of a matrix. Note: eigenvectors stored columnwise. General complex diagonalizer: ComplexEigenSolver in Eigen.

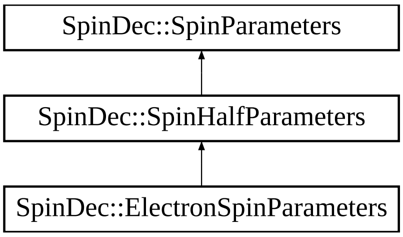
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Eigenspectrum.h
- /home/sbalian/spindec/src/Eigenspectrum.cpp

4.17 SpinDec::ElectronSpinParameters Class Reference

Parameters for an electron spin.

`#include <ElectronSpinParameters.h>`Inheritance diagram for SpinDec::ElectronSpinParameters::



Public Member Functions

- ElectronSpinParameters ()

  Free electron gyromagnetic ratio.

- **ElectronSpinParameters** (const double gyromagnetic_ratio)

4.17.1 Detailed Description

Parameters for an electron spin. Gyromagnetic ratio of the free electron by default.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/ElectronSpinParameters.h
- /home/sbalian/spindec/src/ElectronSpinParameters.cpp

4.18 SpinDec::Errors Class Reference

Error and warning handling.

```
#include <Errors.h>
```

Static Public Member Functions

- static void **quit** ()
- static void **quit** (const string &message)
- static void **warning** (const string &message)

4.18.1 Detailed Description

Error and warning handling.

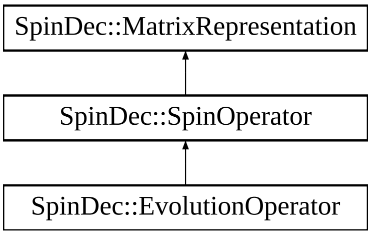
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Errors.h
- /home/sbalian/spindec/src/Errors.cpp

4.19 SpinDec::EvolutionOperator Class Reference

Free evolution operator.

`#include <EvolutionOperator.h>`Inheritance diagram for SpinDec::EvolutionOperator::



Public Member Functions

- EvolutionOperator (const SpinBasis &basis, const ComplexMatrix &eigenvectors, const RealVector &eigenvalues, const double time)
- void set_time (const double time)

  Updates matrix.

- double **get_time** () const

Private Member Functions

- void **set_matrix** ()

Private Attributes

- double **time_**
- ComplexMatrix eigenvectors_
- RealVector eigenvalues_

4.19.1 Detailed Description

Free evolution operator.

4.19.2 Constructor & Destructor Documentation

4.19.2.1 SpinDec::EvolutionOperator::EvolutionOperator (const SpinBasis & *basis*, const ComplexMatrix & *eigenvectors*, const RealVector & *eigenvalues*, const double *time*)

Unitary operator

$$\hat{U} = \sum_n \left(|E_n\rangle \exp[-iE_n t] \langle E_n| \right)$$

- E_n: eigenvalues (real).
- $|E_n\rangle$: eigenvectors.

- t: time (real double) in microseconds (energies in M rad s^{-1}).

For time independent Hamiltonians.

4.19.3 Member Data Documentation

4.19.3.1 RealVector SpinDec::EvolutionOperator::eigenvalues_ [private]

Not for the resulting opertor! These are used to construct the operator, for example from a Hamiltonian.

4.19.3.2 ComplexMatrix SpinDec::EvolutionOperator::eigenvectors_ [private]

Not for the resulting opertor! These are used to construct the operator, for example from a Hamiltonian.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/EvolutionOperator.h
- /home/sbalian/spindec/src/EvolutionOperator.cpp

4.20 SpinDec::FileProperties Class Reference

Static methods for ASCII file properties.

```
#include <FileProperties.h>
```

Static Public Member Functions

- static bool **exists** (const string file_name)
- static UInt num_lines (const string file_name)

  NOTE: empty lines not counted.

4.20.1 Detailed Description

Static methods for ASCII file properties.

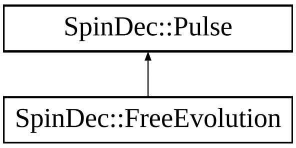
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/FileProperties.h
- /home/sbalian/spindec/src/FileProperties.cpp

4.21 SpinDec::FreeEvolution Class Reference

(Pulse)-free evolution.

`#include <FreeEvolution.h>`Inheritance diagram for SpinDec::FreeEvolution::



Public Member Functions

- FreeEvolution (const EvolutionOperator &evolution_operator)

  "Pulse" duration taken from evolution operator.

4.21.1 Detailed Description

(Pulse)-free evolution.

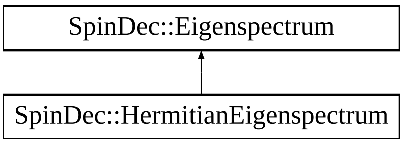
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/FreeEvolution.h
- /home/sbalian/spindec/src/FreeEvolution.cpp

4.22 SpinDec::HermitianEigenspectrum Class Reference

Diagonalizes a Hermitian matrix.

`#include <HermitianEigenspectrum.h>`Inheritance diagram for SpinDec::HermitianEigenspectrum::



Public Member Functions

- **HermitianEigenspectrum** (const ComplexMatrix &matrix)
- virtual ComplexMatrix spectralDecomposition () const

Private Member Functions

- void diagonalize_eigen (const ComplexMatrix &matrix)

  Diagonalizer.

- virtual void **diagonalize** (const ComplexMatrix &matrix)

4.22.1 Detailed Description

Diagonalizes a Hermitian matrix. Eigenvectors are orthonormal, eigenvalues are always real.

4.22.2 Member Function Documentation

4.22.2.1 ComplexMatrix SpinDec::HermitianEigenspectrum::spectralDecomposition () const `[virtual]`

Since eigenvectors orthonormal, $V^{-1} = V^{\dagger}$, use faster (unitary) decomposition.

Reimplemented from SpinDec::Eigenspectrum.

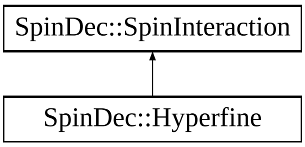
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/HermitianEigenspectrum.h
- /home/sbalian/spindec/src/HermitianEigenspectrum.cpp

4.23 SpinDec::Hyperfine Class Reference

Calculates the electron-nuclear hyperfine interaction in a lattice.

`#include <Hyperfine.h>`Inheritance diagram for SpinDec::Hyperfine::



Public Member Functions

- Hyperfine (const HyperfineParameters &parameters)

  If you wish to calculate.

- Hyperfine (const double strength)

  If you don't wish to calculate.

