Reply to “Comment on ‘Piezoelectricity in planar boron nitride via a geometric phase’”

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In relation to our original paper [M. Droth et al., Phys. Rev. B 94, 075404 (2016)], the Comment by Li et al. [Phys. Rev. B 98, 167403 (2018)] claims to have identified a “mistake in constructing the adiabatic process of the piezoelectricity”. More specifically, they write that in our original work “the erroneous usage of the polarization difference formula in Eq. (4) leads to an invalid analytical expression of piezoelectric constant in Eq. (12) of Reference 1”. We explain below why these and other minor claims in the Comment are unwarranted, and why we maintain that our result is correct and physically sound.

I. CHOICE OF ADIABATIC PARAMETER

The procedure used to obtain the piezoelectric constant in our original paper hinges on a calculation of the bulk polarization as an explicit function of the strain tensor [cf. the original Eq. (9)]. As established by the seminal work of Resta, Vanderbilt and King-Smith, the only well defined physical quantity that is amenable to a controlled calculation is a variation in bulk polarization. This led to the development of the modern theory of polarization according to which such polarization differences are calculated by integrating the varying Berry curvature along an adiabatic path connecting the two states. One of the most typical situations involves computing the absolute bulk polarization of a given system: to exploit this method, one sets up an adiabatic path that connects that target with a reference system having zero bulk polarization. Such an adiabatic path is frequently defined in terms of a parameter of the Hamiltonian that can be continuously tuned between the initial and target state and, in particular, the adiabatic process does not have to necessarily reflect any real physical process. For example, in first-principles implementations it is rather common to obtain the bulk polarization by an adiabatic process that continuously changes the atomic pseudopotentials, or which evolves the lattice from an inversion-symmetric configuration to the target state through a fictitious deformation path (for a specific example where this evolution of a “virtual crystal” is done for a BN-based system see Ref. [4]).

In calculations made with effective Hamiltonians, the earlier paper in the context of nanotubes by Mele and Král relies on exactly the same approach that we used of evolving the gap parameter in an adiabatic path that begins with a strained carbon nanotube and ends with a strained BN nanotube. As our adiabatic parameter is the gap $\Delta$, our adiabatic process begins with strained graphene and ends with strained BN; strain is kept finite and constant throughout. The adiabatic process chosen by Li et al. begins with relaxed BN and ends with strained BN. Since the bulk polarization of the initial state is zero in the two cases (in uniaxially strained graphene because of inversion symmetry, and in relaxed BN because of its $D_{3h}$ point group), they are, in principle, both legitimate adiabatic paths to determine the bulk polarization. It is therefore erroneous, and not in line with the modern formulation of the quantum theory of polarization, to claim that “the correct adiabatic process of piezoelectricity should reflect the deformation-induced polarization difference from the initial state of undeformed h-BN to the final state of deformed h-BN”, as stated in the Comment.

II. THE ANALYTICAL EXPRESSION FOR $e_{222}$

Reinstating the parameter $\kappa$ associated with the electron-phonon coupling, as per our original parametrization, Li et al.’s Eq. (18) should read

$$e_{222} = \frac{e|\beta|\kappa}{2\pi a} \left[ \text{sign}(\Delta) - \frac{\Delta}{\sqrt{3}\pi t^2 + \Delta^2} \right].$$

(1)

In the original paper, we obtain instead [cf. our original Eq. (12)]

$$e_{222} = \frac{e|\beta|\kappa}{\pi^2 a} \tan^{-1} \left[ \frac{\Delta}{\sqrt{2}\omega^2 + \Delta^2} \right].$$

(2)

Before further discussion, it is instructive to verify whether these results satisfy simple limits and symmetries. In the model Hamiltonian that is used to describe the BN monolayer, changing $\Delta \to -\Delta$ amounts to an inversion transformation, since it is equivalent to swapping B with N atoms everywhere. Being a rank-3 tensor, $e_{222}$ should change sign under an inversion transformation, which is indeed satisfied by both results (1) and (2).

