Possible superconducting pairing symmetries in 2H-stacking bilayer $NbSe_2$

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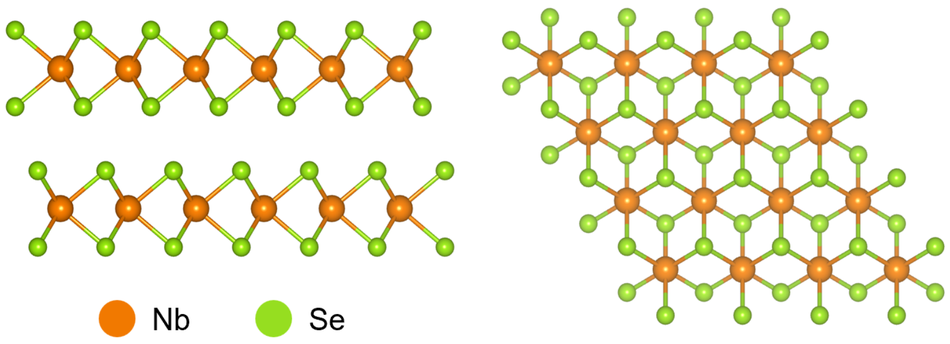
1. Motivation

Motivated by recent experimental breakthroughs of superconducting properties in 2H-stacking $NbSe_2$, this work investigates the **possible pairing symmetries** in **2H-stacking bilayer $NbSe_2$** using Group-Theoretical classification of superconducting states.

In realistic experimental setups, the system is often perturbed by **external experimental factors**, which breaks the inversion symmetry and induces a **Rashba spin-orbit coupling (SOC)** in one. To understand this effect, we compare the superconducting phase diagram in these two scenarios.



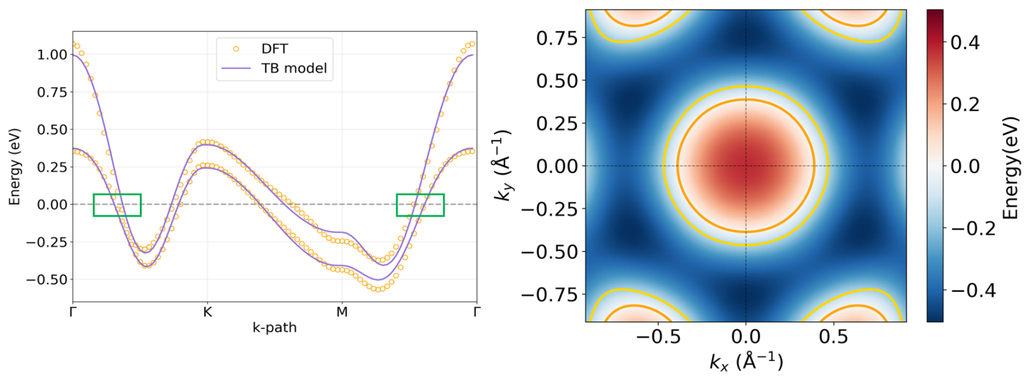
2. Tight-Binding Model and Symmetry

We construct a tight-binding model based on the **Nb d_{z^2} orbitals**. The basis is defined as $\{d_{z^2,1}, d_{z^2,2}\}$, where the indices $1, 2$ denote the layer index.

The monolayer and bilayer Hamiltonians are given by:

$$\hat{H}_{\text{mono}}(\mathbf{k}) = \xi_{\mathbf{k}}\sigma_0 + \Lambda_{\mathbf{k}}\sigma_z, \quad \hat{H}_{\text{bi}}(\mathbf{k}) = \begin{pmatrix} \hat{H}_{\text{mono}}(\mathbf{k}) & \hat{H}_{\text{int}}(\mathbf{k}) \\ \hat{H}^{\dagger}_{\text{int}}(\mathbf{k}) & \hat{H}_{\text{mono}}(-\mathbf{k}) \end{pmatrix}$$

Here, ξ_k denotes the kinetic term, $\Lambda_{\mathbf{k}}$ represents the **Ising SOC** terms.All model parameters are fitted from DFT calculations. Specifically, we consider **intralayer hoppings** up to the 5th nearest neighbor (5NN) and **interlayer hoppings** up to the 3rd nearest neighbor (3NN).



