O_2scl_part - Particle Sub-Library for O_2scl

Version 0.904

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1.2 Particles

These classes in the library `o2scl_part` calculate the thermodynamic properties of interacting and non-interacting quantum and classical particles.

The class part is the basic structure for a particle:

- part::m - mass
- part::g - degeneracy factor (e.g. $2j+1$)
- part::n - number density
- part::ed - energy density
- part::pr - pressure
- part::en - entropy density
- part::ms - effective mass
- part::nu - effective chemical potential
- part::inc_rest_mass - True if the rest mass is included
- part::non_interacting - False if the particle includes interactions

The data members part::ms and part::nu allow one to specify modifications to the mass and the chemical potential due to interactions. This allows one to calculate the properties of particle due to interactions so long as the basic form of the free-particle dispersion relation is unchanged, i.e.

$$\sqrt{k^2+m^2}-\mu \to \sqrt{k^2+m^{*2}}-\nu$$

Typically, if the particle is non-interacting, then part::mu and part::m are copied to part::nu and part::ms, computations are performed with part::nu and part::ms, and then, if necessary, the result for part::nu is copied back to part::mu.

If part::inc_rest_mass is `true` (as is the default in all of the classes except nucleus), then all functions include the rest mass energy density in the energy density, the "mu" functions expect that the rest mass is included in part::mu or part::nu as input and the "density" functions output part::mu or part::nu including the rest mass.

When part::inc_rest_mass is true, antiparticles are implemented by choosing the antiparticle chemical potential to be $-\mu$, and when inc_rest_mass is false, antiparticles are implemented by choosing the chemical potential of the antiparticles to be $-\mu-2m$.

The thermodynamic identity used to compute the pressure for interacting particles is

$$P = -\varepsilon + sT + \nu n$$

where part::nu is used. This way, the particle class doesn't need to know about the structure of the interactions to ensure that the thermodynamic identity is satisfied. Note that in the O_2scl_eos library, where in the equations of state the normal thermodynamic identity is used

$$P = -\varepsilon + sT + \mu n$$

Frequently, the interactions which create an effective chemical potential which is different than part::mu thus create extra terms in the pressure and the energy density for the given equation of state.

At zero temperature, fermions and bosons can be treated exactly in the classes fermion and boson. The quark class is a descendant of the fermion class which contains extra data members for the quark condensate and the contribution to the bag constant. The classical classical is a descendant of both fermion and boson and calculates everything in the classical limit.

At finite temperature, there are different classes corresponding to different approaches to computing the integrals over the distribution functions. The approximation scheme from Johns96 is used in eff_boson, eff_fermion, and eff_quark. An exact method employing direct integration of the distribution functions is used in rel_boson and rel_fermion, but these are necessarily quite a bit slower.

The class nonrel_fermion assumes a non-relativistic dispersion relation for fermions. It includes zero-temperature methods and an exact method for finite temperatures. The non-relativistic integrands are much simpler and nonrel_fermion uses the appropriate GSL functions to compute them.

Units:

Factors of $\hbar, c$ and k_B have been removed everywhere, so that mass, energy, and temperature all have the same units. Number and entropy densities have units of mass cubed (or energy cubed). This particle classes can be used with any system of units which is based on powers of one unit, i.e. $[n] = [T]^3 = [m]^3 = [P]^{3/4} = [\varepsilon]^{3/4}$, etc.

Derivative information:

Sometimes it is useful to know derivatives like \$ds/dT\$ in addition to the energy and pressure. There are three classes which compute these derivatives for fermions and classical particles. The class sn_classical handles the nondegenerate limit, sn_fermion handles fermions and sn_nr_fermion handles nonrelativistic fermions. These classes compute the derivatives

$$\left(\frac{dn}{d\mu}\right)_T, \quad \left(\frac{dn}{dT}\right)_\mu, \quad \text{and} \quad \left(\frac{ds}{dT}\right)_\mu$$

All other first derivatives of the thermodynamic functions can be written in terms of these three. To see how to compute the specific heat, for example, see the discussion in the documentation of deriv_part.

1.3 Atomic nuclei

Nuclei

Atomic nuclei, class nucleus, are implemented as descendants of classical. This class sets the value of nucleus::inc_rest_mass to false by default.

Nuclear mass formulas are given as children of nuclear_mass. The class ame_mass provides the experimental data from Audi95 or Audi03, the class mnmsk_mass provides the mass formula from Moller95, and the class hfb_mass provides the mass formula from Goriely02, Samyn04, or Goriely07. A simple semi-empirical mass formula is given in semi_empirical_mass and this can be fit to experimentally measured masses using mass_fit.

The class nuclear_dist provides an generic base class for a collection of several nuclei with an STL-like iterator. There are two implementations of this base class, simple_dist which provides a simple distribution and full_dist which enumerates all the nuclei for a given mass formula.

1.4 Example source code

1.4.1 exlist_subsect

- Particle example
- Nuclear mass fit example

1.4.2 Particle example

```
/* Example: ex_part.cpp
   -------------------------------------------------------------------
*/

#include <cmath>
#include <o2scl/test_mgr.h>
#include <o2scl/constants.h>
#include <o2scl/eff_fermion.h>
#include <o2scl/rel_fermion.h>
#include <o2scl/classical.h>

using namespace std;
using namespace o2scl;
using namespace o2scl_const;

int main(void) {
  test_mgr t;
  t.set_output_level(1);

  // Create two different electrons, one using the exact method from
  // rel_fermion, and the other from the approximate scheme used in
  // eff_fermion. We work in units of inverse Fermis, so that energy
  // density is fm^{-4}. We also use a classical particle, to compare
  // to the nondegenerate approximation.
  eff_fermion e(o2scl_fm::mass_electron,2.0);
  rel_fermion e2(o2scl_fm::mass_electron,2.0);
  classical e3(o2scl_fm::mass_electron,2.0);

  // Compute the pressure at a density of 0.0001 fm^{-3} and a
  // temperature of 10 MeV. At these temperatures, the electrons are
  // non-degenerate, and Boltzmann statistics nearly applies.
  e.n=0.0001;
  e.calc_density(10.0/hc_mev_fm);
  e2.n=0.0001;
  e2.calc_density(10.0/hc_mev_fm);
  e3.n=0.0001;
  e3.calc_density(10.0/hc_mev_fm);

  cout << e.pr << " " << e2.pr << " " << e3.pr << " "
       << e.n*10.0/hc_mev_fm << endl;

  // Test
  t.test_rel(e.pr,e2.pr,1.0e-2,"EFF vs. exact");
  t.test_rel(e2.pr,e3.pr,4.0e-1,"classical vs. exact");
  t.test_rel(e.n*10.0/hc_mev_fm,e3.pr,1.0e-1,"classical vs. ideal gas law");

  // Compute the pressure at a density of 0.1 fm^{-3} and a
  // temperature of 1 MeV. At these temperatures, the electrons are
  // strongly degenerate
  e.n=0.0001;
  e.calc_density(10.0/hc_mev_fm);
  e2.n=0.0001;
  e2.calc_density(10.0/hc_mev_fm);
  cout << e.pr << " " << e2.pr << endl;

  // Test
  t.test_rel(e.pr,e2.pr,1.0e-2,"EFF vs. exact");
```

```
  // Now add the contribution to the pressure from positrons using the
  // implmentation of part::pair_density()
  e.n=0.0001;
  e.pair_density(10.0/hc_mev_fm);
  e2.n=0.0001;
  e2.pair_density(10.0/hc_mev_fm);
  cout << e.pr << " " << e2.pr << endl;

  // Test
  t.test_rel(e.pr,e2.pr,1.0e-2,"EFF vs. exact");

  t.report();
  return 0;
}
// End of example
```

1.4.3 Nuclear mass fit example

```
/* Example: ex_mass_fit.cpp
   -------------------------------------------------------------------
*/

#include <iostream>
#include <o2scl/test_mgr.h>
#include <o2scl/mass_fit.h>

using namespace std;
using namespace o2scl;
using namespace o2scl_const;
using namespace o2scl_fm;


int main(void) {
  test_mgr t;
  t.set_output_level(1);

  cout.setf(ios::scientific);

  // The RMS deviation of the fit
  double res;
  // The mass formula to be fitted
  semi_empirical_mass sem;
  // The fitting class
  mass_fit mf;

  // Perform the fit
  mf.fit(sem,res);

  // Output the results
  cout << sem.B << " " << sem.Sv << " " << sem.Ss << " "
       << sem.Ec << " " << sem.Epair << endl;
  cout << res << endl;
  t.test_gen(res<4.0,"Successful fit.");

  t.report();
  return 0;
}
// End of example
```

1.5 Bibliography

Some of the references which contain links should direct you to the work referred to directly through dx.doi.org.

Audi95: G. Audi and A. H. Wapstra, Nucl. Phys. A **595** (1995) 409-480.

Audi03: G.Audi, A. H. Wapstra and C. Thibault , Nucl. Phys. A **729** (2003) 337.

Eggleton73: P. P. Eggleton, J. Faulkner, and B. P. Flannery, Astron. and Astrophys. **23** (1973) 325.

Goriely02: S. Goriely, M. Samyn, P.-H. Heenen, J. M. Pearson, and F. Tondeur, Phys. Rev. C **66** (2002) 024326.

Goriely07: S. Goriely, M. Samyn, and J. M. Pearson, Phys. Rev. C **75** (2007) 064312.

Johns96: Johns, P.J. Ellis, and J.M. Lattimer, Astrophys. J. **473** (1996) 1020.

Moller95: P. Moller, J.R. Nix, W.D. Myers, and W.J. Switecki, At. Data Nucl. Data Tables **59** (1995) 185.

Samyn04: M. Samyn, S. Goriely, M. Bender and J. M. Pearson, Phys. Rev. C **70** (2004) 044309.

2 Ideas for future development

Class ame_mass Create a caching and more intelligent search system for the **table**. The **table** is sorted by A and then N, so we could probably just copy the search routine from mnmsk_mass, which is sorted by Z and then N.

Class ame_mass Use the atomic mass unit and other constants defined in the evaulation

Class classical Write a calc_density_zerot() function for completeness?

Class eff_fermion Use bracketing to speed up one-dimensional **root** finding.

Class fermion Use hypot() and other more accurate functions for the analytic expressions for the zero temperature integrals. [Progress has been made, but there are probably other functions which may break down for small but finite masses and temperatures]

Class fermion_T Create a Chebyshev approximation for inverting the the Fermi functions for massless_calc_density() functions?

Global fermion_T::massless_pair_density(const double temper) This could be improved by including more terms in the expansions.

Class mass_fit Convert to a real fit with errors and covariance, etc.

Class nonrel_fermion This could be improved by performing a Chebyshev approximation (for example) to invert the density integral so that we don't need to use a solver.

Class nuclear_mass Make the treatment of the electron binding energy contribution more consistent.

Class nuclear_mass It might be useful to consider a fudge factor to ensure no problems with finite precision arithmetic when converting `double` to `int`.

Global nuclear_mass_info::parse_elstring(std::string ela, int &Z, int &N, int &A) Allow A to precede Z.

Global nuclear_mass_info::parse_elstring(std::string ela, int &Z, int &N, int &A) Right now, `n4` is interpreted incorrectly as Nitrogen-4, rather than the tetraneutron.

Class rel_fermion Allow the user to change the upper limit on the degenerate integration and the hard-coded value of 200 in the integrands.

Class rel_fermion It appears this doesn't compute the uncertainty in the chemical potential or density with calc_density(). This could be fixed.

Class simple_dist Make the vector constructor into a template so it accepts any type. Do the same for set_dist().

Class sn_fermion This class will have difficulty with extremely degenerate or extremely non-degnerate systems. Fix this.

Class sn_fermion Create a more intelligent method for dealing with bad initial guesses for the chemical potential in calc_density().

3 Todo List

Class eff_boson Better documentation (see eff_fermion)

Class eff_boson Remove the 'meth2' stuff

Class eff_boson Remove static variables fix_density and stat_temper

Class eff_fermion There's still def_err_hnd.set_mode(0) in the testing code, probably because the solver has a hard time for extreme values.

Global eff_fermion::calc_mu(const double temper) Should see if the function actually works if $(\mu - m)/T = -199$.

Class eff_quark Add testing.

Class nonrel_fermion Check behaviour of calc_density() at zero density, and compare with that from eff_fermion, rel_fermion, and classical.

Class nonrel_fermion I think calc_mu_zerot() and calc_density_zerot() are missing the proper dependence on the degeneracy, `g`. (8/20/07) (I think this is fixed now, but should be tested, 8/22/07)

Class nonrel_fermion Make sure to test with non-interacting equal to true or false, and document whether or not it works with both inc_rest_mass equal to true or false

Class rel_boson Testing not completely finished.

Class sn_classical This does not work with inc_rest_mass=true

Class sn_fermion This needs to be corrected to calculate $\sqrt{k^2 + m^{*2}} - m$ gracefully when $m^* \approx m$.

Class sn_fermion Call error handler if inc_rest_mass is true or update to properly treat the case when inc_rest_mass is true.

4 Data Structure Documentation

4.1 ame_entry Struct Reference

Atomic mass entry structure.

`#include <nuclear_mass.h>`

4.1.1 Detailed Description

Atomic mass entry structure.

Definition at line 554 of file nuclear_mass.h.

Data Fields

- int NMZ
  N-Z.
- int N
  Neutron number.
- int Z
  Proton number.
- int A
  Atomic number.
- std::string el
  Element name.
- std::string orig
  Data origin.
- double mass
  Mass excess.
- double dmass
  Mass excess uncertainty.
- double be
  Binding energy (given in the '95 data).
- double dbe
  Binding energy uncertainty (given in the '95 data).
- double beoa
  Binding energy / A (given in the '03 data).
- double dbeoa
  Binding energy / A uncertainty (given in the '03 data).
- std::string bdmode
  Beta decay mode.
- double bde
  Beta-decay energy.
- double dbde
  Beta-decay energy uncertainty.
- int A2
  ?
- double amass
  Atomic mass.
- double damass
  Atomic mass uncertainty.

The documentation for this struct was generated from the following file:

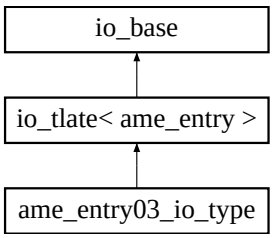
- nuclear_mass.h

4.2 ame_entry03_io_type Class Reference

A support class for I/O of the 2003 AME data.

`#include <nuclear_mass.h>`

Inheritance diagram for ame_entry03_io_type::



4.2.1 Detailed Description

A support class for I/O of the 2003 AME data.

Definition at line 623 of file nuclear_mass.h.

