Spin-currents via the gauge-principle for meta-generalized-gradient exchange-correlation functionals

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The prominence of density functional theory (DFT) in the field of electronic structure computation stems from its ability to usefully balance accuracy and computational effort. At the base of this ability is a functional of the electron density: the exchange-correlation energy. This functional satisfies known exact conditions that guide the derivation of approximations. The strongly-constrainedappropriately-normed (SCAN) approximation stands out as a successful, modern, example. In this work, we demonstrate how the SU(2) gauge-invariance of the exchange-correlation functional in spin current density functional theory allows us to add an explicit dependence on spin currents in the SCAN functional (here called JSCAN) — and similar meta-generalized-gradient functional approximations — solely invoking first principles. In passing, a spin-current dependent generalization of the electron localization function (here called JELF) is also derived. The extended forms are implemented in a developer's version of the CRYSTAL23 program. Applications on molecules and materials confirm the practical relevance of the extensions.

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Introduction. Spin current carrying states have acquired a major role in condensed matter physics and electronic device engineering.¹ Recently, the interest in spin currents has grown further following the discovery of a host of materials which exhibit nontrivial topological properties^{2,3} and the development of new techniques to accurately control the spin of the electrons in spintronic and quantum computing devices.⁴

Commonly, spin currents originate from spin-orbit coupling (SOC). In many situations, SOC can be accounted for via the two-component Pauli equation, which offers formal and computational simplification as compared to the full Dirac equation. Just as an electric potential couples to the particle density and a magnetic field couples to the spin and to the particle (i.e. ordinary) current, SOC can be described as a tensor field which couples to the spin current (SC), i.e., the tensor product of spin and ordinary current. Unlike the ordinary current, the spin current is invariant under time reversal (being the product of two time-reversal odd quantities) and therefore can freely flow in the time-reversal invariant ground state of a non magnetic system.^{5,6}

It is sometimes adequate (for systems composed of light atoms) to include SOC as a small perturbation on top of the Kohn-Sham (KS) potential of ordinary density functional theory (DFT).⁷ This approach can in principle find the particle density and total energy of real *interacting* ground states by solving a single-particle problem in the presence of a self-consistent exchange-correlation (xc) potential, which is a functional of the density. Also, the eigenvalues of the KS single-particle equation provide a useful representation of the band structure and related properties.^{8–11}

However, there is no reason why a pure density func-

tional approximation that was developed for systems lacking spin currents would still yield accurate results when SOC is present. To accomplish this more ambitious task — yet within the two-component Pauli equation we need an exchange-correlation energy functional that depends not only on the density but also — and crucially — on the spin current density, and does so in a universal (i.e., system-independent) manner, as mandated by the original spin-current density functional theory (SCDFT)^{12,13} and its more recent developments.^{14–17} In practice, this means including in the effective potential, not only the "bare" SOC, but also its "dressing" due to many-body effects, in analogy to the dressing of the bare electron-nuclear potential by Hartree and exchangecorrelation (xc) effects.

Crucially, any xc energy functional that depends on the spin current density must be invariant — not only under U(1) gauge transformations^{18,19} — but also under SU(2) transformations^{12,13,20}. The latter can be viewed as local rotations of the spinorial state of the electrons^{21,22}. Failing to satisfy SU(2) invariance would have disastrous consequences for a density functional approximation: it would mean that the approximation does not distinguish between actual variations of the spin current density — which can have physical consequences — and variations arising from gauge transformations, which must have no consequence! Thus the gauge invariance of the exact xc-energy functional acts as a most important exact constraint, which guides the construction of approximate functionals.

While different approximate functionals obviously have different strengths and weaknesses, *they all must satisfy the constraint of gauge-invariance.* Hence, we focus on the strongly-constrained-appropriately-normed (SCAN) functional,²³ which is currently recognized as the least empirical general-purpose approximation in the class of Meta-Generalized-Gradient Approximations (MGGA).^{23–31} However, our procedure is applicable to any approximate functional in this class.

