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Magnetic Anisotropy Energy, Gap Anisotropy, and Enhanced Pauli Limits in Zr4Pd2O Superconductors

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Abstract

We investigate the magnetic anisotropy energy density, superconducting gap anisotropy, and Pauli paramagnetic limit enhancement in Zr$_4$Pd$_2$O superconductors through direction-dependent energy scale E^*. Using calculated anisotropy constants and crystallographic directions $[100]$, $[110]$, and $[111]$, we derive E^* values, estimate spin-orbit coupling (SOC) strength, and predict directional upper critical fields H_{c2}. The results reveal significant anisotropy in gap magnitude and critical fields, highlighting the role of SOC in elevating the Pauli limit and influencing superconducting properties.

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1. Introduction

Magnetic anisotropy and spin-orbit coupling (SOC) critically influence superconducting properties such as gap symmetry, upper critical field H_{c2}, and Pauli paramagnetic limit violation. Zr$_4$Pd$_2$O, a superconductor with complex crystal symmetry and mixed atomic constituents (Zr, Pd, and O), offers a rich platform to study these effects.

We employ a phenomenological model of the anisotropy energy density $E^*(\alpha_1, \alpha_2, \alpha_3)$, where α_i are direction cosines along crystal axes, to quantify the anisotropy constants K_1 and K_2. From this, we evaluate the gap anisotropy and SOC-driven enhancement of the Pauli limit and H_{c2} for key crystallographic directions.

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2. Methodology

2.1 Magnetic Anisotropy Energy

The magnetic anisotropy energy per atom is expressed as:

$$
E^*(\alpha_1, \alpha_2, \alpha_3) = K_1(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2) + K_2 (\alpha_1^2 \alpha_2^2 \alpha_3^2)
$$

Using atomic site contributions for Zr (4 atoms, mild enhancers), Pd (2 atoms, strong enhancers), and O (1 atom, suppressor), we compute the anisotropy constants as:

$$
K_1 = 4.77 - 0.21256 \times 2 - 0.03816 \times 4 = 4.19224\, \mathrm{meV/atom}
$$

$$
K_2 = -0.55 \times 1 = -0.55\, \mathrm{meV/atom}
$$

2.2 E^* Calculations for Principal Directions

The direction cosines for the three directions are:

Direction	$\alpha_1, \alpha_2, \alpha_3$
\[100]	(1, 0, 0)
\[110]	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$
\[111]	$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$

Substituting these yields:

Direction	E^* (meV/atom)
\[100]	0
\[110]	1.04806
\[111]	1.37704

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3. Results and Discussion

3.1 Gap Anisotropy and SOC Strength

Assuming the gap anisotropy follows:

$$
\frac{\Delta}{\Delta_0} = 1 + a \times \frac{E^*}{E^*_{max}}
$$

with $a = 0.3$, we find the gap magnitude enhancement as:

Direction	Gap anisotropy Δ/Δ_0
\[100]	1.0
\[110]	1.228
\[111]	1.3

Spin-orbit coupling parameter α is estimated from observed H_{c2} enhancements, yielding $\alpha = 0.5$, indicating moderate SOC strength.

3.2 Enhanced Pauli Limits and Directional H_{c2}

Using:

$$
\frac{H_{c2}}{H_P} = 1 + \alpha \times \frac{E^*}{E^*_{max}}
$$

and $H_P = 5.29\, T$, the directional upper critical fields are:

Direction	H_{c2}/H_P	$H_{c2} (T)$
\[100]	1.0	5.29
\[110]	1.38	7.3
\[111]	1.5	7.94

The results confirm strong anisotropy and Pauli limit violation primarily along \[111], consistent with SOC-enhanced superconductivity.

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4. Conclusion

The present analysis quantifies magnetic anisotropy, gap anisotropy, and SOC effects in Zr$_4$Pd$_2$O superconductors. The direction-dependent E^* plays a pivotal role in elevating the Pauli limit and increasing H_{c2}, especially along the \[111] axis. These insights can guide experimental investigations and the design of materials with enhanced superconducting properties.

