CCDiag v.1.0

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Contents

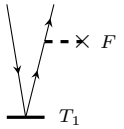
1 Using CCDiag

CCDiag is a TeX file, which allows you to simply draw Coupled Cluster diagrams using TikZ/PGF. Only the *TikZ* package is required; i.e. to include CCDiag in your TeX file use

```
%ccdiag
\usepackage{tikz}
\include{ccdiag}
%
```

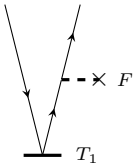
A diagram starts with **\bdiag** and ends with **\ediag**.

```
%<\mu_1|\op F \op T_1 |0>
\bdiag
  \dmoveH{2}
  \dT{1}{t}
  \dF{f}
  \dline{tv1}{t}
  \dline{t}{f}
  \dline{f}{fv2}
\ediag
```



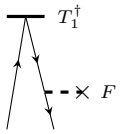
For a symmetric diagram (with Hamilton-operator parts in the middle) use **\bdiags**.

```
%<\mu_1|\op F \op T_1 |0>
\bdiags
  \dmoveH{2}
  \dT{1}{t}
  \dF{f}
  \dline{tv1}{t}
  \dline{t}{f}
  \dline{f}{fv2}
\ediag
```



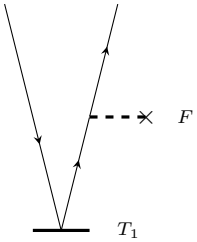
For a non-symmetric diagram with Hamilton-operator parts shifted down use **\bdiagd**.

```
%<0|\op T_1^\dg \op F |\mu_1>
\bdiagd
  \dmoveH{2}
  \dTd{1}{td}
  \dF{f}
  \dline{tdv1}{td}
  \dline{td}{f}
  \dline{f}{fvd2}
\ediag
```



You can scale the diagram by setting a number in the square brackets after **\bdiag** or **\bdiags**.

```
%<\mu_1|\op F \op T_1 |0>
\bdiags[1.5]
  \dmoveH{2}
  \dT{1}{t}
  \dF{f}
  \dline{tv1}{t}
  \dline{t}{f}
  \dline{f}{fv2}
\ediag
```



Or you can scale the diagram vertically and horizontally using
\dvscale{*scaling factor*}
and
\dhscale{*scaling factor*}

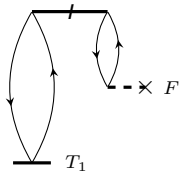
2 Operators

2.1 Excitation and deexcitation operators

2.1.1 Coupled Cluster excitation/deexcitation operators

The usual Coupled Cluster operator with label T_n can be created using the following command:
\dT[*pert.order*]{*exc.level*}{*node*}
Node-names for vertices are generated as *node*1, *node*2, *node*3, ...
The best suitable nodes for external lines are also generated and called *node*1v1 and *node*1v2 (for *node*1) etc
For the complex-conjugated counterpart (with label $T_n^\dagger$) use
\dTd[*pert.order*]{*exc.level*}{*node*}
If the labels are not needed, use
\dTs[*pert.order*]{*exc.level*}{*node*}
\dTds[*pert.order*]{*exc.level*}{*node*}

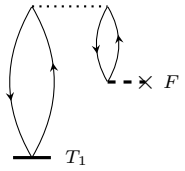
```
%<0|\op T_2^{(1)\dg} \op F \op T_1 |0>
\bdiags
\dmoveH{5}
\dmoveTd{1}
\dTds[1]{2}{td}
\dT{1}{t}
\dF{f}
\dcurcur{td1}{t1}
\dcurcur{td2}{f}
\ediag
```



2.1.2 Bare excitation/deexcitation operators

One can draw the bare excitation/deexcitation operators explicitly and connect external lines to them.
For τ_{μ_i} use
\dTv[*pert.order*]{*exc.level*}{*node*}
And for $\tau_{\mu_i}^\dagger$ use
\dTdv[*pert.order*]{*exc.level*}{*node*}