- virtual void **calculate** (const SpinParameters &electron_parameters, const SpinParameters &nuclear_parameters, const ThreeVector &electron_position, const ThreeVector &nuclear_position, const UniformMagneticField &field)
- virtual void **fill** (ComplexMatrix $*$hamiltonian, const SpinParametersVector &spin_parameters_vector, const SpinBasis &basis, const UInt spin_label1, const UInt spin_label2) const
- virtual auto_ptr< SpinInteraction > **clone** () const
- virtual string **get_type** () const

Private Member Functions

- double **envelope_function** (const UInt index, const ThreeVector &separation) const
- double **n_parameter** () const
- double **n_times_a** () const
- double **n_times_b** () const
- double **scaled_probability_density** (const ThreeVector &separation) const

Private Attributes

- HyperfineParameters **parameters_**

4.23.1 Detailed Description

Calculates the electron-nuclear hyperfine interaction in a lattice. The Hamiltonian is

$$\hat{H}_A = A\hat{S}^z\hat{I}^z + \frac{A}{2}\left[\hat{S}^+\hat{I}^- + \hat{S}^-\hat{I}^+\right]$$

This class calculates A for the above Hamiltonian, $\hat{H}_A$, where $\hat{\mathbf{S}}$ and $\hat{\mathbf{I}}$ are the electronic and nuclear spin operators. Also fills the Hamiltonian matrix elements for $\hat{H}_A$. Uses the Kohn-Luttinger electronic wavefunction. Energy units are M rad s^{-1}.

$$A = pq - D(R)\theta(|R| - na)$$

The first term pq is the isotropic Fermi contact part.

$$p = \frac{16}{9}\pi\hbar\gamma_e\gamma_n\eta$$

where

- $\hbar$: reduced Planck constant [J s].
- γ_e: electron gyromagnetic ratio [M rad $\mathrm{s}^{-1}\mathrm{T}^{-1}$].
- γ_n: nuclear gyromagnetic ratio [M rad $\mathrm{s}^{-1}\mathrm{T}^{-1}$].
- η: charge density.

$$q = (10^{30})|F_1(R)\cos(k_0 x) + F_3(R)\cos(k_0 y) + F_5(R)\cos(k_0 z)|^2$$

where

- R: vector between nucleus and electron ((x, y, z)) components) [Å].
- $k_0 = 0.85 \times 2\pi a_0$ [Å^{-1}]
- $F_{1,2}(R) = \exp[-\sqrt{x^2/(nb)^2 + (y^2 + z^2)/(na)^2}]/\sqrt{\pi(na)^2 nb}$
- $F_{3,4}(R) : xyz \rightarrow yzx.$
- $F_{5,6}(R) : xyz \rightarrow zxy.$
- $n = \sqrt{0.029/E_i}$, E_i: electron ionization energy [eV].
- a and b are lattice parameters [Å].

The second term $[-D(R)\theta(|R| - na)]$ is the dipolar part which requires the direction of the magnetic field and where θ here is the Heaviside step function. See Dipolar.h for $D(R)$, the dipolar interaction (units M rad s^{-1}).

From: arXiv:cond-mat/0211567 (Phys. Rev. B 68, 115322 (2003)).

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Hyperfine.h
- /home/sbalian/spindec/src/Hyperfine.cpp

4.24 SpinDec::HyperfineParameters Class Reference

```
#include <HyperfineParameters.h>
```

Public Member Functions

- **HyperfineParameters** (const double lattice_constant, const double lattice_parameter_a, const double lattice_parameter_b, const double electron_ionization_energy, const double charge_density, const bool ising_only, bool fermi_contact_only_)
- double **get_lattice_constant** () const
- double **get_lattice_parameter_a** () const
- double **get_lattice_parameter_b** () const
- double **get_electron_ionization_energy** () const
- double **get_charge_density** () const
- bool **is_ising_only** () const
- bool **is_fermi_contact_only** () const

Private Attributes

- double lattice_constant_

  Lattice constant in Å.

- double lattice_parameter_a_

  Lattice parameter in Å.

- double lattice_parameter_b_

  Lattice parameter in Å.

- double electron_ionization_energy_

  Donor electron ionization energy in eV.

- double charge_density_

  Charge density (dimensionless).

- bool ising_only_

  Ignore flip-flop part of interaction.

- bool fermi_contact_only_

  ignore dipolar part of hyperfine interaction.

4.24.1 Detailed Description

Parameters to cacluate the hyperfine interaction between an electron spin and a nuclear spin in a lattice.

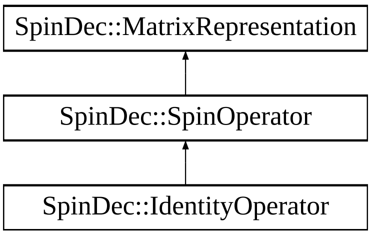
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/HyperfineParameters.h
- /home/sbalian/spindec/src/HyperfineParameters.cpp

4.25 SpinDec::IdentityOperator Class Reference

Identity.

`#include <IdentityOperator.h>`Inheritance diagram for SpinDec::IdentityOperator::



Public Member Functions

- **IdentityOperator** (const SpinBasis &basis)

4.25.1 Detailed Description

Identity.

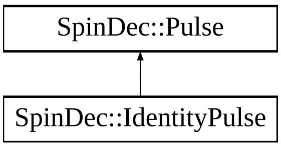
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/IdentityOperator.h
- /home/sbalian/spindec/src/IdentityOperator.cpp

4.26 SpinDec::IdentityPulse Class Reference

Identity pulse (no duration).

`#include <IdentityPulse.h>`Inheritance diagram for SpinDec::IdentityPulse::



Public Member Functions

- **IdentityPulse** (const SpinBasis &basis)

4.26.1 Detailed Description

Identity pulse (no duration).

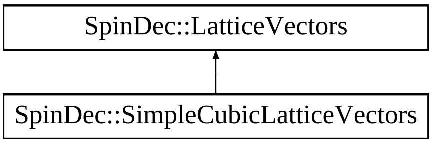
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/IdentityPulse.h
- /home/sbalian/spindec/src/IdentityPulse.cpp

4.27 SpinDec::LatticeVectors Class Reference

Lattice vectors for 3D crystal structures.

`#include <LatticeVectors.h>`Inheritance diagram for SpinDec::LatticeVectors::



Public Member Functions

- **LatticeVectors** (const ThreeVector &a1, const ThreeVector &a2, const ThreeVector &a3)
- const ThreeVector & **get_a1** () const
- const ThreeVector & **get_a2** () const
- const ThreeVector & **get_a3** () const

Protected Member Functions

- bool **linearly_independent** () const
- void **set_lattice_vectors** (const ThreeVector &a1, const ThreeVector &a2, const ThreeVector &a3)

Protected Attributes

- ThreeVector **a1_**
- ThreeVector **a2_**
- ThreeVector **a3_**

4.27.1 Detailed Description

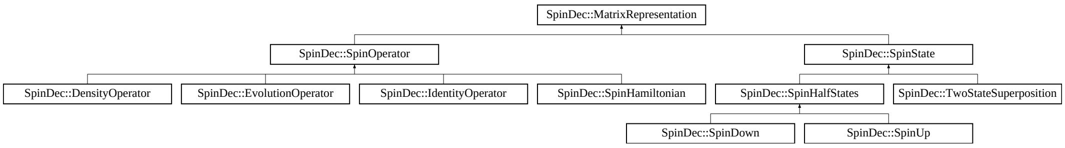
Lattice vectors for 3D crystal structures. Length units: Å. In Cartesian coordinates. Vectors must be linearly independent.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/LatticeVectors.h
- /home/sbalian/spindec/src/LatticeVectors.cpp

4.28 SpinDec::MatrixRepresentation Class Reference

`#include <MatrixRepresentation.h>`Inheritance diagram for SpinDec::MatrixRepresentation::



Public Member Functions

- UInt **get_dimension** () const
- const SpinBasis & **get_basis** () const
- bool **is_basis_equal** (const auto_ptr< MatrixRepresentation > &to_check) const
- virtual void set_zero ()=0

  Set all elements to zero.

