

Identifying optimal magnetic field configurations for decoherence mitigation of boron vacancies in hexagonal boron nitride

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The negatively charged boron vacancy center in two-dimensional (2D) hexagonal boron nitride has emerged as a promising quantum sensor. However, its sensitivity is constrained due to ubiquitous nuclear spins in the environment. The nuclear spins, hyperfine coupled with the central electron spin, effectively behave as magnetic field fluctuators, leading to rapid decoherence. Here, we explore the effectiveness of static magnetic field strength and orientation in realizing peculiar subspaces that can lead to enhanced spin coherence. Specifically, using detailed numerical simulations of the spin Hamiltonian, we identify specific field configurations that minimize energy gradients and, consequently, are expected to facilitate decoherence suppression. We also develop an approximate analytical model based on the perturbation theory that accurately predicts these low-gradient subspaces for magnetic fields aligned with the electron spin quantization axis, applicable not only to boron vacancies but to any spin-1 electronic system coupled to nearby nuclear spins. Furthermore, to stimulate experimental validation, we estimate coherence lifetimes as a function of various bias field configurations and demonstrate that significant decoherence suppression can indeed be achieved in certain regions. These findings and the developed methodology offer valuable insights for mitigating decoherence in a low-field regime.

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I. INTRODUCTION

Optically active spin defects are gaining significant attention due to their potential in various quantum applications [1–3], including quantum sensing [3–8], quantum computing [9–13], and quantum communication [14,15]. A key feature of these defects is their extraordinary sensitivity to external perturbations such as magnetic fields [4–8,16], electric fields [17,18], strain [17,19], and temperature [20,21]. This sensitivity, coupled with the ability to perform optical readout [20,22] of spin states at room temperature, enables the development of ultrasensitive nanoscale sensors. Among the most extensively studied systems is the nitrogen-vacancy center [23–26] in diamond and spin defects in silicon carbide (SiC) [27,28], which have paved the way for practical implementations in quantum sensing and metrology. Despite their success, spin defects in three-dimensional (3D) materials such as diamond and SiC face challenges that limit their applicability. Specifically, their confinement within the bulk

structure prevents spin probes from approaching the target sample with subnanometer resolution. In contrast, spin defects in two-dimensional (2D) materials offer a promising solution. Their atomic-scale thickness allows closer proximity to the sample [29,30], enhancing spatial resolution. Moreover, 2D defects can be seamlessly integrated with photonic nanostructures [30–34] enabling the development of compact, on-chip quantum technologies [35,36]. Among the spin defects in 2D materials [3], the negatively charged boron vacancy (V_B^-) in hexagonal boron nitride (hBN) [20,37–39] has recently emerged as a leading contender. hBN, a Van der Waals material, provides a robust and tunable platform for hosting spin defects. The V_B^- defect has demonstrated remarkable potential due to its optical and spin properties [20,22], making it a promising candidate for high-resolution quantum sensing [19,40–42]. Both theoretical and experimental [43–45] studies have highlighted the potential of V_B^- in applications ranging from nanoscale magnetometry to temperature sensing. A key goal within quantum sensing research is to enhance sensitivities through increasing the coherence time (T_2) of the probe system. In solid-state systems the primary source of decoherence is magnetic field fluctuations in the spin bath surrounding the defect. On the materials engineering side, isotopic purification has been a successful strategy in systems like diamond [46] and SiC [47], however, hBN naturally lacks this avenue for isotopic refinement because of its chemical composition [48]. Therefore, alternative strategies to suppress decoherence are crucial to realize the full potential of V_B^- defects in hBN.

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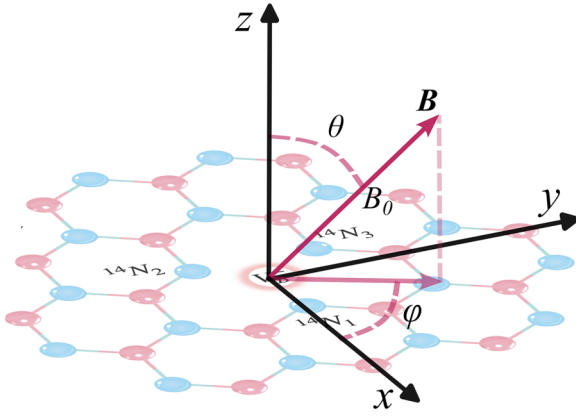


FIG. 1. Structure of the V_B^- defect in hBN, showing the three nearest-neighbor ^{14}N nuclear spins. θ and φ represent the polar and azimuthal angles associated with the applied magnetic field $\mathbf{B}$ of magnitude B_0 . Pink and blue spheres denote boron and nitrogen atoms, respectively, while the red circle marks the boron vacancy site. The coordinate axes and magnetic field orientation are indicated for reference.

Besides conventional dynamical decoupling methods [49,50], a promising approach to address decoherence is identifying subspaces of the system's Hilbert space that are minimally affected by spin fluctuations [51–57] in the bath. This requires a detailed understanding of how external parameters, such as magnetic field, influence the defect's energy level structure and spin-transition properties. Recent experimental and simulation studies [58–60] show that spin coherence in hBN defects is strongly governed by interactions with nearby nuclear spins and the applied magnetic field strength. Our work builds on and extends these recent advances by combining detailed numerical simulations of the spin Hamiltonian with an analytical perturbation theory model. Specifically, we investigate the influence of the strength and the orientation of the static magnetic field on the transition energies of V_B^- defects in hBN. We analyze energy gradient and curvature at low-bias magnetic fields (< 25 mT), identifying regions where decoherence effects can be minimized. We show that these regions with minimal sensitivity to the magnetic fluctuation correspond to highly improved coherence and are critical for a variety of quantum sensing applications.

II. SYSTEM HAMILTONIAN

A missing boron atom in 2D-hBN creates a boron vacancy (V_B) defect. In its negatively charged state, this defect hosts a spin-1 electronic system, surrounded by a spin-full nuclear bath, shown in schematic Fig. 1. The three first shell ^{14}N nuclear spins (spin-1) are strongly coupled with the central V_B^- electron spin (spin-1) via hyperfine interaction. The Hamiltonian of this composite system in the presence of an external magnetic field ($\mathbf{B}$) can be written as

$$H = D \left(S_z^2 - \frac{2}{3} \right) + \epsilon (S_y^2 - S_x^2) + \gamma_e \mathbf{B} \cdot \mathbf{S} + \sum_{i=1}^3 \mathbf{S} \cdot \mathbf{A}^i \cdot \mathbf{I}^i + \sum_{i=1}^3 \gamma_n^i \mathbf{B} \cdot \mathbf{I}^i + \sum_{i=1}^3 \mathbf{I}^i \cdot \mathbf{Q}^i \cdot \mathbf{I}^i. \quad (1)$$

TABLE I. The table outlines all the hyperfine and quadrupolar (in megahertz) tensor elements used in the numerical calculations.

	A_{xx}	A_{yy}	A_{zz}	A_{xy}	Q_{xx}	Q_{yy}	Q_{zz}	Q_{xy}
$^{14}\text{N}_1$	46.944	90.025	48.158	0	-0.46	0.98	-0.52	0
$^{14}\text{N}_2$	79.406	58.170	48.159	-18.391	0.62	-0.1	-0.52	-0.623
$^{14}\text{N}_3$	79.406	58.170	48.159	18.391	0.62	-0.1	-0.52	0.623

Here, $\mathbf{S}$ and $\mathbf{I}$ are electron and nuclear spin operators, respectively. $D = 3.45$ GHz is the zero-field splitting (ZFS) term, ϵ is the strain term, which has been set to zero for this analysis, γ_e and γ_n are the electron and nuclear gyromagnetic ratio, $\mathbf{A}$ is the hyperfine interaction tensor, and $\mathbf{Q}$ is the quadrupole interaction tensor. The z axis is the electron spin quantization axis, perpendicular to the hBN plane. Below, we outline the methodology and key steps involved in the numerical simulation of the composite (V_B^- , ^{14}N) defect system. The hyperfine interaction tensor $\mathbf{A}$ for the first shell ^{14}N nuclear spins as outlined in Table I, is obtained from the parameters reported by Gao *et al.* [61]. As the first shell ^{14}N nuclear spins are arranged symmetrically around the central V_B^- defect, the hyperfine interaction tensors of the other two nuclei can be obtained by rotating the hyperfine tensor of reference nuclei ($^{14}\text{N}_1$) about the symmetry axis (z axis). The quadrupole interaction tensor $\mathbf{Q}$ for the $^{14}\text{N}_1$ nuclear spin as given in Table I, is based on the value reported by Gracheva *et al.* [62]. Using a similar rotational transformation as that used for hyperfine parameters, we derive the quadrupole tensors for the remaining two ^{14}N nuclei. We utilize the quantum toolbox in python (qutip) [63] to construct spin operators for both electronic ($\mathbf{S}$) and nuclear ($\mathbf{I}$) subsystems. The ability to handle high-dimensional Hilbert spaces and define tensor products of spin operators made qutip a natural choice for these calculations. qutip's built-in functions were employed to create the Hamiltonian matrix and compute the eigenenergies and eigenstates of the full spin system [64]. Subsequently, we calculate the gradient and curvature associated with the transition energies (see Appendix A for the in-depth procedure), which quantify the first- and second-order effects of magnetic fluctuations in the surrounding bath.

