SpinDec

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1.1 Class Hierarchy

s inheritance list is sorted roughly, but not completely, alphabetically:	
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SpinDec::ClusterDatabaseEntry	
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Chapter 2

Class Index

2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

SpinDec::AdiabaticLabel (Adiabatic eigenstates of a spin donor)
SpinDec::BoostEigen (Static methods to extend Eigen functionality)
SpinDec::CCE
SpinDec::Cluster
SpinDec::ClusterDatabase
SpinDec::ClusterDatabaseEntry
SpinDec::CPMG
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SpinDec::CrystalBasis
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SpinDec::DensityOperator
SpinDec::DiamondCubic
SpinDec::Dipolar
SpinDec::Eigenspectrum
SpinDec::ElectronSpinParameters
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SpinDec::EvolutionOperator
SpinDec::FileProperties
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SpinDec::IdentityOperator
SpinDec::IdentityPulse
SpinDec::LatticeVectors
SpinDec::MatrixRepresentation
SpinDec::NuclearSpinParameters
SpinDec::PiPulse
SpinDec::Pulse
SpinDec::PulseExperiment
SpinDec::PulseSequence
SpinDec::PulseSequenceBase

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SpinDec::RandomNumberGenerator
SpinDec::ReducedProblem
SpinDec::Sign
SpinDec::SimpleCubicLatticeVectors ?
SpinDec::SpinDown
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SpinDec::SpinInteractionVertex
SpinDec::SpinOperator
SpinDec::SpinParameters
SpinDec::SpinParametersVector
SpinDec::SpinState
SpinDec::SpinSystem
SpinDec::SpinSystemBase
SpinDec::SpinUp
SpinDec::StringOptions
SpinDec::TimeArray
SpinDec::TimeEvolution
SpinDec::TwoStateSuperposition ?
SpinDec::UniformMagneticField
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Chapter 3

Class Documentation

3.1 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)

3.1.1 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.

3.2 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 Complex Vector exp (const Complex Vector &a)

 Element-wise exponentiation for complex vectors.
- static ComplexMatrix tensorProduct (const ComplexMatrix &A, const ComplexMatrix &B)

 Tensor product for complex matrices.
- static Complex Vector tensorProduct (const Complex Vector &a, const Complex Vector &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 is Within Distance (const Three Vector &r, const double distance) $Is |\mathbf{r}| \leq d$?

3.2.1 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/.

3.2.2 Member Function Documentation

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

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

3.2.2.2 double SpinDec::BoostEigen::maxAbsCoeff (const ThreeVector & a) [static]

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

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

Partial trace for complex matrices. Given $C = A \otimes B$, and the dimension of B, this method outputs $Tr_B A$.

3.2.2.4 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.

3.2.2.5 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

$$\mathbf{c} = \begin{pmatrix} a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2 \end{pmatrix}$$

3.2.2.6 ComplexMatrix SpinDec::BoostEigen::tensorProduct (const ComplexMatrix & A, const ComplexMatrix & B) [static]

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

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

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

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

3.3 SpinDec::CCE Class Reference

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

- vector< TimeEvolution > product_correlations_by_order_
- UInt max_truncation_order_
- bool include_one_clusters_
- auto_ptr< PulseExperiment > pulse_experiment_
- ClusterDatabase cluster_database_

3.4 SpinDec::Cluster Class Reference

Public Member Functions

- Cluster (const UIntArray &labels)
- void **add** (const UInt label)
- bool **operator==** (const Cluster &rhs) const
- UInt **num_spins** () const
- UInt get_label (const UInt index) const
- const UIntArray & get_labels () const
- vector< Cluster> subsets () const
- vector< Cluster > proper_subsets () const

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)

3.5 SpinDec::ClusterDatabase Class Reference

Public Member Functions

- ClusterDatabase (const SpinBath &spin_bath, const UInt max_order, const double cluster_cutoff, const string &build_method)
- 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 ()
- void build_ones ()
- void build_with_local_cutoff ()
- void build_with_global_cutoff()
- UInt **get_index** (const **Cluster** &cluster) const
- void add_unsolved_entry (const Cluster &cluster)
- bool **is_order_built** (const UInt order) const
- bool cluster_exists (const Cluster &cluster) const

- UInt max_order_
- SpinBath spin_bath_
- database_map database_
- double cluster_cutoff_

