AUTOMATIC GENERATION OF VACUUM
AMPLITUDE MANY-BODY PERTURBATION SERIES

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An algorithm and a computer program in Fortran 95 are presented which enumerate the
Hugenholtz diagram representation of the many-body perturbation series for the ground
state energy with a two-body interaction. The output is in a form suitable for post-
processing such as automatic code generation. The results of a particular application,
generation of \LaTeX code to draw the diagrams, is shown.

Keywords: Quantum Theory, Perturbation Theory, Many-Body Problem

1. Many-Body Perturbation Theory

Many problems of interest in quantum mechanics have no known analytic solution,
and some approximation is necessary to obtain a solution. A particularly useful
approximation method is perturbation theory, which consists of finding a way of
separating the Hamiltonian into a part which is solvable, either numerically or an-
alytically, and a part which is small (See e.g. \cite{1} for a general treatment). One may
then start from the solution of the solvable part and build in successive orders of
the perturbation in a power series approach to obtain a closer approximation to the
solution of the full problem, providing the series converges.

In many-body quantum mechanics, the perturbation series is conveniently rep-
resented in diagrammatic form, based on the work of Feynman\cite{2}, Goldstone\cite{3}
and Hugenholtz\cite{4}. Diagrams may be prescriptively expressed in algebraic form which
give a complete representation of the perturbation series. One may construct such
series of diagrams and expressions for different observables in Quantum Mechanics.
This paper is concerned with the ground state expectation value of the Hamiltonian
operator that is, the ground state energy, or vacuum amplitude for a many-fermion
system in the special, but common case that the unperturbed problem is given by
the solution of the Hartree-Fock equations and the system is governed by a two-
body interaction. This situation is widely dealt with in textbooks\cite{5,6}. Each order of
correction in perturbation theory for the ground state energy involves, in general,
many diagrams and it is important to be able to enumerate them, order by order, if one is to perform a calculation\textsuperscript{7}.

2. Diagrammatic Representation

The perturbation series for the ground state energy can be given by diagrams in the Hugenholtz vein constructed according to the following rules (see \textsuperscript{5} for a more detailed explanation):

For an \textit{n}\textsuperscript{th} order diagram, \textit{n} dots (vertices) are drawn in a column. These vertices are connected by directed lines subject to the conditions:

1. Each vertex has two lines pointing in and two pointing out
2. Each diagram is connected, i.e. one must be able to go from any one vertex to any other by following some number of lines
3. No line connects a vertex with itself
4. Each diagram is topologically distinct

For each diagram, a simple prescription exists to go from the pictorial representation to an algebraic expression for the contribution to the total energy from the particular diagram\textsuperscript{5}.

Following these rules, one can determine that there are no first order diagrams since a line may not link a vertex with itself. There is one second order diagram, which is shown in figure 1 and three third order diagrams, which are shown in figure 2.

![Figure 1: Second order diagram](image1)

![Figure 2: Third order diagrams](image2)
3. Diagram finding algorithm

A diagram of a given order \( n_{\text{ord}} \) can be fully described by taking all possible (unordered) pairs of distinct vertices, of which there will be

\[
n_{\text{pairs}} = \frac{1}{2} n_{\text{ord}} (n_{\text{ord}} - 1)
\]

and specifying the number of lines linking each pair, along with the direction of each line. It is clear that since the number of lines connected to a given vertex must be four, that no more than four lines may link any pair. In fact, the case of four lines can exist only in the second order diagram shown in figure 1 since any two vertices connected by 4 lines cannot be connected to any other vertices in the diagram, which is inadmissible by point 2 in the above list of rules. Given these facts, the following algorithm can be used to find all possible diagrams:

- Create an ordered list of \( n_{\text{pairs}} \) numbers with a specification for which vertices are associated with each pair: \( 1&2, 1&3, \ldots, 1&n_{\text{ord}}, 2&3, 2&4, \ldots, 2&n_{\text{ord}}, \ldots, (n_{\text{ord}} - 1)&n_{\text{ord}} \).