III. RESULTS AND DISCUSSION

Solid-state spin-based sensing protocols typically involve applying a bias magnetic field parallel to the electron spin quantization axis. Here, we perform a comprehensive analysis of the electronic energy level structure of the composite (V_B^- , ^{14}N) defect as a function of varied bias field amplitude and direction given by

$$\mathbf{B} = B_0 \hat{\mathbf{r}}, \quad \hat{\mathbf{r}} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta). \quad (2)$$

Here, θ and φ are polar and azimuthal angles, respectively, while B_0 is the field strength, as shown in Fig. 1. Firstly, Fig. 2(a) depicts the energy levels of the system as a function of static field strength that is applied along the z axis. Here, the primary splitting observed between the $m_s = 0$ and $m_s = \pm 1$ states is due to the zero-field interaction term. A smaller splitting between the $m_s = +1$ and $m_s = -1$ sublevels

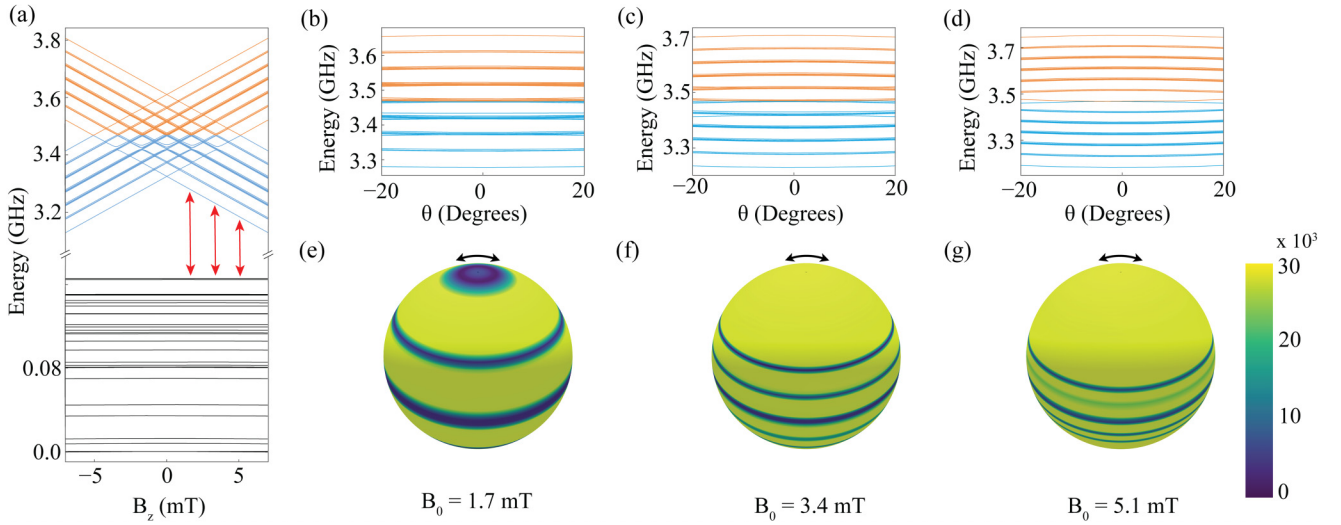


FIG. 2. (a) Energy levels of the system as a function of the magnetic field applied parallel to the quantization axis of the electron spin. The black lines correspond to $m_s = 0$, and orange and blue are for $m_s = \pm 1$ electronic sublevel. These sublevels split into 27 ($3 \times 3 \times 3$) hyperfine levels. The red arrows indicate the chosen magnetic field values. (b)–(d) Energy levels as a function of the polar angle of the applied magnetic field with respect to the quantization axis for 1.7, 3.4, and 5.1 mT magnetic fields, respectively. (e)–(g) The magnitude of energy gradient (in MHz/T), as defined in (A1), corresponding to the spin transition exhibiting the maximum transition probability at the aforementioned fields. The black arrows represent the θ range depicted in (b)–(d). The spherical shell radius, in principle, represents the bias magnetic field magnitude B_0 (in mT); however, for visualization purposes, all spheres are shown with the same size, and the radii do not scale with the field strength. The colorbar indicates the magnitude of the energy gradient.

arises from the hyperfine interaction between the electron spin and the three first shell ^{14}N nuclear spins. If the magnetic field is applied along the spin quantization axis, these nuclear spins can be considered equivalent, effectively giving rise to a spin-3 system. As a result, the energy sublevels can be grouped into seven distinct hyperfine levels, as seen in Fig. 2(a). Additionally, the $m_s = +1$ and $m_s = -1$ levels demonstrate avoided crossings at relatively low fields due to the intricate interplay between Zeeman and hyperfine terms in the system's Hamiltonian; the detailed discussion of this phenomenon is provided in the later part of this section. Secondly, we investigate the energy level variations as a function of the magnetic field orientation (θ) at three distinct anticrossing points. Figures 2(b)–2(d) display the dependence of the electronic energy levels on the polar angle for field strengths of 1.7, 3.4, and 5.1 mT, respectively. In this field regime, the energy levels show minimal dependence on the magnetic field orientation, indicating that they are largely unaffected by local fluctuations. To explore the behavior in detail, we vary both the polar angle (θ) and the azimuthal angles (φ) while keeping the magnitude of the bias field (B_0) constant. The magnitude of gradient of transition energy, f' , defined in (A1), at each (θ, φ) is mapped to a color scale to visualize the magnetic sensitivity of the transition energy across the sphere. Figures 2(e)–2(g) illustrate the gradient of the transition energy for the most probable transitions with a transition probability of more than 30% (see Appendix B for details pertaining to the calculations of transition probabilities). Our analysis reveals that the gradient at low field strengths is minimal near the poles. As the field strength increases, the gradient gradually shifts towards the equator, forming distinctive rings highly dependent on the bias field. This suggests that beyond this regime of a very low static field (≤ 5.1 mT), the low gra-

dient subspaces can be accessed via the application of the field in a transversal direction. In Fig. 3(a) we present the ground state energy levels for transverse applied magnetic fields. In this configuration, the primary splitting between $m_s = 0$ and $m_s = \pm 1$ states remains dominated by crystal field interactions (D). However, applying the transverse field leads to a significant mixing of the $m_s = +1$ and $m_s = -1$ spin states, significantly modifying the energy level landscape. We conduct a magnetic field orientation-dependent analysis following the aforementioned approach. In this case, we investigate the energy levels at three distinct magnetic field strengths, namely, 7.5, 15, and 23.5 mT, as shown in Figs. 3(b), 3(c), and 3(d), respectively. In this orientation, the $m_s = +1$ and $m_s = -1$ levels undergo anticrossing, leading to the low f' , effectively making the spin states less susceptible to fluctuations in the applied field. Figures 3(e)–3(g) depict the energy gradient of a spin transition having the highest transition probability within this field regime. As anticipated, the lowest gradient values occur near the transverse plane at higher fields. This finding suggests that applying a transverse magnetic field becomes increasingly effective in shielding the spin states from magnetic fluctuations as the field strength is increased, providing enhanced stability and protection for the spin system. Figure 4(a) shows the overall gradient of all possible transitions as a function of the applied magnetic field strength oriented parallel to the crystal field axis. At low parallel magnetic fields, the system exhibits notably low gradients at specific field strengths. The sharp dips in the gradient are essentially due to the competing interactions in the Hamiltonian, namely, Zeeman and electron nuclear. To obtain an intuitive description of these features, we develop an approximate analytical approach based on the perturbation theory. Under a parallel bias magnetic field,