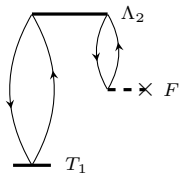
```
%<\mu_2| \op F \op T_1 |0>
\bdiags
\dmoveH{5}
\dmoveTd{1}
\dTdv{2}{td}
\dT{1}{t}
\dF{f}
\dcurcur{td1}{t1}
\dcurcur{td2}{f}
\ediag
```



2.1.3 General excitation/deexcitation operators

One can draw an excitation operator with a custom name using
\dAmp[*name*]{*pert.order*}{*exc.level*}{*node*}
And for an deexcitation operator use
\dAmpD[*name*]{*pert.order*}{*exc.level*}{*node*}

```
%<\Lambda_2| \op F \op T_1 |0>
\bdiags
\dmoveH{5}
\dmoveTd{1}
\dAmpD[$_{\Lambda_2}$]{}{2}{td}
\dT{1}{t}
\dF{f}
\dcurcur{td1}{t1}
\dcurcur{td2}{f}
\ediag
```



2.1.4 Customize excitation/deexcitation operators

It is possible to create custom (de)excitation operators. $\mathbf{U}_n$ and $\mathbf{U}_n^\dagger$ are available already (together with non-labeled versions dUs and dUds):
\dU[*pert.order*]{*exc.level*}{*node*}
\dUd[*pert.order*]{*exc.level*}{*node*}
There is also a transparent version of operators available:
\dTt{*exc.level*}{*node*}
\dTtd{*exc.level*}{*node*}
You can also create your own styles for operator lines (see Section 6).

2.2 Parts of Hamiltonian

2.2.1 Fock operator

For Fock operator use
\dF{*node*}
The best suitable nodes for external lines are called *node*v1 and *node*v2. Nodes for external lines going down are called *node*vd1 and *node*vd2.
For Fock operator without label use
\dFs{*node*}
For a reverse Fock operator line (with × left) use **\dFr** or **\dFsr**.

2.2.2 Fluctuation potential

For fluctuation potential use
\dW{*node1*}{*node2*}
The best suitable nodes for external lines are called *node1*v1 and *node1*v2, and *node2*v1 and *node2*v2. Nodes for external lines going down are called *node1*vd1, *node1*vd2, *node2*vd1, and *node2*vd2.
For fluctuation potential without label use
\dWs{*node1*}{*node2*}
A dressed version of fluctuation potential (with double lines) can be drawn using **\dWbar** and **\dWbars** commands.

2.2.3 Perturbations

For one-electron perturbation use
\dX{*node*}
(**\dXr** for a reverse line)
For two-electron perturbation use
\dXtwo{*node1*}{*node2*}

2.2.4 Custom one- and two-electron parts

For custom one-electron part use
\dHone[*name*]{*node*}
(\dHoner for a reverse line)
and for two-electron part use
\dHtwo[*name*]{*node1*}{*node2*}
You can also create your own styles for operator lines (see Section 6).

2.2.5 Feynman vs Bartlett convention

By default the interaction lines are drawn as dashed lines. If you prefer the usual Feynman's electromagnetic-interaction lines use
\dfeynman
at the beginning of the diagram.

2.3 Scaling of operator lines

The size of operator lines can be influenced using
\dscaleop{*scaling factor*}

3 Hole/Particle lines

3.1 Arrows

By default arrows are placed at 62% of the line. One can change it in the source code ("mark=at position"). Alternatively to set arrows at the end of lines uncomment the corresponding "ph-line-arrow-save".
One can use
\dnoarrow
and
\darrow
in order to switch off and on the arrows.

3.2 Straight lines

In order to connect two vertices with a straight h/p line use
\dline[*index*]{*from-node*}{*to-node*}
If *index* is given, it will be written to the right of the line.

3.3 Curved lines

In order to connect two vertices with a curved h/p line use
\dcurve[*index*]{*from-node*}{*to-node*}
If *index* is given, it will be written to the right of the line.
You can reverse the bend of the line using
\dcurver[*index*]{*from-node*}{*to-node*}
instead.
You can draw a "ring" between two nodes using
\dcurcur{*from-node*}{*to-node*}

3.4 Intelligent lines through three vertices

One can connect three vertices with an intelligent line.
\dcurt{*from-node*}{*through-node*}{*to-node*}
The most appropriate bend will be calculated automatically.