- virtual auto_ptr< MatrixRepresentation > **clone** () const =0

Protected Member Functions

- **MatrixRepresentation** (const SpinBasis &basis)
- virtual void **quit_if_dimension_mismatch** () const =0
- void **quit_if_basis_mismatch** (const auto_ptr< MatrixRepresentation > &to_check) const

Protected Attributes

- UInt dimension_

  Dimension of Hilbert space.

- SpinBasis **basis_**

4.28.1 Detailed Description

Abstract base class for spin states and operators in the matrix representation. Has a SpinBasis (Zeeman basis) and a dimension.

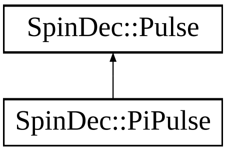
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/MatrixRepresentation.h
- /home/sbalian/spindec/src/MatrixRepresentation.cpp

4.29 SpinDec::PiPulse Class Reference

π-pulse or refocusing pulse.

`#include <PiPulse.h>`Inheritance diagram for SpinDec::PiPulse::



Public Member Functions

- PiPulse (const SpinState &state0, const SpinState &state1)

  Instantaneous.

- PiPulse (const SpinState &state0, const SpinState &state1, const vector< SpinState > &states2_plus)

4.29.1 Detailed Description

π-pulse or refocusing pulse. $|0\rangle\langle 1| + |1\rangle\langle 0|$.

4.29.2 Constructor & Destructor Documentation

4.29.2.1 SpinDec::PiPulse::PiPulse (const SpinState & *state0*, const SpinState & *state1*, const vector< SpinState > & *states2_plus*)

Third parameter: these just add $|n\rangle\langle n|$ for $n = 2, 3, \ldots$

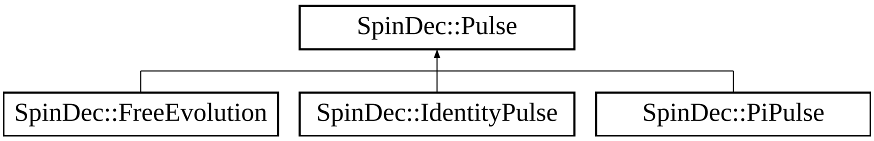
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/PiPulse.h
- /home/sbalian/spindec/src/PiPulse.cpp

4.30 SpinDec::Pulse Class Reference

Pulses in a pulse sequence.

`#include <Pulse.h>`Inheritance diagram for SpinDec::Pulse::



Public Member Functions

- **Pulse** (const double duration, const SpinOperator &pulse_operator)
- const SpinOperator & **get_pulse_operator** () const
- double **get_duration** () const
- Pulse **operator*** (const Pulse &pulse) const
- Pulse **operator^** (const Pulse &pulse) const

Protected Attributes

- double **duration_**
- SpinOperator **pulse_operator_**

4.30.1 Detailed Description

Pulses in a pulse sequence. Includes the no-pulse free evolution.

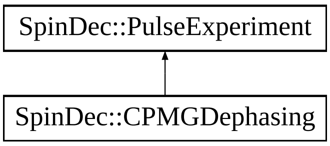
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Pulse.h
- /home/sbalian/spindec/src/Pulse.cpp

4.31 SpinDec::PulseExperiment Class Reference

Abstract base class for a pulse sequence experiment.

`#include <PulseExperiment.h>`Inheritance diagram for SpinDec::PulseExperiment::



Public Member Functions

- **PulseExperiment** (const CSDProblem &csd_problem, const TimeArray &time_array)
- virtual TimeEvolution **time_evolution** (const UIntArray bath_indices)=0
- virtual auto_ptr< PulseExperiment > **clone** () const =0
- const TimeArray & **get_time_array** () const
- const CSDProblem & **get_csd_problem** () const

Protected Attributes

- CSDProblem **csd_problem_**
- TimeArray **time_array_**

4.31.1 Detailed Description

Abstract base class for a pulse sequence experiment.

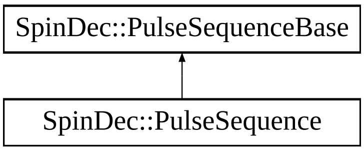
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/PulseExperiment.h
- /home/sbalian/spindec/src/PulseExperiment.cpp

4.32 SpinDec::PulseSequence Class Reference

Concrete general pulse sequence.

`#include <PulseSequence.h>`Inheritance diagram for SpinDec::PulseSequence::



Public Member Functions

- void **clear** ()
- void **add_pulse** (const Pulse &pulse)
- virtual auto_ptr< PulseSequenceBase > **clone** () const

4.32.1 Detailed Description

Concrete general pulse sequence.

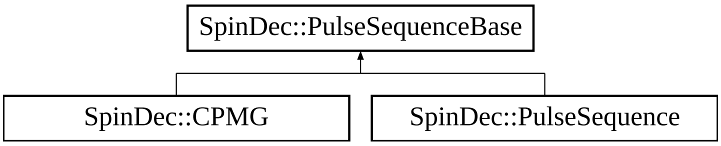
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/PulseSequence.h
- /home/sbalian/spindec/src/PulseSequence.cpp

4.33 SpinDec::PulseSequenceBase Class Reference

Abstract base class for pulse sequences.

`#include <PulseSequenceBase.h>`Inheritance diagram for SpinDec::PulseSequenceBase::



Public Member Functions

- SpinState **final_state** (const SpinState &initial_state) const
- double **get_duration** () const
- UInt **num_pulses** () const
- virtual auto_ptr< PulseSequenceBase > **clone** () const =0

Protected Attributes

- vector< Pulse > **pulses_**
- double **duration_**

4.33.1 Detailed Description

Abstract base class for pulse sequences.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/PulseSequenceBase.h
- /home/sbalian/spindec/src/PulseSequenceBase.cpp

4.34 SpinDec::RandomNumberGenerator Class Reference

Static methods for generating random numbers.

```
#include <RandomNumberGenerator.h>
```

Static Public Member Functions

- static int uniform_c_rand (const int min, const int max)
- static void seed_uniform_c_rand (const int seed)

  If seed is negative, calls clock_seed_uniform_c_rand().

- static void clock_seed_uniform_c_rand ()

  Seed with current time.

- static double **normal_c_rand** (const double mean, const double stdev)

4.34.1 Detailed Description

Static methods for generating random numbers.

4.34.2 Member Function Documentation

4.34.2.1 int SpinDec::RandomNumberGenerator::uniform_c_rand (const int *min*, const int *max*) `[static]`

Random integer $\min \leq i \leq \max$ from a uniform distribution using cstdlib rand().

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/RandomNumberGenerator.h
- /home/sbalian/spindec/src/RandomNumberGenerator.cpp

4.35 SpinDec::ReducedProblem Class Reference

SpinSystemBase and an order.

```
#include <ReducedProblem.h>
```

Public Member Functions

- **ReducedProblem** (const UInt order, const auto_ptr< SpinSystemBase > &spin_system_base)
- **ReducedProblem** (const ReducedProblem &rhs)
- ReducedProblem & **operator=** (const ReducedProblem &rhs)
- UInt **get_order** () const
- auto_ptr< SpinSystemBase > **get_spin_system** () const

Private Attributes

- UInt **order_**
- auto_ptr< SpinSystemBase > **spin_system_base_**

4.35.1 Detailed Description

SpinSystemBase and an order.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/ReducedProblem.h
- /home/sbalian/spindec/src/ReducedProblem.cpp

4.36 SpinDec::Sign Class Reference

±.