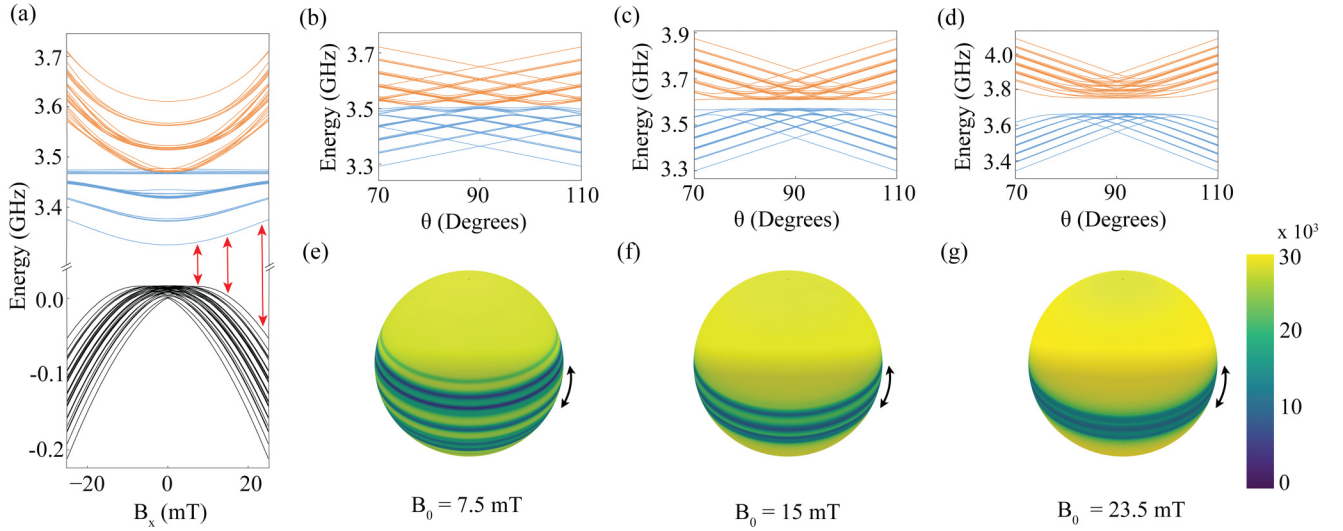


FIG. 3. (a) Energy levels as a function of the transverse magnetic field. The black lines correspond to $m_s = 0$, and orange and blue are for $m_s = \pm 1$ electronic sublevel. The red arrows indicate the chosen magnetic field values. Energy levels as a function of the polar angle of the applied magnetic field with respect to the quantization axis for 7.5, 15, and 23.5 mT magnetic field, respectively. (e)–(g) The magnitude of energy gradient (in MHz/T), as defined in (A1), corresponding to the maximum transition probability at the aforementioned fields. The black arrows represent the θ range depicted in (b)–(d). The spherical shell radius, in principle, represents the bias magnetic field magnitude B_0 (in mT); however, for visualization purposes, all spheres are shown with the same size, meaning the radii do not scale with the field strength. The colorbar indicates the magnitude of the energy gradient.

the three first-shell ^{14}N nuclear spins interact identically to the V_B^- spin. Consequently, the system can be effectively described as an interacting spin-1, spin-3 system. The terms that commute with S_z^2 are treated as the unperturbed Hamiltonian (H^0), while the remaining noncommuting terms are taken as

the perturbation Hamiltonian (H^1):

$$H^0 = DS_z^2 + \gamma_e(B_z + b_z)S_z + A_{zz}S_zI_z, \\ H^1 = \gamma_e(b_xS_x + b_yS_y). \quad (3)$$

Here, b_x, b_y are small fluctuations in the magnetic field components along the x and y directions. Applying second-order perturbation theory to this Hamiltonian, we obtain the approximate transition energies satisfying the conditions $\Delta m_s = \pm 1$, $\Delta m_l = 0$, given by (in-depth calculations are provided in the Appendix C)

$$f = D + m_s \sqrt{[\gamma_e(B_z + b_z) + m_l A_{zz}]^2 + [\gamma_e \sqrt{(b_x^2 + b_y^2)}]^2}. \quad (4)$$

The amplitude of the gradient of these transition energies can be obtained using Eq. (A1). Under small magnetic fluctuation condition, one can obtain the minimal gradient at parallel bias fields,

$$B_z = -\frac{m_l A_{zz}}{\gamma_e}. \quad (5)$$

For the systems comprising multiple nuclear spin shells, Eq. (5) will get extended to $B_z = -\sum_i \frac{m_{li} A_{zzi}}{\gamma_e}$, where i represents the nuclear spin shell index. If the defect is experiencing out-of-plane interactions due to the presence of multiple hBN layers, the hyperfine coupling A_{zz} needs to be replaced with $\sqrt{A_{zx}^2 + A_{zy}^2 + A_{zz}^2}$. The matching condition presented in Eq. (5) will have to be amended to account for the θ dependence of the Zeeman term, if the applied field is not aligned with the quantization axis. However, it is apparent that, as the magnetic field strength increases, the matching between Zeeman and hyperfine splittings occurs at larger θ values.

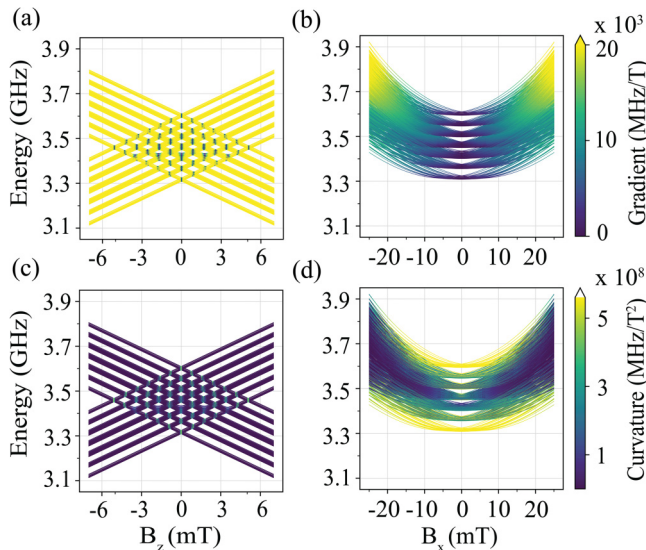


FIG. 4. The magnitude of transition energy gradient [as defined in (A1)] and curvature [as defined in (A2)] associated with all $(2 \times 27 \times 27)$ transitions between $m_s = 0$ and $m_s = \pm 1$ as a function of the magnetic field applied parallel (a),(c), perpendicular (b),(d) to the quantization axis. The color bar corresponds to the magnitude of the gradient and the curvature; In gradient plots values beyond an arbitrary threshold are whitened for visibility purposes.