The exceptional performance of the SCAN is fundamentally due to its ability to satisfy altogether a large number of known exact conditions for the xc-energy functional of DFT. Furthermore, among its crucial ingredients, the KS kinetic-energy density appears in a combination of variables that was originally proposed for the so-called electron localization function (ELF) – a quantity that provides a vivid visualization of molecular bonds and atomic shells (more below).^{32,33}

But regular DFT cannot deal with spin-currents induced by extra interactions. This brings forth the necessity to switch to SCDFT both in principle^{12,13} and in practice.^{14–17,34–36} The dependence of the xc energy functional on spin currents in SCDFT is strongly constrained by the requirement that its form remains invariant under local SU(2) gauge transformations (defined below). Taking as a starting point the SCAN and the ELF forms, in this work we show how to make them functionals of the spin currents while preserving the fundamental SU(2) gauge invariance of the theory. The resulting generalizations are here called JELF and JSCAN. A set of computed results for molecules and materials demonstrates the practical usefulness of our non-empirical extension of the SCAN functional. An implementation is presented in a developer's version of the CRYSTAL23 program.³⁷

SCDFT in a nutshell. We shall consider ground states at geometries that do not magnetize nor host particle currents spontaneously. Furthermore, magnetic couplings (Zeeman field, Abelian vector potential) that break timereversal symmetry are not included. Accounting for non-Abelian vector potentials, however, we must consider together with the particle density, n, the spin currents, $\mathbf{J}^{.6,13,21,38,39}$ The energy density functional of interest, thus, reads as follows:

$$E_{v,\vec{\mathbf{A}}}[n,\vec{\mathbf{J}}] = T_s[n,\vec{\mathbf{J}}] + E_{\mathrm{H}}[n] + E_{\mathrm{xc}}[n,\vec{\mathbf{J}}] + \frac{1}{c} \int d^3r \ \mathbf{J}^a \cdot \mathbf{A}^a + \int d^3r \ n\left(v + \frac{1}{2c^2}\mathbf{A}^a \cdot \mathbf{A}^a\right) \tag{1}$$

where T_s is the kinetic energy of the KS system, while $E_{\rm H}$ and $E_{\rm xc}$ are Hartree and xc energies. Here and in the following, we denote with bold characters, \boldsymbol{v} , quantities with spatial indices (Greek lower indices, v_{μ} , when written explicitly); and use an arrow, \vec{v} , to denote quantities with spin indices (upper Latin indices, v^a , when written explicitly) — μ and a have values x.y.z. Therefore \vec{J} and

 $\mathbf{\tilde{A}}$ have both spatial and spin indices. Contractions over spatial indices are denoted with "." and Einstein convention is used for summing over repeated indices. Unless otherwise stated, we use Hartree atomic units in which $\hbar = m = 1$. The corresponding KS equations are:

$$\left\{\frac{1}{2}\left[-i\nabla + \frac{1}{c}\boldsymbol{\mathcal{A}}_{\mathrm{KS}}\right]^{2} + \left[\left(v + v_{\mathrm{Hxc}}\right) + \frac{1}{2c^{2}}\left(\boldsymbol{\mathcal{A}}^{2} - \boldsymbol{\mathcal{A}}_{\mathrm{KS}}^{2}\right)\right]\right\}\Phi_{\kappa} = \varepsilon_{\kappa}\Phi_{\kappa}$$
(2)

where $\mathcal{A}_{\text{KS}} = \mathcal{A} + \mathcal{A}_{\text{xc}} = \sigma^a \mathbf{A}^a + \sigma^a \mathbf{A}_{\text{xc}}^a$, with $\vec{\sigma}$ being the vector of Pauli matrices, $v_{\text{Hxc}} = \delta E_{\text{Hxc}} / \delta n$ is a Hartreexc-scalar potential (analogous to the Hxc-scalar potential of DFT) and $\frac{1}{c} \vec{\mathbf{A}}_{\text{xc}} = \delta E_{\text{xc}} / \delta \vec{\mathbf{J}}$ is a non-Abelian xc-vector potential (which is specific to SCDFT). The occupied (lowest in energy) two-component KS spinors Φ_k allow us to compute the particle density, $n = \sum_{k=1}^{N} \Phi_k^{\dagger} \Phi_k$, and the spin current $\vec{\mathbf{J}} = \frac{1}{2i} \sum_{k=1}^{N} \Phi_k^{\dagger} \vec{\sigma} \left[\nabla \Phi_k \right] - \left[\nabla \Phi_k^{\dagger} \right] \vec{\sigma} \Phi_k$ of the real state and, thus, the energy as well. All this is exact in principle, while, in practice, we are bound to approximate E_{xc} .