Public Member Functions

- int **input** (**cinput** ∗co, **in_file_format** ∗ins, ame_entry ∗t)
- int **output** (**coutput** ∗co, **out_file_format** ∗outs, ame_entry ∗t)
- virtual const char ∗ **type** ()

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

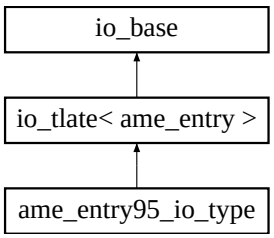
- nuclear_mass.h

4.3 ame_entry95_io_type Class Reference

A support class for I/O of the 1995 AME data.

`#include <nuclear_mass.h>`

Inheritance diagram for ame_entry95_io_type::



4.3.1 Detailed Description

A support class for I/O of the 1995 AME data.

Definition at line 614 of file nuclear_mass.h.

Public Member Functions

- int **input** (**cinput** ∗co, **in_file_format** ∗ins, ame_entry ∗t)
- int **output** (**coutput** ∗co, **out_file_format** ∗outs, ame_entry ∗t)
- virtual const char ∗ **type** ()

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

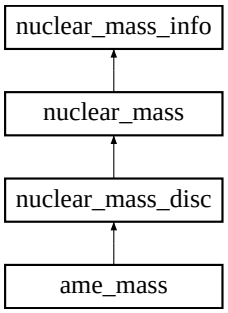
- nuclear_mass.h

4.4 ame_mass Class Reference

Mass formula from the Atomic Mass Evaluation (2005 and 1993).

`#include <nuclear_mass.h>`

Inheritance diagram for ame_mass::



4.4.1 Detailed Description

Mass formula from the Atomic Mass Evaluation (2005 and 1993).

This class provides an interface to the atomic mass **table** using data from Audi95 and Audi03.

There are four data sets, selected by the specification of the `version` string in the constructor.

- "95rmd" - "Recommended" data from Audi95 (ame95rmd.o2)
- "95exp" - "Experimental" data from Audi95 (ame95exp.o2)
- "03round" - "Rounded" data from Audi03 (ame03round.o2)
- "03" - Data from Audi03 (default) (ame03.o2)

If any string other than these four is used, the default data is loaded. If the constructor cannot find the data file (e.g. because of a broken installation), then ame::is_loaded() returns false.

The 1995 data provided the binding energy stored in ame_entry::be and ame_entry::dbe, while the 2003 data provided the binding energy divided by the atomic number stored in ame_entry::beoa and ame_entry::dbeoa. When the 1995 data is used ame_entry::beoa and ame_entry::dbeoa are calculated automatically, and when the 2003 data is used ame_entry::be and ame_entry::dbe are calculated automatically.

Note that blank entries in the original **table** that correspond to columns represented by the type `double` are set to zero arbitrarily.

Note that all uncertainties are 1 sigma uncertainties.

Warning:

There are strict definitions of the atomic mass unit and other constants that are defined by the 1995 and 2003 atomic mass evaluations which are not used at present.

Idea for future

Create a caching and more intelligent search system for the **table**. The **table** is sorted by A and then N, so we could probably just copy the search routine from mnmsk_mass, which is sorted by Z and then N.

Idea for future

Use the atomic mass unit and other constants defined in the evaulation

Definition at line 673 of file nuclear_mass.h.

Public Member Functions

- ame_mass (std::string version="")
  Create a **collection** *specified by* `version`.
- virtual const char * type ()
  Return the type, `"ame_mass"`.
- virtual bool is_included (int Z, int N)
  Return false if the mass formula does not include specified nucleus.
- virtual double mass_excess (int Z, int N)
  Given `Z` *and* `N`*, return the mass excess in MeV.*
- ame_entry get_ZN (int l_Z, int l_N)
  Get element with Z=l_Z and N=l_N (e.g. 82,126).
- ame_entry get_ZA (int l_Z, int l_A)
  Get element with Z=l_Z and A=l_A (e.g. 82,208).
- ame_entry get_elA (std::string l_el, int l_A)
  Get element with name l_el and A=l_A (e.g. "Pb",208).
- ame_entry get (std::string nucleus)
  Get element with string (e.g. "Pb208").
- bool is_loaded ()
  Returns true if the constructor succesfully loaded the data.

Data Fields

- int n
  The number of entries (about 3000).
- std::string * short_names
  The short names of the columns (length 16).
- std::string * col_names
  The long names of the columns (length 16).
- std::string reference
  The reference for the original data.
- ame_entry * mass
  The array containing the mass data of length ame::n.

Protected Attributes

- bool loaded
  True if loading the data was successful.

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

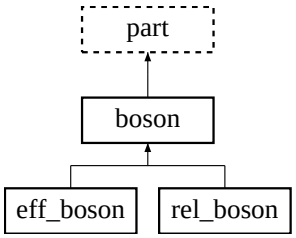
- nuclear_mass.h

4.5 boson Class Reference

Boson class [abstract base].

`#include <boson.h>`

Inheritance diagram for boson::



4.5.1 Detailed Description

Boson class [abstract base].

For bosons:

- if either nu or mu is greater than ms, then they are taken to be equal to ms
- All contributions from any type of condensate are ignored.

This Mathematica notebook contains the series expansions for the bosonic integrals. functions.

```
doc/o2scl/extras/boson.nb
doc/o2scl/extras/boson.pdf
```

Definition at line 66 of file boson.h.

Public Member Functions

- boson (double m=0.0, double g=0.0)
  Create a boson with mass `m` *and degeneracy* `g`.
- virtual int **calc_mu** (const double temper)=0
- virtual int **calc_density** (const double temper)=0
- virtual int **pair_mu** (const double temper)=0
- virtual int **pair_density** (const double temper)=0
- virtual int massless_calc_mu (const double temper)
  Calculate properties of massless bosons.
- virtual const char * type ()
  Return string denoting type ("boson").

Data Fields

- double co
  The condensate.

4.5.2 Member Function Documentation

4.5.2.1 virtual int massless_calc_mu (const double *temper*) [virtual]

Calculate properties of massless bosons.

The expressions used are exact. The chemical potentials are ignored and the scalar density is set to zero

4.5.3 Field Documentation

4.5.3.1 double co

The condensate.

The condensate variable is mostly ignored by class boson and its descendants, and is provided for user storage.

Definition at line 76 of file boson.h.

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

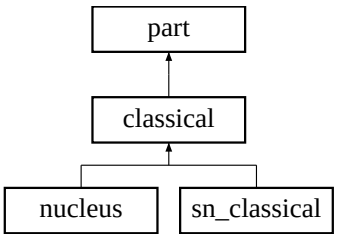
- boson.h

4.6 classical Class Reference

Classical particle class.

`#include <classical.h>`

Inheritance diagram for classical::



4.6.1 Detailed Description

Classical particle class.

Idea for future

Write a calc_density_zerot() function for completeness?

Definition at line 47 of file classical.h.

Public Member Functions

- classical (double m=0.0, double g=0.0)
  Create a classical particle with mass `m` *and degeneracy* `g`.
- virtual int calc_mu (const double temper)
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate properties as function of density.

- virtual const char * type ()
  Return string denoting type ("classical").

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

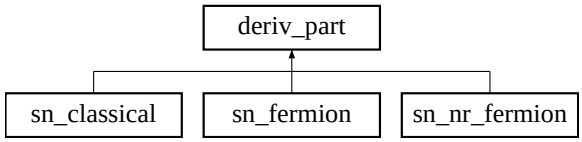
- classical.h

4.7 deriv_part Class Reference

Storage for deriviatives wrt μ and T.

`#include <deriv_part.h>`

Inheritance diagram for deriv_part::



4.7.1 Detailed Description

Storage for deriviatives wrt μ and T.

The variables `dndmu`, `dndT`, and `dsdT` correspond to

$$\left(\frac{dn}{d\mu}\right)_T, \quad \left(\frac{dn}{dT}\right)_\mu, \quad \text{and} \quad \left(\frac{ds}{dT}\right)_\mu$$

respectively.

All other derivatives can be expressed simply in terms of these three.

Derivatives wrt to chemical potential and temperature:

There is a Maxwell relation

$$\left(\frac{ds}{d\mu}\right)_T = \left(\frac{dn}{dT}\right)_\mu$$

The pressure derivatives are trivial

$$\left(\frac{dP}{d\mu}\right)_T = n, \quad \left(\frac{dP}{dT}\right)_\mu = s$$

The energy density derivatives are related through the thermodynamic identity:

$$\left(\frac{d\varepsilon}{d\mu}\right)_T = \mu\left(\frac{dn}{d\mu}\right)_T + T\left(\frac{ds}{d\mu}\right)_T$$

$$\left(\frac{d\varepsilon}{dT}\right)_\mu = \mu\left(\frac{dn}{dT}\right)_\mu + T\left(\frac{ds}{dT}\right)_\mu$$

Other derivatives:

Note that the derivative of the entropy with respect to the temperature above is not the specific heat, c_V. The specific heat is

$$C_V = \frac{T}{N}\left(\frac{\partial S}{\partial T}\right)_{V,N} = \frac{T}{n}\left(\frac{\partial s}{\partial T}\right)_{V,n}$$

To compute the specific heat in terms of the derivatives above, note that the descendants of deriv_part provide all of the thermodynamic functions in terms of μ, V and T, so we have

$$s = s(\mu, V, T) \quad \text{and} \quad n = n(\mu, V, T) \, .$$

We can then construct a function

$$s = s[\mu(n, V, T), V, T]$$

and then write the required derivative directly

$$\left(\frac{\partial s}{\partial T}\right)_{n,V} = \left(\frac{\partial s}{\partial \mu}\right)_{T,V} \left(\frac{\partial \mu}{\partial T}\right)_{n,V} + \left(\frac{\partial s}{\partial T}\right)_{\mu,V} \, .$$

Now we use the identity

$$\left(\frac{\partial \mu}{\partial T}\right)_{n,V} = - \left(\frac{\partial n}{\partial T}\right)_{\mu,V} \left(\frac{\partial n}{\partial \mu}\right)^{-1}_{T,V} \, ,$$

and the Maxwell relation above to give

$$C_V = \frac{T}{n} \left[\left(\frac{\partial s}{\partial T}\right)_{\mu,V} - \left(\frac{\partial n}{\partial T}\right)^2_{\mu,V} \left(\frac{\partial n}{\partial \mu}\right)^{-1}_{T,V} \right]$$

which expresses the specific heat in terms of the three derivatives which are given.

Note that this is the specific heat per particle, and has no units. If specific heat per unit volume is required, you must multiply by the number density.

No derivative with respect to the bare mass is given, since classes cannot know how to relate the effective mass to the bare mass.

Definition at line 136 of file deriv_part.h.

Data Fields

- double dndmu
  Derivative of number density with respect to chemical potential.
- double dndT
  Derivative of number density with respect to temperature.
- double dsdT
  Derivative of entropy density with respect to temperature.
- double dndm
  Derivative of number density with respect to the effective mass.

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

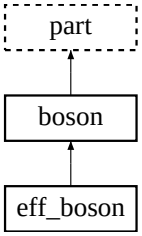
- deriv_part.h

4.8 eff_boson Class Reference

Boson class from fitting method.

`#include <eff_boson.h>`

Inheritance diagram for eff_boson::



4.8.1 Detailed Description

Boson class from fitting method.

Todo

Better documentation (see eff_fermion)

Todo

Remove the 'meth2' stuff

Todo

Remove static variables fix_density and stat_temper

Definition at line 51 of file eff_boson.h.

Public Member Functions

- eff_boson (double m=0.0, double g=0.0)
  Create a boson with mass $\mathtt{m}$ *and degeneracy* $\mathtt{g}$.
- virtual int calc_mu (const double temper)
  Calculate thermodynamic properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate thermodynamic properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate thermodynamic properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate thermodynamic properties with antiparticles as function of density.
- int set_psi_root (**root**< double, **funct**< double > > &rp)
  Set the solver for use in calculating ψ.
- int set_density_mroot (**mroot**< int, **mm_funct**< int > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- int set_meth2_root (**root**< int, **funct**< int > > &rp)
  Set the solver for use in calculating the chemical potential from the density (meth2=true).
- virtual const char * type ()
  Return string denoting type ("boson").

Static Public Member Functions

- static int load_coefficients (int ctype)
  Load coefficients for finite-temperature approximation.

Data Fields

- **gsl_mroot_hybrids**< int, **mm_funct**< int > > def_density_mroot
  The default solver for calc_density() and pair_density().
- **cern_mroot_root**< double, **funct**< double > > def_psi_root
  The default solver for ψ.
- **cern_mroot_root**< int, **funct**< int > > def_meth2_root
  The default solver for calc_density() and pair_density().

Static Public Attributes

- static const int cf_boselat3 = 1
  A set of coefficients from Jim Lattimer.
- static const int cf_bosejel21 = 2
  A set of coefficients from Johns96.
- static const int cf_bosejel22 = 3
  A set of coefficients from Johns96.
- static const int cf_bosejel34 = 4
  A set of coefficients from Johns96.
- static const int cf_bosejel34cons = 5
  The set of coefficients from Johns96 which retains better thermodynamic consistency.

Protected Member Functions

- int solve_fun (double x, double &y, double &psi)
  The function which solves for h from ψ.
- int density_fun (size_t nv, const **ovector_base** &x, **ovector_base** &y, int &pa)
  Fix density for calc_density().
- int pair_density_fun (size_t nv, const **ovector_base** &x, **ovector_base** &y, int &pa)
  Fix density for pair_density().

Protected Attributes

- **mroot**< int, **mm_funct**< int > > * density_mroot
  The solver for calc_density().
- **root**< double, **funct**< double > > * psi_root
  The solver to compute h from ψ.
- **root**< int, **funct**< int > > * meth2_root
  The solver for calc_density().

Static Protected Attributes

- static double ** Pmnb
  The coefficients.
- static int sizem
  The number of coefficient rows.
- static int sizen
  The number of coefficient columns.
- static double parma
  The parameter, a.
- static double fix_density
  Temporary storage.
- static double stat_temper
  Temporary storage.

4.8.2 Member Function Documentation

4.8.2.1 static int load_coefficients (int *ctype*) [static]

Load coefficients for finite-temperature approximation.

Presently acceptable values of `fn` are: `boselat3` from Lattimer's notes `bosejel21`, `bosejel22`, `bosejel34`, and `bosejel34cons` from Johns96.

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

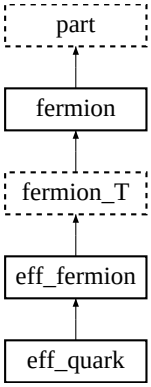
- eff_boson.h

4.9 eff_fermion Class Reference

Fermion class from fitting method.

`#include <eff_fermion.h>`

Inheritance diagram for eff_fermion::



4.9.1 Detailed Description

Fermion class from fitting method.

Based on the fitting method of Johns96 which is an update of the method from Eggleton73 . This method is approximate, but very fast. For a more accurate (but slower) method, use rel_fermion.