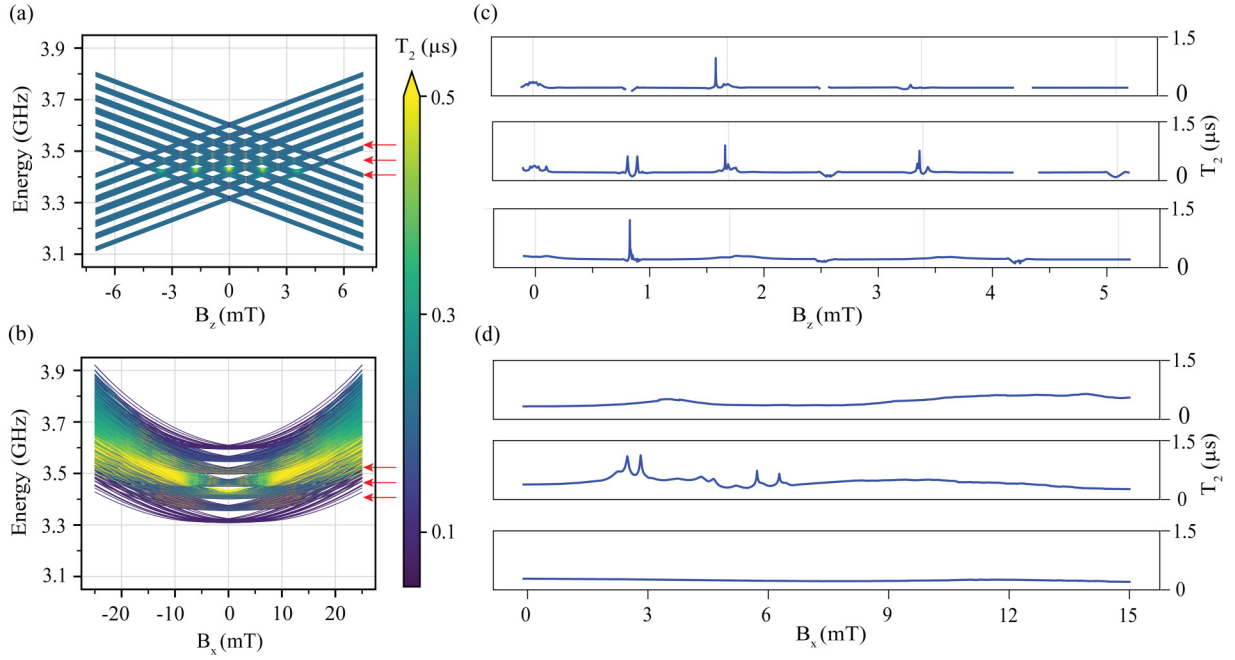


FIG. 5. Estimated coherence lifetime as a function of bias magnetic field for (a) parallel field configuration and (b) transverse field configuration. Here, the upper bound of the color bar has been restricted to $0.5 \mu\text{s}$ for enhancing the visibility of the high T_2 regions. Dependence of T_2 as a function of the applied field corresponding to select transition energies for (c) parallel field configuration and (d) transverse field configuration. The red arrows in (a) and (b) indicate the chosen energies, and the gray lines in (c) indicate the magnetic field values that satisfy Eq. (5).

Consequently, the avoided crossings will shift to larger θ values for higher magnetic field magnitudes as depicted in Figs. 2 and 3. Similar phenomena have been observed in nitrogen-vacancy centers in diamond [57]. Furthermore, we analyze the specific scenario when the magnetic field is applied perpendicular to the crystal field axis. Figure 4(b) shows that the transition gradients are minimal at zero field; however, their rate of increase as a function of the field strength is dramatically suppressed for the transverse field. A lower gradient indicates a reduced first-order response to external perturbations, implying that the system is less affected by small magnetic fluctuations. In such cases, the second-order effect, characterized by the curvature of the transition energy, becomes more relevant. Therefore, we compute the mean curvature for parallel and transverse field variations (detailed calculations are provided in Appendix A). The curvature (i.e., second-order effect due to magnetic fluctuations) of transition energies for fields applied in parallel and transverse orientations are shown in Figs. 4(c) and 4(d), respectively. As anticipated from the geometry of the problem, the curvature is larger at the anticrossing points compared to the other field regions. Besides the anticrossing points, the curvature increases as a function of the field strength for the parallel field; nonetheless, the magnitude and variations are considerably lower as compared to the transverse field scenario. Moreover, for the transverse field application, although the magnitude of the curvature is frequency dependent, it decreases with magnetic field strength. Although our analysis does not explicitly facilitate evaluation of the exact T_2 values, we implement the following route to illustrate coherence enhancement corresponding to the investigated scenarios. Assuming that T_2 is inversely proportional to the frequency broadening caused by

the magnetic field perturbations, its dependence on energy gradients and curvatures can be expressed as

$$T_2 \approx \frac{1}{\sqrt{[f'(B_0)\sigma_B]^2 + \frac{1}{2}[f''(B_0)\sigma_B^2]^2}}, \quad (6)$$

where σ_B is the standard deviation of the external field noise, assuming the normal distribution (for more details, see Appendix D). Here, we assume that magnetic noise is the leading source of decoherence, which is the case for V_B^- in hBN due to the nuclear spin dominated bath. Taking into consideration the reported values T_2 , both experimental as well as those obtained via Cluster Correlation Expansion (CCE) [58], we estimate σ_B to be $172.6 \mu\text{T}$ at 15 mT . This allows for the calculation of T_2 associated with each of the transition energies at various field configurations using Eq. (6). It is important to note that although σ_B depends on the magnetic field, its value is effectively constant over the range investigated here [58]. The color plots of T_2 for the parallel and perpendicular magnetic field scenarios are presented in Figs. 5(a) and 5(b). Moreover, the cross sections taken at specific transition energies are shown in Figs. 5(c) and 5(d). Here, the cross sections have a width of 10 MHz on each side of the central transition energy. For the parallel fields, we obtain extremely long coherence lifetimes at the peculiar points that satisfy Eq. (5). Additionally, some extra features are observed at frequencies where the approximate analytical solution becomes inadequate to capture the complex energy level structure. The linewidths of the individual T_2 peaks are of the order of a few tens of microtesla, thus requiring a relatively high control over the bias field for the practical realization. On the other hand, the transverse field configurations appear to be much less

sensitive to the bias field amplitude, though the T_2 enhancement factor is not as high as the one observed for the parallel cases. In an actual experiment, we expect the enhanced T_2 features to be less pronounced due to the broadening effects arising from factors such as interactions with the rest of the bath, bias field inhomogeneities, and the finite bandwidth of the experimental probe pulse. The transition probability of the probed transitions will also influence the outcome of the experiment. Nonetheless, we anticipate noticeably higher coherence lifetimes close to the predicted configurations.

IV. SUMMARY AND OUTLOOK

Our comprehensive investigation of the magnetic field dependent properties of the composite (V_B^- , ^{14}N) defect uncovers rich physics. In particular, by performing an in-depth numerical simulation of the system's spin Hamiltonian, we identify distinct anticrossing points, corresponding to specific field strengths and orientations where the energy gradients reach their minimum value. Furthermore, we derive an approximate analytical expression to estimate conditions under which gradient minimization occurs when the magnetic field is oriented along the quantization axis. This model is widely applicable as the low-gradient regions can be evaluated for an arbitrary spin-1 electronic system coupled to an arbitrary nuclear spin. Additionally, we compute curvatures of the transition energies that can play an important role in certain low-gradient regions. Finally, we estimate experimentally observable T_2 values and demonstrate that coherence can be improved substantially if specific field configurations are realized. More broadly, the analysis in this study provides a framework for interpreting magnetic field dependent T_2 measurements across diverse systems and is expected to encourage further exploration of such coherence-preserving configurations, both experimentally and through advanced numerical methods such as CCE. Furthermore, our results have significant implications for low-field quantum sensing, where decoherence mitigation remains a critical challenge. Specifically, the identified gradient dips and field-insensitive regions highlight potential pathways for improving spin coherence in V_B^- defects, thus advancing the development of quantum sensing applications such as electrometry and thermometry, based on 2D materials.

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DATA AVAILABILITY

The data that support the findings of this article, the code for Hamiltonian diagonalization, as well as gradient and

curvature evaluation are openly available in the public GitHub repository [64].

APPENDIX A: COMPUTATION OF GRADIENT AND CURVATURE

The workflow of gradient calculation is as follows:

(1) At each point on the shell, defined by (θ, φ) , we introduce small fluctuations $\delta\mathbf{b}$ in magnetic field $\mathbf{B}_0$. Hence, total field strength $\mathbf{B} = \mathbf{B}_0 \pm \delta\mathbf{b}$.

(2) We then find the eigenenergies of the full Hamiltonian and transition energy (f) for all possible transitions, at each of these points.

(3) Subsequently, we calculate the gradient of the transition energy ($\partial f/\partial b_x, \partial f/\partial b_y, \partial f/\partial b_z$) along each direction using a central difference method and finally, evaluate the magnitude of the gradient as follows:

$$f'(B_0) = \sqrt{\left(\frac{\partial f}{\partial b_x}\right)^2 + \left(\frac{\partial f}{\partial b_y}\right)^2 + \left(\frac{\partial f}{\partial b_z}\right)^2}. \quad (\text{A1})$$

The steps for evaluating the curvature are as follows:

(1) At each magnetic field, we introduce small fluctuations directed along six principal axes ($\pm x, \pm y, \pm z$).

(2) We then calculate the eigenenergies of the full Hamiltonian and transition energy (f) for all possible transitions.