Invoking a MGGA, it is convenient to switch to the

so-called generalized-KS (GKS) approach to SCDFT.¹⁷ This means that for generating the single-particle equations, we differentiate the energy functional expression explicitly w.r.t. the orbitals rather than w.r.t. to the densities⁴⁰ — nowadays, this has become a standard procedure in DFT.⁴¹

A central property of the xc-energy functional in SCDFT is its form invariance under local SU(2) transformations, i.e., transformations that act on the KS spinors as follows: $\Phi(\mathbf{r}) \rightarrow U_S(\mathbf{r})\hat{\Psi}(\mathbf{r})$, where $U_S(\mathbf{r}) =$ $\exp\left[\frac{i}{c}\sigma^a\lambda^a(\mathbf{r})\right]$, i.e., subjecting them to different rotations at different points in space. This invariance is expressed by the equation

$$E_{\rm xc}[n', \vec{\mathbf{J}}'] = E_{\rm xc}[n, \vec{\mathbf{J}}]$$
(3)

where $n \to n' = n$, $\mathbf{J}^a \to \mathbf{J'}^a = R^{ab} [\mathbf{J}^b + \frac{n}{c} \mathbf{G}^b]$, R^{ab} is a 3 × 3 matrix describing a rotation in \mathbb{R}^3 around the direction $\hat{\lambda}$ by an angle $\varphi = -2\lambda/c$, and $\mathbf{\vec{G}} = -\frac{ic}{2} \text{Tr} (\vec{\sigma} U_{\rm S}^{\dagger} \nabla U_{\rm S})^{.42}$

It is important to notice that $\vec{\mathbf{J}}$ is not a gauge invariant quantity since it can appear as a consequence of a generic SU(2) transformation acting on a state in which $\vec{\mathbf{J}} = 0$. The invariance of $E_{\rm xc}$ stated in Eq. (3), implies that only certain gauge-invariant combinations of $\vec{\mathbf{J}}$ with other KS quantities can legitimately appear in E_{xc} . We now tackle the task of generalizing the SCAN functional (and the closely related ELF) to include a dependence on spin currents that complies with Eq. (3).

Extension of SCAN and ELF to spin-current carrying states. Recent works have moved valuable steps in developing extended DFT approaches to non-collinear magnetism and SOC.^{17,20,43,44} But Ref. 20 does not carry out applications, Ref. 43 does not work with full SU(2)invariant xc-functionals, Ref. 44 does not include an xcvector potential in the solution, and Ref. 17 does not include spin-current explicitly beyond exchange.

Here, we focus on MGGAs. The SCAN functional, for example, sets²³ $E_{\rm xc} = \int d^3 r \ n(\mathbf{r}) \epsilon_{\rm xc}^{\rm SCAN}(\mathbf{r})$ where $\epsilon_{\rm xc}^{\rm SCAN} = \epsilon_{\rm xc}^1 + (\epsilon_{\rm xc}^0 - \epsilon_{\rm xc}^1) f_{\rm xc}(\alpha)$ interpolates between the semi-local energy densities for single-orbital densities ($\epsilon_{\rm xc}^0$) and for slowly-varying densities ($\epsilon_{\rm xc}^1$), which only depend on n (a gauge-invariant quantity). The interpolation function $f_{\rm xc}$ is controlled by the variable $\alpha = (\tau - \tau_{\rm W})/\tau_{\rm unif}$. The latter quantity entails three kinetic energy densities: the positive-definite conventional $\tau = 1/2 \sum_{i}^{\rm occ.} |\nabla \phi_i|^2$ defined in terms of the occupied (one-component) KS orbitals $\{\phi_i\}$, the von Weizsäcker $\tau_W = |\nabla n|^2/(8n)$ — that is the *bosonic* expression of τ — where $n = \sum_{i}^{\rm occ.} |\phi_i|^2$, and the kinetic energy of the noninteracting Fermi gas at uniform density n: $\tau_{\rm unif} = \frac{3}{10} (3\pi^2)^{2/3} n^{5/3}$.

The success of the SCAN is explained not only by the fact that it satisfies a large set of known exact conditions but also by the fact that it uses, specifically, α as a key variable. The α tends to zero in the iso-orbital limit (i.e., when the density is dominated by a single occupied orbital), tends to one in the uniform-density limit, and tends to infinity in regions dominated by density overlap between closed shells. In fact, α is a useful building block of density functional approximations,^{24,25,45} and it is the main ingredient of the electron localization function,^{33,46,47} ELF = $1/(1+\alpha^2)$ – a simple but effective descriptor of molecular bonds and atomic shells.