Given the chemical potential and the temperature the functions calc_mu() and pair_mu() work by solving the equation

$$\psi = 2\sqrt{1+f/a} + \log\left(\frac{\sqrt{1+f/a}-1}{\sqrt{1+f/a}+1}\right)$$

for f given $\psi = (\mu - m)/T$. If $f/a < 10^{-10}$, then the alternative expression

$$\psi = 2\left(1+f/(2a)\right) + \log\left[\frac{f/(2a)}{(1+f/(2a))}\right]$$

is used. The pressure, energy density, and entropy, are determined as polynomials in f with a set of precomputed coefficients as done in Johns96 .

If ψ is too small (less than about -200), the above procedure fails. To handle this, this class uses the classical result if $\psi <$ min_psi, where min_psi defaults to -200.

When the density and temperature is given instead (calc_density() and pair_density()), then there are two ways to proceed.

- Use the density to solve for f .
- Use the density to solve for the chemical potential.

Because the density is a complicated polynomial in f, the former procedure does not work very well even though it might be less time consuming. In this class, the density is solved for the effective chemical potential instead. The initial guess is just taken from the present value of part::nu .

Note:

It is important to note that the coefficients are static and apply to all objects of type eff_fermion.

Todo

There's still def_err_hnd.set_mode(0) in the testing code, probably because the solver has a hard time for extreme values.

Idea for future

Use bracketing to speed up one-dimensional **root** finding.

Definition at line 93 of file eff_fermion.h.

Coefficients for finite-temperature approximation

- static const int cf_fermilat3 = 1
  A set of coefficients from Jim Lattimer.
- static const int cf_fermijel2 = 2
  The smaller set of coefficients from Johns96.
- static const int cf_fermijel3 = 3
  The larger set of coefficients from Johns96.
- static const int cf_fermijel3cons = 4
  The set of coefficients from Johns96 which retains better thermodynamic consistency.
- static int load_coefficients (int ctype)
  Load coefficients.

Public Member Functions

- eff_fermion (double mass=0.0, double dof=0.0)
  Create a fermion with mass `mass` *and degeneracy* `dof`.
- virtual int calc_mu (const double temper)
  Calculate thermodynamic properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate thermodynamic properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate thermodynamic properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate thermodynamic properties with antiparticles as function of density.
- int set_psi_root (**root**< double, **funct**< double > > &rp)
  Set the solver for use in calculating ψ.
- int set_density_root (**root**< double, **funct**< double > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- virtual const char * type ()
  Return string denoting type ("eff_fermion").

Data Fields

- double tlimit
  If the temperature is less than `tlimit` *then the zero-temperature functions are used (default 0).*
- **cern_mroot_root**< double, **funct**< double > > def_psi_root
  The default solver for ψ.
- **cern_mroot_root**< double, **funct**< double > > def_density_root
  The default solver for calc_density() and pair_density().
- double min_psi
  The minimum value of ψ (default -200).

Protected Member Functions

- int solve_fun (double x, double &y, double &psi)
  The function which solves for f from ψ.
- int density_fun (double x, double &y, double &temper)
  Fix density for calc_density().
- int pair_density_fun (double x, double &y, double &temper)
  Fix density for pair_density().

Protected Attributes

- **root**< double, **funct**< double > > * psi_root
  The solver for ψ.
- **root**< double, **funct**< double > > * density_root
  The other solver for calc_density().

Static Protected Attributes

- static double ** Pmnf
  The matrix of coefficients.
- static double parma
  The parameter a.
- static int sizem
  The array row size.
- static int sizen
  The array column size.

4.9.2 Member Function Documentation

4.9.2.1 virtual int calc_density (const double *temper*) [virtual]

Calculate thermodynamic properties as function of density.

Warning:

This function needs a guess for the chemical potential, and will fail if that guess is not sufficiently accurate.

Implements fermion_T.

Reimplemented in eff_quark.

4.9.2.2 virtual int calc_mu (const double *temper*) [virtual]

Calculate thermodynamic properties as function of chemical potential.

If the quantity $(\mu - m)/T$ (or $(\nu - m^*)/T$ in the case of interacting particles) is less than -200, then this quietly sets the density, the scalar density, the energy density, the pressure and the entropy to zero and exits.

Todo

Should see if the function actually works if $(\mu - m)/T = -199$.

Implements fermion_T.

Reimplemented in eff_quark.

4.9.2.3 static int load_coefficients (int *ctype*) [static]

Load coefficients.

The argument `ctype` Should be one of the constants below.

4.9.2.4 virtual int pair_mu (const double *temper*) [virtual]

Calculate thermodynamic properties with antiparticles as function of chemical potential.

Warning:

This function needs a guess for the chemical potential, and will fail if that guess is not sufficiently accurate.

Implements fermion_T.

Reimplemented in eff_quark.

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

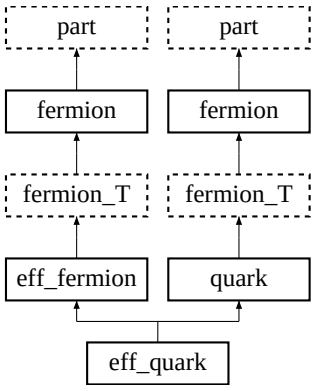
- eff_fermion.h

4.10 eff_quark Class Reference

Quark class from fitting method.

`#include <eff_quark.h>`

Inheritance diagram for eff_quark::



4.10.1 Detailed Description

Quark class from fitting method.

Todo

Add testing.

Definition at line 45 of file eff_quark.h.

Public Member Functions

- eff_quark (double m=0.0, double g=0.0)

Create a quark with mass m *and degeneracy* g.

- virtual int calc_mu (const double temper)
  Calculate thermodynamic properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate thermodynamic properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate thermodynamic properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate thermodynamic properties with antiparticles as function of density.
- virtual const char * type ()
  Return string denoting type ("eff_quark").

4.10.2 Member Function Documentation

4.10.2.1 virtual int calc_density (const double *temper*) [virtual]

Calculate thermodynamic properties as function of density.

Warning:

This function needs a guess for the chemical potential, and will fail if that guess is not sufficiently accurate.

Reimplemented from eff_fermion.

4.10.2.2 virtual int calc_mu (const double *temper*) [virtual]

Calculate thermodynamic properties as function of chemical potential.

If the quantity $(\mu - m)/T$ (or $(\nu - m^*)/T$ in the case of interacting particles) is less than -200, then this quietly sets the density, the scalar density, the energy density, the pressure and the entropy to zero and exits.

Todo

Should see if the function actually works if $(\mu - m)/T = -199$.

Reimplemented from eff_fermion.

4.10.2.3 virtual int pair_mu (const double *temper*) [virtual]

Calculate thermodynamic properties with antiparticles as function of chemical potential.

Warning:

This function needs a guess for the chemical potential, and will fail if that guess is not sufficiently accurate.

Reimplemented from eff_fermion.

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

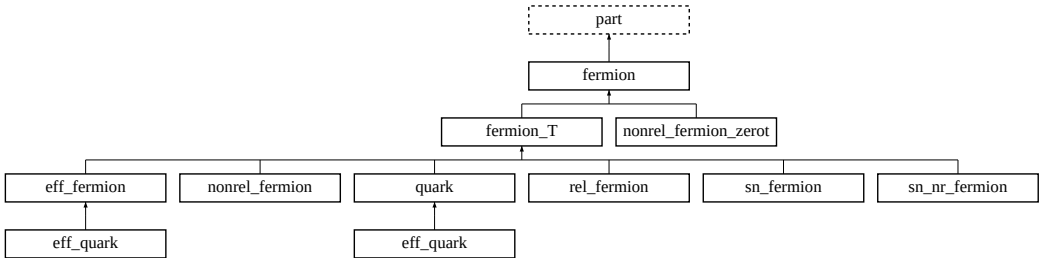
- eff_quark.h

4.11 fermion Class Reference

Fermion class.

`#include <fermion.h>`

Inheritance diagram for fermion::



4.11.1 Detailed Description

Fermion class.

This is a base class for the computation of fermionic statistics at zero temperature. The more general case of finite temperature is taken care of by fermion_T objects. The primary functions are calc_mu_zerot() and calc_density_zerot() which compute all the thermodynamic quantities as a function of the chemical potential, or the density, respectively.

This class also adds two member data variables, kf and del, for the Fermi momentum and the gap.

Idea for future

Use hypot() and other more accurate functions for the analytic expressions for the zero temperature integrals. [Progress has been made, but there are probably other functions which may break down for small but finite masses and temperatures]

Definition at line 63 of file fermion.h.

Public Member Functions

- fermion (double mass=0, double dof=0)
  Create a fermion with mass `mass` *and degeneracy* `dof`.
- virtual const char * type ()
  Return string denoting type ("fermion").

Zero-temperature fermions

- int kf_from_density ()
  Calculate the Fermi momentum from the density.
- int energy_density_zerot ()
  Energy density at T=0 from kf and ms.
- int pressure_zerot ()
  Pressure at T=0 from kf and ms.
- virtual int calc_mu_zerot ()
  Zero temperature fermions from nu and ms.
- virtual int calc_density_zerot ()
  Zero temperature fermions from n and ms.

Data Fields

- double kf
  Fermi momentum.
- double del
  Gap.

4.11.2 Member Function Documentation

4.11.2.1 virtual int calc_density_zerot () [virtual]

Zero temperature fermions from n and ms.

This function always returns gsl_success.

Reimplemented in nonrel_fermion, and nonrel_fermion_zerot.

4.11.2.2 virtual int calc_mu_zerot () [virtual]

Zero temperature fermions from nu and ms.

This function always returns gsl_success.

Reimplemented in nonrel_fermion, and nonrel_fermion_zerot.

4.11.2.3 int energy_density_zerot ()

Energy density at T=0 from kf and ms.

Calculates the integral

$$\varepsilon = \frac{g}{2\pi^2}\int_0^{k_F} k^2\sqrt{k^2+m^{*2}}dk$$

4.11.2.4 int kf_from_density ()

Calculate the Fermi momentum from the density.

Uses the relation $k_F = (6\pi^2 n/g)^{1/3}$

4.11.2.5 int pressure_zerot ()

Pressure at T=0 from kf and ms.

Calculates the integral

$$P = \frac{g}{6\pi^2}\int_0^{k_F} \frac{k^4}{\sqrt{k^2+m^{*2}}}dk$$

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

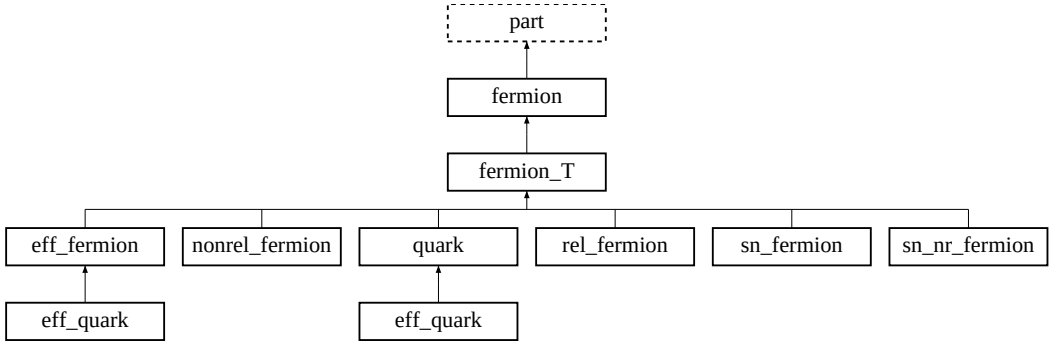
- fermion.h

4.12 fermion_T Class Reference

Fermion with finite-temperature thermodynamics [abstract base].

`#include <fermion.h>`

Inheritance diagram for fermion_T::



4.12.1 Detailed Description

Fermion with finite-temperature thermodynamics [abstract base].

This is an abstract base for the computation of finite-temperature fermionic statistics. Different children (e.g. eff_fermion and rel_fermion) use different techniques to computing the momentum integrations.

Because massless fermions at finite temperature are much simpler, there are separate member functions included in this class to handle them. The functions massless_calc_density() and massless_calc_mu() compute the thermodynamics of massless fermions at finite temperature given the density or the chemical potentials. The functions massless_pair_density() and massless_pair_mu() perform the same task, but automatically include antiparticles.

The function massless_calc_density() uses a **root** object to solve for the chemical potential as a function of the density. The default is an object of type **cern_mroot_root**. The function massless_pair_density() does not need to use the **root** object because of the simplification afforded by the inclusion of antiparticles.

Idea for future

Create a Chebyshev approximation for inverting the the Fermi functions for massless_calc_density() functions?

This Mathematica notebook contains the derivations of related series expansions and some algebra for the massless_pair() functions.

```
doc/o2scl/extras/fermion.nb
doc/o2scl/extras/fermion.pdf
```

Definition at line 174 of file fermion.h.

Public Member Functions

- fermion_T (double mass=0, double dof=0)
  Create a fermion with mass `mass` *and degeneracy* `dof`.
- virtual int calc_mu (const double temper)=0
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)=0
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)=0
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)=0
  Calculate properties with antiparticles as function of density.
- int set_massless_root (**root**< const double, **funct**< const double > > &rp)
  Set the solver for use in massless_calc_density().
- virtual const char * type ()
  Return string denoting type ("fermion_T").

Massless fermions

- virtual int massless_calc_mu (const double temper)
  Finite temperature massless fermions.
- virtual int massless_calc_density (const double temper)
  Finite temperature massless fermions.
- int massless_pair_mu (const double temper)
  Finite temperature massless fermions and antifermions.
- int massless_pair_density (const double temper)
  Finite temperature massless fermions and antifermions.

Data Fields

- **cern_mroot_root**< const double, **funct**< const double > > def_massless_root
  The default solver for massless_calc_density().

4.12.2 Member Function Documentation

4.12.2.1 int massless_pair_density (const double *temper*)

Finite temperature massless fermions and antifermions.

In the cases $n^3 >> T$ and $T >> n^3$, expansions are used instead of the exact formulas to avoid loss of precision.