(3) Subsequently, we calculate first-order (f_x, f_y, f_z) and second-order (f_{xx}, f_{yy}, f_{zz}) derivatives of the transition energy at each magnetic field and finally, evaluate the magnitude of the curvature.

$$f''(B_0) = \sqrt{\left(\frac{\partial^2 f}{\partial b_x^2}\right)^2 + \left(\frac{\partial^2 f}{\partial b_y^2}\right)^2 + \left(\frac{\partial^2 f}{\partial b_z^2}\right)^2}. \quad (\text{A2})$$

APPENDIX B: CALCULATION OF TRANSITION PROBABILITIES

The transition probabilities between spin states in the presence of an oscillating microwave field are computed numerically from the eigenstates of the full spin Hamiltonian. Given initial and final eigenstates $|\psi_i\rangle$ and $|\psi_f\rangle$, the transition probability $P_{i \rightarrow f}$ for a microwave excitation polarized perpendicular to the quantization axis is evaluated as the squared matrix element of the electronic spin operators transverse to the field:

$$P_{i \rightarrow f} = |\langle \psi_f | S_x | \psi_i \rangle|^2 + |\langle \psi_f | S_y | \psi_i \rangle|^2.$$

The transition probabilities for the most probable transitions discussed in Figs. 2 and 3 are presented in Fig. 6. To further illustrate the relative strength of these transitions, in Fig. 7 These maps highlight the eminence of the selected transitions across varying field strengths and orientations.

APPENDIX C: PERTURBATION ANALYSIS

Under a parallel bias magnetic field, three first shell ^{14}N nuclear spins are identical to V_B^- spin. Therefore, the system can be considered as an interacting spin-1, spin-3 system. The unperturbed Hamiltonian,

$$H^0 = DS_z^2 + (B_z + b_z)S_z + A_{zz}S_zI_z, \quad (\text{C1})$$

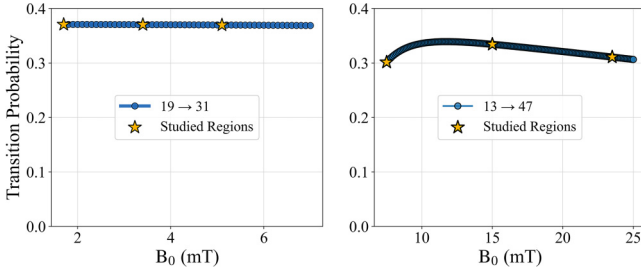


FIG. 6. Transition probability under (left) parallel and (right) transverse magnetic fields. The star-marked points indicate the field values at which a detailed analysis of the energy spectra and gradient variations with respect to the magnetic field orientation was performed, which is displayed in Figs. 2 and 3.

where B_z is the bias magnetic field and b_z is the magnetic field fluctuation along the z axis, D and A_{zz} are parallel ZFS and hyperfine constants. The terms that do not commute with S_z^2 are considered as part of the perturbation Hamiltonian (H^1),

$$H^1 = \gamma_e(b_x S_x + b_y S_y),$$

$$H^1 = \gamma_e \left[b_x \left(\frac{S_+ + S_-}{2} \right) + b_y \left(\frac{S_+ - S_-}{2i} \right) \right]. \quad (C2)$$

Here, b_x, b_y are small fluctuations in the magnetic field components along the x and y directions, and $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$ are the spin raising and lowering operators. The unperturbed energy levels corresponding to H^0 are given by

$$E_{|m_s, m_I\rangle}^0 = Dm_s^2 + \gamma_e(B_z + b_z)m_s + A_{zz}m_s m_I, \quad (C3)$$

where m_s , the electron spin projection quantum number, can take value $\{m_s = 0, \pm 1\}$ and m_I , the nuclear spin projection quantum number, can take value $\{m_I = -3, \dots, 0, \dots, 3\}$. As the $|m_s = 0, m_I\rangle$ states are degenerate, we apply first-order degenerate perturbation theory, where the corrections to the energies are obtained from the eigenvalues of the perturbation matrix $W^0 = [w]_{7 \times 7}$. The diagonal and off-diagonal elements of this matrix are

$$w_{m_I, m_I}^0 = \langle 0, m_I | H^1 | 0, m_I \rangle = 0, \quad (C4a)$$

$$w_{m_I, m_I'}^0 = \langle 0, m_I | H^1 | 0, m_I' \rangle = 0. \quad (C4b)$$

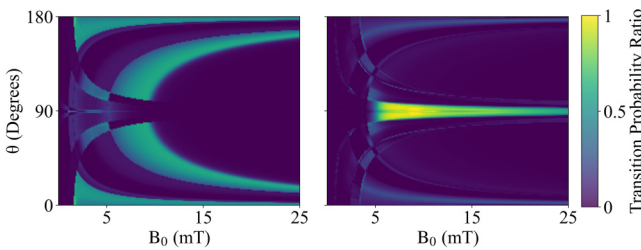


FIG. 7. Heatmaps illustrating the transition-probability ratios for the two representative transitions discussed in Figs. 2 and 3. The ratio was obtained by dividing the actual transition probability by the probability of the maximally allowed transition within the $m_s = 0$ and $m_s = -1$ manifolds. The magnetic field magnitude B_0 and polar angle θ are varied while the azimuthal angle is fixed ($\phi = 0$).

For the $|m_s = \pm 1, m_I\rangle$ states, which are nondegenerate, we use first-order nondegenerate perturbation theory, yielding the energy corrections,

$$\langle \pm 1, m_I | H^1 | \pm 1, m_I \rangle = 0. \quad (C5)$$

Thus, in both the degenerate and the nondegenerate cases, all first-order corrections vanish,

$$E_{|m_s, m_I\rangle}^1 = 0. \quad (C6)$$

Since the degeneracy of the $|m_s = 0, m_I\rangle$ states is not lifted at first order, we proceed with second-order degenerate perturbation theory. The effective perturbation matrix is given as

$$\Lambda^0 = [\lambda]_{7 \times 7}, \quad (C7)$$

where matrix elements are

$$\lambda_{ij}^0 = \sum_{n \neq m} \frac{\langle \varphi_{n,i} | H^1 | \psi_m \rangle \langle \psi_m | H^1 | \varphi_{n,j} \rangle}{E_n^{(0)} - E_m^{(0)}} = 0. \quad (C8)$$

Here, φ_n are the degenerate states and ψ_m represent all other states, and $E_n^{(0)}, E_m^{(0)}$ are the zeroth-order energies of the n th and m th eigenstates. Thus, the second-order energy correction for the $|m_s = 0, m_I\rangle$ states also vanishes,

$$E_{|m_s=0, m_I\rangle}^2 = 0. \quad (C9)$$

For the $|m_s = \pm 1, m_I\rangle$ states, which are nondegenerate, we apply second-order nondegenerate perturbation theory. The general expression for the second-order correction is

$$E_{|m_s, m_I\rangle}^2 = \sum_{n \neq m} \frac{|\langle \psi_m | H^1 | \varphi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}}. \quad (C10)$$

For instance, the correction for the state $|1, 3\rangle$ is

$$E_{|1,3\rangle}^2 = \frac{|\langle 0, 3 | H^1 | 1, 3 \rangle|^2}{\gamma_e(B_z + b_z) + 3A_{zz}}$$

$$= \frac{\gamma_e^2}{2} \frac{b_x^2 + b_y^2}{\gamma_e(B_z + b_z) + 3A_{zz}}. \quad (C11)$$

More generally, the second-order energy correction for $|m_s, m_I\rangle$ can be expressed as

$$E_{|m_s, m_I\rangle}^2 = \frac{m_s^2 \gamma_e^2 (b_x^2 + b_y^2)}{2[m_s \gamma_e (B_z + b_z) + m_s m_I A_{zz}]}. \quad (C12)$$

The total energy of the system reads

$$E = E^0 + E^1 + E^2$$

$$= m_s^2 D + m_s Y, \quad (C13)$$

where

$$Y = \sqrt{[\gamma_e(B_z + b_z) + m_I A_{zz}]^2 + [\gamma_e \sqrt{b_x^2 + b_y^2}]^2}. \quad (C14)$$

The transition frequency is defined under the condition $\Delta m_s = \pm 1$ and $\Delta m_I = 0$, and is given by

$$f = D + m_s \sqrt{[\gamma_e(B_z + b_z) + m_I A_{zz}]^2 + [\gamma_e \sqrt{b_x^2 + b_y^2}]^2}. \quad (C15)$$