More in general, the kinetic energy density must be expressed in terms of the occupied two-component KS spinors $\tau = 1/2 \sum_{k}^{\text{occ.}} \nabla \Phi_k^{\dagger} \cdot \nabla \Phi_k$. Crucially, let us next consider the transformation of the kinetic energy under a local SU(2) transformation, $U_{\rm S}$, of the spinors. For 3

the states considered in this work, one readily finds:²⁰ $\tau \to \tau' = \tau + \frac{1}{c} \mathbf{J}^a \cdot \mathbf{G}^a + \frac{n}{2c^2} \mathbf{G}^a \cdot \mathbf{G}^a$; for the definition of \mathbf{G} see below Eq. (3). As a consequence of which, it is apparent that α will change, too. Hence, neither the SCAN functional nor the ELF are SU(2)-form invariant. Such an invariance, however, is not only an exact mathematical property of the xc-energy functional in SCDFT but — because a local SU(2) transformation may be regarded as part of an overall gauge transformation (i.e., a change in the description which cannot change the physics) — it is also a proper feature for any quantity that should carry direct chemical-physical information. Fortunately, in one stroke, the substitution $\tau \to \tilde{\tau} = \tau - \frac{\mathbf{J}^a \cdot \mathbf{J}^a}{2n}$, solves both issues: i.e., it introduces an explicit dependence on the spin currents and enforces the sought form invariance. In detail.

$$\alpha \to \widetilde{\alpha} = \alpha - \frac{\mathbf{J}^a \cdot \mathbf{J}^a}{2n\tau_{\text{unif}}} \tag{4}$$

implies

$$\epsilon_{\rm xc}^{\rm JSCAN} := \epsilon_{\rm xc}^1 + \left(\epsilon_{\rm xc}^0 - \epsilon_{\rm xc}^1\right) f_{\rm xc}(\widetilde{\alpha}),\tag{5}$$

and

$$\text{JELF} := \frac{1}{1 + \tilde{\alpha}^2} . \tag{6}$$

Note that, under the restriction to time-reversal symmetric states, the rest of the SCAN only depends on the particle density (a fully invariant quantity) and, thus, shall not be modified here. Also note that $\tilde{\alpha} \geq 0$, as for the original quantity. Importantly, the above substitution should *not* be confused with the analogous well-known substitution that involves the (paramagnetic) particle current:¹⁹ $\tau \rightarrow \tilde{\tau} = \tau - \frac{j \cdot j}{2n}$. The latter derives from the consideration of local U(1) transformations. The importance of the dependence of xc functionals on the particle current has been already largely demonstrated.^{19,48–58}

For the states considered in this work as for any gaugeinvariant MGGA within GKS, we stress that \vec{A}_{xc}^{JSCAN} does not transform covariantly and does not exert a torque on the spin current. In fact, from Eq. (5), taking a functional derivative with respect to \vec{J} , we obtain

$$\frac{1}{c}\vec{\mathbf{A}}_{\mathrm{xc}}^{\mathrm{JSCAN}} = -\vec{\mathbf{J}}\left[\frac{\left(\epsilon_{\mathrm{xc}}^{0} - \epsilon_{\mathrm{xc}}^{1}\right)f_{\mathrm{xc}}'(\widetilde{\alpha})}{n\tau_{\mathrm{unif}}}\right],\qquad(7)$$

where f'_{xc} denotes the derivative of f_{xc} wrt its own argument. This is a non-Abelian effective connection; i.e., an xc-spin-vector potential. This expression shows that $\vec{\mathbf{A}}_{xc}^{\text{JSCAN}}$ is parallel to $\vec{\mathbf{J}}$ at each point in space and, therefore,

$$\frac{1}{c}\vec{A}_{\mathrm{xc},\mu}^{\mathrm{_{JSCAN}}} \times \vec{J}_{\mu} = 0.$$
(8)

Yet, the role of $\vec{\mathbf{A}}_{xc}^{\text{JSCAN}}$ is far from negligible (more below). The GKS equations for the JSCAN are reported in the supporting information 59 in a form which is handy for numerical implementations.