In particular, using the parameter

$$\alpha = \frac{g^2 \pi^2 T^6}{243 n^2}$$

and defining the expression

$$\mathrm{cbt} = \alpha^{-1/6} \left(-1 + \sqrt{1+\alpha}\right)^{1/3}$$

we can write the chemical potential as

$$\mu = \frac{\pi T}{\sqrt{3}} \left(\frac{1}{\mathrm{cbt}} - \mathrm{cbt} \right)$$

These expressions, however, do not work well when α is very large or very small, so series expansions are used whenever $\alpha > 10^4$ or $\alpha < 3 \times 10^{-4}$. For large α,

$$\left(\frac{1}{\mathrm{cbt}} - \mathrm{cbt} \right) \approx \frac{2^{1/3}}{\alpha^{1/6}} - \frac{\alpha^{1/6}}{2^{1/3}} + \frac{\alpha^{5/6}}{6\, 2^{2/3}} + \frac{\alpha^{7/6}}{12\, 2^{1/3}} - \frac{\alpha^{11/6}}{18\, 2^{2/3}} - \frac{5\alpha^{13/6}}{144\, 2^{1/3}} + \frac{77\alpha^{17/6}}{2592\, 2^{2/3}}$$

and for small α,

$$\left(\frac{1}{\mathrm{cbt}} - \mathrm{cbt} \right) \approx \frac{2}{3}\sqrt{\frac{1}{\alpha}} - \frac{8}{81}\left(\frac{1}{\alpha}\right)^{3/2} + \frac{32}{729}\left(\frac{1}{\alpha}\right)^{5/2}$$

This approach works to within about 1 part in 10^{12}, and is tested in `fermion_ts.cpp`.

Idea for future

This could be improved by including more terms in the expansions.

4.12.3 Field Documentation

4.12.3.1 cern_mroot_root<const double, funct<const double> > def_massless_root

The default solver for massless_calc_density().

We default to **cern_mroot_root** here since we don't have a bracket or a derivative.

Definition at line 304 of file fermion.h.

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

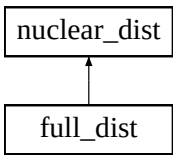
- fermion.h

4.13 full_dist Class Reference

Full distribution including all nuclei from a discrete mass formula.

`#include <nuclear_dist.h>`

Inheritance diagram for full_dist::



4.13.1 Detailed Description

Full distribution including all nuclei from a discrete mass formula.

For example, to create a collection of all nuclei from the most recent (2003) Atomic Mass Evaluation, and then output all the nuclei in the collection

```
ame_mass ame;
full_dist fd(&ame);
for(nuclear_dist::iterator ndi=fd.begin();ndi!=fd.end();ndi++) {
  cout << ndi->Z << " " << ndi->A << " " << ndi->m << endl;
}
```

Definition at line 250 of file nuclear_dist.h.

Public Member Functions

- full_dist (nuclear_mass &nm, int maxA=400, bool include_neutron=false)
  Create a distribution including all nuclei with atomic numbers less than `maxA` *from the mass formula* `nm`.
- int set_dist (nuclear_mass &nm, int maxA=400, bool include_neutron=false)
  Set the distribution to all nuclei with atomic numbers less than `maxA` *from the mass formula* `nm`.
- virtual iterator begin ()
  The beginning of the distribution.
- virtual iterator end ()
  The end of the distribution.
- virtual size_t size ()
  The number of nuclei in the distribution.

4.13.2 Member Function Documentation

4.13.2.1 int set_dist (nuclear_mass & *nm*, int *maxA* = `400`, bool *include_neutron* = `false`)

Set the distribution to all nuclei with atomic numbers less than `maxA` from the mass formula `nm`.

The information for the previous distribution is cleared before a new distribution is set.

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

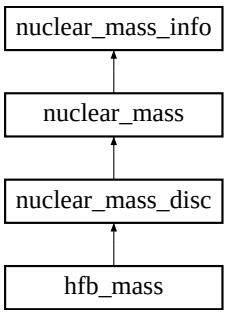
- nuclear_dist.h

4.14 hfb_mass Class Reference

HFB Mass formula.

`#include <nuclear_mass.h>`

Inheritance diagram for hfb_mass::



4.14.1 Detailed Description

HFB Mass formula.

Definition at line 1019 of file nuclear_mass.h.

Public Member Functions

- hfb_mass (size_t model=14)
  Create a new mass formula object using the specified model number.
- virtual bool is_included (int Z, int N)
  Return false if the mass formula does not include specified nucleus.
- virtual double mass_excess (int Z, int N)
  Given `Z` *and* `N`*, return the mass excess in MeV.*
- hfb_mass_entry get_ZN (int l_Z, int l_N)
  Get the entry for the specified proton and neutron number.
- bool is_loaded ()
  Verify that the constructor properly loaded the **table**.
- double blank ()
  The value which corresponds to a blank entry.
- virtual const char * type ()
  Return the type, `"hfb_mass"`.

Data Fields

- int n
  The number of **table** *entries.*
- hfb_mass_entry * mass
  The array containing the **table**.

Protected Attributes

- bool loaded
  True if the **table** *was successfully loaded.*
- int last
  The last **table** *index for caching.*

4.14.2 Constructor & Destructor Documentation

4.14.2.1 hfb_mass (size_t *model* = 14)

Create a new mass formula object using the specified model number.

Valid values of `model` at present are 2, 8, and 14, corresponding to the HFB2 (Goriely02), HFB8 (Samyn04), and HFB14 (Goriely07). If a number other than these three is given, the error handler is called.

4.14.3 Member Function Documentation

4.14.3.1 hfb_mass_entry get_ZN (int *l_Z*, int *l_N*)

Get the entry for the specified proton and neutron number.

This method searches the **table** using a cached binary search algorithm. It is assumed that the **table** is sorted first by proton number and then by neutron number.

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

- nuclear_mass.h

4.15 hfb_mass_entry Struct Reference

Mass formula entry structure for HFB mass formula.

`#include <nuclear_mass.h>`

4.15.1 Detailed Description

Mass formula entry structure for HFB mass formula.

Definition at line 976 of file nuclear_mass.h.

Data Fields

- int N
  Neutron number.
- int Z
  Proton number.
- int A
  Atomic number.
- double bet2
  Beta 2 deformation.
- double bet4
  Beta 4 deformation.
- double Rch
  RMS charge radius.
- double def_wig
  Deformation and Wigner energies.
- double Sn
  Neutron separation energy.
- double Sp
  Proton separation energy.
- double Qbet
  Beta-decay energy.
- double Mcal

Calculated mass excess.
- double Err
  Error between experimental and calculated mass excess.

The documentation for this struct was generated from the following file:

- nuclear_mass.h

4.16 mass_fit Class Reference

Fit a nuclear mass formula.

`#include <mass_fit.h>`

4.16.1 Detailed Description

Fit a nuclear mass formula.

There is an example of the usage of this class given in Nuclear mass fit example.

Idea for future

Convert to a real fit with errors and covariance, etc.

Definition at line 46 of file mass_fit.h.

Public Member Functions

- virtual int fit (nuclear_mass_fit &n, double &res)
  Fit the nuclear mass formula.
- virtual int eval (nuclear_mass &n, double &res)
  Evaluate quality without fitting.
- int set_mmin (**multi_min**< int, **multi_funct**< int > > &umm)
  Change the minimizer for use in the fit.
- int set_dist (nuclear_dist &uexp)
  Set the distribution of nuclei to fit.

Data Fields

- bool even_even
  If true, then only fit doubly-even nuclei (default false).
- int minZ
  Minimum proton number to fit (default 8).
- int minN
  Minimum neutron number to fit (default 8).
- **gsl_mmin_simp**< int, **multi_funct**< int > > def_mmin
  The default minimizer.
- full_dist def_dist
  The default distribution of nuclei to fit (defaults to all nuclei in def_exp_mass).
- ame_mass def_exp_mass
  The default experimental nuclear mass object for def_dist.

4.16.2 Field Documentation

4.16.2.1 gsl_mmin_simp<int,multi_funct<int> > def_mmin

The default minimizer.

The value of def_mmin::ntrial is automatically multiplied by 10 in the constructor because the minimization frequently requires more trials than the default.

Definition at line 77 of file mass_fit.h.

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

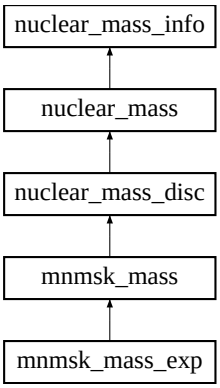
- mass_fit.h

4.17 mnmsk_mass Class Reference

Mass formula from Moller, Nix, Myers and Swiatecki.

`#include <nuclear_mass.h>`

Inheritance diagram for mnmsk_mass::



4.17.1 Detailed Description

Mass formula from Moller, Nix, Myers and Swiatecki.

The data containing an object of type moller_mass_entry for 8979 nuclei is automatically loaded by the constructor. If the file (nucmass/mnmsk.o2) is not found, then is_loaded() will return false and all calls to get_ZN() will return an object with `N=Z=0`.

There are several entries in the original **table** which are blank because they are in some way not known, measured, or computable. To distinguish these values from zero, blank entries have been replaced by the number `1.0e99`. For convenience, this value is returned by blank().

Definition at line 874 of file nuclear_mass.h.

Public Member Functions

- virtual bool is_included (int Z, int N)
  Return false if the mass formula does not include specified nucleus.
- virtual double mass_excess (int Z, int N)
  Given `Z` and `N`, return the mass excess in MeV.
- mnmsk_mass_entry get_ZN (int l_Z, int l_N)
  Get the entry for the specified proton and neutron number.

- bool is_loaded ()
  Verify that the constructor properly loaded the **table**.
- double blank ()
  The value which corresponds to a blank entry.
- double neither ()
  Neither beta+ or beta- is possible.
- double beta_stable ()
  The value which corresponds to a blank entry.
- double beta_plus_and_minus ()
  Both beta+ and beta- are possible.
- double greater_100 ()
  The value is greater than 100.
- double very_large ()
  The value is greater than 10^{20}.
- virtual const char * type ()
  Return the type, `"mnmsk_mass"`.

Data Fields

- int n
  The number of **table** *entries.*
- mnmsk_mass_entry * mass
  The array containing the **table**.

Protected Attributes

- bool loaded
  True if the **table** *was successfully loaded.*
- int last
  The last **table** *index for caching.*

4.17.2 Member Function Documentation

4.17.2.1 mnmsk_mass_entry get_ZN (int *l_Z*, int *l_N*)

Get the entry for the specified proton and neutron number.

This method searches the **table** using a cached binary search algorithm. It is assumed that the **table** is sorted first by proton number and then by neutron number.

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

- nuclear_mass.h

4.18 mnmsk_mass_entry Struct Reference

Mass formula entry structure for Moller, et al.

`#include <nuclear_mass.h>`

4.18.1 Detailed Description

Mass formula entry structure for Moller, et al.

Definition at line 740 of file nuclear_mass.h.

Data Fields

- int N
  Neutron number.
- int Z
  Proton number.
- int A
  Atomic number.
- double Emic
  The ground-state microscopic energy.
- double Mth
  The theoretical mass excess (in MeV).
- double Mexp
  The experimental mass excess (in MeV).
- double sigmaexp
  Experimental mass excess error.
- double EmicFL
  The ground-state microscopic energy in the FRLDM.
- double MthFL
  The theoretical mass excess in the FRLDM.
- std::string spinp
  Spin and pairity of odd proton.
- std::string spinn
  Spin and pairity of odd neutron.
- double gapp
  Lipkin-Nogami proton gap.
- double gapn
  Lipkin-Nogami neutron gap.
- double be
  Total binding energy.
- double S1n
  One neutron separation energy.
- double S2n
  Two neutron separation energy.
- double PA
  Percentage of daughters generated in beta decay after beta-delayed neutron emission.
- double PAm1
  Desc.
- double PAm2
  Desc.
- double Qbeta
  Energy released in beta-decay.
- double Tbeta
  Half-life w.r.t. GT beta-decay.
- double S1p
  One proton separation energy.
- double S2p
  Two proton separation energy.
- double Qalpha
  Energy released in alpha-decay.
- double Talpha
  Half-life w.r.t. alpha-decay.

Ground state deformations (perturbed-spheroid parameterization)

- double eps2
  Quadrupole.
- double eps3

Octupole.
- double eps4
  Hexadecapole.
- double eps6
  Hexacontatetrapole.
- double eps6sym
  Hexacontatetrapole without mass asymmetry.

Ground state deformations in the spherical-harmonics expansion

- double beta2
  Quadrupole.
- double beta3
  Octupole.
- double beta4
  Hexadecapole.
- double beta6
  Hexacontatetrapole.

The documentation for this struct was generated from the following file:

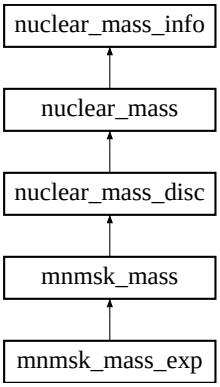
- nuclear_mass.h

4.19 mnmsk_mass_exp Class Reference

The experimental values from Moller, Nix, Myers and Swiatecki.

`#include <nuclear_mass.h>`

Inheritance diagram for mnmsk_mass_exp::



4.19.1 Detailed Description

The experimental values from Moller, Nix, Myers and Swiatecki.

Definition at line 953 of file nuclear_mass.h.

Public Member Functions

- virtual bool is_included (int Z, int N)
  Return false if the mass formula does not include specified nucleus.
- virtual double mass_excess (int Z, int N)

Given Z *and* N*, return the mass excess in MeV.*

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

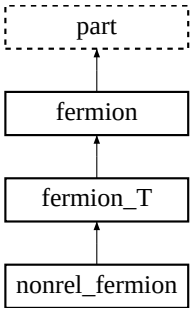
- nuclear_mass.h

4.20 nonrel_fermion Class Reference

Nonrelativistic fermion class.

`#include <nonrel_fermion.h>`

Inheritance diagram for nonrel_fermion::



4.20.1 Detailed Description

Nonrelativistic fermion class.

The rest mass energy density is given by n∗m not n∗ms. Note that the effective mass here is the Landau mass, not the Dirac mass.

Pressure is computed with

$$P = 2\varepsilon/3$$

and entropy density with

$$s = \frac{5\varepsilon}{3T} - \frac{n\mu}{T}$$

These relations can be verified with an integration by parts. See, e.g. Callen's "Thermodynamics and an introduction to thermostatistics", 2nd edition, pg. 403 or Landau and Lifshitz, Stat. Phys. 3rd edition, part 1, pg. 164.

The functions fermion::pair_density() and pair_mu() have not been implemented.

Todo

Check behaviour of calc_density() at zero density, and compare with that from eff_fermion, rel_fermion, and classical.

Todo

I think calc_mu_zerot() and calc_density_zerot() are missing the proper dependence on the degeneracy, g. (8/20/07) (I think this is fixed now, but should be tested, 8/22/07)

Todo

Make sure to test with non-interacting equal to true or false, and document whether or not it works with both inc_rest_mass equal to true or false

Idea for future

This could be improved by performing a Chebyshev approximation (for example) to invert the density integral so that we don't need to use a solver.

Definition at line 91 of file nonrel_fermion.h.