The partial derivatives of the transition frequency with respect to b_x , b_y , and b_z are as follows:

$$\frac{\partial f}{\partial b_x} = \frac{m_s \gamma_e^2 b_x}{\sqrt{[\gamma_e(B_z + b_z) + m_I A_{zz}]^2 + [\gamma_e \sqrt{b_x^2 + b_y^2}]^2}}, \quad (\text{C16})$$

$$\frac{\partial f}{\partial b_y} = \frac{m_s \gamma_e^2 b_y}{\sqrt{[\gamma_e(B_z + b_z) + m_I A_{zz}]^2 + [\gamma_e \sqrt{b_x^2 + b_y^2}]^2}}, \quad (\text{C17})$$

and

$$\frac{\partial f}{\partial b_z} = \frac{m_s \gamma_e [\gamma_e(B_z + b_z) + m_I A_{zz}]}{\sqrt{[\gamma_e(B_z + b_z) + m_I A_{zz}]^2 + [\gamma_e \sqrt{b_x^2 + b_y^2}]^2}}. \quad (\text{C18})$$

The gradient of the transition energies is then given by

$$\left| \frac{df}{db} \right| = \sqrt{\left(\frac{\partial f}{\partial b_x} \right)^2 + \left(\frac{\partial f}{\partial b_y} \right)^2 + \left(\frac{\partial f}{\partial b_z} \right)^2}. \quad (\text{C19})$$

The gradient is minimized when

$$\left| \frac{df}{db} \right| = 0, \Rightarrow \gamma_e B_z + m_I A_{zz} = 0. \quad (\text{C20})$$

Under the condition of small perturbation i.e., $\gamma_e B_z, A_{zz} \gg \gamma_e b_x, \gamma_e b_y, \gamma_e b_z$, the bias magnetic field B_z satisfies

$$B_z = -\frac{m_I A_{zz}}{\gamma_e}. \quad (\text{C21})$$

APPENDIX D: DETAILED DERIVATION OF T_2 FORMULAS

Consider the transition energy $f(\mathbf{B})$ as a function of the magnetic field $\mathbf{B}$, which fluctuates around a mean-field value

$\mathbf{B}_0$. Expanding $f(\mathbf{B})$ using a Taylor series about $\mathbf{B}_0$ gives

$$f(\mathbf{B}) \approx f(\mathbf{B}_0) + \nabla f(\mathbf{B}_0) \cdot (\mathbf{B} - \mathbf{B}_0) + \frac{1}{2} (\mathbf{B} - \mathbf{B}_0)^T H_f(\mathbf{B}_0) (\mathbf{B} - \mathbf{B}_0) + \dots, \quad (\text{D1})$$

where $\nabla f(\mathbf{B}_0)$ is the gradient of f at $\mathbf{B}_0$ and $H_f(\mathbf{B}_0)$ is the Hessian matrix at $\mathbf{B}_0$. Assuming the magnetic field fluctuations $\delta \mathbf{b} = \mathbf{B} - \mathbf{B}_0$ are described by a Gaussian distribution with zero mean value and standard deviation σ_B . The variance of the energy fluctuations $\sigma_f^2 = \text{Var}(f)$ can be approximated by truncating higher-order terms:

$$\begin{aligned} \sigma_f^2 &= \text{Var} \left(f(\mathbf{B}_0) + \nabla f(\mathbf{B}_0) \cdot \delta \mathbf{b} + \frac{1}{2} \delta \mathbf{b}^T H_f(\mathbf{B}_0) \delta \mathbf{b} \right) \\ &= 0 + \left[\left(\frac{\partial f}{\partial b_x} \right)^2 + \left(\frac{\partial f}{\partial b_y} \right)^2 + \left(\frac{\partial f}{\partial b_z} \right)^2 \right] \sigma_B^2 \\ &\quad + \frac{1}{2} \left[\left(\frac{\partial^2 f}{\partial b_x^2} \right)^2 + \left(\frac{\partial^2 f}{\partial b_y^2} \right)^2 + \left(\frac{\partial^2 f}{\partial b_z^2} \right)^2 \right] \sigma_B^4, \end{aligned} \quad (\text{D2})$$

where we have used the fact that for a Gaussian variable δb , $\text{Var}(\delta b) = \sigma_B^2$ and $\text{Var}[(\delta b)^2] = 2\sigma_B^4$.

The coherence time T_2 can then be approximated as

$$T_2 \approx \frac{1}{\sigma_f} = \frac{1}{\sqrt{[f'(\mathbf{B}_0)\sigma_B]^2 + \frac{1}{2}[f''(\mathbf{B}_0)\sigma_B^2]^2}}. \quad (\text{D3})$$

Here,

$$\begin{aligned} f'(\mathbf{B}_0) &= \sqrt{\left(\frac{\partial f}{\partial b_x} \right)^2 + \left(\frac{\partial f}{\partial b_y} \right)^2 + \left(\frac{\partial f}{\partial b_z} \right)^2}, \\ f''(\mathbf{B}_0) &= \sqrt{\left(\frac{\partial^2 f}{\partial b_x^2} \right)^2 + \left(\frac{\partial^2 f}{\partial b_y^2} \right)^2 + \left(\frac{\partial^2 f}{\partial b_z^2} \right)^2}. \end{aligned}$$

This expression [Eq. (6) in the main text] quantifies how both linear (gradient) and quadratic (curvature) sensitivities of the transition energy to magnetic field fluctuations influence the spin coherence time.

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- [1] G. Wolfowicz, F. J. Heremans, C. P. Anderson, S. Kanai, H. Seo, A. Gali, G. Galli, and D. D. Awschalom, Quantum guidelines for solid-state spin defects, *Nat. Rev. Mater.* **6**, 906 (2021).
 - [2] D. D. Awschalom, R. Hanson, J. Wrachtrup, and B. B. Zhou, Quantum technologies with optically interfaced solid-state spins, *Nat. Photonics* **12**, 516 (2018).
 - [3] H.-H. Fang, X.-J. Wang, X. Marie, and H.-B. Sun, Quantum sensing with optically accessible spin defects in van der Waals layered materials, *Light Sci. Appl.* **13**, 303 (2024).
 - [4] G. Balasubramanian, I. Y. Chan, R. Kolesov, M. Al-Hmoud, J. Tisler, C. Shin, C. Kim, A. Wojcik, P. R. Hemmer, A. Krueger, T. Hanke, A. Leitenstorfer, R. Bratschitsch, F. Jelezko, and J. Wrachtrup, Nanoscale imaging magnetometry with diamond spins under ambient conditions, *Nature (London)* **455**, 648 (2008).
 - [5] J. R. Maze, P. L. Stanwix, J. S. Hodges, S. Hong, J. M. Taylor, P. Cappellaro, L. Jiang, M. V. Dutt, E. Togan, A. S. Zibrov, A. Yacoby, R. L. Walsworth, and M. D. Lukin, Nanoscale magnetic sensing with an individual electronic spin in diamond, *Nature (London)* **455**, 644 (2008).
 - [6] H. Kraus, V. A. Soltamov, F. Fuchs, D. Simin, A. Sperlich, P. G. Baranov, G. V. Astakhov, and V. Dyakonov, Magnetic field and temperature sensing with atomic-scale spin defects in silicon carbide, *Sci. Rep.* **4**, 5303 (2014).
 - [7] D. Simin, V. A. Soltamov, A. V. Poshakinskiy, A. N. Anisimov, R. A. Babunts, D. O. Tolmachev, E. N. Mokhov, M. Trupke, S. A. Tarasenko, A. Sperlich, P. G. Baranov, V. Dyakonov, and G. V. Astakhov, All-optical dc nanoscale magnetometry using silicon vacancy fine structure in isotopically purified silicon carbide, *Phys. Rev. X* **6**, 031014 (2016).
 - [8] S. T. Alsidd, J. M. Schloss, M. H. Steinecker, J. F. Barry, A. C. Maccabe, G. Wang, P. Cappellaro, and D. A. Braje, Solid-state microwave magnetometer with Picotesla-level sensitivity, *Phys. Rev. Appl.* **19**, 054095 (2023).