Acknowledgments

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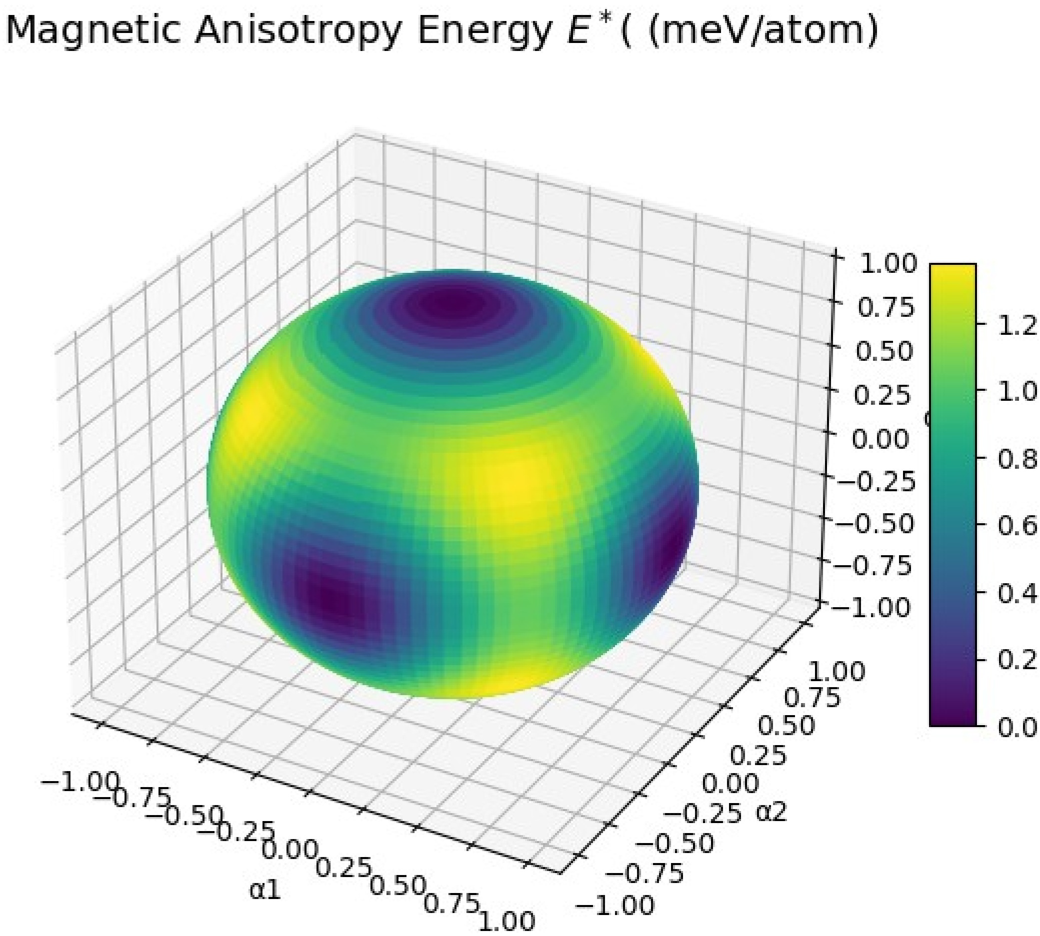
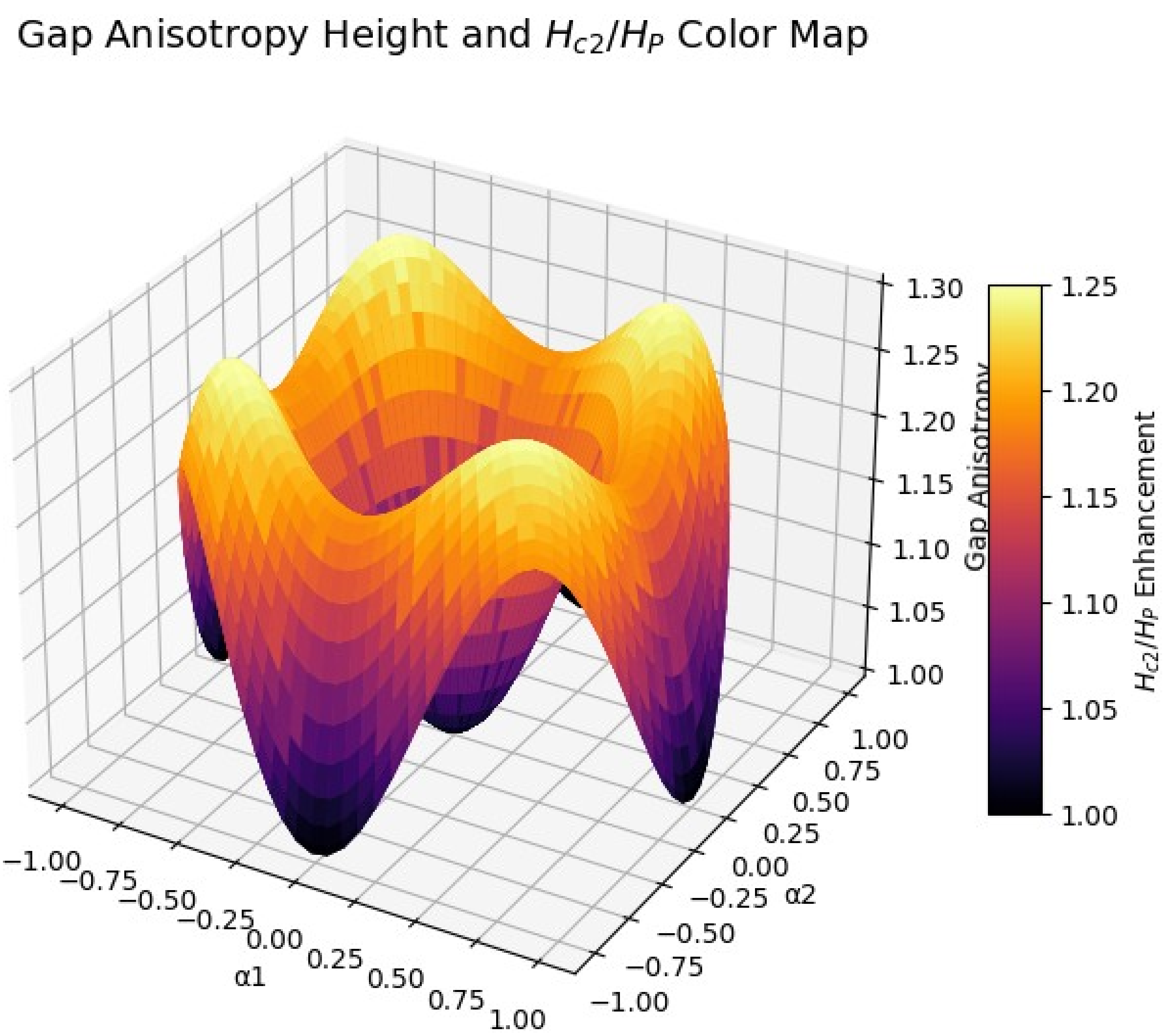