4 Shifting operators

Often in order to improve the diagram-look you have to shift the operator lines. There are four shift-commands available:

- shift excitation operators to the right:
  \dmoveT{*shift*}
- shift deexcitation operators to the right:
  \dmoveTd{*shift*}
- shift Hamiltonian-operators to the right:
  \dmoveH{*shift*}
- shift deexcitation operators up:
  \dmovac{*shift*}
- shift Hamiltonian-operators up:
  \dvmoveH{*shift*}

shift= 1 in the horizontal direction corresponds to a shift of a half length of single excitation operator (or of a quarter of doubles operator)

5 Text in diagrams

\dname{*text*} – write *text* (e.g. diagram name) over the diagram
\dtext{*shift*}{*text*} – write *text* in the diagram (with a horizontal shift).

5.1 Named nodes

Use operators
\dTone[*pert.order*]{*node*}{*node name*}
\dTtwo[*pert.order*]{*node*}{*node1 name*}{*node2 name*}
\dFn{*node*}{*node name*}
\dWn{*node1*}{*node2*}{*node1 name*}{*node2 name*}
to name individual nodes. Versions **\dTsone**, **\dTstwo**, **\dTdone**, **\dTdtwo**, **\dTdsone**, **\dTdstwo**, **\dTdvone**, **\dTdvtwo**, **\dUone**, **\dUtwo**, **\dUsone**, **\dUstwo**, **\dFsn**, **\dFrn**, **\dFsrn**, **\dWsn** are also available.

6 Styles

Change **exoper-line-save**, **exvac-line-save**, **hoper-line-save**, **ph-line-arrow-save**(or **ph-line-noarrow-save**) in order to change excitation operator, bare excitation operator, H-operator, or h/p line styles.
You can create your own operator style for a custom operator (see how **\dU** or **\dTv** are defined).

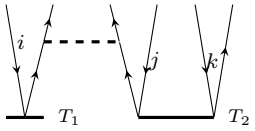
7 Generating external graphics

put
\beginpgfgraphicnamed{*Name-of-diagram*}
and
\endpgfgraphicnamed
before and after a block of diagrams that can be put outside, and
\pgfrealjobname{*Real-name of the tex document*}
in the preamble (e.g., after **\include{ccdiag}**).
Now you can use provided script **makediags** to generate all diagrams:

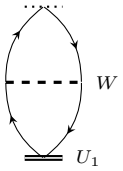
makediags *Real-name of the tex document.tex*
The resulting pdf files will be included by pdflatex instead of diagram-generation by later compilations (which can considerably speed up the compilation!) .

8 Examples

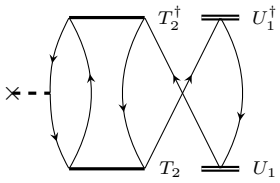
```
\bdiag
\dmoveH{2}
\dT{1}{t}
\dmoveT{2}
\dT{2}{tt}
\dWs{wn1}{wn2}
\dline[\raisebox{0.5cm}{$i$}]{t1v1}{t1}
\dline{t1}{wn1}
\dline{wn1}{wn1v2}
\dline[$j$]{tt1v2}{tt1}
\dline{tt1}{wn2}
\dline{wn2}{wn2v1}
\dline[$k$]{tt2v1}{tt2}
\dline{tt2}{tt2v2}
\ediag
```



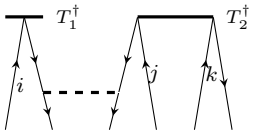

```
\bdiags
\dmoveT{1}
\dmoveTd{1}
\dU{1}{t}
\dTdv{1}{td}
\dW{w1}{w2}
\dcurt{t}{w1}{td}
\dcurt{td}{w2}{t}
\ediag
```




```
\bdiags
\dmoveT{3}
\dmoveTd{3}
\dTd{2}{td}
\dUd{1}{ud}
\dFsr{f}
\dT{2}{t}
\dU{1}{u}
\dcurt{td1}{f}{t1}
\dcurve{t1}{td1}
\dcurve{td2}{t2}
\dline{t2}{ud}
\dcurver{ud}{u}
\dline{u}{td2}
\ediag
```