3.6 SpinDec::ClusterDatabaseEntry Class Reference

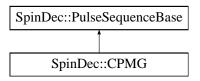
Public Member Functions

- ClusterDatabaseEntry (const Cluster &cluster)
- const Cluster & get_cluster () const
- bool is_solved () const
- const TimeEvolution & get_time_evolution () const
- void **set_time_evolution** (const **TimeEvolution** &time_evolution)

- Cluster cluster_
- TimeEvolution time_evolution_
- bool is_solved_

3.7 SpinDec::CPMG Class Reference

Inheritance diagram for SpinDec::CPMG::



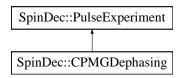
Public Member Functions

- 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

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

3.8 SpinDec::CPMGDephasing Class Reference

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

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

3.9 SpinDec::CrystalBasis Class Reference

Public Member Functions

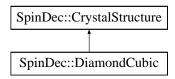
- void **add_basis_vector** (const ThreeVector &basis_vector)
- const std::vector< ThreeVector > & get_basis_vectors () const
- const ThreeVector & **get_basis_vector** (const UInt index) const
- UInt num_basis_vectors () const

Protected Attributes

• std::vector < ThreeVector > basis_vectors_

3.10 SpinDec::CrystalStructure Class Reference

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)
- CrystalStructure (const string &file_name)
- **CrystalStructure** (const vector< ThreeVector > &site_vectors)
- const std::vector < Three Vector > & 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
- 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)
- void **add_site_vector** (const ThreeVector &site_vector)
- void **scale_site_vectors** (const double scale_factor)
- std::vector< Three Vector > cartesian_basis_vectors (const Lattice Vectors & lattice_vectors, const CrystalBasis & basis) const

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)

3.11 SpinDec::CSDProblem Class Reference

Public Member Functions

- CSDProblem (const CSDProblem &csd_problem)
- CSDProblem & operator= (const CSDProblem &csd_problem)
- CSDProblem (const auto_ptr< SpinSystemBase > ¢ral_spin_system_base, const SpinBath &spin_bath, const vector< SpinInteractionEdge > &system_bath_edges, const UniformMagnetic-Field &field)
- CSDProblem (const auto_ptr< SpinSystemBase > ¢ral_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

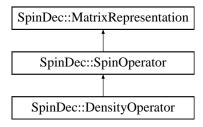
Private Member Functions

- void **init** (const auto_ptr< SpinSystemBase > ¢ral_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

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

3.12 SpinDec::DensityOperator Class Reference

Inheritance diagram for SpinDec::DensityOperator::



Public Member Functions

- DensityOperator (const SpinState &state, const SpinState &state0, const SpinState &state1)
- DensityOperator reduced () const
- CDouble off_diagonal_reduced () const

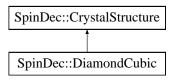
Private Member Functions

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

- SpinState state0_
- SpinState state1_

3.13 SpinDec::DiamondCubic Class Reference

Inheritance diagram for SpinDec::DiamondCubic::



Public Member Functions

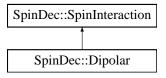
- DiamondCubic (const double lattice_constant, const double side_length)
- **DiamondCubic** (const double lattice_constant, const double side_length, const double fractional_abundance)
- void make_sphere (const double radius)
- void make_shell (const double min_radius, const double max_radius)

Private Member Functions

- SimpleCubicLatticeVectors construct_lattice_vectors (const double lattice_constant) const
- CrystalBasis construct_basis_vectors () const
- int int_range_centred_cube (const double side_length, const double lattice_constant) const

3.14 SpinDec::Dipolar Class Reference

Inheritance diagram for SpinDec::Dipolar::

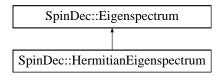


Public Member Functions

- **Dipolar** (const double strength)
- 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

3.15 SpinDec::Eigenspectrum Class Reference

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

Protected Member Functions

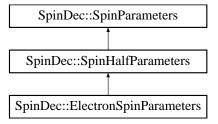
• virtual void diagonalize (const ComplexMatrix &matrix)

Protected Attributes

- ComplexMatrix eigenvectors_
- Complex Vector eigenvalues_

3.16 SpinDec::ElectronSpinParameters Class Reference

Inheritance diagram for SpinDec::ElectronSpinParameters::



Public Member Functions

• ElectronSpinParameters (const double gyromagnetic_ratio)