However, it is clear that when $\Delta \to 0$, our result (2) decreases and ultimately becomes zero in the limit of graphene ($\Delta = 0$). This is just as expected, because the six-fold rotational symmetry of the latter precludes...
a piezoelectric response \((e_{ijk} = 0 \text{ in graphene by symmetry})\). In contrast, the expression (1) obtained by Li et al. remains finite as \(\Delta \rightarrow 0\). In fact, according to their result, \(e_{222}\) increases monotonically when \(\Delta\) decreases. In addition to failing to recover the graphene case in the limit \(\Delta \rightarrow 0\), this is contrary to physical intuition because, even if the gap remains finite, when it decreases, the charge transfer between B and N decreases as well. Even though in the modern theory the macroscopic polarization is not defined in terms of local properties, one expects its magnitude to qualitatively follow the trend of the bond polarity. Hence, the dipole moment induced by a finite deformation in this system is expected to decrease when the gap parameter \(\Delta\) is brought to zero. Seeing this from another perspective, if one makes an infinitesimal perturbation to graphene that breaks its intrinsic sublattice symmetry, one is breaking the inversion symmetry of the system only by an infinitesimal amount as well, and expects the induced polarization to be small. But the result by Li et al. predicts otherwise, namely a gap-independent value of \(P\) (and, by extension, of \(e_{222}\) as well) in the limit where the gap is much smaller than the bandwidth (\(\Delta \ll t\)), and a finite discontinuity in \(e_{222}\) when \(\Delta\) varies infinitesimally between \(0^-\) and \(0^+\).

Therefore, our original work is suitable to characterize, in an entirely analytical way, the behavior of both the electronic contribution to the bulk polarization and the piezoelectric constant in BN, as intended and stated in our original paper. Moreover, relying on an analytical model Hamiltonian, it is only useful if it captures the qualitative trends of these quantities, in particular when transitioning from BN to the graphene limit, which is not the case with the result in the Comment.

### III. TWO DIFFERENT ANALYTICAL RESULTS

There are two aspects related to the different results obtained for \(e_{222}\) in Eqs. (1) and (2). The first one is a superficial difference related to the approximation used for the effective Brillouin zone (BZ) in the momentum integrations. Whereas our original paper uses a square, total-state-conserving effective BZ, the Comment uses a circular one. If \(e_{222}\) is computed in a circular BZ domain (using polar coordinates for the integrations) we obtain

\[
e_{222} = \frac{e|\beta|\kappa}{4\pi a} \frac{\Delta}{\sqrt{q_t^2 + \Delta^2}}.
\]

As expected, this expression agrees with Eq. (2) to leading order when \(\Delta \gg \{q_t, w\}\), up to a factor \(\sim 1\) arising from the circular-vs-square geometry difference [note that \(4\pi^2 = \pi q_t^2 = 4\pi^2/(3\sqrt{3}a^2)\), see the original paper]. Moreover, it corresponds precisely\(^a\) to the second term in the result (1) above, which is the proposed analytical form in the Comment.

The second aspect has to do with the essential difference that makes the result proposed in the Comment a constant as \(\Delta \rightarrow 0\), thus failing to capture the correct graphene (gapless) limit. The method followed in the Comment relies on two steps that are mathematically unsafe when combined: using strain as the adiabatic parameter and, in practice, differentiating the integral that yields the polarization with respect to strain beforehand. As a result, in the Comment, \(e_{222}\) is expressed as the integral stated in their Eq. (9), where the derivatives with respect to the strain components appear in the integrand. The problem with this approach is that the original integrand that yields the polarization \(P\) is not a continuous function over the domain of the multiple integral. Hence, “passing” the derivative from the outside to the inside of the multiple integral (Leibniz’s rule) is not warranted. In Appendix A, we show explicitly that, doing so, we obtain the result stated in the Comment (still using the gap as adiabatic parameter), but it arises only because of a blind application of Leibniz’s rule.

In addition, to corroborate the mathematical robustness of our original result, we provide in the Supplemental Material\(^b\) a Mathematica notebook that verifies the steps involved in the calculations reported in our original paper.