Nb d_{z^2} orbitals are predominant at the Γ point in Density of States (DOS) calculations. Consequently, we restrict our analysis to the pairing instabilities on the Fermi surface pockets surrounding the Γ point (highlighted by the green box above). Here we enforce an active pairing energy window of **15 meV** around the Fermi level.

Classification of spin-singlet and spin-triplet basis gap functions based on D_{3d} symmetry. The basis function are generated from C_{3v} irrep A_1, A_2, E, where $C(\mathbf{k}) = \frac{1}{\sqrt{3}}(\cos k_1 + \cos k_2 + \cos k_3)$, $C_+(\mathbf{k}) = \frac{1}{\sqrt{3}}(\cos k_1 + e^{i\frac{2\pi}{3}}\cos k_2 + e^{i\frac{4\pi}{3}}\cos k_3)$, $S(\mathbf{k}) = \frac{1}{\sqrt{3}}(\sin k_1 + \sin k_2 + \sin k_3)$, $S_+(\mathbf{k}) = \frac{1}{\sqrt{3}}(\sin k_1 + e^{i\frac{2\pi}{3}}\sin k_2 + e^{i\frac{4\pi}{3}}\sin k_3)$, and τ matrix represent layer degree.

Γ	Singlet basis	Singlet τ	Triplet basis	Triplet τ
A_{1g}	$\Psi^{A_1,on} = 1$ $\Psi^{A_1,nn} = C(\mathbf{k})$	τ_0	$d^{A_1,z} = S(\mathbf{k})\, z$ $d^{A_1,xy} = [S_-(\mathbf{k})\,\mathbf{x}_+ - S_+(\mathbf{k})\,\mathbf{x}_-]$	τ_z
A_{2g}	–	–	$d^{A_2,xy} = S_-(\mathbf{k})\,\mathbf{x}_+ + S_+(\mathbf{k})\,\mathbf{x}_-$	τ_z
Eg	$\Psi_1^{E,nn} = C_+(\mathbf{k})$ $\Psi_2^{E,nn} = C_-(\mathbf{k})$	τ_0	$d_1^{E,z} = S_+(\mathbf{k})\, z$ $d_2^{E,z} = S_-(\mathbf{k})\, z$	τ_z
A_{1u}	$\Psi^{A_1,on} = 1$ $\Psi^{A_1,nn} = C(\mathbf{k})$	τ_z	$d^{A_1,z} = S(\mathbf{k})\, z$ $d^{A_1,xy} = [S_-(\mathbf{k})\,\mathbf{x}_+ - S_+(\mathbf{k})\,\mathbf{x}_-]$	τ_0
A_{2u}	–	–	$d^{A_2,xy} = S_-(\mathbf{k})\,\mathbf{x}_+ + S_+(\mathbf{k})\,\mathbf{x}_-$	τ_0
Eu	$\Psi_1^{E,nn} = C_+(\mathbf{k})$ $\Psi_2^{E,nn} = C_-(\mathbf{k})$	τ_z	$d_1^{E,z} = S_+(\mathbf{k})\, z$ $d_2^{E,z} = S_-(\mathbf{k})\, z$	τ_0