Public Member Functions

- nonrel_fermion (double m=0.0, double g=0.0)
  Create a nonrelativistic fermion with mass 'm' and degeneracy 'g'.
- virtual int calc_mu_zerot ()
  Zero temperature fermions.
- virtual int calc_density_zerot ()
  Zero temperature fermions.
- virtual int calc_mu (const double temper)
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate properties with antiparticles as function of density.
- virtual int nu_from_n (const double temper)
  Calculate effective chemical potential from density.
- int set_density_root (**root**< double, **funct**< double > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- virtual const char * type ()
  Return string denoting type ("nonrel_fermion").

Data Fields

- **cern_mroot_root**< double, **funct**< double > > def_density_root
  The default solver for calc_density().

4.20.2 Member Function Documentation

4.20.2.1 virtual int calc_density (const double *temper*) [virtual]

Calculate properties as function of density.

If the density is zero, this function just sets part::mu, part::nu, part::ed, part::pr, and part::en to zero and returns without calling the error handler (even though at zero density and finite temperature, the chemical potentials formally are equal to $-\infty$).

Implements fermion_T.

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

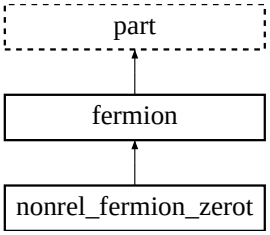
- nonrel_fermion.h

4.21 nonrel_fermion_zerot Class Reference

A zero temperature non-relativistic fermion.

`#include <nonrel_fermion.h>`

Inheritance diagram for nonrel_fermion_zerot::



4.21.1 Detailed Description

A zero temperature non-relativistic fermion.

Definition at line 170 of file nonrel_fermion.h.

Public Member Functions

- nonrel_fermion_zerot (double m=0.0, double g=0.0)
  Create a nonrelativistic fermion with mass 'm' and degeneracy 'g'.
- virtual int calc_mu_zerot ()
  Zero temperature fermions.
- virtual int calc_density_zerot ()
  Zero temperature fermions.
- virtual const char * type ()
  Return string denoting type ("nonrel_fermion_zerot").

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

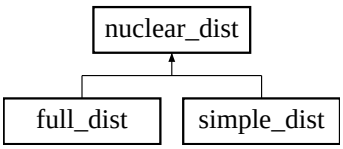
- nonrel_fermion.h

4.22 nuclear_dist Class Reference

A distribution of nuclei.

`#include <nuclear_dist.h>`

Inheritance diagram for nuclear_dist::



4.22.1 Detailed Description

A distribution of nuclei.

The virtual base class for a collection of objects of type nucleus . See simple_dist and full_dist for implmentations of this base class.

Definition at line 41 of file nuclear_dist.h.

Data Structures

- class iterator
  An iterator for the nuclear distribution.

Public Member Functions

- virtual iterator begin ()=0
  The beginning of the distribution.
- virtual iterator end ()=0
  The end of the distribution.
- virtual size_t size ()=0
  The number of nuclei in the distribution.

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

- nuclear_dist.h

4.23 nuclear_dist::iterator Class Reference

An iterator for the nuclear distribution.

`#include <nuclear_dist.h>`

4.23.1 Detailed Description

An iterator for the nuclear distribution.

The standard usage of this iterator is something of the form:

```
mnmsk_mass mth;
simple_dist sd(5,6,10,12,&mth);
for(nuclear_dist::iterator ndi=sd.begin();ndi!=sd.end();ndi++) {
// do something here for each nucleus
}
```

which would create a list consisting of three isotopes (A=10, 11, and 12) of boron and three isotopes carbon for a total of six nuclei.

Definition at line 70 of file nuclear_dist.h.

Public Member Functions

- iterator (nuclear_dist *ndpp, nucleus *npp)
  Create an iterator from the given distribution using the nucleus specified in `npp`.
- iterator operator++ ()
  Proceed to the next nucleus.
- iterator operator++ (int unused)
  Proceed to the next nucleus.
- nucleus * operator → () const
  Dereference the iterator.

Protected Attributes

- nucleus * np
  A pointer to the current nucleus.
- nuclear_dist * ndp
  A pointer to the distribution.

Friends

- bool operator== (const nuclear_dist::iterator &i1, const nuclear_dist::iterator &i2)
  Give access to the == operator.
- bool operator!= (const nuclear_dist::iterator &i1, const nuclear_dist::iterator &i2)
  Give access to the != operator.

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

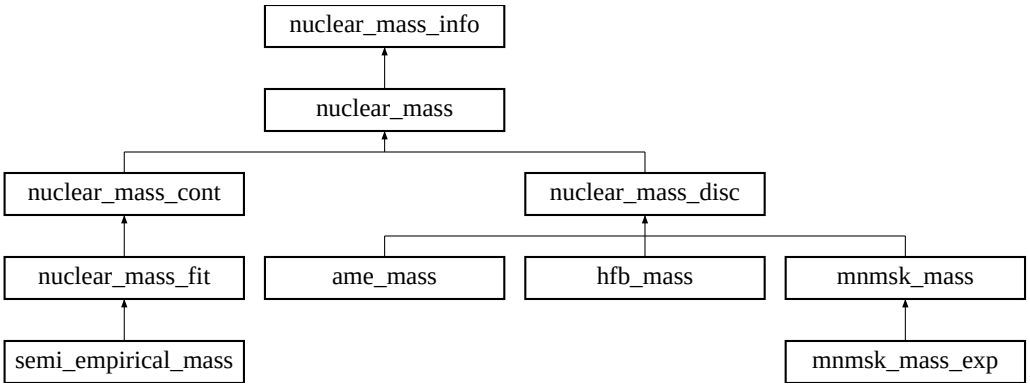
- nuclear_dist.h

4.24 nuclear_mass Class Reference

Nuclear mass formula base [abstract base].

`#include <nuclear_mass.h>`

Inheritance diagram for nuclear_mass::



4.24.1 Detailed Description

Nuclear mass formula base [abstract base].

This base class provides some default functionality for the nuclear mass formulas. For typical usage, use ame_mass, mnmsk_mass, mnmsk_mass_exp, or semi_empirical_mass.

Elements 112-118 are named "Uub", "Uut", "Uuq", "Uup", "Uuh", "Uus", and "Uuo", respectively.

The binding energy is defined by

$$\mathrm{BE} = Zm_H + Nm_n - m_{\mathrm{nuclide}}$$

where m_{nuclide} is the mass of the nucleus including the mass of the electrons. The mass excess is defined by

$$m_{\mathrm{excess}} = m_{\mathrm{nuclide}} - Am_u$$

For example, for U^{238}, the binding energy is 1801.695 MeV, the mass excess is 47.30366 MeV, and m_{nuclide} is 221742.9 MeV. This is consistent with the above, as m_H is 938.7830 MeV, m_n is 939.5650 MeV, and m_u is 931.494 MeV.

Some mass formulas are undefined for sufficiently exotic nuclei. You can use the function is_included() to find if a particular nucleus is included or not.

Warning:

The treatment of the electron binding energy contribution is not necessarily consistent at present.

Some common reaction Q-values and separation energies:

$\mathrm{Q}(\beta^-) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A},\mathrm{Z}+1)$: Beta-decay energy

$\mathrm{Q}(2\beta^-) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A},\mathrm{Z}+2)$: Double beta-decay energy

$\mathrm{Q}(4\beta^-) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A},\mathrm{Z}+4)$: Four beta-decay energy

$\mathrm{Q}(\alpha) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A}-4,\mathrm{Z}-2) - \mathrm{M}(\mathrm{He}^4)$: Alpha-decay energy

$\mathrm{Q}(\beta - n) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A}-1,\mathrm{Z}+1) - \mathrm{M}(\mathrm{n})$: Beta-delayed neutron emission decay energy

$\mathrm{Q}(d,\alpha) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A}-2,\mathrm{Z}-1) - \mathrm{M}(\mathrm{He}^4) - \mathrm{M}(\mathrm{H}^2)$: (d,α) reaction energy

$\mathrm{Q}(\mathrm{EC}) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A},\mathrm{Z}-1)$: Electron capture decay energy

$\mathrm{Q}(\mathrm{ECp}) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A}-1,\mathrm{Z}-2)$: Electron capture with delayed proton emission decay energy

$\mathrm{Q}(n,\alpha) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A}-3,\mathrm{Z}-2) - \mathrm{M}(\mathrm{He}^4) + \mathrm{M}(\mathrm{n})$: (n,α) reaction energy

$\mathrm{Q}(p,\alpha) = \mathrm{M}(\mathrm{A},\mathrm{Z}) - \mathrm{M}(\mathrm{A}-3,\mathrm{Z}-1) - \mathrm{M}(\mathrm{He}^4) + \mathrm{M}(\mathrm{p})$: (p,α) reaction energy

$\mathrm{S}(n) = -\mathrm{M}(\mathrm{A},\mathrm{Z}) + \mathrm{M}(\mathrm{A}-1,\mathrm{Z}) + \mathrm{M}(\mathrm{n})$: Neutron separation energy

$\mathrm{S}(p) = -\mathrm{M}(\mathrm{A},\mathrm{Z}) + \mathrm{M}(\mathrm{A}-1,\mathrm{Z}-1) + \mathrm{H}^1$: Proton separation energy

$\mathrm{S}(2n) = -\mathrm{M}(\mathrm{A},\mathrm{Z}) + \mathrm{M}(\mathrm{A}-2,\mathrm{Z}) + 2\mathrm{M}(\mathrm{n})$: Two neutron separation energy

$\mathrm{S}(2p) = -\mathrm{M}(\mathrm{A},\mathrm{Z}) + \mathrm{M}(\mathrm{A}-2,\mathrm{Z}-2) + 2\mathrm{M}(\mathrm{H}^{1)}$: Two proton separation energy

Idea for future

Make the treatment of the electron binding energy contribution more consistent.

Idea for future

It might be useful to consider a fudge factor to ensure no problems with finite precision arithmetic when converting `double` to `int`.

Definition at line 290 of file nuclear_mass.h.

Public Member Functions

- virtual const char * type ()
  Return the type, `"nuclear_mass"`.
- virtual bool is_included (int Z, int N)
  Return false if the mass formula does not include specified nucleus.
- int get_nucleus (int Z, int N, nucleus &n)
  Fill `n` *with the information from nucleus with the given neutron and proton number.*
- virtual double mass_excess (int Z, int N)=0
  Given `Z` *and* `N`*, return the mass excess in MeV.*
- virtual double mass_excess_d (double Z, double N)=0
  Given `Z` *and* `N`*, return the mass excess in MeV.*
- virtual double binding_energy (int Z, int N)
  Return the binding energy in MeV.
- virtual double binding_energy_d (double Z, double N)
  Return the binding energy in MeV.
- virtual double total_mass (int Z, int N)
  Return the total mass of the nucleus (without the electrons) in MeV.
- virtual double total_mass_d (double Z, double N)
  Return the total mass of the nucleus (without the electrons) in MeV.

4.24.2 Member Function Documentation

4.24.2.1 virtual double binding_energy (int *Z*, int *N*) [inline, virtual]

Return the binding energy in MeV.

The binding energy is defined to be negative for bound nuclei, thus the binding energy per baryon of Pb-208 is about -8∗208 = -1664 MeV.

Definition at line 351 of file nuclear_mass.h.

4.24.2.2 virtual double binding_energy_d (double *Z*, double *N*) [inline, virtual]

Return the binding energy in MeV.

The binding energy is defined to be negative for bound nuclei, thus the binding energy per baryon of Pb-208 is about -8∗208 = -1664 MeV.

Definition at line 365 of file nuclear_mass.h.

4.24.2.3 int get_nucleus (int *Z*, int *N*, nucleus & *n*) [inline]

Fill n with the information from nucleus with the given neutron and proton number.

All masses are given in fm^{-1}. The total mass (withouth the electrons) is put in part::m and part::ms, the binding energy is placed in nucleus::be, the mass excess in nucleus::mex and the degeneracy (part::g) is arbitrarily set to 1 for even A nuclei and 2 for odd A nuclei.

Warning:

The spin degeneracy is not handled particularly intelligently. This function simply assumes 0 spin for even A and spin 1/2 for odd A.

Definition at line 325 of file nuclear_mass.h.

4.24.2.4 virtual bool is_included (int *Z*, int *N*) [inline, virtual]

Return false if the mass formula does not include specified nucleus.

Note:

By default, this returns false, so that children must overload this function if they do not provide masses for arbitrary nuclei.

Reimplemented in ame_mass, mnmsk_mass, mnmsk_mass_exp, and hfb_mass.

Definition at line 308 of file nuclear_mass.h.

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

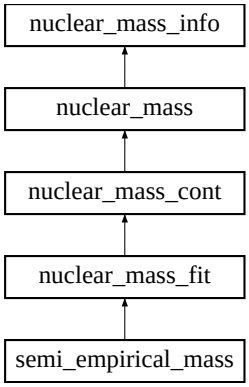
- nuclear_mass.h

4.25 nuclear_mass_cont Class Reference

Continuous nuclear mass formula [abstract base].

`#include <nuclear_mass.h>`

Inheritance diagram for nuclear_mass_cont::



4.25.1 Detailed Description

Continuous nuclear mass formula [abstract base].

Definition at line 421 of file nuclear_mass.h.

Public Member Functions

- virtual double mass_excess (int Z, int N)
  Given `Z` *and* `N`*, return the mass excess in MeV.*
- virtual double mass_excess_d (double Z, double N)=0
  Given `Z` *and* `N`*, return the mass excess in MeV.*

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

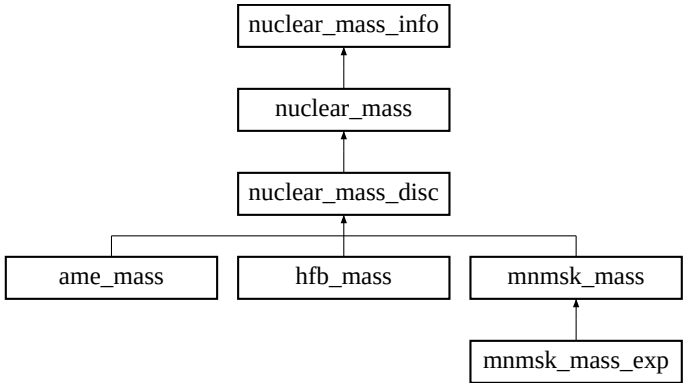
- nuclear_mass.h

4.26 nuclear_mass_disc Class Reference

Discrete nuclear mass formula [abstract base].

`#include <nuclear_mass.h>`

Inheritance diagram for nuclear_mass_disc::



4.26.1 Detailed Description

Discrete nuclear mass formula [abstract base].

This uses simple linear interpolation to obtain masses of nuclei with non-integer Z and N which may be particularly sensitive to the form of the pairing.

Definition at line 398 of file nuclear_mass.h.