### IV. SYMMETRY CONSTRAINTS ON \(e_{ijk}\)

The discussion presented in the Comment in connection to its Eqs. (19-20) implicitly suggests that Eq. (10) in our paper, which states

\[
e_{211} = e_{112} = e_{121} = -e_{222},
\]

is incorrect and should instead read as the Comment’s Eq. (20). However, the relations (4) must be satisfied by any rank-3 physical tensor in a system containing a threefold rotational axis, and with the mirror plane parallel to the direction \(u_2\) (refer to any textbook covering symmetry aspects of crystals, such as our original Ref. [47]). This is the case of monolayer BN in the orientation shown in our Fig. 1, which has point group symmetry \(D_{3h}\). Our definition in Eq. (9) of the paper ensures \(e_{ijk}\) is a Cartesian tensor. Hence, it is clear that Eq. (20) in the Comment violates the symmetry-imposed constraint among the nonzero components of \(e_{ijk}\). The error stems from the flawed considerations in the text preceding Eq. (19) of the Comment, namely because \(\epsilon_{ij}\) defined there is not a physical tensor (i.e., its components do not transform as those of a Cartesian tensor) due to the factor of 2 included in the definition of \(\varepsilon_{12}\). Eq. (4) above is a relation involving components of a tensor which should be adapted if one is using a Voigt representation, and not the other way around as stated in the Comment.

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\(^a\) A blind application of Leibniz’s rule.

\(^b\) Mathematica notebook.
V. BETTER AGREEMENT WITH THE DFT RESULT

The authors of the Comment emphasize that they obtain a very good numerical agreement between their numerical result for $\varepsilon_{222}$ and the one arising from first-principles in a clamped-ion calculation of the electronic contributions associated with the $\pi$ and $\sigma$ bands. This is misleading because such an agreement is simply a numerical coincidence, especially in view of the approximations involved in the effective (Dirac) Hamiltonian and the uncertainty associated with the estimates of the logarithmic derivative of the hopping parameter under strain. Moreover, those estimates were not based on the specific bandstructure predicted by the quoted density functional theory (DFT) calculation.

The authors of the Comment also refer to Ref. [11] as an alternative approach to check their calculation. However, piezoelectricity in BN is not discussed in that reference and it also does not offer an alternative approach. Instead, the calculation shown there is very similar to an alternative approach to check their calculation. Howver, piezoelectricity in BN is not discussed in that reference and it also does not offer an alternative approach. Instead, the calculation shown there is very similar to the one in their Comment, adapted to transition metal dichalcogenides.

VI. CONCLUSION

In summary, we trust that our methodology and calculations reported originally in Ref. [1] are sound and physically well justified.

MD acknowledges funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) within Project No. 317796071. MD and GB thank the European Science Foundation and the DFG for support within the EuroGRAPHENE project CONGRAN and the DFG for funding within SFB 767 and FOR 912.

Appendix A: Differentiating beforehand

There is an apparent advantage in performing the derivatives

$$\left. \frac{\partial P_x}{\partial A_y} \right|_{A=0} \quad \text{and} \quad \left. \frac{\partial P_y}{\partial A_x} \right|_{A=0} ,$$

required to compute $\varepsilon_{222}$, before performing the adiabatic and BZ integrals since, in this way, the integrand becomes a simpler algebraic function and the shifted Dirac point disappears. This is, in effect, what is implied by the procedure followed in the Comment by Li et al. when using strain as the adiabatic parameter.

However, there is a technical subtlety in doing so which we illustrate following our approach that uses the gap as the adiabatic parameter. The $i$-th Cartesian component of the polarization is obtained as

$$P_i = \int_0^\Delta d\lambda \left[ 2e \sum_{\tau} \frac{\partial}{\partial A_x} \int_{BZ/2} dq \Omega^{(\tau)}_{q_i,\lambda} \right] ,$$

which is our original Eq. (4). To obtain the piezoelectric constant we need to compute, for example, [cf. Eq. (11) in the paper]

$$\varepsilon_{222} \propto \frac{\partial}{\partial A_x} \int_0^\Delta d\lambda \int_{BZ/2} dq \Omega^{(\tau)}_{q_2,\lambda} .$$

Whether or not one can safely employ Leibniz’s rule and pass the derivative to the inside of the integral depends on $\Omega^{(\tau)}_{q_2,\lambda}$ being a continuous function of $(q_x, q_y, \lambda)$ in the domain of the multiple integral. However,

$$\Omega^{(\tau)}_{q_2,\lambda} = \frac{x - A_x}{\left((q_x - A_x)^2 + (q_y - A_y)^2 + \lambda^2\right)^{3/2}}$$

has a clear discontinuity at the point $(q_x, q_y, \lambda) = (A_x, A_y, 0)$ and, therefore, the conditions of Leibniz’s rule are not fulfilled [the singularity is integrable though — to zero —, as we demonstrate in Appendix B]. As a result of this discontinuity, even though the integral of $\partial \Omega^{(\tau)}_{q_2,\lambda} / \partial A_x$ converges, its value depends on the sequence of the partial integrations. We now show this explicitly.

