

matri element m_zmel

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!! -----
cold  ntqxx--->nqmax
cold  nbmax -->nmmax
!!note: For usual correlation mode, I think nctot=0
!!note: For self-energy mode; we calculate <iq1|\Sigma |iq2> , where
iq1 and iq2 are in nqmax.
!!      nstate = nctot+nmmax
!!      allocate(zmelt(MPB, intermediate phi nstate, external state
phi ntqxx))
!!      zmelt= < MPB      phi    | phi    >
!!              <rkvec q-rkvec | q      >
!              cphim    | cphiq
!              ispm     | ispq
!      nctot+  nmini:nmmax | ncc + nqini:ntqxx
!              middle state| end state
!
!!--- For dielectric funciton, we use irot=1 kvec=rkvec=q. We calulate
\chi(q).
!!      q      rkvec      | q + rkvec
!      nkmin:nkmax | nkqmin:nkqmax
!      (we fix nkmin=1)
!
!      or
!      nt0=nkmax-nkmin+1 | ntp0=nkqmax-nkqmin+1
!      1:nt0      | 1:ntp0
!      occ      | unocc
!      (cphi_k   | cphi_kq !in x0kf)
!      middle state| end state
!
!! NOTE: dimension
!!      nmtot = nctot+ nmmax-mnini+1
!!      nqtot = ncc + ntqxx-nqini+1
!!      <q 1:ngb,      q-rkvec, 1:nmtot | rkvec, 1:nqtot>
!!      <end state,      middle state | MPB      >
!!      rkvec =mutmul(symops(:, :, irot), kvec)
!! -----
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PROF

Space group rotation of ecalj

- basic routines for spherical harmonics rotation.
/home/takao/ecalj/SRC/subroutines/rdpp.F: call rotcg(nl-1,symope,ng,grp,cgr)
/home/takao/ecalj/SRC/subroutines/rotcg.F: call rotldmm(symops, ng, 2*lmxax+1,dlmm)
rotcg --> rotldmm (rotation matrix of Ylm)
m_zmel->rdpp --> rotcg (rotated CG coefficients)

- eigenfunction rotation on the PMT basis
/home/takao/ecalj/SRC/main/hsfp0.sc.m.F: call rotwvigg(igrp,q(:,iqxx),q(:,iqxx),nhdim,
- m_zmel matrix elements
mt part readcphif -> readeigen -> rotmto
ipw part drvmelp melpl2 -> readgeigf -> rotipw
mptauf_zmel, ppbafp_v2->cgr ---->ppbir
 - eigenfunction (MT+IPW expansion) rotation
readeigen->rotipw,rotmto
/home/takao/ecalj/SRC/subroutines/readeigen.F: call rotipw(qtt(:,iqq),
/home/takao/ecalj/SRC/subroutines/readeigen.F: call rotmto(qtt(:,iqq),cphifr,ldim2,nband,
 - gvector rotation rotgvec
/home/takao/ecalj/SRC/subroutines/ppbafp.fal.F: call rotgvec(symope, 1, ngc, ngcs, qbas,
ngvecc,

(wannier-based matrix element are implemented in wannier/wmatK_mpi.F(in principle, only readeigenW, cphieigW are different)

- MPB rotation. symmetrization of x0
x0kf->rotMPB2->rotmto2,rotipw2
/home/takao/ecalj/SRC/subroutines/x0kf_v4h.F: call rotMPB2(nbloch,ngb,q,ig,itime,ginv,zrotm)
/home/takao/ecalj/SRC/subroutines/m_rotMPB.F: call rotmto2(qin,nbloch,ngbb,
/home/takao/ecalj/SRC/subroutines/m_rotMPB.F: call rotipw2(qin,qout,ngcx,ngbb,
/home/takao/ecalj/SRC/subroutines/m_rotMPB.F: call rotdlmm(symops,ngrp,nl,dlmm)
- Self-energy Sigma rotation. Read sigm.* which is expanded by MTO basis only (neglecting IPW components)
/home/takao/ecalj/SRC/subroutines/rdsigm2.F: call
rotsig(qin,q1,ndimh,napw_in,ldim,hq,gfbz(i1,i2,i3,: 🤔),ierr,iaf)

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/home/takao/ecalj/SRC/subroutines/m_hamindex.F: call rotdlmm(symops,ngrp, nl, dlmm)
/home/takao/ecalj/SRC/subroutines/m_hamindex.F: call rotdlmm(symops,ngrp, nl, dlmm)
/home/takao/ecalj/SRC/subroutines/m_q0p.F: call rotcg(lmxax,
(/1d0,0d0,0d0,0d0,1d0,0d0,0d0,0d0,1d0/),1,cg)
/home/takao/ecalj/SRC/subroutines/mptauof.F: call rotcg(lmxax,(/1d0,0d0,0d0,0d0,1d0,0d0,0d
/home/takao/ecalj/SRC/wanniergw/hpsig.F: call rotcg(nl-1,symope,ngrp,cg)
/home/takao/ecalj/SRC/wanniergw/hpsig_MPI.F: call rotcg(nl-1,symope,ngrp,cg)
/home/takao/ecalj/SRC/wanniergw/humat.F: call rotcg(nl-1,symope,ngrp,cg)
/home/takao/ecalj/SRC/wanniergw/humat_MPI.F: call rotcg(nl-1,symope,ngrp,cg)
/home/takao/ecalj/SRC/wanniergw/hwmatK.F:c call rotgvec(symgg(:,irot), nqibz,
/home/takao/ecalj/SRC/wanniergw/hwmatK_MPI.F:c call rotgvec(symgg(:,irot), nqibz,
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/home/takao/ecalj/SRC/subroutines/a2rotm.F: call rotma(phi,theta,angle,rotj)
/home/takao/ecalj/SRC/subroutines/chkdmu.F: call rotycs(-1,vorb,nbas,nsp,lmaxu,sspec,ssite,lldau)
/home/takao/ecalj/SRC/subroutines/sudmtu.F: call rotycs(2*idvsh-
1,dmatu,nbas,nsp,lmaxu,sspec,ssite,lldau)
/home/takao/ecalj/SRC/subroutines/mkplat.F: call rotmat(-1,.false.,nrot(m),mat,vecg)
/home/takao/ecalj/SRC/subroutines/rothrm.F: call rothrm(2,ndimh,iprmb,rotm,1,nbas,ndimh,uz,uz)
/home/takao/ecalj/SRC/subroutines/rothrm.F: call rothph(02,qpr,delT,ndimh,iprmb,1,nbas,ndimh,sq1)
/home/takao/ecalj/SRC/subroutines/rsmsym.F: call rotpnt(v,rv,g(1,ig))
/home/takao/ecalj/SRC/subroutines/symdmu.F: call rotspu(0,1,1,eula,1,u(1,1,ig))
/home/takao/ecalj/SRC/subroutines/symiax.F: call rotpnt(v,rv,g(1,ig))
/home/takao/ecalj/SRC/wanniergw/hmaxloc.F: call rot_hmnk(umnk,eunk,