`#include <Sign.h>`

Public Member Functions

- int **as_int** () const
- bool **isPlus** () const
- bool **isMinus** () const
- bool **operator==** (const Sign &rhs) const

Static Public Attributes

- static const Sign **Plus**
- static const Sign **Minus**

Private Member Functions

- **Sign** (const int value)

Private Attributes

- int **value_**

Friends

- std::ostream & operator<< (std::ostream &os, Sign const &sign)

  Print with cout.

4.36.1 Detailed Description

±.

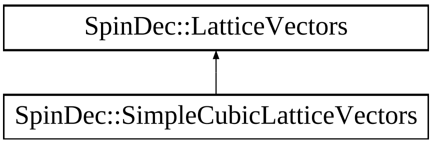
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/Sign.h
- /home/sbalian/spindec/src/Sign.cpp

4.37 SpinDec::SimpleCubicLatticeVectors Class Reference

Simple cubic lattice vectors.

`#include <SimpleCubicLatticeVectors.h>`Inheritance diagram for SpinDec::SimpleCubicLatticeVectors::



Public Member Functions

- SimpleCubicLatticeVectors (const double lattice_constant)

  Lattice constant a_0 in Å.

4.37.1 Detailed Description

Simple cubic lattice vectors. $|\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3| = a_0$ and $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ mutually orthogonal (parallel to x, y, z respectively in Cartesian coordinates).

Source: `http://en.wikipedia.org/wiki/Cubic_crystal_system.`

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SimpleCubicLatticeVectors.h
- /home/sbalian/spindec/src/SimpleCubicLatticeVectors.cpp

4.38 SpinDec::SpinBasis Class Reference

Holds magnetic quantum numbers for (in general) multiple spins.

`#include <SpinBasis.h>`

Public Member Functions

- SpinBasis (const SpinParametersVector &spin_parameters_vector)

  Automatically build using spin multiplicities.

- SpinBasis (const SpinParameters &spin_parameters)

  Automatically build using spin multiplicity.

- SpinBasis (const Eigen::ArrayXXd &basis_as_array)

  Custom build.

- const Eigen::ArrayXXd & **get_basis_as_array** () const
- UInt **num_basis_states** () const
- UInt **num_spins** () const
- double **get_element** (const UInt index, const UInt slot) const
- SpinBasis operator+ (const SpinBasis &to_append) const
- SpinBasis operator^ (const SpinBasis &to_combine) const
- bool operator== (const SpinBasis to_compare) const

  Check if bases are identical.

- bool **is_equal** (const SpinBasis &basis) const

Private Member Functions

- Eigen::ArrayXXd build (const SpinParametersVector &spin_parameters_vector)

  Automatically build using spin multiplicities.

- Eigen::ArrayXXd build (const SpinParameters &spin_parameters)

  Build using multiplicity.

Private Attributes

- Eigen::ArrayXXd **basis_as_array_**

Friends

- std::ostream & operator<< (std::ostream &os, SpinBasis const &basis)

  Print with cout.

4.38.1 Detailed Description

Holds magnetic quantum numbers for (in general) multiple spins. Implements the Zeeman basis and includes build methods.

Columns: spins. Rows: magnetic quantum numbers.

For example, for two electrons, this is

$$\begin{array}{cc} 0.5 & 0.5 \\ 0.5 & -0.5 \\ -0.5 & 0.5 \\ -0.5 & 0.5 \end{array}$$

For example, the first row corresponds to $|m_{S1} = 0.5, m_{S2} = 0.5\rangle$.

4.38.2 Member Function Documentation

4.38.2.1 SpinBasis SpinDec::SpinBasis::operator+ (const SpinBasis & *to_append*) const

For example,

$$\text{basis1} = \begin{array}{c} 0.5 \\ -0.5 \end{array}$$

and

$$\text{basis2} = \begin{array}{c} 4.5 \\ -4.5 \end{array}$$

basis1 + basis2 gives

$$\begin{array}{cc} 0.5 & 4.5 \\ -0.5 & -4.5 \end{array}$$

4.38.2.2 SpinBasis SpinDec::SpinBasis::operator^ (const SpinBasis & *to_combine*) const

Like tensor product. For example,

$$\text{basis1} = \begin{array}{c} 4.5 \\ -4.5 \end{array}$$

and

$$\text{basis2} = \begin{array}{c} 0.5 \\ -0.5 \end{array}$$

basis1^(basis2) is

$$\begin{array}{cc} 4.5 & 0.5 \\ 4.5 & -0.5 \\ -4.5 & 0.5 \\ -4.5 & -0.5 \end{array}$$

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinBasis.h
- /home/sbalian/spindec/src/SpinBasis.cpp

4.39 SpinDec::SpinBath Class Reference

Public Member Functions

- **SpinBath** (const CrystalStructure &crystal_structure, const auto_ptr< SpinSystemBase > &spin_system_base, const vector< SpinInteractionEdge > &intrabath_edges)
- **SpinBath** (const CrystalStructure &crystal_structure, const auto_ptr< SpinSystemBase > &spin_system_base, const SpinInteractionEdge &intrabath_edge)
- **SpinBath** (const SpinBath &spin_bath)
- SpinBath & **operator=** (const SpinBath &spin_bath)
- const SpinState & **get_bath_state** (const UInt index) const
- UInt **num_bath_states** () const
- SpinState **get_bath_product_state** (const UIntArray &indices) const
- const CrystalStructure & **get_crystal_structure** () const
- const vector< SpinInteractionEdge > & **get_intrabath_edges** () const
- auto_ptr< SpinSystemBase > **get_spin_system** () const
- SpinInteractionGraph **reduced_problem_graph** (const UInt order) const
- ThreeVector **get_position** (const UInt vertex_label, const UInt bath_index) const
- void **set_bath_state** (const UInt index, const UInt level)

Private Member Functions

- void **init** (const CrystalStructure &crystal_structure, const auto_ptr< SpinSystemBase > &spin_system_base, const vector< SpinInteractionEdge > &intrabath_edges)
- vector< SpinInteractionEdge > **make_intrabath_edges** (const UInt order, const SpinInteractionEdge &intrabath_edge) const
- vector< SpinInteractionEdge > **make_intrabath_edges** (const UInt order) const

Private Attributes

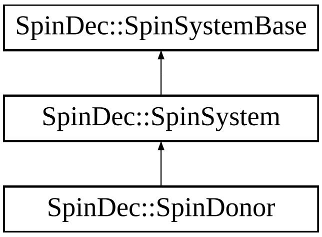
- vector< SpinState > **bath_states_**
- CrystalStructure **crystal_structure_**
- auto_ptr< SpinSystemBase > **spin_system_base_**
- vector< SpinInteractionEdge > **intrabath_edges_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinBath.h
- /home/sbalian/spindec/src/SpinBath.cpp

4.40 SpinDec::SpinDonor Class Reference

Inheritance diagram for SpinDec::SpinDonor::