Public Member Functions

- virtual double mass_excess (int Z, int N)=0
  Given `Z` *and* `N`*, return the mass excess in MeV.*
- virtual double mass_excess_d (double Z, double N)
  Given `Z` *and* `N`*, return the mass excess in MeV.*

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

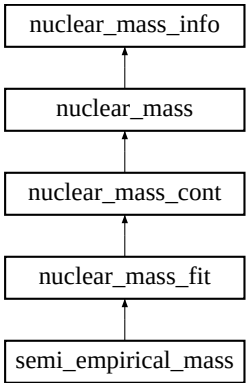
- nuclear_mass.h

4.27 nuclear_mass_fit Class Reference

Fittable mass formula.

`#include <nuclear_mass.h>`

Inheritance diagram for nuclear_mass_fit::



4.27.1 Detailed Description

Fittable mass formula.

Nuclear mass formulas which are descendants of this class can be fit to experiment using mass_fit.

Definition at line 441 of file nuclear_mass.h.

Public Member Functions

- virtual const char * type ()
  Return the type, `"nuclear_mass_fit"`.
- virtual int fit_fun (size_t nv, const **ovector_base** &x)
  Fix parameters from an array for fitting.

- virtual int guess_fun (size_t nv, **ovector_base** &x)
  Fill array with guess from present values for fitting.

Data Fields

- size_t nfit
  Number of fitting parameters.

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

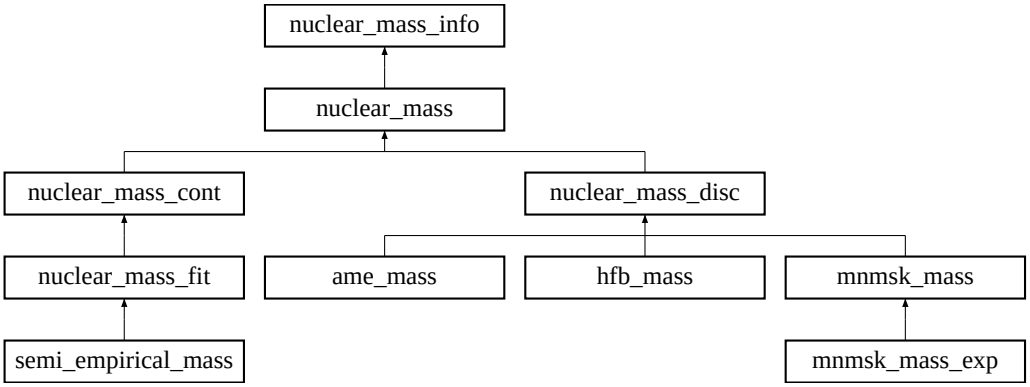
- nuclear_mass.h

4.28 nuclear_mass_info Class Reference

Nuclear mass info.

`#include <nuclear_mass.h>`

Inheritance diagram for nuclear_mass_info::



4.28.1 Detailed Description

Nuclear mass info.

Definition at line 39 of file nuclear_mass.h.

Data Structures

- struct string_less_than
  String comparison operator for element_table.

Public Member Functions

- int parse_elstring (std::string ela, int &Z, int &N, int &A)
  Parse a string representing an element.
- int eltoZ (std::string el)
  Return Z given the element name.
- std::string Ztoel (size_t Z)
  Return the element name given Z.
- std::string tostring (size_t Z, size_t N)
  Return a string of the form "Pb208" for a given Z and N.

Protected Types

- typedef std::map< std::string, int, string_less_than >::iterator table_it
  A convenient typedef for an iterator for element_table.

Protected Attributes

- std::map< std::string, int, string_less_than > element_table
  A map containing the proton numbers organized by element name.
- std::string element_list [nelements]
  The list of elements organized by proton number.

Static Protected Attributes

- static const int nelements = 119
  The number of elements (proton number).

4.28.2 Member Function Documentation

4.28.2.1 int eltoZ (std::string *el*) [inline]

Return Z given the element name.

If the string parameter `el` is invalid, the error handler is called and the value -1 is returned.

Definition at line 143 of file nuclear_mass.h.

4.28.2.2 int parse_elstring (std::string *ela*, int & *Z*, int & *N*, int & *A*) [inline]

Parse a string representing an element.

Accepts strings of one of the following forms:

- `Pb208`
- `pb208`
- `Pb 208`
- `Pb-208`
- `pb 208`
- `pb-208` or one of the special strings `n`, `p`, `d` or `t` for the neutron, proton, deuteron, and triton, respectively.

Note:

At present, this allows nuclei which don't make sense because A<Z, such as Carbon-5.

Idea for future

Allow A to precede Z.

Idea for future

Right now, `n4` is interpreted incorrectly as Nitrogen-4, rather than the tetraneutron.

Definition at line 66 of file nuclear_mass.h.

4.28.2.3 std::string tostring (size_t *Z*, size_t *N*) [inline]

Return a string of the form "Pb208" for a given Z and N.

Note that if `Z` is zero, then and `'n'` is used to indicate the a nucleus composed entirely of neutrons and if the argument `Z` is greater than 118, an empty string is returned (independ.

Definition at line 176 of file nuclear_mass.h.

4.28.2.4 std::string Ztoel (size_t *Z*) [inline]

Return the element name given Z.

Note:

This function returns `"n"` indicating the neutron for Z=0, and if the argument `Z` is greater than 118, an empty string is returned after calling the error handler.

Definition at line 160 of file nuclear_mass.h.

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

- nuclear_mass.h

4.29 nuclear_mass_info::string_less_than Struct Reference

String comparison operator for element_table.

`#include <nuclear_mass.h>`

4.29.1 Detailed Description

String comparison operator for element_table.

Definition at line 189 of file nuclear_mass.h.

Public Member Functions

- bool **operator()** (const std::string s1, const std::string s2) const

The documentation for this struct was generated from the following file:

- nuclear_mass.h

4.30 nuclear_reaction Class Reference

A simple nuclear reaction specification.

`#include <reaction_lib.h>`

4.30.1 Detailed Description

A simple nuclear reaction specification.

Definition at line 41 of file reaction_lib.h.

Public Member Functions

- std::string to_string ()
  Convert the reaction to a string for screen output.
- int clear ()
  Clear the rate.
- nuclear_reaction (const nuclear_reaction &nr)
  Copy constructor.
- nuclear_reaction & operator= (const nuclear_reaction &nr)
  Copy constructor.
- double rate (double T9)
  Compute the reaction rate from the temperature in units of $10^9 K$.

Data Fields

- size_t chap
  Chapter.
- std::string name [6]
  Names of the participating nuclei.
- std::string ref
  Reference.
- char type
  Type of rate (resonant/non-resonant/weak).
- char rev
  Forward or reverse.
- double Q
  Q value.
- double a [7]
  Coefficients.
- size_t Z [6]
  Proton number of participating nuclei.
- size_t A [6]
  Mass number of participating nuclei.
- size_t isomer [6]
  Isomer designation of participating nuclei.

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

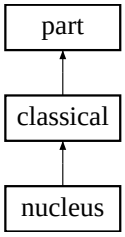
- reaction_lib.h

4.31 nucleus Class Reference

A simple nucleus class.

`#include <nucleus.h>`

Inheritance diagram for nucleus::



4.31.1 Detailed Description

A simple nucleus class.

The variable part::m is typically used for the mass of the nucleus with no electrons.

The binding energy of the nucleus (be) is typically defined as the mass of the nucleus (without the electrons) minus Z times the mass of the proton minus N times the mass of the neutron.

The mass excess (be) is defined as the mass of the nucleus including the electron contribution minus a times the mass of the atomic mass unit.

The variable part::inc_rest_mass is set to `false` by default, to insure that energies and chemical potentials do not include the rest mass. This is typically appropriate for nuclei.

Definition at line 51 of file nucleus.h.

Data Fields

- int Z
  Proton number.
- int N
  Neutron number.
- int A
  Atomic number.
- double mex
  Mass excess in fm^{-1}.
- double be
  Binding energy in fm^{-1} *(with a minus sign for bound nuclei).*

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

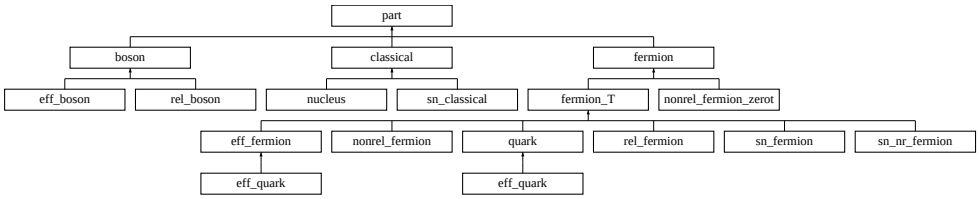
- nucleus.h

4.32 part Class Reference

Particle base class.

`#include <part.h>`

Inheritance diagram for part::



4.32.1 Detailed Description

Particle base class.

Calculate the properties of particles from their chemical potential (calc_mu() and pair_mu()) or from the density (calc_density() and pair_density()).

When non-interacting is false, the thermodynamic integrals need both a value of "mu" and "nu". "nu" is an effective chemical potential which appears in the argument of the exponential of the Fermi-function.

Keep in mind, that the pair functions use anti(), which assumes that nu -> -nu and mu -> -mu for the anti-particles, which might not be true for interacting particles. When non-interacting is true, then "ms" is set equal to "m", and "nu" is set equal to "mu", everywhere.

The "density" functions use the value of nu (or mu when non_interacting is true) for an initial guess. Zero is very likely a bad guess, but these functions will not warn you about this.

Definition at line 94 of file part.h.

Public Member Functions

- part (double m=0.0, double g=0.0)
  make a particle of mass `m` *and degeneracy* `g`.
- virtual int init (double m, double g)
  Set the mass `m` *and degeneracy* `g`.
- virtual int anti (part &ax)
  Make an anti-particle.
- virtual const char * type ()
  Return string denoting type ("part").

Data Fields

- double g
  degeneracy
- double m
  mass
- double n
  density
- double ed
  energy density
- double pr
  pressure
- double mu
  chemical potential
- double en
  entropy
- double ms
  effective mass (Dirac unless otherwise specified)
- double nu
  effective chemical potential
- bool inc_rest_mass
  derivative of energy with respect to effective mass
- bool non_interacting
  True if the particle is non-interacting (default true).

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

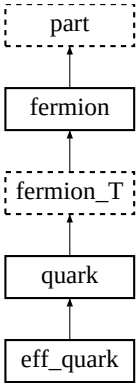
- part.h

4.33 quark Class Reference

Quark base [abstract base].

`#include <quark.h>`

Inheritance diagram for quark::



4.33.1 Detailed Description

Quark base [abstract base].

Definition at line 43 of file quark.h.

Public Member Functions

- quark (double mass=0.0, double dof=0.0)
  Create a quark with mass `m` *and degeneracy* `g`.
- virtual int calc_mu (const double temper)=0
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)=0
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)=0
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)=0
  Calculate properties with antiparticles as function of density.
- virtual const char * type ()
  Return string denoting type ("quark").

Data Fields

- double B
  Contribution to the bag constant.
- double qq
  Quark condensate.

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

- quark.h

4.34 reaction_lib Class Reference

Simple reaction library.

`#include <reaction_lib.h>`

4.34.1 Detailed Description

Simple reaction library.

Units:

- Chapters 1,2,3, and 11: 1/s
- Chapters 4,5,6, and 7: cm^3/g/s
- Chapter 8 and 9: cm^6/g^2/s
- Chapter 10: cm^9/g^3/s

Chapters:

- 1: nuc1 -> nuc2
- 2: nuc1 -> nuc2 + nuc3
- 3: nuc1 -> nuc2 + nuc3 + nuc4
- 4: nuc1 + nuc2 -> nuc3
- 5: nuc1 + nuc2 -> nuc3 + nuc4
- 6: nuc1 + nuc2 -> nuc3 + nuc4 + nuc5
- 7: nuc1 + nuc2 -> nuc3 + nuc4 + nuc5 + nuc6
- 8: nuc1 + nuc2 + nuc3 -> nuc4
- 9: nuc1 + nuc2 + nuc3 -> nuc4 + nuc5
- 10: nuc1 + nuc2 + nuc3 + nuc4 -> nuc5 + num6
- 11: nuc1 -> nuc2 + nuc3 + nuc4 + nuc5

Original FORTRAN format:

```
FORMAT(i1,4x,6a5,8x,a4,a1,a1,3x,1pe12.5)
FORMAT(4e13.6)
FORMAT(3e13.6)
```

Definition at line 202 of file reaction_lib.h.

Public Member Functions

- int read_file_reaclib2 (std::string fname)
  Read from a file in the REACLIB2 format.
- int find_in_chap (std::vector< nuclear_reaction > &nrl, size_t chap, std::string nuc1, std::string nuc2="", std::string nuc3="", std::string nuc4="", std::string nuc5="", std::string nuc6="")
  Find a set of nuclear reactions in a specified chapter.

Data Fields

- std::vector< nuclear_reaction > lib
  The library.

Protected Member Functions

- bool matches (size_t ul, size_t ri)
  Test if entry `ul` *in the arrays matches the library reaction.*

Protected Attributes

- int fN [6]
  Storage for the find function.
- int **fZ** [6]
- int **fA** [6]
- size_t **fi**

4.34.2 Member Function Documentation

4.34.2.1 int read_file_reaclib2 (std::string *fname*)

Read from a file in the REACLIB2 format.

Note:

This function does not check that the chapter numbers are correct for the subsequent reaction.

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

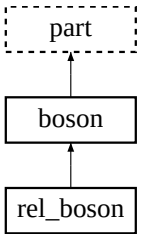
- reaction_lib.h

4.35 rel_boson Class Reference

Equation of state for a relativistic boson.

`#include <rel_boson.h>`

Inheritance diagram for rel_boson::



4.35.1 Detailed Description

Equation of state for a relativistic boson.

Todo

Testing not completely finished.

Definition at line 48 of file rel_boson.h.

Public Member Functions

- rel_boson (double m=0.0, double g=0.0)
  Create a boson with mass `m` *and degeneracy* `g`.
- virtual int calc_mu (const double temper)
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate properties with antiparticles as function of density.
- virtual int nu_from_n (const double temper)
  Calculate effective chemical potential from density.
- int set_inte (**inte**< const double, **funct**< const double > > &l_nit, **inte**< const double, **funct**< const double > > &l_dit)
  Set **inte** *object.*
- int set_density_root (**root**< const double, **funct**< const double > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- virtual const char * type ()
  Return string denoting type ("rel_boson").

Data Fields

- int mroot_err
  The error value from **mroot**.
- int inte_err
  The error value from **inte**.
- **cern_mroot_root**< const double, **funct**< const double > > def_density_root
  The default solver for calc_density().
- **gsl_inte_qagiu**< const double, **funct**< const double > > def_nit
  Default nondegenerate integrator.
- **gsl_inte_qag**< const double, **funct**< const double > > def_dit
  Default degenerate integrator.