We are interested in the integral

$$I = \int_0^\Delta d\lambda \int_{BZ/2} dq \frac{\partial \Omega^{(\tau)}_{q_2,\lambda}}{\partial A_x} ,$$

where

$$\left. \frac{\partial \Omega^{(\tau)}_{q_2,\lambda}}{\partial A_x} \right|_{A=0} = \frac{2q_x^2 - q_y^2 - \lambda^2}{(q_x^2 + q_y^2 + \lambda^2)^{3/2}} .$$

Since we are focusing on the technical aspect here, for simplicity, we drop all the non-essential prefactors and, for definiteness, consider $\Delta > 0$ in the remainder of this appendix. Computing (A5) by integrating first over the BZ and $\lambda$ last, we obtain

$$I_{\lambda \text{ last, } \square} = -2\tan^{-1} \left( \frac{\Delta}{\sqrt{2u^2 + \Delta^2}} \right) .$$

With the prefactors, this is our result (12) in the original paper, where the BZ integral has been performed over a square-shaped, state-conserving BZ, as discussed in the paper. For completeness, if one opts to use a circularly shaped domain with cutoff momentum $q_c$ (the choice made in the Comment), the result for $I$ becomes

$$I_{\lambda \text{ last, } \square} = -\frac{\pi \Delta}{2\sqrt{u^2 + \Delta^2}} .$$

On the other hand, if one performs the adiabatic integral first by that over the BZ, one obtains

$$I_{\lambda \text{ first, } \square} = \pi - 2\tan^{-1} \left( \frac{\Delta}{\sqrt{2u^2 + \Delta^2}} \right) .$$
for the square BZ, and

\[ I_{\text{last}} = \pi \frac{\Delta}{2} \frac{\pi\Delta}{2\sqrt{q_x^2 + \Delta^2}} \]  

(A8b)

for the circular BZ. Note that this last result is the one reported in Eq. (18) of the Comment once the prefactors are restored\(^9\). Therefore, computing (A5) by performing the adiabatic integral first followed by that over the BZ, introduces a constant, independent of \(\Delta\).

Mathematically, this dependence of the result on the order of the multiple integrations arises because Eq. (A5) does not converge absolutely and, consequently, it is sensitive to whether one performs the \(q_x\) integration before or after the one over \(\lambda\) (changing to polar coordinates does not change this, of course)\(^{12}\). This non-uniform convergence is, of course, a consequence of having erroneously used Leibniz’s rule when the integrand of (A3) is not a continuous function (incidentally, performing the \(\lambda\) integral last, which is physically motivated, yields the correct result).

In order to avoid these pitfalls, the method of calculation used in our original paper keeps \(A_x\) and \(A_y\) finite until the triple integral that yields \(P\) is obtained. We only linearize the result in \(A\) afterwards. In this way, the result is mathematically well defined, irrespective of the sequence used for the triple integration\(^9\).

### Appendix B: Singularity of the Berry curvature

In spherical coordinates,

\[
q_x - A_x = r \sin(\theta) \cos(\phi),
\]

\[
q_y - A_y = r \sin(\theta) \sin(\phi),
\]

\[
\lambda = r \cos(\theta),
\]

the Berry curvature given in Eq. (A4) reads

\[
\Omega_{q_y, \lambda}^{(\tau)} \propto \frac{r \sin(\theta) \cos(\phi)}{r^3} = \frac{\sin(\theta) \cos(\phi)}{r^2}.
\]  

(B2)

This expression has a discontinuity at \(r=0\), i.e., at \((q_x, q_y, \lambda)=(A_x, A_y, 0)\), which lies in the integration domain of Eq. (A2). The support of this point is 0 but the Berry curvature diverges so one must, in principle, verify whether there is a finite contribution to the integral. This contribution can be checked as follows:

\[
\lim_{\delta \to 0} \int_0^\delta \int_0^{\pi/2} \int_0^{2\pi} \frac{r^2 \sin^2(\theta) d\theta \cdot \int_0^{2\pi} \cos(\phi) d\phi}{(q_y - A_y)^2 + \lambda^2} = \lim_{\delta \to 0} (\delta - 0) \cdot \frac{\pi}{4} \cdot 0 = 0.
\]  

(B3)

This means that the singularity at the shifted Dirac points integrates to 0 and does not add any particular contribution to the result of Eq. (A2).