In summary, Eqs. (4)-(8) are the key equations of this

work — Eqs. (4), (7) and (8) apply to any MGGA which uses τ through α (for example the TASK functional).⁶⁰



FIG. 1: (a) Effect of SOC on the ELF and JELF (isosurface at 0.005) in the I₂ molecule. Δ SOC (J)ELF is the difference between calculations with and without SOC on the (J)ELF. The rightmost panel reports the difference JELF-ELF (isosurface at 0.002). Positive (negative) isosurfaces are in yellow (blue), while the atoms are represented as purple balls. (b) (top) Valence bands of single-layer MoSe₂ and (bottom) bulk α -MoTe₂ Rashba materials without SOC (black) and with SOC, employing the r²SCAN and J-r²SCAN xc models (dashed and continuous blue lines, respectively).

Applications. We have implemented a self-consistent treatment of the JSCAN functional, including effective non-Abelian vector potentials, as well as the JELF in a developer's version of the CRYSTAL23 code.³⁷ Computational and implementation details are provided in the supporting information⁵⁹ (see also Refs. 61–77 therein). In the calculations, we employ the restored-regularized r^2 -SCAN, rather than the original SCAN functional, to improve numerical stability and performance.⁷⁸

We apply our SU(2) gauge-invariant J-r²SCAN approach to molecules on reproducing the SOC-induced modification of the valence electronic structure in halogen diatoms and hydrides, which have served as model systems in previous studies.^{81–83} Values of the SOC-induced modification to the HOMO-LUMO gap are reported in Table I, first at the exchange-only level of theory, and then including effects of exchange and correlation. Values are presented with exchange-only (gauge-invariant) J-r²SCAN functional, and numbers in parentheses represent corresponding results with the standard (gauge-dependent) r²SCAN approach.

TABLE I: We report the effect of SOC on the HOMO-LUMO gap at the level of Exchange-only and Exchange-Correlation using J(SCAN) and the SOC effect on the optical gap at the RPAx level.^{79,80} The results show that these effects are comparable, and the agreement is improved when spin currents are included in the MGGA. All values are reported in eV.

| | Exx-Only | | | Exx & Corr | | |
|---------------|-------------------------------|---------|-------|-----------------------|-------|--|
| | \mathbf{J} - \mathbf{r}^2 | SCAN | HF | J-r ² SCAN | RPAx | |
| \mathbf{FI} | 0.248 | (0.225) | 0.322 | 0.232(0.222) | 0.360 | |
| $_{\rm HI}$ | 0.337 | (0.276) | 0.343 | 0.324(0.281) | 0.343 | |
| I_2 | 0.333 | (0.276) | 0.364 | 0.317(0.278) | 0.396 | |
| HAt | 0.927 | (0.675) | 0.891 | 0.884(0.213) | 0.887 | |
| | | | | | | |

Inclusion of the spin currents in the functional greatly improves the agreement with Hartree-Fock (HF) results. In the case of the HI molecule, for example, the HOMO-LUMO gap is increased from 0.276 eV to 0.337 eV; which reduces the relative error from 20% to 2%. In the case of HAt, the effect of SOC on the HOMO-LUMO gap is increased from 0.675 eV to 0.927 eV; relative error decreased from 24% to 4%.

At the xc level of theory, values are benchmarked against the random phase approximation including the dynamical response of Fock exchange (RPAx).⁸⁴ In detail, this comparison assumes that the effect of SOC on the fundamental gap is to a good approximation the same as the effect of SOC on the optical gap. In all cases, inclusion of currents in the xc model improves agreement against the RPAx. The most extreme case is HAt where the effect of SOC on the gap is increased from 0.213 eV to 0.884 eV by inclusion of spin-currents in the MGGA, essentially coinciding with the RPAx value of 0.887 eV.

Next, we discuss electron localization through the JELF [see Eq. (6)]. We recall that large values of $\tilde{\alpha}$, corresponding to a (J)ELF close to one, indicate that electrons are highly localized. Here we look at the effect of SOC on the (J)ELF. For the I₂ molecule, after a self-consistent solution with J-r²SCAN, including both exchange and correlation effects, in Fig. 1(a) we plot the ELF and JELF indicators as differences w.r.t. the calculation without SOC.