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

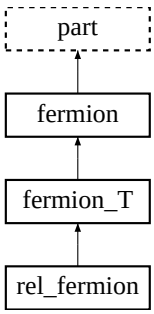
- rel_boson.h

4.36 rel_fermion Class Reference

Equation of state for a relativistic fermion.

`#include <rel_fermion.h>`

Inheritance diagram for rel_fermion::



4.36.1 Detailed Description

Equation of state for a relativistic fermion.

This implements an equation of state for a relativistic fermion using direct integration. Define the degeneracy parameter

$$\psi = (\nu - m^*)/T$$

where ν is the effective chemical potential and m^* is the effective mass. For ψ greater than deg_limit (degenerate regime), a finite interval integrator is used and for ψ less than deg_limit (non-degenerate regime), an integrator over the interval from $[0, \infty)$ is used. The upper limit on the degenerate integration is given by

$$\sqrt{(20T + \nu)^2 - m^{*,2}}$$

The default integrators are **gsl_inte_qag** (for degenerate particles) and **gsl_inte_qagiu** (for non-degenerate particles).

When the integrators provide numerical uncertainties, these uncertainties are stored in unc. In the case of calc_density() and pair_density(), the uncertainty from the numerical accuracy of the solver is not included. (There is also a relatively small inaccuracy due to the mathematical evaluation of the integrands which is not included in unc.)

One way to improve the accuracy of the computation is just to decrease the tolerances on the default integration objects. This can be done, using, for example

```
rel_fermion rf(1.0,2.0);
rf.def_dit.tolx/=1.0e2;
rf.def_dit.tolf/=1.0e2;
rf.def_nit.tolx/=1.0e2;
rf.def_nit.tolf/=1.0e2;
```

which decreases the both the relative and absolute tolerances for both the degenerate and non-degenerate integrators. If one is using either the calc_density() or pair_density() functions, one may also have to improve the accuracy of the solver which determines the chemical potential from the density. For the default solver, this could be done with

```
rf.def_density_root.tolx/=1.0e2;
rf.def_density_root.tolf/=1.0e2;
```

Of course if these tolerances are too small, the calculation may fail.

Note:

This does not work with inc_rest_mass=false (3/30/09: There is a significant amount of testing code to ensure that it does work with inc_rest_mass=false, so this may have been fixed already.)

Idea for future

Allow the user to change the upper limit on the degenerate integration and the hard-coded value of 200 in the integrands.

Idea for future

It appears this doesn't compute the uncertainty in the chemical potential or density with calc_density(). This could be fixed.

Definition at line 107 of file rel_fermion.h.

Public Member Functions

- rel_fermion (double m=0.0, double g=0.0)
  Create a fermion with mass `m` *and degeneracy* `g`.
- virtual int calc_mu (const double temper)

Calculate properties as function of chemical potential.

- virtual int calc_density (const double temper)
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate properties with antiparticles as function of density.
- virtual int nu_from_n (const double temper)
  Calculate effective chemical potential from density.
- int set_inte (**inte**< double, **funct**< double > > &non_it, **inte**< double, **funct**< double > > &deg_it)
  Set integrators.
- int set_density_root (**root**< double, **funct**< double > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- virtual const char * type ()
  Return string denoting type ("rel_fermion").

Data Fields

- double deg_limit
  The critical degeneracy at which to switch integration techniques.
- fermion unc
  Storage for the uncertainty.
- bool guess_from_nu
  If true, use the present value of the chemical potential as a guess for the new chemical potential.
- **cern_mroot_root**< double, **funct**< double > > def_density_root
  The default solver for calc_density().
- **gsl_inte_qag**< double, **funct**< double > > def_dit
  The default integrator for degenerate fermions.
- **gsl_inte_qagiu**< double, **funct**< double > > def_nit
  The default integrator for non-degenerate fermions.

Protected Member Functions

- double density_fun (double u, double &pa)
  The integrand for the density for non-degenerate fermions.
- double energy_fun (double u, double &pa)
  The integrand for the energy density for non-degenerate fermions.
- double entropy_fun (double u, double &pa)
  The integrand for the entropy density for non-degenerate fermions.
- double deg_density_fun (double u, double &pa)
  The integrand for the density for degenerate fermions.
- double deg_energy_fun (double u, double &pa)
  The integrand for the energy density for degenerate fermions.
- double deg_entropy_fun (double u, double &pa)
  The integrand for the entropy density for degenerate fermions.
- int solve_fun (double x, double &yy, double &pa)
  Solve for the chemical potential given the density.
- int pair_fun (double x, double &yy, double &pa)
  Solve for the chemical potential given the density with antiparticles.

Protected Attributes

- **inte**< double, **funct**< double > > * nit
  The non-degenerate integrator.
- **inte**< double, **funct**< double > > * dit
  The degenerate integrator.

- **root**< double, **funct**< double > > * density_root
  The solver for calc_density().

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

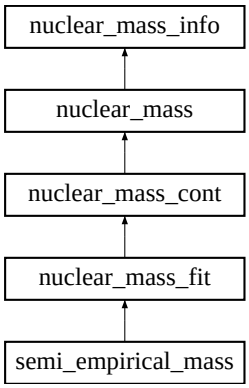
- rel_fermion.h

4.37 semi_empirical_mass Class Reference

Semi-empirical mass formula.

`#include <nuclear_mass.h>`

Inheritance diagram for semi_empirical_mass::



4.37.1 Detailed Description

Semi-empirical mass formula.

A simple semi-empirical mass formula of the form

$$E/A = B + S_s \frac{1}{A^{1/3}} + E_c \frac{Z^2}{A^{4/3}} + S_v \left(1 - \frac{2Z}{A}\right)^2 + E_{\rm pair}(Z,N)$$

where

$$E_{\rm pair}(Z,N) = \frac{E_{\rm pair}}{A^{3/2}} \times \begin{cases} -1 & \text{N and Z even} \\ +1 & \text{N and Z odd} \\ 0 & \text{otherwise} \end{cases}$$

Note:

The default parameters are arbitrary, and are not determined from a fit.

There is an example of the usage of this class given in Nuclear mass fit example.

Definition at line 491 of file nuclear_mass.h.

Public Member Functions

- virtual const char * type ()
  Return the type, `"semi_empirical_mass"`.
- virtual double mass_excess_d (double Z, double N)

Given Z *and* N*, return the mass excess in MeV.*

- virtual int fit_fun (size_t nv, const **ovector_base** &x)
  Fix parameters from an array for fitting.
- virtual int guess_fun (size_t nv, **ovector_base** &x)
  Fill array with guess from present values for fitting.

Data Fields

- double B
  Binding energy (negative and in MeV, default -16).
- double Sv
  Symmetry energy (in MeV, default 23.7).
- double Ss
  Surface energy (in MeV, default 18).
- double Ec
  Coulomb energy (in MeV, default 0.7).
- double Epair
  Pairing energy (MeV, default 13.0).

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

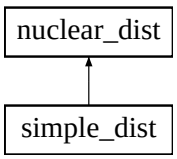
- nuclear_mass.h

4.38 simple_dist Class Reference

A simple nuclear distribution given a range in A and Z.

`#include <nuclear_dist.h>`

Inheritance diagram for simple_dist::



4.38.1 Detailed Description

A simple nuclear distribution given a range in A and Z.

The iterator for this distribution begins with the nucleus with the lowest Z and A, and increases A before incrementing Z and beginning again with the lowest A for that value of Z. In other words, it proceeds through all the isotopes of an element first, and then proceeds to the next element.

For example, to create a collection of isotopes of Carbon, Nitrogen and Oxygen using the most recent (2003) Atomic Mass Evaluation, and then output the nuclei in the collection

```
ame_mass ame;
simple_dist fd(6,8,2,30,&ame);
for(nuclear_dist::iterator ndi=fd.begin();ndi!=fd.end();ndi++) {
  cout << ndi->Z << " " << ndi->A << " " << ndi->m << endl;
}
```

Idea for future

Make the vector constructor into a template so it accepts any type. Do the same for set_dist().

Definition at line 166 of file nuclear_dist.h.

Public Member Functions

- simple_dist ()
  Create an empty distribution.
- simple_dist (int minZ, int maxZ, int minA[ ], int maxA[ ], nuclear_mass &nm)
  Create a distribution from ranges in A specified for each Z.
- simple_dist (int minZ, int maxZ, int minA, int maxA, nuclear_mass &nm)
  Create a square distribution in A and Z.
- virtual iterator begin ()
  The beginning of the distribution.
- virtual iterator end ()
  The end of the distribution.
- virtual size_t size ()
  The number of nuclei in the distribution.
- int set_dist (int minZ, int maxZ, int minA[ ], int maxA[ ], nuclear_mass &nm)
  Set the distribution from ranges in A specified for each Z.
- int set_dist (int minZ, int maxZ, int minA, int maxA, nuclear_mass &nm)
  Set a square distribution in A and Z.

4.38.2 Constructor & Destructor Documentation

4.38.2.1 simple_dist (int *minZ*, int *maxZ*, int *minA*[ ], int *maxA*[ ], nuclear_mass & *nm*)

Create a distribution from ranges in A specified for each Z.

The length of the arrays minA and maxA should be exactly $\mathrm{maxZ} - \mathrm{minZ} + 1$.

4.38.3 Member Function Documentation

4.38.3.1 int set_dist (int *minZ*, int *maxZ*, int *minA*[ ], int *maxA*[ ], nuclear_mass & *nm*)

Set the distribution from ranges in A specified for each Z.

The length of the arrays minA and maxA should be exactly $\mathrm{maxZ} - \mathrm{minZ} + 1$.

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

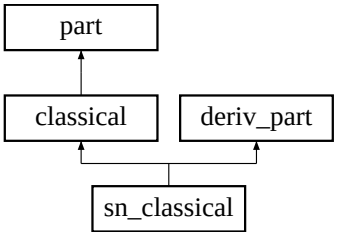
- nuclear_dist.h

4.39 sn_classical Class Reference

Equation of state for a classical particle with derivatives.

`#include <sn_classical.h>`

Inheritance diagram for sn_classical::



4.39.1 Detailed Description

Equation of state for a classical particle with derivatives.

Todo

This does not work with inc_rest_mass=true

Definition at line 42 of file sn_classical.h.

Public Member Functions

- sn_classical (double m=0.0, double g=0.0)
  Create a fermion with mass `m` *and degeneracy* `g`.
- virtual int calc_mu (const double temper)
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate properties as function of density.
- virtual const char * type ()
  Return string denoting type ("sn_classical").

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

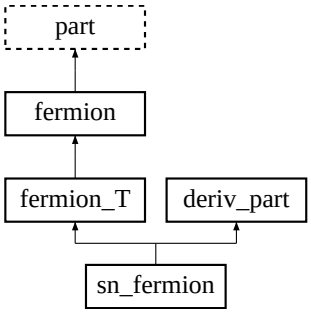
- sn_classical.h

4.40 sn_fermion Class Reference

Equation of state for a relativistic fermion.

`#include <sn_fermion.h>`

Inheritance diagram for sn_fermion::



4.40.1 Detailed Description

Equation of state for a relativistic fermion.

Note:

This class does not work with inc_rest_mass=true.

This implements an equation of state for a relativistic fermion using direct integration. After subtracting the rest mass from the chemical potentials, the distribution function is

$$\left\{1+\exp[(\sqrt{k^2+m^{*2}}-m-\nu)/T]\right\}^{-1}$$

where k is the momentum, ν is the effective chemical potential, m is the rest mass, and m^* is the effective mass. For later use, we define $E^* = \sqrt{k^2 + m^{*2}}$. The degeneracy parameter is

$$\psi = (\nu + (m - m^*))/T$$

For ψ greater than deg_limit (degenerate regime), a finite interval integrator is used and for ψ less than deg_limit (non-degenerate regime), an integrator over the interval from $[0, \infty)$ is used. Typical choices are Gauss-Legendre integration for the degenerate regime and Gauss-Laguerre integration for the non-degenerate regime. The upper limit on the degenerate integration is given by the solution of

$$(\sqrt{k^2 + m^{*,2}} - m - \nu)/T = \text{flimit}$$

which is

$$\sqrt{(m + \mathcal{L})^2 - m^{*2}}$$

where $\mathcal{L} \equiv \text{flimit} \times T + \nu$.

In the non-degenerate regime, we make the substitution $u = k/T$ to ensure that the variable of integration does not have units.

Uncertainties are given in unc.

Todo

This needs to be corrected to calculate $\sqrt{k^2 + m^{*2}} - m$ gracefully when $m^* \approx m$.

Todo

Call error handler if inc_rest_mass is true or update to properly treat the case when inc_rest_mass is true.

Evaluation of the derivatives

The relevant derivatives of the distribution function are

$$\frac{\partial f}{\partial T} = f(1-f)\frac{E^* - m - \nu}{T^2}$$

$$\frac{\partial f}{\partial \nu} = f(1-f)\frac{1}{T}$$

$$\frac{\partial f}{\partial k} = -f(1-f)\frac{k}{E^* T}$$

$$\frac{\partial f}{\partial m^*} = -f(1-f)\frac{m^*}{E^* T}$$

We also need the derivative of the entropy integrand w.r.t. the distribution function, which is

$$\mathcal{S} \equiv f \ln f + (1-f)\ln(1-f) \qquad \frac{\partial \mathcal{S}}{\partial f} = \ln\left(\frac{f}{1-f}\right) = \left(\frac{\nu - E^* + m}{T}\right)$$

where the entropy density is

$$s = -\frac{g}{2\pi^2}\int_0^\infty \mathcal{S} k^2 dk$$

The derivatives can be integrated directly (method = direct) or they may be converted to integrals over the distribution function through an integration by parts (method = byparts)

$$\int_a^b f(k)\frac{dg(k)}{dk}dk = f(k)g(k)|_{k=a}^{k=b} - \int_a^b g(k)\frac{df(k)}{dk}dk$$

using the distribution function for $f(k)$ and 0 and ∞ as the limits, we have

$$\frac{g}{2\pi^2}\int_0^\infty \frac{dg(k)}{dk} f dk = \frac{g}{2\pi^2}\int_0^\infty g(k) f(1-f)\frac{k}{E^* T}dk$$

as long as $g(k)$ vanishes at $k = 0$. Rewriting,

$$\frac{g}{2\pi^2}\int_0^\infty h(k)f(1-f)dk = \frac{g}{2\pi^2}\int_0^\infty f\frac{T}{k}\left[h'E^* - \frac{hE^*}{k} + \frac{hk}{E^*}\right]dk$$

as long as $h(k)/k$ vanishes at $k = 0$.