Public Member Functions

- **SpinDonor** (const double field_strength, const double nuclear_quantum_number, const double electron_gyromagnetic_ratio, const double nuclear_gyromagnetic_ratio, const double hyperfine_strength, const unsigned int lower_level_label, const unsigned int upper_level_label, const ThreeVector &electron_position, const ThreeVector &nuclear_position, const bool complete_basis)
- const ElectronSpinParameters & **get_electron_parameters** () const
- const SpinParameters & **get_nuclear_parameters** () const
- const Hyperfine & **get_hyperfine** () const
- int **max_quantum_number** () const
- virtual UInt **dimension** () const
- UInt **total_multiplicity** () const
- virtual SpinState **eigenstate** (const UInt level_label)
- virtual double **energy** (const UInt level_label)
- double **polarization** (const UInt level_label) const
- const SpinInteractionVertex & **electron_vertex** () const
- const SpinInteractionVertex & **nuclear_vertex** () const
- const UIntArray **get_orthogonal_level_labels** () const
- SpinState **get_lower_level** ()
- SpinState **get_upper_level** ()
- vector< SpinState > **get_orthogonal_levels** ()
- virtual PiPulse **pi_pulse** (const UInt level_label1, const UInt level_label2)
- virtual auto_ptr< SpinSystemBase > **clone** () const

Private Member Functions

- void **sort_level_labels** ()
- UInt **level_label_index** (const UInt level_label) const
- virtual void **check_level_label** (const UInt level_label) const
- void **calc_adiabatic_level_labels** ()
- double **delta** () const
- double **omega** () const
- double **scaled_omega** () const
- double **D** (const int quantum_number) const
- double **O** (const int quantum_number) const
- double **R** (const int quantum_number) const
- double **energy** (const AdiabaticLabel &adiabatic_level_label) const

- UInt **adiabatic_label_to_int_label** (const AdiabaticLabel &adiabatic_level_label) const
- AdiabaticLabel **int_label_to_adiabatic_label** (const UInt level_label) const
- AdiabaticLabel **orthogonal_adiabatic_level_label** (AdiabaticLabel adiabatic_level_label) const
- double **cos_theta** (const int quantum_number) const
- double **sin_theta** (const int quantum_number) const
- double **a** (const int quantum_number) const
- double **b** (const int quantum_number) const
- double **polarization** (const AdiabaticLabel &adiabatic_level_label) const
- SpinBasis **build_basis** (const AdiabaticLabel &adiabatic_level_label) const
- SpinBasis **build_basis** (const std::vector< AdiabaticLabel > &adiabatic_level_labels) const
- SpinBasis **build_basis** (const UIntArray &level_labels) const
- SpinBasis **build_truncated_basis** () const
- void **set_transition** (const UInt lower_level_label, const UInt upper_level_label)
- void **set_orthogonal_level_labels** (const UInt lower_level_label, const UInt upper_level_label)
- UIntArray **get_orthogonal_level_labels** (const UInt lower_level_label, const UInt upper_level_label) const
- UInt **orthogonal_level_label** (const UInt level_label) const
- void **init** (const double field_strength, const double nuclear_quantum_number, const double electron_gyromagnetic_ratio, const double nuclear_gyromagnetic_ratio, const double hyperfine_strength, const unsigned int lower_level_label, const unsigned int upper_level_label, const ThreeVector &electron_position, const ThreeVector &nuclear_position, const bool complete_basis)

Private Attributes

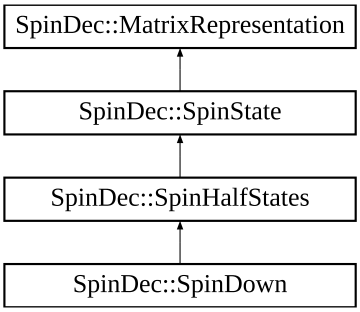
- bool **complete_basis_**
- ElectronSpinParameters **electron_parameters_**
- SpinParameters **nuclear_parameters_**
- Hyperfine **hyperfine_**
- UInt **transition_level_labels_** [2]
- UIntArray **orthogonal_level_labels_**
- UIntArray **sorted_level_labels_**
- std::vector< AdiabaticLabel > **adiabatic_level_labels_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinDonor.h
- /home/sbalian/spindec/src/SpinDonor.cpp

4.41 SpinDec::SpinDown Class Reference

Inheritance diagram for SpinDec::SpinDown::



Public Member Functions

- **SpinDown** (const SpinHalfParameters &spin_half_parameters)

Private Member Functions

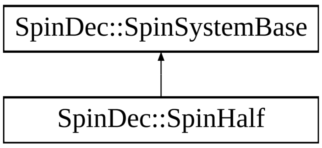
- virtual void **init** (const double gyromagnetic_ratio)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinDown.h
- /home/sbalian/spindec/src/SpinDown.cpp

4.42 SpinDec::SpinHalf Class Reference

Inheritance diagram for SpinDec::SpinHalf::



Public Member Functions

- **SpinHalf** (const double gyromagnetic_ratio, const double field_strength, const ThreeVector &position)
- virtual UInt **dimension** () const
- virtual auto_ptr< SpinSystemBase > **clone** () const

Private Member Functions

- virtual void **solve_once** ()
- virtual void **check_level_label** (const UInt level_label) const

Private Attributes

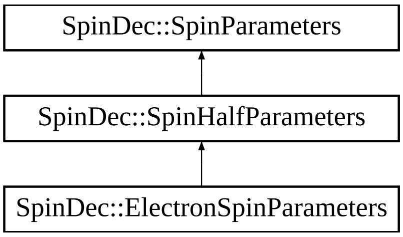
- double **gyromagnetic_ratio_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinHalf.h
- /home/sbalian/spindec/src/SpinHalf.cpp

4.43 SpinDec::SpinHalfParameters Class Reference

Inheritance diagram for SpinDec::SpinHalfParameters::



Public Member Functions

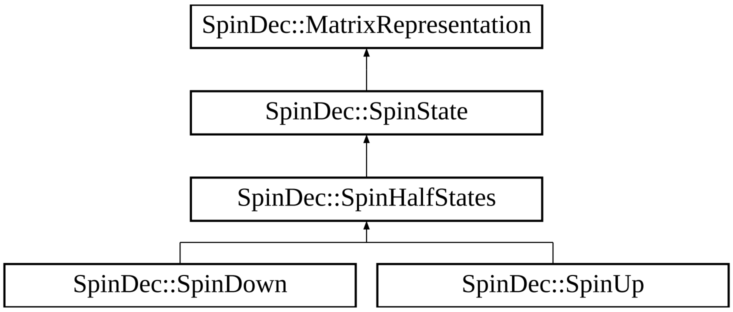
- **SpinHalfParameters** (const double gyromagnetic_ratio)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinHalfParameters.h
- /home/sbalian/spindec/src/SpinHalfParameters.cpp

4.44 SpinDec::SpinHalfStates Class Reference

Inheritance diagram for SpinDec::SpinHalfStates::



Protected Member Functions

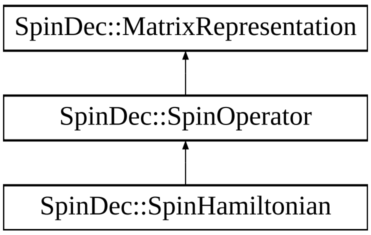
- virtual void **init** (const double gyromagnetic_ratio)=0
- virtual void **set_state_vector** (const ComplexVector &state_vector)
- virtual void **set_element** (const UInt index, const CDouble &element)
- virtual void **set_element** (const UInt index, const double element)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinHalfStates.h
- /home/sbalian/spindec/src/SpinHalfStates.cpp

4.45 SpinDec::SpinHamiltonian Class Reference

Inheritance diagram for SpinDec::SpinHamiltonian::