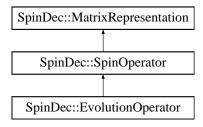
3.17 SpinDec::Errors Class Reference

Static Public Member Functions

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

3.18 SpinDec::EvolutionOperator Class Reference

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)
- double **get_time** () const

Private Member Functions

• void set_matrix ()

- double time_
- ComplexMatrix eigenvectors_
- RealVector eigenvalues_

3.19 SpinDec::FileProperties Class Reference

Static Public Member Functions

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

3.20 SpinDec::FreeEvolution Class Reference

Inheritance diagram for SpinDec::FreeEvolution::

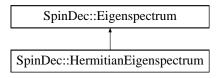


Public Member Functions

• FreeEvolution (const EvolutionOperator &evolution_operator)

3.21 SpinDec::HermitianEigenspectrum Class Reference

Inheritance diagram for SpinDec::HermitianEigenspectrum::



Public Member Functions

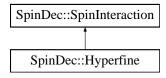
- **HermitianEigenspectrum** (const ComplexMatrix &matrix)
- virtual ComplexMatrix spectralDecomposition () const

Private Member Functions

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

3.22 SpinDec::Hyperfine Class Reference

Inheritance diagram for SpinDec::Hyperfine::



Public Member Functions

- Hyperfine (const HyperfineParameters ¶meters)
- **Hyperfine** (const double strength)
- 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_

3.23 SpinDec::HyperfineParameters Class Reference

Public Member Functions

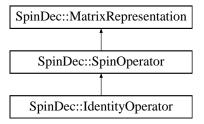
• **HyperfineParameters** (const double lattice_constant, const double lattice_parameter_a, const double lattice_parameter_b, const double electron_ionization_energy, const double charge_density, const bool ising_only, bool fermi_contact_only_)

- 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

- double lattice_constant_
- double lattice_parameter_a_
- double lattice_parameter_b_
- double electron_ionization_energy_
- double charge_density_
- bool ising_only_
- bool fermi_contact_only_

3.24 SpinDec::IdentityOperator Class Reference

Inheritance diagram for SpinDec::IdentityOperator::

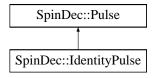


Public Member Functions

• IdentityOperator (const SpinBasis &basis)

3.25 SpinDec::IdentityPulse Class Reference

Inheritance diagram for SpinDec::IdentityPulse::

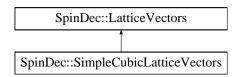


Public Member Functions

• IdentityPulse (const SpinBasis &basis)

3.26 SpinDec::LatticeVectors Class Reference

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_

3.27 SpinDec::MatrixRepresentation Class Reference

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

Protected Member Functions

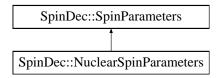
- MatrixRepresentation (const SpinBasis &basis)
- virtual void quit_if_dimension_mismatch () const =0
- void quit_if_basis_mismatch (const auto_ptr< MatrixRepresentation > &to_check) const

Protected Attributes

- UInt dimension_
- SpinBasis basis_

3.28 SpinDec::NuclearSpinParameters Class Reference

Inheritance diagram for SpinDec::NuclearSpinParameters::

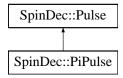


Public Member Functions

• NuclearSpinParameters (const double quantum_number, const double gyromagnetic_ratio)

3.29 SpinDec::PiPulse Class Reference

Inheritance diagram for SpinDec::PiPulse::

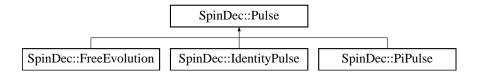


Public Member Functions

- PiPulse (const SpinState &state0, const SpinState &state1)
- **PiPulse** (const SpinState &state0, const SpinState &state1, const vector< SpinState > &states2_-plus)

3.30 SpinDec::Pulse Class Reference

Inheritance diagram for SpinDec::Pulse::



Public Member Functions

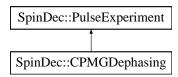
- Pulse (const double duration, const SpinOperator &pulse_operator)
- const SpinOperator & get_pulse_operator () const
- double **get_duration** () const
- Pulse operator* (const Pulse &pulse) const
- Pulse operator (const Pulse &pulse) const

Protected Attributes

- double duration_
- SpinOperator pulse_operator_

3.31 SpinDec::PulseExperiment Class Reference

Inheritance diagram for SpinDec::PulseExperiment::