- [9] S. Simmons, R. M. Brown, H. Riemann, N. V. Abrosimov, P. Becker, H. J. Pohl, M. L. Thewalt, K. M. Itoh, and J. J. Morton, Entanglement in a solid-state spin ensemble, *Nature (London)* **470**, 69 (2011).
- [10] T. H. Taminiau, J. Cramer, T. V. D. Sar, V. V. Dobrovitski, and R. Hanson, Universal control and error correction in multi-qubit spin registers in diamond, *Nat. Nanotechnol.* **9**, 171 (2014).
- [11] J. Cramer, N. Kalb, M. A. Rol, B. Hensen, M. S. Blok, M. Markham, D. J. Twitchen, R. Hanson, and T. H. Taminiau, Repeated quantum error correction on a continuously encoded qubit by real-time feedback, *Nat. Commun.* **7**, 11526 (2016).
- [12] C. E. Bradley, J. Randall, M. H. Abobeih, R. C. Berrevoets, M. J. Degen, M. A. Bakker, M. Markham, D. J. Twitchen, and T. H. Taminiau, A ten-qubit solid-state spin register with quantum memory up to one minute, *Phys. Rev. X* **9**, 031045 (2019).
- [13] A. Bourassa, C. P. Anderson, K. C. Miao, M. Onizhuk, H. Ma, A. L. Crook, H. Abe, J. Ul-Hassan, T. Ohshima, N. T. Son, G. Galli, and D. D. Awschalom, Entanglement and control of single nuclear spins in isotopically engineered silicon carbide, *Nat. Mater.* **19**, 1319 (2020).
- [14] G. Wolfowicz, H. Maier-Flaig, R. Marino, A. Ferrier, H. Vezin, John J. L. Morton, and P. Goldner, Coherent storage of microwave excitations in rare-earth nuclear spins, *Phys. Rev. Lett.* **114**, 170503 (2015).
- [15] B. Hensen, H. Bernien, A. E. Dreaú, A. Reiserer, N. Kalb, M. S. Blok, J. Ruitenbergh, R. F. Vermeulen, R. N. Schouten, C. Abellán, W. Amaya, V. Pruneri, M. W. Mitchell, M. Markham, D. J. Twitchen, D. Elkouss, S. Wehner, T. H. Taminiau, and R. Hanson, Loophole-free bell inequality violation using electron spins separated by 1.3 kilometres, *Nature (London)* **526**, 682 (2015).
- [16] P. Lamba, A. Rana, S. Halder, S. Dhomkar, D. Suter, and R. K. Kamineni, Vector detection of ac magnetic fields by nitrogen vacancy centers of single orientation in diamond, *Phys. Rev. B* **109**, 195424 (2024).
- [17] P. Udvarhelyi, T. Clua-Provost, A. Durand, J. Li, J. H. Edgar, B. Gil, G. Cassaboiss, V. Jacques, and A. Gali, A planar defect spin sensor in a two-dimensional material susceptible to strain and electric fields, *npj Comput. Mater.* **9**, 150 (2023).
- [18] F. Dolde, H. Fedder, M. W. Doherty, T. Nöbauer, F. Rempp, G. Balasubramanian, T. Wolf, F. Reinhard, L. C. Hollenberg, F. Jelezko, and J. Wrachtrup, Electric-field sensing using single diamond spins, *Nat. Phys.* **7**, 459 (2011).
- [19] X. Lyu, Q. Tan, L. Wu, C. Zhang, Z. Zhang, Z. Mu, J. Zúñiga-Pérez, H. Cai, and W. Gao, Strain quantum sensing with spin defects in hexagonal boron nitride, *Nano Lett.* **22**, 6553 (2022).
- [20] A. Gottscholl, M. Kianinia, V. Soltamov, S. Orlinskii, G. Mamin, C. Bradac, C. Kasper, K. Krambrock, A. Sperlich, M. Toth, I. Aharonovich, and V. Dyakonov, Initialization and read-out of intrinsic spin defects in a van der Waals crystal at room temperature, *Nat. Mater.* **19**, 540 (2020).
- [21] P. Neumann, I. Jakobi, F. Dolde, C. Burk, R. Reuter, G. Waldherr, J. Honert, T. Wolf, A. Brunner, J. H. Shim, D. Suter, H. Sumiya, J. Isoya, and J. Wrachtrup, High-precision nanoscale temperature sensing using single defects in diamond, *Nano Lett.* **13**, 2738 (2013).
- [22] H. L. Stern, Q. Gu, J. Jarman, S. E. Barker, N. Mendelson, D. Chugh, S. Schott, H. H. Tan, H. Sirringhaus, I. Aharonovich, and M. Atatüre, Room-temperature optically detected magnetic resonance of single defects in hexagonal boron nitride, *Nat. Commun.* **13**, 618 (2022).
- [23] F. Jelezko and J. Wrachtrup, Single defect centres in diamond: A review, *Phys. Status Solidi A* **203**, 3207 (2006).
- [24] L. Rondin, J. P. Tetienne, T. Hingant, J. F. Roch, P. Maletinsky, and V. Jacques, Magnetometry with nitrogen-vacancy defects in diamond, *Rep. Prog. Phys.* **77**, 056503 (2014).
- [25] R. Schirhagl, K. Chang, M. Loretz, and C. L. Degen, Nitrogen-vacancy centers in diamond: Nanoscale sensors for physics and biology, *Annu. Rev. Phys. Chem.* **65**, 83 (2014).
- [26] J. F. Barry, J. M. Schloss, E. Bauch, M. J. Turner, C. A. Hart, L. M. Pham, and R. L. Walsworth, Sensitivity optimization for NV-diamond magnetometry, *Rev. Mod. Phys.* **92**, 015004 (2020).
- [27] S. Castelletto, C. T. Lew, W. X. Lin, and J. S. Xu, Quantum systems in silicon carbide for sensing applications, *Rep. Prog. Phys.* **87**, 014501 (2024).
- [28] Z. Jiang, H. Cai, R. Cernansky, X. Liu, and W. Gao, Quantum sensing of radio-frequency signal with NV centers in sic, *Sci. Adv.* **9**, eadg2080 (2023).
- [29] B. Huang, M. A. McGuire, A. F. May, D. Xiao, P. Jarillo-Herrero, and X. Xu, Emergent phenomena and proximity effects in two-dimensional magnets and heterostructures, *Nat. Mater.* **19**, 1276 (2020).
- [30] A. Reserbat-Plantey, I. Epstein, I. Torre, A. T. Costa, P. A. Gonçalves, N. A. Mortensen, M. Polini, J. C. Song, N. M. Peres, and F. H. Koppens, Quantum nanophotonics in two-dimensional materials, *ACS Photonics* **8**, 85 (2021).
- [31] M. Rao, F. Shi, Z. Rao, J. Yang, C. Song, X. Chen, J. Dong, Y. Yu, and S. Yu, Single photon emitter deterministically coupled to a topological corner state, *Light Sci. Appl.* **13**, 19 (2024).
- [32] T. T. H. Do, M. Nonahal, C. Li, V. Valuckas, H. H. Tan, A. I. Kuznetsov, H. S. Nguyen, I. Aharonovich, and S. T. Ha, Room-temperature strong coupling in a single-photon emitter-metasurface system, *Nat. Commun.* **15**, 2281 (2024).
- [33] L. Sortino, A. Gale, L. Kühner, C. Li, J. Biechteler, F. J. Wendisch, M. Kianinia, H. Ren, M. Toth, S. A. Maier, I. Aharonovich, and A. Tittl, Optically addressable spin defects coupled to bound states in the continuum metasurfaces, *Nat. Commun.* **15**, 2008 (2024).
- [34] M. Atatüre, D. Englund, N. Vamivakas, S. Y. Lee, and J. Wrachtrup, Material platforms for spin-based photonic quantum technologies, *Nat. Rev. Mater.* **3**, 38 (2018).
- [35] A. Branny, S. Kumar, R. Proux, and B. D. Gerardot, Deterministic strain-induced arrays of quantum emitters in a two-dimensional semiconductor, *Nat. Commun.* **8**, 15053 (2017).
- [36] C. Palacios-Berraquero, D. M. Kara, A. R. Montblanch, M. Barbone, P. Latawiec, D. Yoon, A. K. Ott, M. Loncar, A. C. Ferrari, and M. Atatüre, Large-scale quantum-emitter arrays in atomically thin semiconductors, *Nat. Commun.* **8**, 15093 (2017).
- [37] T. T. Tran, K. Bray, M. J. Ford, M. Toth, and I. Aharonovich, Quantum emission from hexagonal boron nitride monolayers, *Nat. Nanotechnol.* **11**, 37 (2016).
- [38] A. L. Exarhos, D. A. Hopper, R. N. Patel, M. W. Doherty, and L. C. Bassett, Magnetic-field-dependent quantum emission in hexagonal boron nitride at room temperature, *Nat. Commun.* **10**, 222 (2019).