Public Member Functions

- **SpinHamiltonian** (const SpinInteractionGraph &graph, const UniformMagneticField &field)
- UniformMagneticField **get_field** () const
- const SpinInteractionGraph & **get_graph** () const
- void **update_positions** (const UIntArray &vertex_labels, const vector< ThreeVector > &positions)

Private Member Functions

- void **fill_zeeman** ()
- void **fill_interactions** ()
- void **init_terms** ()
- void **sum_zeeman_terms** ()
- void **sum_interaction_terms** ()
- void **fill_zeeman** (const UInt vertex_label)
- void **fill_interaction** (const UInt edge_index)

Private Attributes

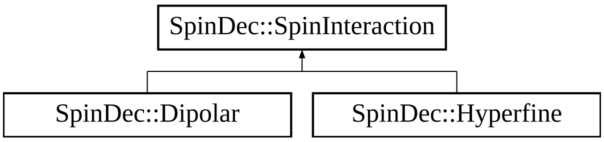
- UniformMagneticField **field_**
- SpinInteractionGraph **graph_**
- vector< ComplexMatrix > **zeeman_terms_**
- vector< ComplexMatrix > **interaction_terms_**
- ComplexMatrix **zeeman_hamiltonian_**
- ComplexMatrix **interaction_hamiltonian_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinHamiltonian.h
- /home/sbalian/spindec/src/SpinHamiltonian.cpp

4.46 SpinDec::SpinInteraction Class Reference

Inheritance diagram for SpinDec::SpinInteraction::



Public Member Functions

- virtual void **calculate** (const SpinParameters &spin_parameters1, const SpinParameters &spin_parameters2, const ThreeVector &position1, const ThreeVector &position2, const UniformMagneticField &field)=0
- double **get_strength** () const
- bool **strength_preset** () const
- virtual void **fill** (ComplexMatrix ∗hamiltonian, const SpinParametersVector &spins, const SpinBasis &basis, const UInt spin_label1, const UInt spin_label2) const =0
- virtual auto_ptr< SpinInteraction > **clone** () const =0
- virtual string **get_type** () const =0

Protected Member Functions

- **SpinInteraction** (const double strength)
- void **fill_ising_flipflop** (ComplexMatrix ∗hamiltonian, const SpinParametersVector &spin_parameters_vector, const SpinBasis &basis, const UInt spin_label1, const UInt spin_label2, const bool ising_only, const CDouble &flipflop_form) const
- void **warn_if_preset_then_calculated** () const

Protected Attributes

- double **strength_**
- bool **strength_preset_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinInteraction.h
- /home/sbalian/spindec/src/SpinInteraction.cpp

4.47 SpinDec::SpinInteractionEdge Class Reference

Public Member Functions

- **SpinInteractionEdge** (const SpinInteractionEdge &other)
- **SpinInteractionEdge** (const UInt label1, const UInt label2, const auto_ptr< SpinInteraction > &interaction)
- UInt **get_label1** () const
- UInt **get_label2** () const
- auto_ptr< SpinInteraction > **get_interaction** () const
- SpinInteractionEdge & **operator=** (const SpinInteractionEdge &other)

Private Attributes

- pair< UInt, UInt > **labels_**
- auto_ptr< SpinInteraction > **interaction_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinInteractionEdge.h
- /home/sbalian/spindec/src/SpinInteractionEdge.cpp

4.48 SpinDec::SpinInteractionGraph Class Reference

Public Member Functions

- void **set_basis** (const SpinBasis &basis)
- void **add_vertex** (const SpinParameters &spin_parameters, const ThreeVector &position)
- void **add_vertex** (const SpinParameters &spin_parameters, const SpinBasis &basis, const ThreeVector &position)
- void **add_vertex_appending_basis** (const SpinParameters &spin_parameters, const ThreeVector &position)
- void **add_vertex_appending_basis** (const SpinParameters &spin_parameters, const SpinBasis &basis, const ThreeVector &position)
- void **add_edge** (unsigned int label1, unsigned int label2, const auto_ptr< SpinInteraction > &interaction)
- void **add_edges** (const vector< SpinInteractionEdge > &edges)
- unsigned int **num_vertices** () const
- unsigned int **num_edges** () const
- void **clear** ()
- const SpinBasis & **get_basis** () const
- const SpinParameters & **get_spin_parameters** (const unsigned int label) const
- const ThreeVector & **get_position** (const unsigned int label) const
- auto_ptr< SpinInteraction > **get_interaction** (const unsigned int index) const
- void **set_interaction** (const unsigned int index, const auto_ptr< SpinInteraction > &interaction)
- SpinParametersVector **spin_parameters_vector** () const
- const SpinInteractionVertex & **get_vertex** (const unsigned int label) const
- const SpinInteractionEdge & **get_edge** (const unsigned int index) const
- void **join_in_place** (const SpinInteractionGraph &to_join)
- void **join_in_place** (const SpinInteractionGraph &to_join, const std::vector< SpinInteractionEdge > &edges)
- SpinInteractionGraph **join** (const SpinInteractionGraph &to_join) const
- SpinInteractionGraph **join** (const SpinInteractionGraph &to_join, const std::vector< SpinInteractionEdge > &edges) const
- void **set_position** (const UInt label, const ThreeVector &position)
- const SpinInteractionVertex & **get_vertex1** (const UInt index) const
- const SpinInteractionVertex & **get_vertex2** (const UInt index) const
- void **set_positions** (const UIntArray &vertex_labels, const vector< ThreeVector > &positions)

Private Member Functions

- void **quit_if_vertex_label_out_of_bounds** (const unsigned int label) const
- void **quit_if_edge_index_out_of_bounds** (const unsigned int index) const
- void **set_vertex** (const unsigned int label, const SpinInteractionVertex &vertex)
- void **set_edge** (const unsigned int index, const SpinInteractionEdge &edge)

Private Attributes

- vector< SpinInteractionVertex > **vertices_**
- vector< SpinInteractionEdge > **edges_**
- SpinBasis **basis_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinInteractionGraph.h
- /home/sbalian/spindec/src/SpinInteractionGraph.cpp

4.49 SpinDec::SpinInteractionVertex Class Reference

Public Member Functions

- **SpinInteractionVertex** (const UInt label, const SpinParameters &spin_parameters, const ThreeVector &position)
- **SpinInteractionVertex** (const UInt label, const SpinParameters &spin_parameters, const SpinBasis &basis, const ThreeVector &position)
- UInt **get_label** () const
- const SpinParameters & **get_spin_parameters** () const
- const SpinBasis & **get_basis** () const
- const ThreeVector & **get_position** () const
- void **set_position** (const ThreeVector &position)

Private Attributes

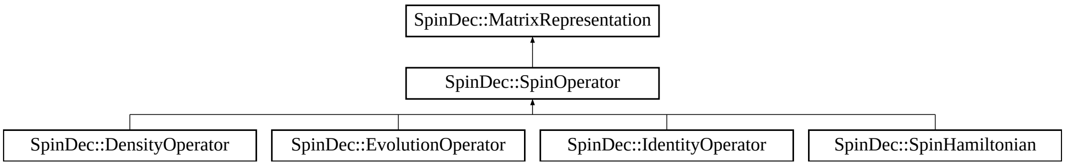
- UInt **label_**
- SpinParameters **spin_parameters_**
- SpinBasis **basis_**
- ThreeVector **position_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinInteractionVertex.h
- /home/sbalian/spindec/src/SpinInteractionVertex.cpp

4.50 SpinDec::SpinOperator Class Reference

Inheritance diagram for SpinDec::SpinOperator::