Yellow contours indicate that SOC localizes the electron. Blue contours indicate that the electron is delocalized by SOC. The leftmost panel, containing the Δ SOC JELF shows that electrons are localized along the bond axis by SOC. On the other hand, we observe two blue "onion rings" around the atomic centers. Thus, SOC localizes electrons along the bond and delocalizes them in the orthogonal directions. Although this analysis is consistent with previous reports,^{85,86} the degree of delocalization is largely overestimated by the gauge-dependent ELF, compared to the SU(2) form-invariant JELF, see their difference in the rightmost panel of Fig. 1(a). The JELF displays more localization on the bonding compared to the (gauge-dependent) ELF.

We proceed to apply our approach to the description of the electronic band structure of infinite periodic systems. In Table II, we provide values of the splitting of the valence band at the **K** high-symmetry point in molybdenum dichalcogenide Rashba systems: the inversion asymmetric hexagonal single layer MoSe₂ and the inversionsymmetric hexagonal bulk α -MoTe₂. The valence band structure is provided in panel (b) of Figure 1.

For both systems, about one third of the total effect of SOC on the splitting is accounted for through many-body effects by inclusion of spin currents in the functional. Low-temperature experimental values on the transport gap are available from Refs. 87-90, while band splittings are provided in Refs. 91-96. The values of valence band splittings are considerably enhanced by including spin-current in the xc form (from 0.14 eV to 0.20 eV in MoSe₂, and from 0.28 eV to 0.32 eV in MoTe₂), leading to an improved agreement with experiment (relative

error decreased from 29% to 10% in MoSe₂ and leading to an exact coincidence with the mean experimental value in MoTe₂). Overall, the accuracy of the J-r²SCAN approach is comparable to more involved hybrid-GGA SCDFT treatments (which provide splittings of 0.17 and 0.32 eV, respectively for MoSe₂ and MoTe₂ using optimal fractions of Fock exchange) — without requiring the determination of an optimal fraction of Fock exchange:¹⁷ a step that involves either empiricism or extra/external ab initio calculations.⁹⁷

TABLE II: Splitting of the valence band at \mathbf{K} and band gap of molybdenum dichalcogenide Rashba systems.

| | 2D [| $MoSe_2$ | $3D \alpha$ -MoTe ₂ | |
|-------------|-------|-----------|--------------------------------|------|
| | split | gap | split | gap |
| r^2SCAN | 0.14 | 1.57 | 0.28 | 0.82 |
| $J-r^2SCAN$ | 0.20 | 1.53 | 0.32 | 0.81 |
| Exp. | 0.18 | 1.6 - 2.3 | 0.3-0.34 | 1.03 |

Finally, we report on the application of our SU(2) form-invariant approach to topological materials. We consider the case of Weyl semi-metals. We report on the splitting of Weyl nodes in the orthorhombic TaAs phase (W1 node pair, along the $k_z = 0$ mirror plane). The pair of nodes is located at $k_y = 0.5066$ (in units of π/\mathbf{b}), in excellent agreement with the experimental value of $k_y = 0.5173.^{98,99}$ Spin-current dependent terms in the xc functional account for 21% of the total splitting along k_x . See Fig. S1 of the supplementary material.

Conclusions. Focusing on the prominent example of the SCAN functional and the ELF, we have shown how to include a dependence on spin currents in meta-GGA functional forms while fulfilling SU(2) gauge invariance for time-reversal symmetric systems. For the states considered in this work, the current-dependent form of the approximation is furthermore strongly suggested by previous studies on the structure of the exact exchange hole (see Ref. 20), which incidentally, also motivate the inclusion of the kinetic energy density as a variable on which the functional must depend. A large body of works have highlighted the usefulness of the kinetic energy in combination with other quantities as in the ELF (and, thus, as in the iso-orbital indicator α of SCAN) as a practical means for capturing relevant local features of the manyelectron state in correlated regimes beyond exchangeonly effects.

Of course, the question of including the "right physics" beyond the minimalistic yet *necessary* approach presented here remains open. Looking ahead, it will help disentangle the role of the SU(2) invariance in density functional approximations from questions more directly related to the physics of the electron-electron interaction. It is particularly appealing to explore the consequence of a full (compound) U(1)×SU(2) gauge-invariance on general states that may *also* break time-reversal symmetry.

This may help solve standing difficulties of present DFT methodologies for magnetized systems. $^{30,100-107}$

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