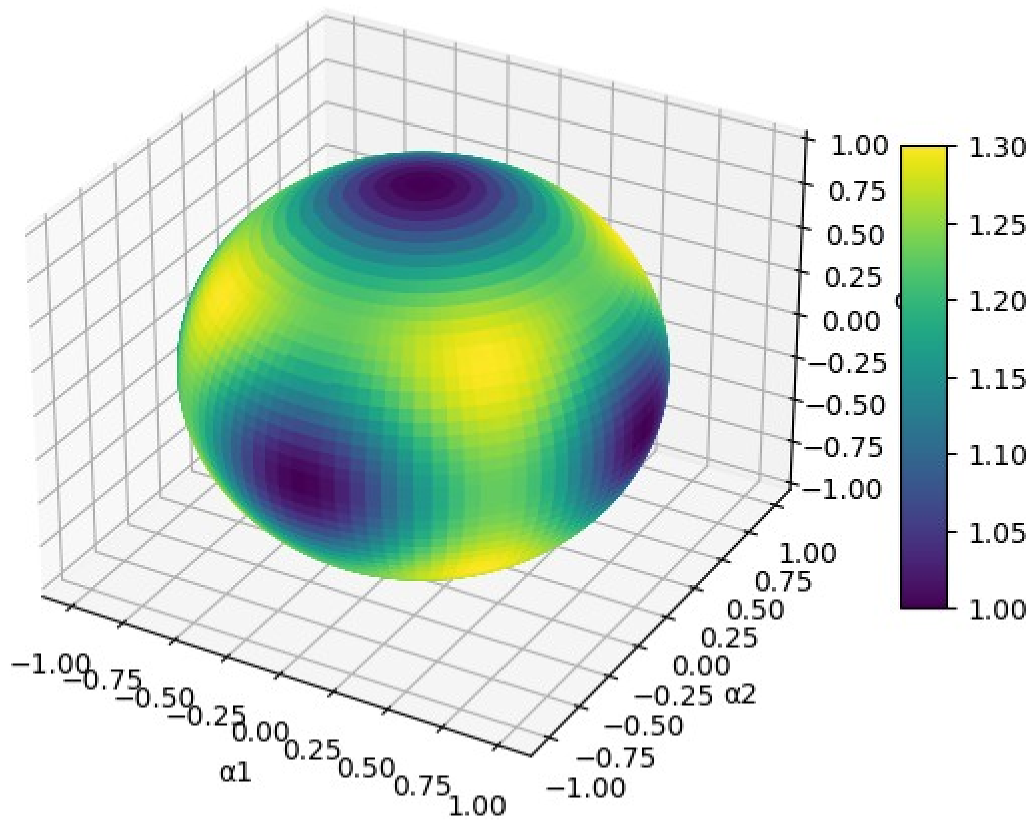
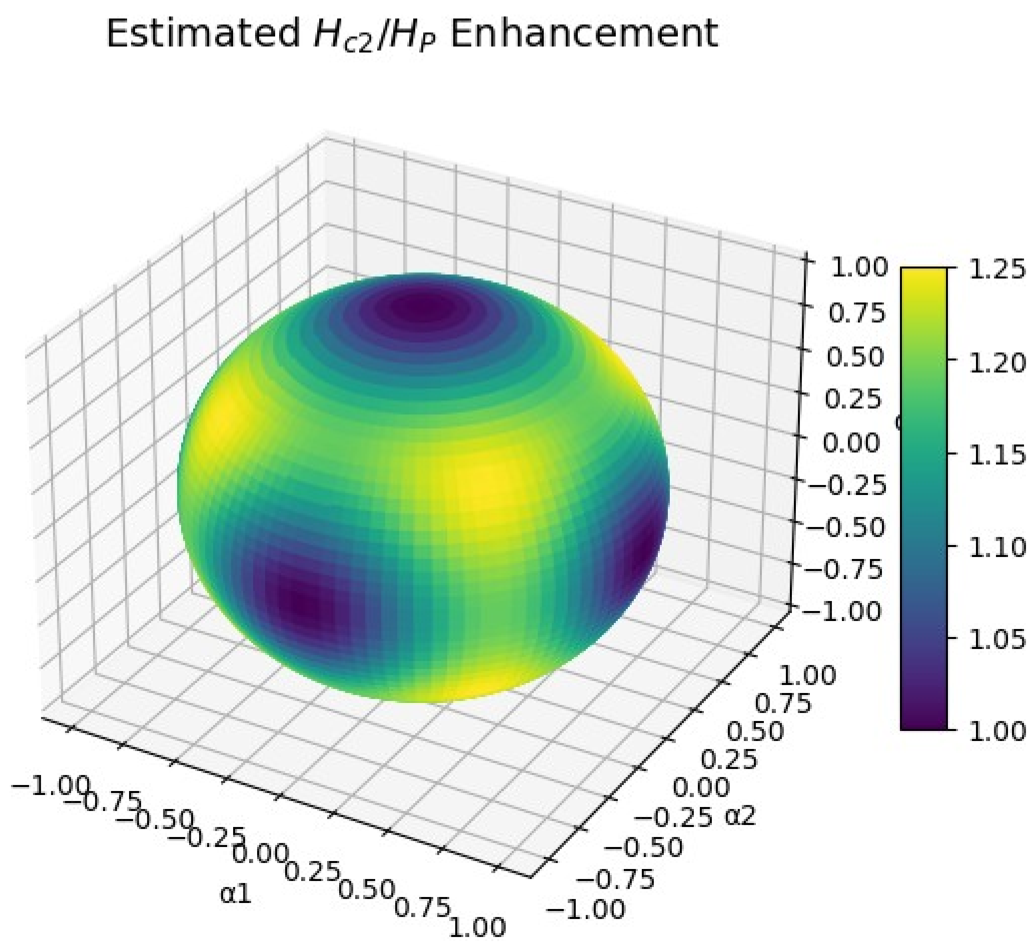