3. Linear Gap Equation

We define the basis pairing matrices as $\Psi^{(r)}_{\Gamma,m}(\mathbf{k}) = \psi^{(r)}_{\Gamma,m}(\mathbf{k})i\sigma_y$ and $D^{(r)}_{\Gamma,m}(\mathbf{k}) = \mathbf{d}^{(r)}_{\Gamma,m}(\mathbf{k})\cdot\boldsymbol{\sigma}i\sigma_y$. According to symmetry constrain, the interaction is then expanded in terms of coupling constants $\{v_r(\Gamma)\}$:

$$V_{s's s_1 s_2}(\mathbf{k},\mathbf{k}') = -\sum_{r,m,\Gamma}\frac{v_r(\Gamma)}{A}\times\left\{[\Psi^{(r)}_{\Gamma,m}(\mathbf{k})]_{ss'}[\Psi^{(r)}_{\Gamma,m}(\mathbf{k}')]^*_{s_1s_2} + [D^{(r)}_{\Gamma,m}(\mathbf{k})]_{ss'}[D^{(r)}_{\Gamma,m}(\mathbf{k}')]^*_{s_1s_2}\right\}$$

Substituting this expansion, the linearized gap equation transforms into:

$$\Delta(\mathbf{k}) = -\frac{k_BT_c}{A}\sum_{n,\mathbf{k}',r,m,\Gamma} v_r(\Gamma)\times\{\Psi^{(r)}_{\Gamma,m}(\mathbf{k})\,\mathrm{tr}[\Psi^{(r)}_{\Gamma,m}(\mathbf{k}')^\dagger G_e(\mathbf{k}',i\omega_n)\Delta(\mathbf{k}')G_h(\mathbf{k}',i\omega_n)] + D^{(r)}_{\Gamma,m}(\mathbf{k})\,\mathrm{tr}[D^{(r)}_{\Gamma,m}(\mathbf{k}')^\dagger G_e(\mathbf{k}',i\omega_n)\Delta(\mathbf{k}')G_h(\mathbf{k}',i\omega_n)]\Big\}$$

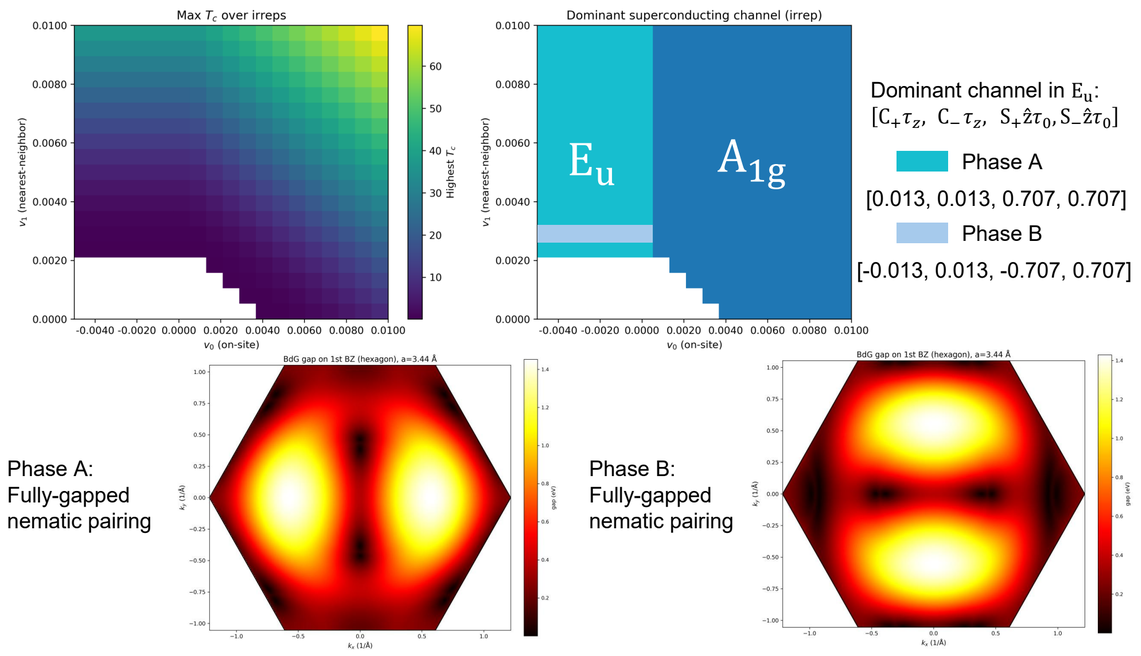
Meanwhile, the pairing field can be expressed in terms of the order parameters s_n and t_n:

$$\Delta_\Gamma(\mathbf{k}) = \sum_{r,m}\left[s_r(\Gamma,m)\Psi^{(r)}_{\Gamma,m}(\mathbf{k}) + t_r(\Gamma,m)D^{(r)}_{\Gamma,m}(\mathbf{k})\right]$$

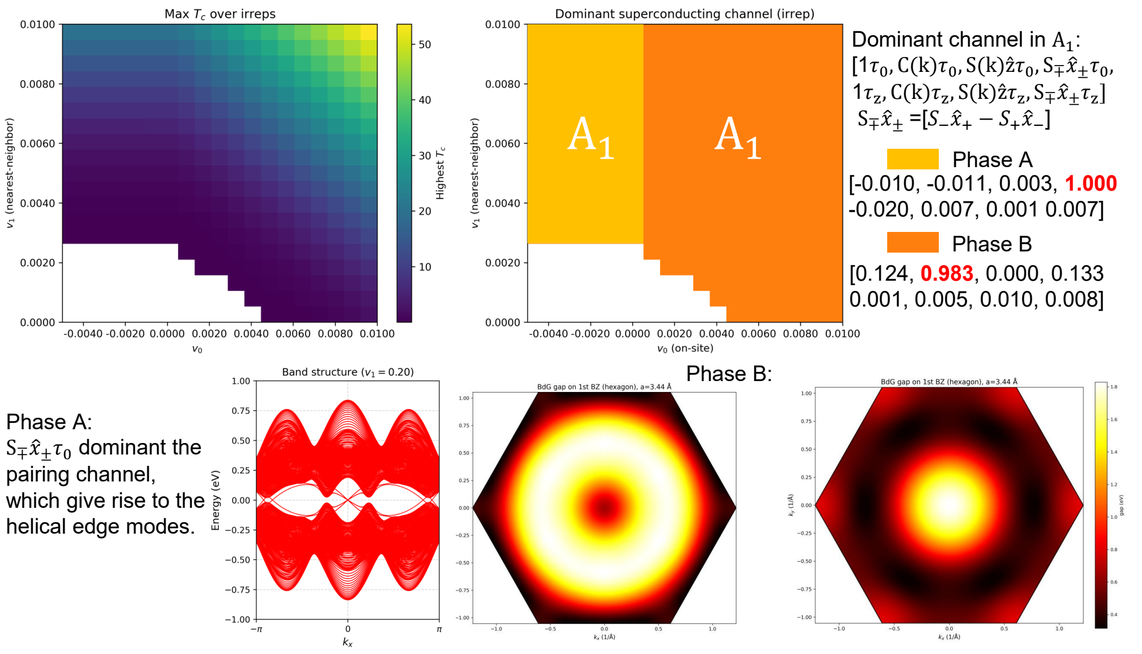
By substituting this expansion into the linearized gap equation, we can solve the system self-consistently.

4. Phase Diagram

Possible pairing phase diagram of bilayer 2H-$NbSe_2$ without Rashba SOC:



Possible pairing phase diagram of bilayer 2H-$NbSe_2$ with Rashba SOC at one layer(C_{3v}):



Conclusions:

1. In the absence of Rashba SOC, a negative interaction strength ($v_1 < 0$) leads to a nematic pairing state that preserves time-reversal symmetry.
2. With Rashba SOC applied to one layer, the $S_-\hat{x}_+ - S_+\hat{x}_-$ channel becomes dominant due to its alignment parallel to the Rashba spin-orbit coupling vector.

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