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1. M. Droth, G. Burkard, and V. M. Pereira, Phys. Rev. B 94, 075404 (2016).
2. R. Resta, Ferroelectrics 136, 51 (1992), R. Resta, Rev. Mod. Phys. 66, 899 (1994).
3. D. Vanderbilt, Phys. Rev. B 41, 7892 (1990), R. D. King-Smith and D. Vanderbilt, Phys. Rev. B 47, 1651 (1993).
4. S. M. Nakhmanson et al., Phys. Rev. B 67, 235406 (2003).
5. E. J. Mele and P. Král, Phys. Rev. Lett. 88, 056803 (2002).
6. J. Li, Y. Wang, Z. Wang, J. Tan, B. Wang, and Y. Liu, Phys. Rev. B 98, 167403 (2018).
7. H. Suzuura and T. Ando, Phys. Rev. B 65, 235412 (2002).
8. When comparing, note that in our notation the gap is \(\hbar v_F \Delta\), while it is simply represented by \(\Delta\) in the notation of the Comment (we maintain the original notations of each).
9. See Supplemental Material for a verification of our calculations using Mathematica.
10. K.-A. N. Duerloo, M. T. Ong, and E. J. Reed, J. Phys. Chem. B 3, 2871 (2012).
11. Y. Wang, Z. Wang, J. Li, J. Tan, B. Wang, and Y. Liu, Phys. Rev. B 98, 125402 (2018).
12. The integral in question has precisely the same pathology as the double integral \(\int_0^1 \int_0^1 \frac{x^2+y^2}{(x^2+y^2)^2} \, dx \, dy\), which is a common counterexample to the interchangeability in the order of integrations in the absence of absolute convergence. In this case, the result is \(+\pi/4\) \((-\pi/4\) if \(y \neq x\) is integrated first.)
Utility functions and definitions

Generic assumptions and functions handy to perform simplifications below:

```math
MyAss = qx \in \text{Reals} \land qy \in \text{Reals} \land Ax \in \text{Reals} \land Ay \in \text{Reals} \land \lambda \in \text{Reals} \land \Delta \in \text{Reals} \land w > 0;
```

```math
FS[x_] := \text{FullSimplify}[x, \text{Assumptions} \rightarrow \text{MyAss}]
```

```math
SS[x_] := \text{Simplify}[x, \text{Assumptions} \rightarrow \text{MyAss}]
```

Utility to output an expression with a label and an enclosing frame:

```math
ClearAll[myFrame];
myFrame[label_, x_, color_: LightMagenta] := Framed[label <> ToString[x, TraditionalForm],
  Background -> color, FrameMargins -> Large, FrameStyle -> Thin]
myFrame["Result = ", \pi, LightOrange]
```

Prefactors

In the calculations below we will leave out the prefactors of all the above expressions. To recover them for $P_{\alpha\nu}$ multiply by

```math
prefactorP = \frac{e}{\pi^2};
```

and, for $e_{222}$, multiply $\partial_a \Omega_a$ by

```math
prefactorE222 = \frac{\beta \kappa}{2a} \times \text{prefactorP};
```

The Berry curvatures

Begin with the results in Eq. (6) of the paper, which can be easily shown to be correctly calculated:
\[\Omega y = \frac{qy}{2 (q^2 + y^2 + \Delta^2)^{3/2}} \quad / \quad (q \to q - Ax, y \to y - Ay)\]

\[\Omega y = \frac{qx}{2 (q^2 + x^2 + \Delta^2)^{3/2}} \quad / \quad (x \to x - Ay, y \to y - Ax)\]

\[\int (...) \, d\lambda = \frac{\Delta (Ay - qy)}{2 \left( (Ax - qx)^2 + (Ay - qy)^2 \right) \sqrt{(Ax - qx)^2 + (Ay - qy)^2 + \Delta^2}}\]

**Adiabatic integral**

Following exactly the sequence described in the paper, we begin with the adiabatic integral.