- Allow each number in the list to take on independently the values 0, 1, 2, 3 corresponding to the number of lines linking the pairs. There will be \( n_{\text{pairs}}^4 \) such combinations. The case of \( n_{\text{order}} = 2 \) is treated specially by allowing the number of lines linking pairs to take the value 4.

- For each combination of number of lines linking pairs, rule 2 from the above list is checked along with the condition that four lines emanate from each vertex (due to rule 1). Any combination not satisfying the rules is rejected. Any combination which does satisfy these rules is a valid unlabelled diagram. The diagram is labelled in all possible ways by adding arrows to the lines in all possible permutations of upward- and downward-going arrows and checking these permutations against rule 1. Those which pass are valid (labelled) Hugenholz diagrams. The diagram is completely specified by the ordered list of numbers of lines connecting the pairs, and by a second list which gives the number of such lines which are pointing up; the rest must point down.

This provides an exhaustive search and is guaranteed to find all diagrams, at the cost of potential slowness as the number of permutations to check grows rapidly with order. The two lists of numbers given in the output may be post-processed to give, for example, Fortran code which implements the algebraic form of the diagrams. Note that condition 3 is automatically satisfied by the fact that in the specification of the pairs, we don’t consider pairing a vertex with itself. Similarly condition 4 is automatically satisfied by the specification of the problem in terms of vertices being ordered in a column in space.

4. Description of Code
A Fortran 95 code to calculate valid diagrams using the approach described in the previous section has been written and is presented in Appendix A. The code is described in terms of the subprograms as follows.

4.1. program hugenholz

\( n_{ord} \) is read in, from which \( n_{pairs} \) is calculated. The pairs structure is set up so that the first pair links vertices one and two and so on as described in section 3. A structure of \( n_{pairs} \) numbers is initialized with all numbers zero and passed to subroutine new to enumerate the diagrams.

4.2. subroutine new

Given a diagram specification, a loop is made over the first number of pairs over possible allowed values (0...3 or 4). The remainder of the diagram specification is then passed recursively to the subroutine new for the further numbers to be looped over. If we are at the last element of the specification, the diagram is checked for consistency using the function consistent and then printed out prepended by ‘+’. Finally a call is made to label to find all ways of labelling the lines with arrows.

4.3. function consistent

This function, which returns a logical, takes a possible configuration of lines connecting pairs of vertices, and checks first that it satisfies the condition from rule 1 that each vertex has four lines connected to it. Then the diagram is checked for being fully connected by starting at the bottom of the diagram, at vertex 1 and following lines until all vertices have been reached, in which case the diagram is consistent, or all lines have been followed without reaching some vertices, in which case it is inconsistent with rule 2 and we reject it.

4.4. subroutine label

A new array is set up which stores the number of upward-pointing lines for each pair of vertices. This is initialized to zero and passed to newlabel.

4.5. subroutine newlabel

Like new, this subroutine loops over all possible numbers of upward-pointing lines that each pair may admit given the number of total lines. The looping is again recursive, and once the last pair of lines is reached, the labelled diagram is tested with the function testlab. If it passes the number of upward-pointing arrows is printed prepended by ‘*’.

4.6. function testlab

This function tests for rule 2. The number of lines entering and leaving each vertex is calculated. If, for every vertex, both these numbers are two, then the
5. Sample output

The output of the program for second order diagrams is
+ 4
* 2
which says that there is one unlabelled diagram, which has one pair linked by four lines. There is furthermore only one way of labelling it, with two of the lines pointing up, as shown in figure 1. The output for \( n_{\text{ord}} = 3 \) is
+ 222
* 020
* 111
* 202
which says that there is again only one unlabelled diagram, which has three pairs, each linked by two lines. This time there are three possible ways of labelling the lines with arrows; 020 in which all lines point down except those linking vertices 1 and 3, 111 in which each pair of vertices is connected by one upgoing and one downgoing line, and 202 in which all lines point up except those linking vertices 1 and 3. These three possibilities are shown in figure 2 from left to right in the order given here.