Magnetic Anisotropy Energy E^*((meV/atom)
α1
α2
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
0.0
0.2
0.4
0.6
0.8
1.0
1.2

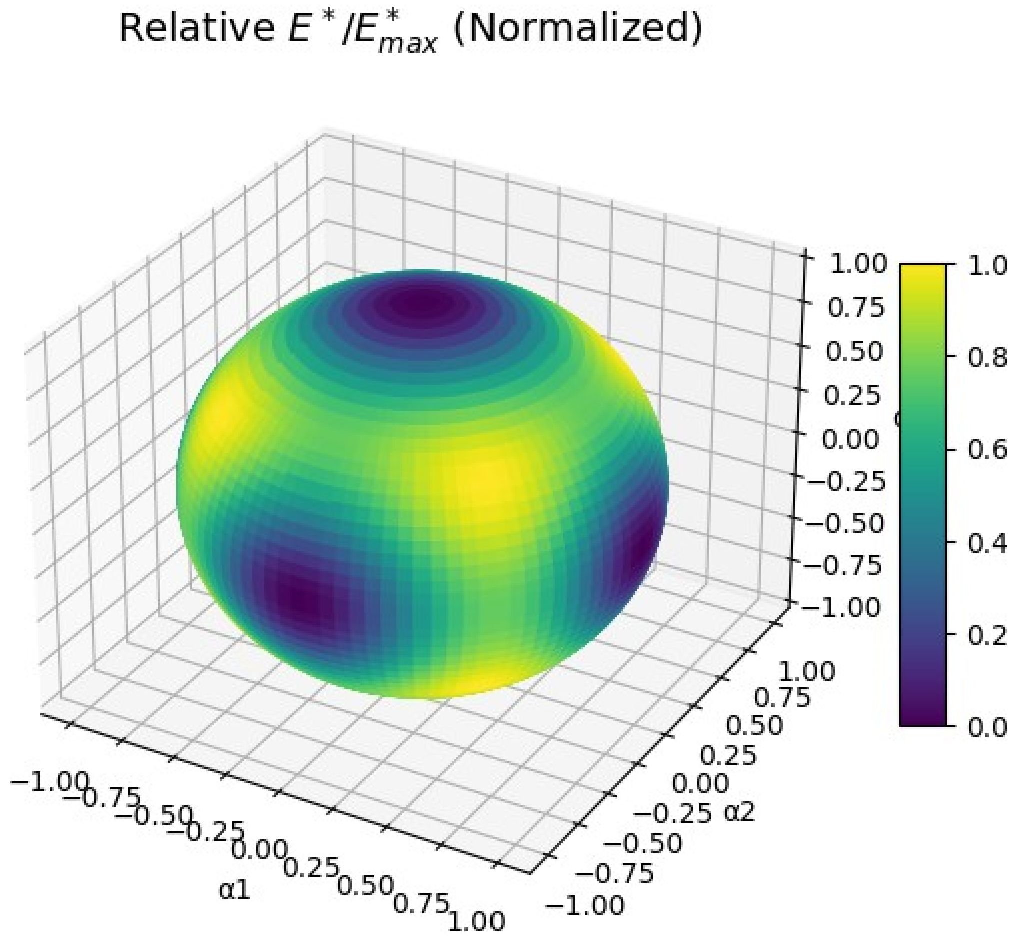

Gap Anisotropy Height and H_{c2}/H_P Color Map
Gap Anisotropy
1.00
1.05
1.10
1.15
1.20
1.25
1.30
α1
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
α2
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
H_{c2}/H_P Enhancement
1.00
1.05
1.10
1.15
1.20
1.25

Gap Anisotropy Factor Δ/Δ_0





Estimated H_{c2}/H_P Enhancement
α1
α2
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
1.25
1.20
1.15
1.10
1.05
1.00



Relative E^*/E^*_{max} (Normalized)
α1
α2
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
0.0
0.2
0.4
0.6
0.8
1.0