- [39] W. Liu, N. J. Guo, S. Yu, Y. Meng, Z. P. Li, Y. Z. Yang, Z. A. Wang, X. D. Zeng, L. K. Xie, Q. Li, J. F. Wang, J. S. Xu, Y. T. Wang, J. S. Tang, C. F. Li, and G. C. Guo, Spin-active defects in hexagonal boron nitride, *Mater. Quantum Technol.* **2**, 032002 (2022).
- [40] A. Gottscholl, M. Diez, V. Soltamov, C. Kasper, D. Krauß, A. Sperlich, M. Kianinia, C. Bradac, I. Aharonovich, and V. Dyakonov, Spin defects in hBN as promising temperature, pressure and magnetic field quantum sensors, *Nat. Commun.* **12**, 4480 (2021).
- [41] A. J. Healey, S. C. Scholten, T. Yang, J. A. Scott, G. J. Abrahams, I. O. Robertson, X. F. Hou, Y. F. Guo, S. Rahman, Y. Lu, M. Kianinia, I. Aharonovich, and J. P. Tetienne, Quantum microscopy with van der Waals heterostructures, *Nat. Phys.* **19**, 87 (2023).
- [42] W. Liu, Z. P. Li, Y. Z. Yang, S. Yu, Y. Meng, Z. A. Wang, Z. C. Li, N. J. Guo, F. F. Yan, Q. Li, J. F. Wang, J. S. Xu, Y. T. Wang, J. S. Tang, C. F. Li, and G. C. Guo, Temperature-dependent energy-level shifts of spin defects in hexagonal boron nitride, *ACS Photonics* **8**, 1889 (2021).
- [43] V. Ivády, G. Barcza, G. Thiering, S. Li, H. Hamdi, J. P. ChouŒrs Legeza, and A. Gali, *Ab initio* theory of the negatively charged boron vacancy qubit in hexagonal boron nitride, *npj Comput. Mater.* **6**, 41 (2020).
- [44] S. Vaidya, X. Gao, S. Dikshit, I. Aharonovich, and T. Li, Quantum sensing and imaging with spin defects in hexagonal boron nitride, *Adv. Phys. X* **8**, 2206049 (2023).
- [45] D. M. Daly, N. R. Reed, S. J. DeVience, Z. Yin, J. Cremer, A. J. Beling, J. W. Blanchard, and R. L. Walsworth, Prospects for ultralow-mass nuclear magnetic resonance using spin defects in hexagonal boron nitride, [arXiv:2505.00383](https://arxiv.org/abs/2505.00383).
- [46] G. Balasubramanian, P. Neumann, D. Twitchen, M. Markham, R. Kolesov, N. Mizuochi, J. Isoya, J. Achard, J. Beck, J. Tissler, V. Jacques, P. R. Hemmer, F. Jelezko, and J. Wrachtrup, Ultra-long spin coherence time in isotopically engineered diamond, *Nat. Mater.* **8**, 383 (2009).
- [47] A. M. Tyryshkin, S. Tojo, J. J. Morton, H. Riemann, N. V. Abrosimov, P. Becker, H. J. Pohl, T. Schenkel, M. L. Thewalt, K. M. Itoh, and S. A. Lyon, Electron spin coherence exceeding seconds in high-purity silicon, *Nat. Mater.* **11**, 143 (2012).
- [48] J. Lee, H. Park, and H. Seo, First-principles theory of extending the spin qubit coherence time in hexagonal boron nitride, *npj 2D Mater. Appl.* **6**, 60 (2022).
- [49] E. L. Hahn and E. L. Hahn, Spin echoes, *Phys. Rev.* **80**, 580 (1950).
- [50] H. Y. Carr and E. M. Purcell, Effects of diffusion on free precession in nuclear magnetic resonance experiments, *Phys. Rev.* **94**, 630 (1954).
- [51] G. Wolfowicz, A. M. Tyryshkin, R. E. George, H. Riemann, N. V. Abrosimov, P. Becker, H. J. Pohl, M. L. Thewalt, S. A. Lyon, and J. J. Morton, Atomic clock transitions in silicon-based spin qubits, *Nat. Nanotechnol.* **8**, 561 (2013).
- [52] S. J. Balian, R. B. Liu, and T. S. Monteiro, Keeping a spin qubit alive in natural silicon: Comparing optimal working points and dynamical decoupling, *Phys. Rev. B* **91**, 245416 (2015).
- [53] C. S. Shin, C. E. Avalos, M. C. Butler, H. J. Wang, S. J. Seltzer, R. B. Liu, A. Pines, and V. S. Bajaj, Suppression of electron spin decoherence of the diamond NV center by a transverse magnetic field, *Phys. Rev. B* **88**, 161412(R) (2013).
- [54] D. L. McAuslan, J. G. Bartholomew, M. J. Sellars, and J. J. Longdell, Reducing decoherence in optical and spin transitions in rare-earth-ion doped materials, *Phys. Rev. A* **85**, 032339 (2012).
- [55] L. Nicolas, M. Businger, T. S. Mejia, A. Tiranov, T. Chanelière, E. Lafitte-Houssat, A. Ferrier, P. Goldner, and M. Afzelius, Coherent optical-microwave interface for manipulation of low-field electronic clock transitions in $^{171}\text{Yb}^{3+}:\text{Y}_2\text{SiO}_5$, *npj Quantum Inf.* **9**, 21 (2023).
- [56] J. Davidsson, M. Onizhuk, C. Vorwerk, and G. Galli, Discovery of atomic clock-like spin defects in simple oxides from first principles, *Nat. Commun.* **15**, 4812 (2024).
- [57] K. R. K. Rao and D. Suter, Level anti-crossings of a nitrogen-vacancy center in diamond: Decoherence-free subspaces and 3d sensors of microwave magnetic fields, *New J. Phys.* **22**, 083035 (2020).
- [58] A. Tárkányi and V. Ivády, Understanding decoherence of the boron vacancy center in hexagonal boron nitride, *Adv. Funct. Mater.* **e11300** (2025).
- [59] J. Lee, H. Kim, H. Park, and H. Seo, Magnetic-field dependent vb- spin decoherence in hexagonal boron nitrides: A first-principles study, *Adv. Funct. Mater.* **e11274** (2025).
- [60] S. Mahajan, R. Kumar, A. Xhameni, G. Venu, B. Mistri, F. Donaldson, T. Taniguchi, K. Watanabe, S. Dhomkar, A. Lombardo, and J. J. L. Morton, Impact of irradiation conditions on the magnetic field sensitivity of spin defects in hBN nano flakes, [arXiv:2510.13991](https://arxiv.org/abs/2510.13991).
- [61] X. Gao, S. Vaidya, K. Li, P. Ju, B. Jiang, Z. Xu, A. E. Allcca, K. Shen, T. Taniguchi, K. Watanabe, S. A. Bhave, Y. P. Chen, Y. Ping, and T. Li, Nuclear spin polarization and control in hexagonal boron nitride, *Nat. Mater.* **21**, 1024 (2022).
- [62] I. N. Gracheva, F. F. Murzakhanov, G. V. Mamin, M. A. Sadovnikova, B. F. Gabbasov, E. N. Mokhov, and M. R. Gafurov, Symmetry of the hyperfine and quadrupole interactions of boron vacancies in a hexagonal boron nitride, *J. Phys. Chem. C* **127**, 3634 (2023).
- [63] N. Lambert, E. Giguère, P. Menczel, B. Li, P. Hopf, G. Suárez, M. Gali, J. Lishman, R. Gadhvi, R. Agarwal, A. Galicia, N. Shammah, P. Nation, J. R. Johansson, S. Ahmed, S. Cross, A. Pitchford, and F. Nori, Qutip 5: The quantum toolbox in python, [arXiv:2412.04705](https://arxiv.org/abs/2412.04705).
- [64] B. Mistri, Code for hamiltonian diagonalization, gradient, and curvature evaluation, GitHub, 2025, https://github.com/Basanta-iitm-git/Decoherence_mapping.