Explicit forms

1) The derivative of the density wrt the chemical potential

$$\left(\frac{dn}{d\mu}\right)_T = \frac{g}{2\pi^2}\int_0^\infty \frac{k^2}{T}f(1-f)dk$$

Using $h(k) = k^2/T$ we get

$$\left(\frac{dn}{d\mu}\right)_T = \frac{g}{2\pi^2}\int_0^\infty \left(\frac{k^2+E^{*2}}{E^*}\right)fdk$$

2) The derivative of the density wrt the temperature

$$\left(\frac{dn}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty \frac{k^2(E^*-m-\nu)}{T^2}f(1-f)dk$$

Using $h(k) = k^2(E^* - \nu)/T^2$ we get

$$\left(\frac{dn}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty \frac{f}{T}\left[2k^2 + E^{*2} - E^*\left(\nu+m\right) - k^2\left(\frac{\nu+m}{E^*}\right)\right]dk$$

3) The derivative of the entropy wrt the chemical potential

$$\left(\frac{ds}{d\mu}\right)_T = \frac{g}{2\pi^2}\int_0^\infty k^2 f(1-f)\frac{(E^*-m-\nu)}{T^2}dk$$

This verifies the Maxwell relation

$$\left(\frac{ds}{d\mu}\right)_T = \left(\frac{dn}{dT}\right)_\mu$$

4) The derivative of the entropy wrt the temperature

$$\left(\frac{ds}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty k^2 f(1-f)\frac{(E^*-m-\nu)^2}{T^3}dk$$

Using $h(k) = k^2(E^* - \nu)^2/T^3$

$$\left(\frac{ds}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty \frac{f(E^*-m-\nu)}{E^*T^2}\left[E^{*3} + 3E^*k^2 - (E^{*2}+k^2)(\nu+m)\right]dk$$

5) The derivative of the density wrt the effective mass

$$\left(\frac{dn}{dm^*}\right)_{T,\mu} = -\frac{g}{2\pi^2}\int_0^\infty \frac{k^2m^*}{E^*T}f(1-f)dk$$

Using $h(k) = -(k^2m^*)/(E^*T)$ we get

$$\left(\frac{dn}{dm^*}\right)_{T,\mu} = -\frac{g}{2\pi^2}\int_0^\infty m^* f dk$$

Note:

The dsdT integration doesn't work well if the system is very degenerate. When method is byparts, the integral involves a large cancellation between the regions from $k \in (0, \mathrm{ulimit}/2)$ and $k \in (\mathrm{ulimit}/2, \mathrm{ulimit})$. Switching to method=direct and setting the lower limit to llimit, may help, but recent testing on this gave negative values for dsdT. For very degenerate systems, an expansion is probably better than trying to perform the integration.

Idea for future

This class will have difficulty with extremely degenerate or extremely non-degnerate systems. Fix this.

Idea for future

Create a more intelligent method for dealing with bad initial guesses for the chemical potential in calc_density().

Definition at line 225 of file sn_fermion.h.

Method of computing derivatives

- int method
  Method (default is byparts).
- static const int direct = 1
  In the form containing $f(1-f)$.
- static const int byparts = 2
  Integrate by parts.

Public Member Functions

- sn_fermion (double m=0.0, double g=0.0)
  Create a fermion with mass m *and degeneracy* g.
- virtual int calc_mu (const double temper)
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate properties with antiparticles as function of density.
- virtual int nu_from_n (const double temper)
  Calculate effective chemical potential from density.
- int set_inte (**inte**< const double, **funct**< const double > > &unit, **inte**< const double, **funct**< const double > > &udit)
  Set **inte** *objects.*
- int set_density_root (**root**< const double, **funct**< const double > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- virtual const char * type ()
  Return string denoting type ("sn_fermion").

Data Fields

- double deg_limit
  The critical degeneracy at which to switch integration techniques (default 2.0).
- double flimit
  The limit for the Fermi functions (default 20.0).
- fermion unc
  Storage for the most recently calculated uncertainties.
- deriv_part dunc
  Storage for the most recently calculated uncertainties.
- **gsl_inte_qagiu**< const double, **funct**< const double > > def_nit
  The default integrator for the non-degenerate regime.
- **gsl_inte_qag**< const double, **funct**< const double > > def_dit
  The default integrator for the degenerate regime.
- **cern_mroot_root**< const double, **funct**< const double > > def_density_root
  The default solver for npen_density() and pair_density().

4.40.2 Member Function Documentation

4.40.2.1 int set_inte (inte< const double, funct< const double > > & *unit*, inte< const double, funct< const double > > & *udit*)

Set **inte** objects.

The first integrator is used for non-degenerate integration and should integrate from 0 to ∞ (like **gsl_inte_qagiu**). The second integrator is for the degenerate case, and should integrate between two finite values.

4.40.3 Field Documentation

4.40.3.1 double flimit

The limit for the Fermi functions (default 20.0).

sn_fermion will ignore corrections smaller than about $\exp(-\mathrm{flimit})$.

Definition at line 244 of file sn_fermion.h.

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

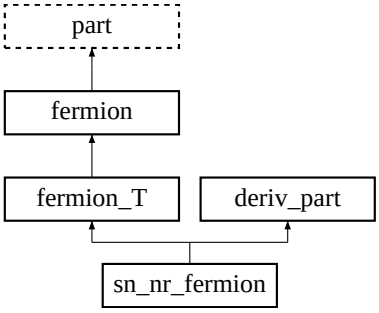
- sn_fermion.h

4.41 sn_nr_fermion Class Reference

Equation of state for a nonrelativistic fermion.

`#include <sn_nr_fermion.h>`

Inheritance diagram for sn_nr_fermion::



4.41.1 Detailed Description

Equation of state for a nonrelativistic fermion.

This does not include the rest mass energy in the chemical potential or the rest mass energy density in the energy density to alleviate numerical precision problems at low densities

This implements an equation of state for a nonrelativistic fermion using direct integration. After subtracting the rest mass from the chemical potentials, the distribution function is

$$\left\{1+\exp\left[\left(\frac{k^2}{2m^*}-\nu\right)/T\right]\right\}^{-1}$$

where ν is the effective chemical potential, m is the rest mass, and m^* is the effective mass. For later use, we define $E^*=k^2/2/m^*$.

Uncertainties are given in unc.

Evaluation of the derivatives

The relevant derivatives of the distribution function are

$$\frac{\partial f}{\partial T} = f(1-f)\frac{E^* - \nu}{T^2}$$

$$\frac{\partial f}{\partial \nu} = f(1-f)\frac{1}{T}$$

$$\frac{\partial f}{\partial k} = -f(1-f)\frac{k}{m^* T}$$

$$\frac{\partial f}{\partial m^*} = f(1-f)\frac{k^2}{2m^{*2}T}$$

We also need the derivative of the entropy integrand w.r.t. the distribution function, which is quite simple

$$\mathcal{S} \equiv f\ln f + (1-f)\ln(1-f) \qquad \frac{\partial \mathcal{S}}{\partial f} = \ln\left(\frac{f}{1-f}\right) = \left(\frac{\nu - E^*}{T}\right)$$

where the entropy density is

$$s = -\frac{g}{2\pi^2}\int_0^\infty \mathcal{S}k^2 dk$$

The derivatives can be integrated directly or they may be converted to integrals over the distribution function through an integration by parts

$$\int_a^b f(k)\frac{dg(k)}{dk}dk = f(k)g(k)|_{k=a}^{k=b} - \int_a^b g(k)\frac{df(k)}{dk}dk$$

using the distribution function for $f(k)$ and 0 and ∞ as the limits, we have

$$\frac{g}{2\pi^2}\int_0^\infty \frac{dg(k)}{dk} f dk = \frac{g}{2\pi^2}\int_0^\infty g(k) f(1-f)\frac{k}{E^* T}dk$$

as long as $g(k)$ vanishes at $k = 0$. Rewriting,

$$\frac{g}{2\pi^2}\int_0^\infty h(k) f(1-f)dk = \frac{g}{2\pi^2}\int_0^\infty f\frac{Tm^*}{k}\left[h' - \frac{h}{k}\right]dk$$

as long as $h(k)/k$ vanishes at $k = 0$.

Explicit forms

1) The derivative of the density wrt the chemical potential

$$\left(\frac{dn}{d\mu}\right)_T = \frac{g}{2\pi^2}\int_0^\infty \frac{k^2}{T} f(1-f)dk$$

Using $h(k) = k^2/T$ we get

$$\left(\frac{dn}{d\mu}\right)_T = \frac{g}{2\pi^2}\int_0^\infty m^* f dk$$

2) The derivative of the density wrt the temperature

$$\left(\frac{dn}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty \frac{k^2(E^* - \nu)}{T^2} f(1-f)dk$$

Using $h(k) = k^2(E^* - \nu)/T^2$ we get

$$\left(\frac{dn}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty \frac{f}{T}\left[m^*\left(E^* - \nu\right) - k^2\right]dk$$

3) The derivative of the entropy wrt the chemical potential

$$\left(\frac{ds}{d\mu}\right)_T = \frac{g}{2\pi^2}\int_0^\infty k^2 f(1-f)\frac{(E^*-\nu)}{T^2}dk$$

This verifies the Maxwell relation

$$\left(\frac{ds}{d\mu}\right)_T = \left(\frac{dn}{dT}\right)_\mu$$

4) The derivative of the entropy wrt the temperature

$$\left(\frac{ds}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty k^2 f(1-f)\frac{(E^*-\nu)^2}{T^3}dk$$

Using $h(k) = k^2(E^*-\nu)^2/T^3$

$$\left(\frac{ds}{dT}\right)_\mu = \frac{g}{2\pi^2}\int_0^\infty f\frac{m^*}{T^2}\left[(E^*-\nu)^2 + \frac{2k^2}{m^*}(E^*-\nu)\right]dk$$

5) The derivative of the density wrt the effective mass

$$\left(\frac{dn}{dm^*}\right)_{T,\mu} = \frac{g}{2\pi^2}\int_0^\infty \frac{k^2}{2m^{*2}T}f(1-f)k^2dk$$

Using $h(k) = k^4/(2m^{*2}T)$ we get

$$\left(\frac{dn}{dm^*}\right)_{T,\mu} = \frac{g}{2\pi^2}\int_0^\infty f\frac{3k^2}{2m^*}dk$$

New section

$u = k^2/2/m^*/T$ and $y = \mu/T$, so

$$kdk = m^*Tdu$$

or

$$dk = \frac{m^*T}{\sqrt{2m^*Tu}}du = \sqrt{\frac{m^*T}{2u}}du$$

1) The derivative of the density wrt the chemical potential

$$\left(\frac{dn}{d\mu}\right)_T = \frac{gm^{*3/2}\sqrt{T}}{2^{3/2}\pi^2}\int_0^\infty u^{-1/2}fdu$$

2) The derivative of the density wrt the temperature

$$\left(\frac{dn}{dT}\right)_\mu = \frac{gm^{*3/2}\sqrt{T}}{2^{3/2}\pi^2}\int_0^\infty fdu\left[3u^{1/2} - yu^{-1/2}\right]$$

4) The derivative of the entropy wrt the temperature

$$\left(\frac{ds}{dT}\right)_\mu = \frac{gm^{*3/2}T^{1/2}}{2^{3/2}\pi^2}\int_0^\infty f\left[5u^{3/2} - 6yu^{1/2} + y^2u^{-1/2}\right]du$$

5) The derivative of the density wrt the effective mass

$$\left(\frac{dn}{dm^*}\right)_{T,\mu} = \frac{3gm*1/2T^{3/2}}{2^{3/2}\pi^2}\int_0^\infty u^{1/2}fdu$$

Definition at line 221 of file sn_nr_fermion.h.

Public Member Functions

- sn_nr_fermion (double m=0.0, double g=0.0)
  Create a fermion with mass $\mathtt{m}$ *and degeneracy* $\mathtt{g}$.
- virtual int calc_mu (const double temper)
  Calculate properties as function of chemical potential.
- virtual int calc_density (const double temper)
  Calculate properties as function of density.
- virtual int pair_mu (const double temper)
  Calculate properties with antiparticles as function of chemical potential.
- virtual int pair_density (const double temper)
  Calculate properties with antiparticles as function of density.
- virtual int nu_from_n (const double temper)
  Calculate effective chemical potential from density.
- int set_density_root (**root**< const double, **funct**< const double > > &rp)
  Set the solver for use in calculating the chemical potential from the density.
- virtual const char * type ()
  Return string denoting type ("sn_nr_fermion").

Data Fields

- double flimit
  The limit for the Fermi functions (default 20.0).
- fermion unc
  Storage for the most recently calculated uncertainties.
- deriv_part dunc
  Storage for the most recently calculated uncertainties.
- bool guess_from_nu
  If true, use the present value of the chemical potential as a guess for the new chemical potential.
- **cern_mroot_root**< const double, **funct**< const double > > def_density_root
  The default solver for npen_density() and pair_density().

Protected Member Functions

- int solve_fun (double x, double &yy, const double &temper)
  Function to compute chemical potential from density.
- int pair_fun (double x, double &yy, const double &temper)
  Function to compute chemical potential from density when antiparticles are included.

Protected Attributes

- **root**< const double, **funct**< const double > > * density_root
  Solver to compute chemical potential from density.

4.41.2 Field Documentation

4.41.2.1 double flimit

The limit for the Fermi functions (default 20.0).

sn_nr_fermion will ignore corrections smaller than about $\exp(-\mathrm{flimit})$.

Definition at line 235 of file sn_nr_fermion.h.

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

- sn_nr_fermion.h

4.42 thermo Class Reference

A class for the thermodynamical variables (energy density, pressure, entropy density).

`#include <part.h>`

4.42.1 Detailed Description

A class for the thermodynamical variables (energy density, pressure, entropy density).

Definition at line 46 of file part.h.

Public Member Functions

- const char * type ()
  Return string denoting type ("thermo").

Data Fields

- double pr
  pressure
- double ed
  energy density
- double en
  entropy density

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

- part.h

5 File Documentation

5.1 part.h File Reference

File for definitions for thermo and part.

`#include <string>`

`#include <iostream>`

`#include <cmath>`

`#include <o2scl/constants.h>`

`#include <o2scl/inte.h>`

`#include <o2scl/collection.h>`

`#include <o2scl/funct.h>`

`#include <o2scl/mroot.h>`

Data Structures

- class thermo
  A class for the thermodynamical variables (energy density, pressure, entropy density).
- class part
  Particle base class.

Functions

- thermo operator+ (const thermo &left, const thermo &right)
  Addition operator.
- thermo operator- (const thermo &left, const thermo &right)
  Subtraction operator.
- thermo operator+ (const thermo &left, const part &right)
  Addition operator.
- thermo operator- (const thermo &left, const part &right)
  Subtraction operator.

5.1.1 Detailed Description

File for definitions for thermo and part.

Definition in file part.h.

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