The graphical representation of the diagrams in this paper were automatically generated from the output of the Fortran program hugenholtz by means of a perl program\(^*\) which outputs \LaTeX\ source using the FeynMF package\(^8\). While it would have been quite easy to work out second and third order diagrams by hand, the ability to automatically enumerate and represent all diagrams for higher orders becomes very useful. For example, the number of (labelled) diagrams at fourth, fifth, sixth and seventh orders are 39, 840, 27,300 and 1,232,280 respectively, which would be tedious to say the least to enumerate by hand. As an example of a less trivial result, the fourth order diagrams, as generated from the output of hugenholtz are shown in figure 3.

6. Summary

An algorithm has been presented and implemented which enumerates and represents Hugenholtz diagrams for the ground state perturbation series for a many-body system interacting under the influence of a two-body interaction. The representation is in a form suitable for post-processing. An example was given whereby \LaTeX\ code was automatically generated to draw the diagrams. A suggested further application is automatic code generation to evaluate the series in specific cases.

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Appendix A

module hug
    type pair
        integer :: v1, v2
    end type pair

type diagram
    integer, dimension(:), pointer :: occ
end type diagram

integer :: npairs, norder

contains

logical function consistent(diag, nlines, pairs)
    implicit none
    type(diagram), intent(in) :: diag
    integer, intent(in) :: nlines
    type(pair), dimension(:), intent(in) :: pairs
    integer :: linesum, i, vertex, lines, j, start, fin
    integer, allocatable, dimension(:) :: link
    logical, allocatable, dimension(:) :: linked, to_try, tried
    logical :: isdiaglinked

    consistent = .true.
    ! check each vertex for correct number of lines:
    allocate(link(norder))
    link = 0
    do i = 1, size(diag%occ(:))
        link(pairs(i)%v1) = link(pairs(i)%v1) + diag%occ(i)
        link(pairs(i)%v2) = link(pairs(i)%v2) + diag%occ(i)
    end do

    do i = 1, norder
        if (link(i) /= 4) then
            consistent = .false. ; return
        end if
    end do

deallocate(link)

    ! Test for unlinked diagrams.
    isdiaglinked = .false.
    allocate(linked(norder), to_try(norder), tried(norder))
    linked = .false. ; to_try = .false. ; tried = .false.
linked(i) = .true. ; to_try(i) = .true.
do
  vertex = 0
  do i = norder, 1, -1
    if (to_try(i) .eqv. .true.) vertex = i
  end do
  if (vertex == 0) exit
  do i = 1, size(pairs)
    if (diag%occ(i) /= 0) then
      if (pairs(i)%v1 == vertex) then
        linked(pairs(i)%v2) = .true.
        if (tried(pairs(i)%v2) .eqv. .false.) then
          to_try(pairs(i)%v2) = .true.
        end if
      else if (pairs(i)%v2 == vertex) then
        linked(pairs(i)%v1) = .true.
        if (tried(pairs(i)%v1) .eqv. .false.) then
          to_try(pairs(i)%v1) = .true.
        end if
      end if
    end if
  end do
  tried(vertex) = .true.
  to_try(vertex) = .false.
  isdiaglinked = .true.
  do i = 1, norder
    if (linked(i) .eqv. .false.) isdiaglinked = .false.
  end do
end do
deallocate(linked, to_try, tried)
if (isdiaglinked .eqv. .false.) consistent = .false.
end function consistent

subroutine label(diag, pairs)
  implicit none
  type(diagram) :: diag
  type(pair), dimension(::), intent(in) :: pairs
  integer, dimension(::), allocatable :: nups
  integer :: offset = 0