Public Member Functions

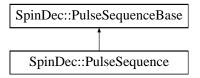
- PulseExperiment (const CSDProblem &csd_problem, const TimeArray &time_array)
- virtual TimeEvolution time_evolution (const UIntArray bath_indices)=0
- virtual auto_ptr< PulseExperiment > clone () const =0
- const TimeArray & get_time_array () const
- const CSDProblem & get_csd_problem () const

Protected Attributes

- CSDProblem csd_problem_
- TimeArray time_array_

3.32 SpinDec::PulseSequence Class Reference

Inheritance diagram for SpinDec::PulseSequence::

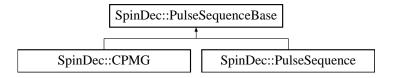


Public Member Functions

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

3.33 SpinDec::PulseSequenceBase Class Reference

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_

3.34 SpinDec::RandomNumberGenerator Class Reference

Static Public Member Functions

- static int uniform_c_rand (const int min, const int max)
- static void **seed_uniform_c_rand** (const int seed)
- static void clock_seed_uniform_c_rand ()
- static double **normal_c_rand** (const double mean, const double stdev)

3.35 SpinDec::ReducedProblem Class Reference

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

- UInt order_
- auto_ptr< SpinSystemBase > spin_system_base_

3.36 SpinDec::Sign Class Reference

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

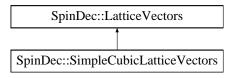
• int value_

Friends

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

3.37 SpinDec::SimpleCubicLatticeVectors Class Reference

Inheritance diagram for SpinDec::SimpleCubicLatticeVectors::



Public Member Functions

• SimpleCubicLatticeVectors (const double lattice_constant)

3.38 SpinDec::SpinBasis Class Reference

Public Member Functions

- SpinBasis (const SpinParametersVector &spin_parameters_vector)
- SpinBasis (const SpinParameters &spin_parameters)
- **SpinBasis** (const Eigen::ArrayXXd &basis_as_array)
- 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
- bool is_equal (const SpinBasis &basis) const

Private Member Functions

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

Private Attributes

• Eigen::ArrayXXd basis_as_array_

Friends

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

3.39 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)

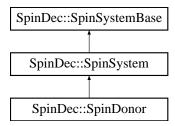
Private Member Functions

- 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

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

3.40 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 Three-Vector &electron_position, const Three-Vector &nuclear_position, const bool complete_basis)
- const ElectronSpinParameters & get_electron_parameters () const
- const NuclearSpinParameters & 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

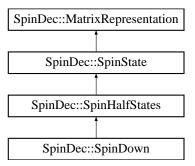
- void sort_level_labels ()
- UInt level_label_index (const UInt level_label) const
- virtual void check_level_label (const UInt level_label) const
- void calc_adiabatic_level_labels ()
- double delta () const
- double omega () const
- double scaled_omega () const
- double **D** (const int quantum_number) 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 Three-Vector &electron_position, const Three-Vector &nuclear_position, const bool complete_basis)

- bool complete_basis_
- ElectronSpinParameters electron_parameters_
- NuclearSpinParameters nuclear_parameters_
- Hyperfine hyperfine_
- UInt transition_level_labels_[2]
- UIntArray orthogonal_level_labels_
- UIntArray sorted level labels
- std::vector< AdiabaticLabel > adiabatic_level_labels_

3.41 SpinDec::SpinDown Class Reference

Inheritance diagram for SpinDec::SpinDown::



Public Member Functions

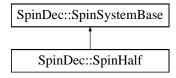
• SpinDown (const SpinHalfParameters &spin_half_parameters)

Private Member Functions

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

3.42 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

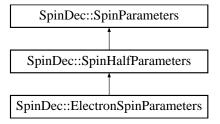
- virtual void solve once ()
- virtual void check_level_label (const UInt level_label) const

Private Attributes

• double gyromagnetic_ratio_

3.43 SpinDec::SpinHalfParameters Class Reference

Inheritance diagram for SpinDec::SpinHalfParameters::

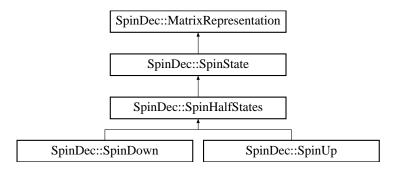


Public Member Functions

• SpinHalfParameters (const double gyromagnetic_ratio)

3.44 SpinDec::SpinHalfStates Class Reference

Inheritance diagram for SpinDec::SpinHalfStates::