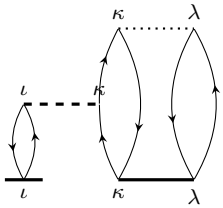
```
\bdiagd
\dmoveH{2}
\dTd{1}{t}
\dmoveTd{2}
\dTd{2}{tt}
\dWs{wn1}{wn2}
\dline[\raisebox{-0.5cm}{$i$}]{t1v1}{t1}
\dline{t1}{wn1}
\dline{wn1}{wn1vd2}
\dline[$j$]{tt1v2}{tt1}
\dline{tt1}{wn2}
\dline{wn2}{wn2vd1}
\dline[$k$]{tt2v1}{tt2}
\dline{tt2}{tt2v2}
\ediag
```



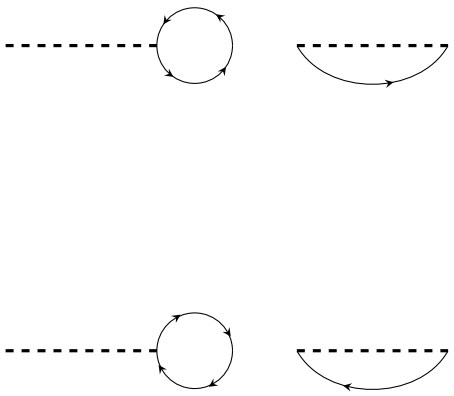

```
% transparent operators
\bdiagd
\dTtd{1}{t}
\dTt{1}{tt}
\dline{t1}{tt1}
\ediag
```



```
% named nodes
% and an external graphic "ExampleDiag"
\beginpgfgraphicnamed{ExampleDiag}
\bdiags
\dmoveH{1}
\dmoveTd{6}
\dTdvtwo{t}{$\kappa$}{$\lambda$}
\dWsn{w1}{w2}{$\iota$}{$\kappa$}
\dTsone{tt}{$\iota$}
\dmoveT{2}
\dTstwo{ttt}{$\kappa$}{$\lambda$}
\dcurcur{tt}{w1}
\dcurt{ttt1}{w2}{t1}
\dcurver{t1}{ttt1}
\dcurcur{ttt2}{t2}
\ediag
\endpgfgraphicnamed
```



```
% bubble and oyster
% and the p/h counterparts
\bdiags[2]
\dWs{w1}{w2}
\dbubble{w2}{1}
\ediag
\bdiags[2]
\dWs{w1}{w2}
\doyster{w1}{w2}
\ediag
\bdiags[2]
\dWs{w1}{w2}
\dbubbler{w2}{1}
\ediag
\bdiags[2]
\dWs{w1}{w2}
\doysterr{w1}{w2}
\ediag
```



8.1 DCD

```
\bdiags[1.5]
\dvscale{0.5}
\dfeynman \dnoarrow
\dvmoveH{-2}
\dTdv{2}{td}
\dWbars{w1}{w2}
\dcurcur{w1}{td1}
\dcurcur{w2}{td2}
\ediag
\bdiags[1.5]
\dvscale{0.5}
\dfeynman \dnoarrow
\dTdv{2}{td}
\dmoveH{4.6}
\dFbars{f}
\dTs{2}{tt}
\dcurcur{tt1}{td1}
\dcurve{td2}{tt2}
\dcurt{tt2}{f}{td2}
\ediag
\bdiags[1.5]
\dvscale{0.5}
\dfeynman \dnoarrow
\dTdv{2}{td}
\dmoveH{1.2}
\dscaleop{0.7}
\dWs{w1}{w2}
\dscaleop{1}
\dTs{2}{tt}
\dcurve{td1}{tt1}
\dcurt{tt1}{w1}{td1}
\dcurve{tt2}{td2}
\dcurt{td2}{w2}{tt2}
\ediag
\bdiags[1.5]
\dvscale{0.5}
\dfeynman \dnoarrow
\dmoveH{4.5}
\dTdv{2}{td}
\dTs{2}{tt}
\dscaleop{0.37}
\dWs{w1}{w2}
\dscaleop{1}
\dcurcur{tt1}{td1}
\dcurt{tt2}{w1}{td2}
\dcurt{td2}{w2}{tt2}
\ediag
```