  allocate(nups(npairs))
call newlabel(offset, nups, diag%occ(::), pairs)
deallocate(nups)
end subroutine label

logical function testlab(nuparray, pairs, occarray)
    implicit none
    type(pair), dimension(:), intent(in) :: pairs
    integer, dimension(:), intent(in) :: nuparray, occarray
    integer :: vstart, vend, i
    integer, dimension(:), allocatable :: enter

    allocate(enter(norder))
    enter=0
    do i=1,npairs
        vstart = pairs(i)%v1
        vend = pairs(i)%v2
        if (vstart < vend) then
            enter(vend) = enter(vend)+nuparray(i)
            enter(vstart) = enter(vstart)+ occarray(i)-nuparray(i)
        else
            enter(vstart) = enter(vstart)+nuparray(i)
            enter(vend) = enter(vend)+ occarray(i)-nuparray(i)
        end if
    end do
    testlab=.false.
    if(all(enter==2)) testlab = .true.
    deallocate(enter)
end function testlab

recursive subroutine newlabel(offset, nuparray, occarray, pairs)
    implicit none
    integer :: offset
    integer, dimension(:) :: nuparray, occarray
    integer :: nuplo, nuphi, n, j
    type(pair), dimension(:), intent(in) :: pairs

    if(offset==npairs) then
        if (testlab(nuparray, pairs, occarray).eqv..true.) then
            write (*,'(a1,1x,100(i1))') '*',(nuparray(j),j=1,npairs)
        end if
        return
    end if
    offset=offset+1
    nuplo = max(occarray(offset)-2,0)
    nuphi = min(occarray(offset),2)
do n = nuplo,nuphi
    nuparray(offset) = n
    call newlabel(offset,nuparray,occarray, pairs)
end do
offset=offset-1
end subroutine newlabel

recursive subroutine new(nlines, offset, temp, pairs)
implicit none
integer, intent(in) :: nlines
type(diagram) :: temp
integer, intent(inout) :: offset
type(pair), dimension(:), intent(in) :: pairs
integer :: i, maxlinks = 3, j, ilo = 0

if(offset==nlines/2-1 .and. sum(temp%occ(1:offset)).ne.4) return
if(offset==npairs) then
  ! We have got to the end of the array - check for consistency:
  if(consistent(temp,nlines,pairs)) then
    write (*,'(a1,1x,100(i1))') '+',(temp%occ(j),j=1,npairs)
    call label(temp, pairs)
  end if
  return
end if
if(npairs==1) maxlinks = 4
do i=ilo,maxlinks
  temp%occ(1+offset)=i
  if(sum(temp%occ(1:offset+1))>nlines) cycle
  offset=offset+1
  call new(nlines, offset, temp, pairs)
  offset=offset-1
end do
end subroutine new

end module hug

program hugenholtz
use hug
implicit none
integer :: nfixed, nlines, index, i, j, offset = 0
type(pair), dimension(:), allocatable :: pairs
type(diagram) :: temp

write(unit=*,fmt='("Input order of diagrams: ")',advance='no')
Automatic Generation of Vacuum Amplitude

read(unit=*,fmt=*) norder
npairs = norder * (norder - 1) / 2
allocate(pairs(1:npairs),temp%occ(1:npairs))
nlines = 2 * norder
index = 1
do i = 1, norder
    do j = i + 1, norder
        pairs(index)%v1 = i ; pairs(index)%v2 = j
        index = index + 1
    end do
end do
temp%occ(:) = 0
call new(nlines, offset, temp, pairs)
d/deallocate(temp%occ,pairs)
end program hugenholtz

References

1. A. Messiah, Quantum Mechanics (North Holland, Amsterdam, 1966)
4. N. M. Hugenholtz, Physica 23, 481 (1957)
5. A. Szabo and N. Ostlund, Modern Quantum Chemistry (Dover, New York, 1996)
Figure 3: The 39 fourth order diagrams