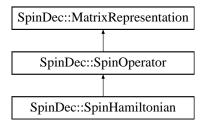


Protected Member Functions

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

3.45 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)

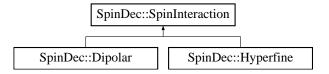
Private Member Functions

- 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)

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

3.46 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_

3.47 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)

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

3.48 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 Three-Vector &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)

- vector< SpinInteractionVertex > vertices_
- vector < SpinInteractionEdge > edges
- SpinBasis basis

3.49 SpinDec::SpinInteractionVertex Class Reference

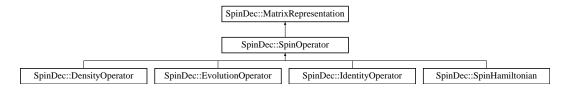
Public Member Functions

- **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)

- UInt label
- SpinParameters spin_parameters_
- SpinBasis basis_
- ThreeVector **position**_

3.50 SpinDec::SpinOperator Class Reference

Inheritance diagram for SpinDec::SpinOperator::



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

Protected Member Functions

• virtual void quit_if_dimension_mismatch () const

Protected Attributes

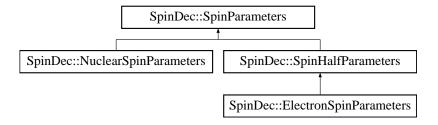
• ComplexMatrix matrix_

Friends

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

3.51 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)

3.52 SpinDec::SpinParametersVector Class Reference

Public Member Functions

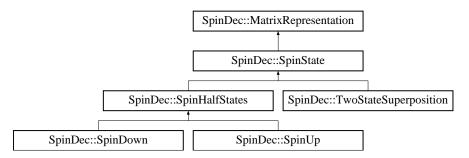
- **SpinParametersVector** (const **SpinParameters** &spin_parameters)
- SpinParameters & operator[] (const UInt index)
- const SpinParameters & operator[] (const UInt index) const
- void **push_back** (const **SpinParameters** &spin_parameters)
- UInt size () const
- void clear ()
- UInt multiplicity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

Private Attributes

• std::vector< SpinParameters > spin_parameters_vector_

3.53 SpinDec::SpinState Class Reference

Inheritance diagram for SpinDec::SpinState::



Public Member Functions

- SpinState (const Complex Vector & state_vector, const SpinBasis & basis)
- SpinState (const SpinBasis &basis)
- const Complex Vector & get_state_vector () const
- virtual void **set_state_vector** (const Complex Vector & 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 ()
- void normalize ()
- SpinState normalized () const
- virtual auto_ptr< MatrixRepresentation > clone () const

Protected Member Functions

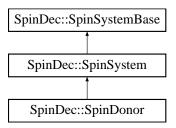
• virtual void quit if dimension mismatch () const

Protected Attributes

• Complex Vector state_vector_

3.54 SpinDec::SpinSystem Class Reference

Inheritance diagram for SpinDec::SpinSystem::



Public Member Functions

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

Protected Member Functions

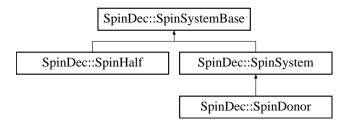
- virtual void solve_once ()
- virtual void check_level_label (const UInt level_label) const

Protected Attributes

• HermitianEigenspectrum eigenspectrum_

3.55 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

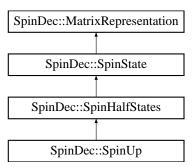
- virtual void **solve_once** ()=0
- virtual void **check_level_label** (const UInt level_label) const =0

Protected Attributes

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

3.56 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)

3.57 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_

3.58 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)

3.59 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

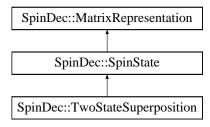
Private Member Functions

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

- TimeArray time_array_
- CDoubleArray evolution_

3.60 SpinDec::TwoStateSuperposition Class Reference

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

- SpinState state0_
- SpinState state1_
- CDouble **c0**_
- CDouble c1_

3.61 SpinDec::UniformMagneticField Class Reference

Public Member Functions

- UniformMagneticField (const double magnitude)
- UniformMagneticField (const double magnitude, const ThreeVector &direction)
- double get_magnitude () const
- ThreeVector $\mathbf{get_direction}$ () const
- void **set_magnitude** (const double magnitude)
- void **set_direction** (const ThreeVector &direction)

- double magnitude_
- ThreeVector direction_