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from __future__ import annotations
from typing import Union
from dataclasses import dataclass
from collections.abc import Sequence
from functools import cached_property
import numpy as np
from gpaw.response.kpoints import KPointDomainGenerator
@dataclass
class QSymmetries(Sequence):
    """Symmetry operations for a given q-point.
    We operate with several different symmetry indices:
      * u: indices the unitary symmetries of the system. Length is nU.
      * S: extended symmetry index. In addition to the unitary symmetries
           (first nU indices) it includes also symmetries generated by a
           unitary symmetry transformation *followed* by a time-reversal.
           Length is 2 * nU.
      * s: reduced symmetry index. Includes all the "S-symmetries" which map
           the q-point in question onto itself (up to a reciprocal lattice
           vector). May be reduced further, if some of the symmetries have been
           disabled. Length is q-dependent and depends on user input.
    q_c: np.ndarray
    U_ucc: np.ndarray # unitary symmetry transformations
    S_s: np.ndarray # extended symmetry index for each q-symmetry
    shift sc: np.ndarray # reciprocal lattice shifts, G = (T)Ug - g
    def __post_init__(self):
        self.nU = len(self.U_ucc)
    def __len__(self):
        return len(self.S_s)
    def getitem (self, s):
        return self.U_scc[s], self.sign_s[s], self.shift_sc[s]
    def unioperator(self, S):
        return self.U ucc[S % self.nU]
    def timereversal(self, S):
        """Does the extended index S involve a time-reversal symmetry?"""
        return bool(S // self.nU)
    def sign(self, S):
        """Flip the sign under time-reversal."""
        if self.timereversal(S):
           return -1
        return 1
    @cached property
    def U scc(self):
        return np.array([self.unioperator(S) for S in self.S s])
    @cached property
    def sign s(self):
        return np.array([self.sign(S) for S in self.S s])
    @cached property
    def ndirect(self):
        """Number of direct symmetries."""
        return sum(np.array(self.S_s) < self.nU)</pre>
    @property
    def nindirect(self):
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"""Number of indirect symmetries."""
        return len(self) - self.ndirect
    def description(self) -> str:
        """Return string description of symmetry operations."""
        isl = ['\n']
        nx = 6 # You are not allowed to use non-symmorphic syms (value 3)
        y = 0
        for y in range((len(self) + nx - 1) // nx):
            for c in range(3):
                 tisl = []
                 for x in range(nx):
                     s = x + y * nx
if s == len(self):
                         break
                     U_cc, sign, _ = self[:
op_c = sign * U_cc[c]
                                   = self[s]
                     tisl.append(f' ({op_c[0]:2d} {op_c[1]:2d} {op_c[2]:2d})')
            tisl.append('\n')
isl.append(''.join(tisl))
isl.append('\n')
        return ''.join(isl[:-1])
QSymmetryInput = Union['QSymmetryAnalyzer', dict, bool]
@dataclass
class QSymmetryAnalyzer:
    """Identifies symmetries of the k-grid, under which q is invariant.
    Parameters
    point_group : bool
        Use point group symmetry.
    time_reversal : bool
    Use time-reversal symmetry (if applicable).
    point group: bool = True
    time_reversal: bool = True
    @staticmethod
    def from input(gsymmetry: QSymmetryInput) -> QSymmetryAnalyzer:
        if not isinstance(qsymmetry, QSymmetryAnalyzer):
            if isinstance(qsymmetry, dict):
                 qsymmetry = QSymmetryAnalyzer(**qsymmetry)
             else:
                 qsymmetry = QSymmetryAnalyzer(
                     point_group=qsymmetry, time_reversal=qsymmetry)
        return qsymmetry
    @property
    def disabled(self):
        return not (self.point group or self.time reversal)
    @property
    def disabled_symmetry_info(self):
        if self.disabled:
            txt = ''
        elif not self.point_group:
            txt = 'point-group
        elif not self.time reversal:
            txt = 'time-reversal
        else:
        txt += 'symmetry has been manually disabled'
        return txt
    def analysis_info(self, symmetries):
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dsinfo = self.disabled symmetry info
    return '\n'.join([
        f'Symmetries of q_c{f" ({dsinfo})" if len(dsinfo) else ""}:',
        f'
              Direct symmetries (Uq -> q): {symmetries.ndirect}'
              Indirect symmetries (TUq -> q): {symmetries.nindirect}',
        f'In total {len(symmetries)} allowed symmetries.',
        symmetries.description()])
def analyze(self, q_c, kpoints, context):
    """Analyze symmetries and set up KPointDomainGenerator."""
    symmetries = self.analyze symmetries(q c, kpoints.kd)
    generator = KPointDomainGenerator(symmetries, kpoints)
    context.print(self.analysis_info(symmetries))
    context.print(generator.get_infostring())
    return symmetries, generator
def analyze symmetries(self, q c, kd):
    r"""Determine allowed symmetries.
    An direct symmetry U must fulfill::
      U \neq 0 
   Under time-reversal (indirect) it must fulfill::
      -U \mathbb{q} = q + \mathbb{q}
    where :math: \Delta is a reciprocal lattice vector.
    # Map q-point for each unitary symmetry
    U_ucc = kd.symmetry.op_scc # here s is the unitary symmetry index
   Uq\_uc = np.dot(U\_ucc, q\_c)
    # Direct and indirect -> global symmetries
    nU = len(U ucc)
    nS = 2 * n\overline{U}
    shift_Sc = np.zeros((nS, 3), int)
    is qsymmetry S = np.zeros(nS, bool)
    # Identify direct symmetries
    # Check whether U q - q is integer (reciprocal lattice vector)
    dshift_uc = Uq_uc - q_c[np.newaxis]
is_direct_symm_u = (dshift_uc == dshift_uc.round()).all(axis=1)
    is_qsymmetry_S[:nU][is_direct_symm_u] = True
    shift_Sc[:nU] = dshift_uc
    # Identify indirect symmetries
    # Check whether -U q - q is integer (reciprocal lattice vector)
    idshift_uc = -Uq_uc - q_c
is_indirect_symm_u = (idshift_uc == idshift_uc.round()).all(axis=1)
    is_qsymmetry_S[nU:][is_indirect_symm_u] = True
    shift_Sc[nU:] = idshift_uc
    # The indices of the allowed symmetries
    S_s = is_qsymmetry_S.nonzero()[0]
    # Set up symmetry filters
    def is not point group(S):
        return (U_ucc[S % nU] == np.eye(3)).all()
    def is not time reversal(S):
        return not bool(S // nU)
    def is not non symmorphic(S):
        return not bool(kd.symmetry.ft_sc[S % nU].any())
    # Filter out point-group symmetry, if disabled
    if not self.point_group:
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S_s = list(filter(is_not_point_group, S_s))
# Filter out time-reversal, if inapplicable or disabled
if not kd.symmetry.time_reversal or \
    kd.symmetry.has_inversion or \
    not self.time_reversal:
    S_s = list(filter(is_not_time_reversal, S_s))
# We always filter out non-symmorphic symmetries
S_s = list(filter(is_not_non_symmorphic, S_s))
return QSymmetries(q_c, U_ucc, S_s, shift_Sc[S_s])
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