First note that

\[\Omega x = -qy \quad \frac{qy}{(q^2 + y^2)} \quad / \quad (q \to q - Ax, y \to y - Ay)\]

\[\Omega y = \frac{qx}{2 (q^2 + y^2 + \Delta^2)^{3/2}} \quad / \quad (x \to x - Ay, y \to y - Ax)\]

which means that the result has the same parity as \(\Delta\) itself. For that reason, we can look only at the case \(\Delta > 0\) from now on, and we will do so. Incorporate this into the assumptions:

\[\text{MyAss} = \text{Reduce} \{\text{MyAss} \&\& \Delta > 0\}\]

\[Ax \in \mathbb{R} \&\& Ay \in \mathbb{R} \&\& qx \in \mathbb{R} \&\& qy \in \mathbb{R} \&\& \lambda \in \mathbb{R} \&\& \Delta > 0 \&\& w > 0\]

The adiabatic integral is then

\[\int (...) \, d\lambda = \frac{\Delta (Ay - qy)}{2 \left( (Ax - qx)^2 + (Ay - qy)^2 \right) \sqrt{(Ax - qx)^2 + (Ay - qy)^2 + \Delta^2}}\]

The singularity at the Dirac point is integrable

The previous result must now be integrated over the BZ, but the integrand is singular at the shifted Dirac point where \((Ax - qx)^2 + (Ay - qy)^2 = 0\). Let us confirm that it is an integrable singularity.

Change to polar coordinates with respect to the shifted Dirac point:
The angular integration goes via \( q \, d\theta \), so the factor \( q \) in the nominator cancels out and the remaining integrand is finite. Performing the integration over \( \sin[\theta] \) obviously gives zero. Hence, the integral over the BZ is well defined and, in addition, this shows that there is no singular nor finite "topological" contribution from the displaced Dirac point.

### BZ integration for \( P_x \)

**Over \( q_x \)**

Integrate over \( q_x \) but, to fulfil the condition \((Ax - qx)^2 + (Ay - qy)^2 > 0\), split into two integrals over \([-w, Ax]\) plus \((Ax, w]\). As we have just shown, the divergence at \( qx = Ax \) does not give a contribution and thus can be left out.

```
In[19]:= Integrate[I1 /. {qx -> Ax + q Cos[\[Theta]], qy -> Ay + q Sin[\[Theta]]} // FS

Out[19]= ConditionalExpression[-\[LeftFraction]1/2\[RightFraction] ArcTan[\[LeftFraction]Ax + w\[RightFraction] \[LeftFraction](Ax + w) \[Delta]\[RightFraction] qy \sqrt{qy^2 + (Ax + w)^2 + \[Delta]^2}], qy \[NotEqual] 0]

Out[20]= ConditionalExpression[\[LeftFraction]1/2\[RightFraction] ArcTan[\[LeftFraction]Ax - w\[RightFraction] \[LeftFraction](Ax - w) \[Delta]\[RightFraction] qy \sqrt{qy^2 + (Ax - w)^2 + \[Delta]^2}], qy \[NotEqual] 0]
```

This result is now the integrand for the integration over \( q_y \). But note that it has a discontinuity at \( q_y = Ay \) where \( \tan^{-1} \) changes branch:

\[
\int (...) \, dq_x = \frac{1}{2} \left( \tan^{-1} \left( \frac{\Delta (Ax - w)}{(qy - Ay) \sqrt{(Ax - w)^2 + (qy - Ay)^2 + \Delta^2}} \right) - \tan^{-1} \left( \frac{\Delta (Ax + w)}{(qy - Ay) \sqrt{(Ax + w)^2 + (qy - Ay)^2 + \Delta^2}} \right) \right)
\]
Over \(q_y\)

It's not easy to make Mathematica perform the definite integral over \(q_y\) keeping \(A_x\) and \(A_y\) arbitrary (more on this below). So we'll use primitives taking explicitly into account the step discontinuity at \(q_y = A_y\) in that process.