SpinDec::MatrixRepresentation
SpinDec::SpinOperator
SpinDec::DensityOperator
SpinDec::EvolutionOperator
SpinDec::IdentityOperator
SpinDec::SpinHamiltonian

Public Member Functions

- **SpinOperator** (const ComplexMatrix &matrix, const SpinBasis &basis)
- **SpinOperator** (const SpinBasis &basis)
- const ComplexMatrix & **get_matrix** () const
- void **set_matrix** (const ComplexMatrix &matrix)
- const CDouble & **get_element** (const UInt i, const UInt j) const
- void **set_element** (const UInt i, const UInt j, const CDouble &element)
- void **set_element** (const UInt i, const UInt j, const double element)
- void **add_to_element** (const UInt i, const UInt j, const CDouble &to_add)
- SpinOperator **operator^** (const SpinOperator &rhs) const
- SpinState **operator*** (const SpinState &operand) const
- SpinOperator **operator+** (const SpinOperator &rhs) const
- SpinOperator **operator-** (const SpinOperator &rhs) const
- virtual void set_zero ()

  Set all elements to zero.

- virtual auto_ptr< MatrixRepresentation > **clone** () const

Protected Member Functions

- virtual void **quit_if_dimension_mismatch** () const

Protected Attributes

- ComplexMatrix **matrix_**

Friends

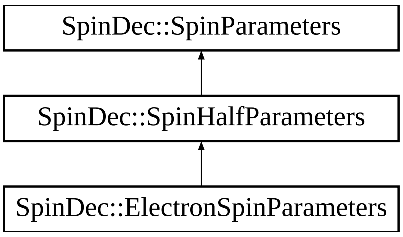
- std::ostream & **operator<<** (std::ostream &os, SpinOperator const &spin_operator)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinOperator.h
- /home/sbalian/spindec/src/SpinOperator.cpp

4.51 SpinDec::SpinParameters Class Reference

Inheritance diagram for SpinDec::SpinParameters::



Public Member Functions

- **SpinParameters** (const double quantum_number, const double gyromagnetic_ratio)
- double **get_quantum_number** () const
- double **get_gyromagnetic_ratio** () const
- UInt **get_multiplicity** () const

Protected Member Functions

- UInt **multiplicity** (const double quantum_number) const

Protected Attributes

- double **quantum_number_**
- double **gyromagnetic_ratio_**
- UInt **multiplicity_**

Friends

- std::ostream & **operator**<< (std::ostream &os, SpinParameters const &spin_parameters)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinParameters.h
- /home/sbalian/spindec/src/SpinParameters.cpp

4.52 SpinDec::SpinParametersVector Class Reference

Public Member Functions

- **SpinParametersVector** (const SpinParameters &spin_parameters)
- SpinParameters & **operator[ ]** (const UInt index)
- const SpinParameters & **operator[ ]** (const UInt index) const
- void **push_back** (const SpinParameters &spin_parameters)
- UInt **size** () const
- void **clear** ()
- UInt **multiplicity** () const

Private Attributes

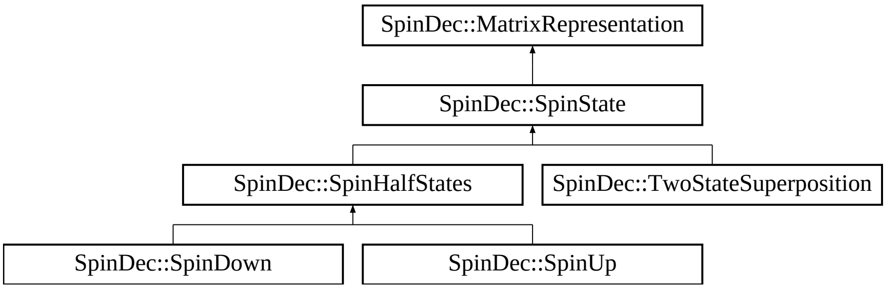
- std::vector< SpinParameters > **spin_parameters_vector_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinParametersVector.h
- /home/sbalian/spindec/src/SpinParametersVector.cpp

4.53 SpinDec::SpinState Class Reference

Inheritance diagram for SpinDec::SpinState::



Public Member Functions

- **SpinState** (const ComplexVector &state_vector, const SpinBasis &basis)
- **SpinState** (const SpinBasis &basis)
- const ComplexVector & **get_state_vector** () const
- virtual void **set_state_vector** (const ComplexVector &state_vector)
- const CDouble & **get_element** (const UInt index) const
- virtual void **set_element** (const UInt index, const CDouble &element)
- virtual void **set_element** (const UInt index, const double element)
- SpinState **operator^** (const SpinState &rhs) const
- CDouble **operator∗** (const SpinState &rhs) const
- SpinOperator **operator%** (const SpinState &rhs) const
- SpinState **operator+** (const SpinState &rhs) const
- SpinState **operator-** (const SpinState &rhs) const
- SpinState **operator∗** (const CDouble &c) const
- void **time_evolve** (const ComplexMatrix &unitary_evolution_matrix)
- virtual void set_zero ()

  Set all elements to zero.

- void **normalize** ()
- SpinState **normalized** () const
- virtual auto_ptr< MatrixRepresentation > **clone** () const

Protected Member Functions

- virtual void **quit_if_dimension_mismatch** () const

Protected Attributes

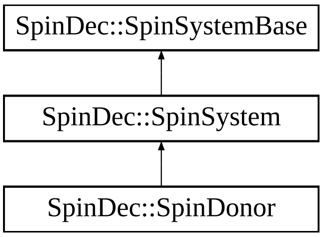
- ComplexVector **state_vector_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinState.h
- /home/sbalian/spindec/src/SpinState.cpp

4.54 SpinDec::SpinSystem Class Reference

Inheritance diagram for SpinDec::SpinSystem::



Public Member Functions

- **SpinSystem** (const SpinHamiltonian &hamiltonian)
- virtual UInt **dimension** () const
- virtual auto_ptr< SpinSystemBase > **clone** () const

Protected Member Functions

- virtual void **solve_once** ()
- virtual void **check_level_label** (const UInt level_label) const

Protected Attributes

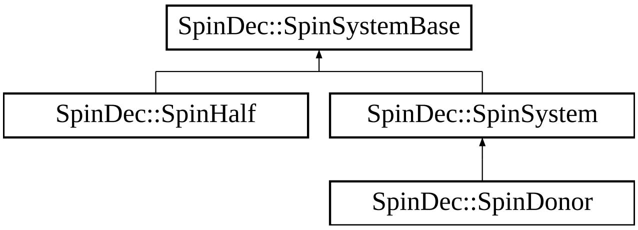
- HermitianEigenspectrum **eigenspectrum_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinSystem.h
- /home/sbalian/spindec/src/SpinSystem.cpp

4.55 SpinDec::SpinSystemBase Class Reference

Inheritance diagram for SpinDec::SpinSystemBase::