Compute the primitive:

\[
\begin{align*}
\text{In[24]:=} & \quad I3 = \text{Integrate}[I2, qy]; \\
\text{Out[24]=} & \quad \frac{q_y}{-0.2} + \frac{q_y}{-0.1} + \frac{q_y}{-0.5} + \frac{q_y}{1}
\end{align*}
\]

which looks like this:

\[
\begin{align*}
\text{In[25]:=} & \quad \text{Plot}[I3 /. \{Ay \rightarrow 0.2, Ax \rightarrow 0.1, \Delta \rightarrow 0.5, w \rightarrow 1\}, \{qy, -2, 2\}]
\end{align*}
\]

Note that, instead of a kink at \(q_y = A_y\) we see a discontinuity which means the primitive has jumped during the branch change of \(\text{ArcTan}\). We must be careful in computing the integral from this primitive. In particular, we cannot compute the integral as the difference in primitives at \(\pm w\) straight away.

To be on the safe side, we'll consider separately the integrals in \([-w, A_y]\) and \([A_y, w]\). Each of them is well defined in terms of the difference of primitives. But we must be careful in evaluating the primitives at \(A_y + \epsilon\) and \(A_y - \epsilon\) staying in the correct branch.

Begin by computing the left and right limits of the primitive as \(q_y \to A_y\):
In[26]:= limLeft[x_] := Limit[x, {qy -> Ay}, Direction -> "FromBelow", Assumptions -> MyAss && -w < Ax < w && -w < Ay < w && w > 0]

limRight[x_] := Limit[x, {qy -> Ay}, Direction -> "FromAbove", Assumptions -> MyAss && -w < Ax < w && -w < Ay < w && w > 0]

I3left = Map[limLeft, Expand[I3]]
I3right = Map[limRight, Expand[I3]];

We can confirm that there is indeed the (spurious) discontinuity at $A_y$ we saw in the previous plot:

In[30]:= I3right - I3left // SS
Out[30]= $-A_y \pi$

which is proportional to $A_y$ (this must be handled with care because, in order to get $\varepsilon_222$, one needs to perform a derivative w.r.t. $A_y$)

Compute then the $q_y$ integral by combining the primitives on each side:

In[31]:= I4 = I3left - (I3 /. {qy -> w}) + (I3 /. {qy -> -w}) - I3right;

Finally, linearize in $A$ [can take 1-2 minutes to complete...]:

Out[35]= $2 A_y \tan^{-1} \left( \frac{\Delta}{\sqrt{2 w^2 + \Delta^2}} \right) - \arctan \left( \frac{\Delta}{\sqrt{2 w^2 + \Delta^2}} \right) + \arctan \left( \frac{\Delta}{\sqrt{\Delta^2 + 2 w^2}} \right)$

We can now invoke the addition formula for the arctan:

$$\tan^{-1}(x) + \tan^{-1}(y) = \begin{cases} 
\tan^{-1} \left( \frac{x + y}{1 - xy} \right), & xy < 1 \\
\tan^{-1} \left( \frac{x + y}{1 - xy} \right) + \pi, & xy > 1 \land \{x, y\} > 0 \\
\tan^{-1} \left( \frac{x + y}{1 - xy} \right) - \pi, & xy > 1 \land \{x, y\} < 0 
\end{cases}$$

Apply this identity and display the final result:

Out[36]= $P_x (\text{paper}) = 2 A_y \tan^{-1} \left( \frac{\Delta}{\sqrt{2 w^2 + \Delta^2}} \right)$

... with the expression obtained here for $P_x$: 

Supplement.nb

Supplement.nb
... and it matches perfectly.

Adding the prefactors, we get the result for $P_x$ stated in Eq. (8) of the paper:

In[38]:= myFrame["$P_x (\text{here}) = \frac{2Ay}{\pi^2} \tan^{-1}\left(\frac{\Delta}{\sqrt{\Delta^2 + 2w^2}}\right)\]",
prefactorP*PxHere, LightOrange]

Out[38]= $P_x (\text{here}) = \frac{2Ay}{\pi^2} \tan^{-1}\left(\frac{\Delta}{\sqrt{\Delta^2 + 2w^2}}\right)$

A posteriori confirmation

Since the result does not depend on $A_x$, we can take a step back and work with $A_x = 0$ from the beginning. Going back to the result of integrating over $\lambda$, we do that and obtain

In[39]:= J1 = I1 /. (Ax -> 0)

Out[39]= \[
\frac{(Ay - qy) \Delta}{2 \left(qx^2 + (Ay - qy)^2\right) \sqrt{qx^2 + (Ay - qy)^2 + \Delta^2}}
\]

Integrate over $q_x$:

In[40]:= Integrate[J1 /. (Ax -> 0), {qx, -w, w}, Assumptions -> MyAss]
ComplexExpand[Normal[%, TargetFunctions -> {Re, Im}];
J2 = FS[%, {qy -> qy - Ay}, Assumptions -> MyAss]

Out[40]= \[
\frac{1}{4} \left(-i \pi + 2 \log\left[\frac{2i}{qy}\right] + 2 \log[qy] - 2 \log\left[\frac{4i\left(qy^2 - \sqrt{qy^2 + w^2 + \Delta^2}\right) + (qy^2 + w^2 + \Delta^2)}{qy - i w}\right]ight)
\]

Out[42]= \[
\frac{1}{4} \left(-i \pi + 4 \text{ArcCot}\left[\frac{w \Delta}{(Ay - qy) \sqrt{(Ay - qy)^2 + w^2 + \Delta^2}}\right] + 2 \text{ArcTan}\left[\theta, \frac{1}{Ay - qy}\right] + 2 \text{ArcTan}\left[-Ay + qy, \theta\right]\right)
\]
See that we have the same discontinuous behavior as above:

```plaintext
In[43]:= Plot[J2 /. {Ay -> 0.2, Ax -> 0.1, \[Delta] -> 0.5, w -> 1}, {qy, -2, 2}, Epilog -> {PointSize[Large], Point[{0.2, 0}]}]
```

Now integrate the two halves of the domain separately [each can take a few minutes to complete...]:

```plaintext
In[44]:= J3left = Integrate[J2, {qy, -w, Ay}, Assumptions -> MyAss && -w < qy < Ay];
In[45]:= J3right = Integrate[J2, {qy, Ay, w}, Assumptions -> MyAss && Ay < qy < w];
```

and combine them into the final result (up to now, valid for any finite Ay):

```plaintext
In[46]:= J4 = Expand[J3left + J3right];
```

Linearize in Ay:

```plaintext
In[47]:= Series[J4, {Ay, 0, 1}] // Normal;
```

```plaintext
Out[50]= 2 Ay ArcTan[\[Delta]/\[Sqrt][2 w^2 + \[Delta]^2]] + ArcTan[\[Delta]/\Sqrt[2 w^2 + \[Delta]^2]]
```

This is the combination of two ArcTan we encountered above. Proceeding in the same way,

```plaintext
In[51]:= J6 = J5 /. {HoldPattern[-ArcTan[x_] + ArcTan[y_]] -> ArcTan[-x + y]/(1 + x y)} // FS
```

```plaintext
Out[51]= 2 Ay ArcTan[\[Delta]/\Sqrt[2 w^2 + \[Delta]^2]]
```

which is the result we sought:

```plaintext
In[52]:= J6 = PxPaper
Out[52]= True
```

---

**BZ integration for Py**

Given the symmetry in the expressions of the Berry curvatures,
it is clear that the expression for \( P_y \) will be formally the same as that obtained for \( P_x \), with \( A_y \) replaced by \( A_x \) and an extra “–” sign. We thus obtain the result in Eq. (8) of the paper.

**Piezoelectric constant**

Using Eq. (12) of the paper, it now follows immediately that

\[
\text{In[55]:=} -\partial_{A_y} P_x \text{Here}
\]

\[
\text{Out[55]=} -2 \arctan \left( \frac{\Delta}{\sqrt{2w^2 + \Delta^2}} \right)
\]

or, with the prefactors,

\[
\text{In[56]:=} \text{myFrame}[^{\text{"e}_{222}} \text{ (here)} = ^{\text{"}, \text{ prefactorE222} \ast (-\partial_{A_y} P_x \text{Here}), LightOrange}]
\]

\[
\text{Out[56]=} \frac{\beta \varepsilon \tan^{-1} \left( \frac{\Delta}{\sqrt{2w^2}} \right)}{\pi^2 a}
\]

which is precisely the result in Eq. (12) of the paper (recall that \( \beta < 0 \), see text below Eq. (3) of the paper).