Public Member Functions

- **SpinSystemBase** (const SpinHamiltonian &hamiltonian)
- const SpinHamiltonian & **get_hamiltonian** () const
- virtual SpinState **eigenstate** (const UInt level_label)
- virtual double **energy** (const UInt level_label)
- void **set_state** (const SpinState &state)
- void **set_state** (const UInt level_label)
- void **set_state** (const CDouble &c0, const UInt level_label0, const CDouble &c1, const UInt level_label1)
- const SpinState & **get_state** () const
- EvolutionOperator **evolution_operator** (const double time)
- virtual UInt **dimension** () const =0
- const ComplexMatrix & **get_eigenvector_matrix** ()
- const RealVector & **get_eigenvalue_vector** ()
- virtual PiPulse **pi_pulse** (const UInt level_label1, const UInt level_label2)
- void **print** (const char option)
- virtual auto_ptr< SpinSystemBase > **clone** () const =0
- void **update_positions** (const UIntArray &vertex_labels, const vector< ThreeVector > &positions)

Protected Member Functions

- virtual void **solve_once** ()=0
- virtual void **check_level_label** (const UInt level_label) const =0

Protected Attributes

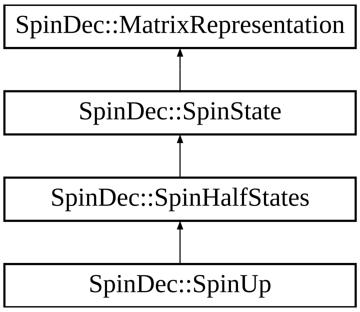
- SpinHamiltonian **hamiltonian_**
- RealVector **energies_**
- ComplexMatrix **eigenstates_**
- SpinState **state_**
- bool **is_solved_**
- bool **is_state_set_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinSystemBase.h
- /home/sbalian/spindec/src/SpinSystemBase.cpp

4.56 SpinDec::SpinUp Class Reference

Inheritance diagram for SpinDec::SpinUp::



Public Member Functions

- **SpinUp** (const SpinHalfParameters &spin_half_parameters)

Private Member Functions

- virtual void **init** (const double gyromagnetic_ratio)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/SpinUp.h
- /home/sbalian/spindec/src/SpinUp.cpp

4.57 SpinDec::StringOptions Class Reference

Public Member Functions

- **StringOptions** (const string &options)
- bool **found_option** (const char option) const
- bool **is_empty** () const

Private Attributes

- string **options_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/StringOptions.h
- /home/sbalian/spindec/src/StringOptions.cpp

4.58 SpinDec::TimeArray Class Reference

Public Member Functions

- **TimeArray** (const double initial_time, const double final_time, const UInt num_steps)
- **TimeArray** (const double single_time)
- bool **operator==** (const TimeArray &time_array) const
- void **logarithmic_time** ()
- double **get_time** (const UInt index) const
- const DoubleArray & **get_time_vector** () const
- UInt **num_steps** () const
- UInt **get_dimension** () const
- void **scale_time** (const double scalar)

Private Member Functions

- void **clear** ()
- void **initialize** (const double initial_time, const double final_time, const UInt num_steps)

Private Attributes

- DoubleArray **time_vector_**
- UInt **dimension_**

Friends

- std::ostream & **operator**<< (std::ostream &os, TimeArray const &time_array)

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/TimeArray.h
- /home/sbalian/spindec/src/TimeArray.cpp

4.59 SpinDec::TimeEvolution Class Reference

Public Member Functions

- **TimeEvolution** (const TimeArray &time_array, const CDoubleArray &evolution)
- **TimeEvolution** (const TimeArray &time_array)
- const CDouble & **evolution** (const UInt index) const
- void **set_evolution_zeros** ()
- void **set_evolution_ones** ()
- const CDoubleArray & **get_evolution** () const
- const TimeArray & **get_time_array** () const
- UInt **dimension** () const
- TimeEvolution **operator+** (const TimeEvolution &to_add) const
- TimeEvolution **operator**∗ (const TimeEvolution &to_multiply) const
- TimeEvolution **operator/** (const TimeEvolution &to_divide) const
- void **print** () const
- void **print_real** () const
- void **print_imag** () const
- void **print_abs** () const
- void **print** (const string &file_name) const
- void **print_real** (const string &file_name) const
- void **print_imag** (const string &file_name) const
- void **print_abs** (const string &file_name) const
- void **scale_time** (const double scalar)
- void **finite_zeros** ()
- bool **has_greater_than_one** () const

Private Member Functions

- void **print** (const char option) const
- void **print** (const string &file_name, const char option) const

Private Attributes

- TimeArray **time_array_**
- CDoubleArray **evolution_**

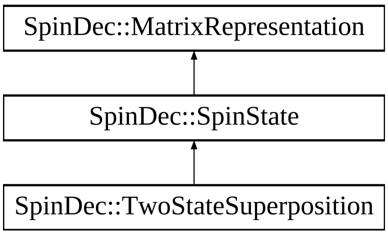
The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/TimeEvolution.h
- /home/sbalian/spindec/src/TimeEvolution.cpp

4.60 SpinDec::TwoStateSuperposition Class Reference

2-level superposition state.

`#include <TwoStateSuperposition.h>`Inheritance diagram for SpinDec::TwoStateSuperposition::



Public Member Functions

- **TwoStateSuperposition** (const CDouble &c0, const SpinState &state0, const CDouble &c1, const SpinState &state1)
- const SpinState & **get_state0** () const
- const SpinState & **get_state1** () const
- const CDouble & **get_c0** () const
- const CDouble & **get_c1** () const

Private Attributes

- SpinState **state0_**
- SpinState **state1_**
- CDouble **c0_**
- CDouble **c1_**

4.60.1 Detailed Description

2-level superposition state.

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/TwoStateSuperposition.h
- /home/sbalian/spindec/src/TwoStateSuperposition.cpp

4.61 SpinDec::UniformMagneticField Class Reference

Public Member Functions

- **UniformMagneticField** (const double magnitude)
- **UniformMagneticField** (const double magnitude, const ThreeVector &direction)
- double **get_magnitude** () const
- ThreeVector **get_direction** () const
- void **set_magnitude** (const double magnitude)
- void **set_direction** (const ThreeVector &direction)

Private Attributes

- double **magnitude_**
- ThreeVector **direction_**

The documentation for this class was generated from the following files:

- /home/sbalian/spindec/include/SpinDec/UniformMagneticField.h
- /home/sbalian/spindec/src/UniformMagneticField.cpp

Chapter 5

File Documentation

5.1 /home/sbalian/spindec/include/SpinDec/typedefs.h File Reference

typedefs and "usings" `#include "SpinDec/config.h"`

```
#include <Eigen/Dense>
#include <complex>
#include <vector>
#include <string>
#include <iostream>
#include <memory>
#include <utility>
#include <map>
```

Typedefs

- typedef unsigned int SpinDec::UInt

  Unsigned int.

- typedef Eigen::Vector3d SpinDec::ThreeVector

  Real 3-vector.

- typedef std::complex< double > SpinDec::CDouble

  Complex double.

- typedef Eigen::MatrixXcd SpinDec::ComplexMatrix

  Matrix of complex doubles.

- typedef Eigen::VectorXcd SpinDec::ComplexVector

  Vector of complex doubles.

- typedef Eigen::VectorXd SpinDec::RealVector

Vector of doubles.

- typedef std::vector< double > SpinDec::DoubleArray

  STL vector of doubles.

- typedef std::vector< int > SpinDec::IntArray

  STL vector of integers.

- typedef std::vector< unsigned int > SpinDec::UIntArray

  STL vector of unsigned integers.

- typedef std::vector< CDouble > SpinDec::CDoubleArray

  STL vector of complex doubles.

5.1.1 Detailed Description

typedefs and "usings" Custom STL and Eigen typedefs for SpinDec. Also includes some usings, all in the SpinDec namespace.

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