Superconducting dome driven by intervalley phonon scattering in monolayer MoS₂

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Abstract

We combine first-principles calculations, a three-band tight-binding model, and Bardeen–Cooper–Schrieffer theory to explore the physical mechanism for a dome-shaped dependence of superconducting transition temperature of monolayer MoS₂ on electron doping concentration, which has been observed experimentally (2012 Science 338 1193). We find that in the process of doping more electrons contribute to superconducting pairing, but above some doping value the effective attractive interaction decreases so greatly that it starts to reduce the pairing strength, forming a superconducting dome. Therefore, the dome behavior can be attributed to the competition between the growing Fermi pocket (corresponding to an increase of the number of intervalley phonon scatterings) and the screened intervalley phonon scattering (corresponding to a decrease of scattering probability).

1. Introduction

Molybdenum disulfide (MoS₂) is a layered transition-metal dichalcogenide with a weak interlayer interaction. Its bulk and monolayer are direct and indirect band-gap semiconductors, respectively. The former has shown novel tribological [1], catalytic [2, 3], and photovoltaic [4] properties. Recently, several experimental groups have reported a gate-induced superconducting state at the surface of gated MoS₂ flakes [5–8]. Particularly, an interesting field-doping-induced superconducting dome was observed in a temperature-doping phase diagram of monolayer MoS₂ [5]. Upon raising carrier concentration of the MoS₂ monolayer, the superconductivity sharply appears at $6.8 \times 10^{13}$ cm$^{-2}$, peaks with a maximum $T_c = 10.8$ K at $1.2 \times 10^{14}$ cm$^{-2}$ and then the critical temperature decreases as doping increase. Actually, this dome phenomenon is often observed near the quantum critical point of a magnetic ground state of unconventional superconductors, such as cuprates, pnictides, and heavy fermions. A widely accepted explanation is that the unconventional superconductivity is driven by critical phase fluctuations of the intertwined electronic order [9]. For conventional superconductors, such a dome is not a general feature. But it has also been observed in several systems, including Li [10] and Fe [11] metals under pressure, doped SrTiO₃ [12, 13], gated LaAlO₃/SrTiO₃ interface [14], XSe₂ ($X = Ti$ and Nb) families [15–17], o-TaS₃ [18], and the MoS₂ monolayer [5]. Because of the diversity on lattice structure, dimension, and external factors, there is still no a solid and unifying theoretical explanation. Therefore, it is highly desirable to study what the physical mechanism is for such a superconducting dome in conventional superconductors.

Several groups have theoretically studied the superconducting dome of MoS₂ in a similar approach [19–21]. They first obtain electron–phonon coupling constants from first-principles calculations, and then estimate superconducting transition temperatures using the Allen–Dynes formula based on Eliashberg theory [22, 23]. In this work, we use a more fundamental and direct approach (tight-binding model and Bardeen–Cooper–Schrieffer (BCS) theory) to explain the dome behavior. Our results show that the superconducting dome is driven by intervalley phonon scattering. With increasing electron doping concentration there is more carriers near the Fermi level in each
conduction-band valley, while the total attractive interaction from intervalley phonon scattering decreases. Their competition leads to the superconducting dome. In addition, we introduce a superconducting pairing term into the Hamiltonian. Through analyzing effective interactions from BCS theory and solving superconducting order parameters self-consistently, we obtain a superconducting dome theoretically, which is in agreement with the experimental measurement. Finally, we conclude this work with a brief summary in section 4.

2. First-principles calculations, tight-binding fitting and superconducting hamiltonian

Figure 1(a) shows the monolayer MoS₂ lattice structure in top view. It is a two-dimensional rhombic lattice with a \( D_{3h} \) point-group symmetry, and each unit cell contains one Mo atom and two S atoms. Our first-principles calculations were carried out using the WIEN2K package with a full-potential augmented plane wave method [24]. The electronic structures were calculated using standard density functional theory (DFT) based on the Perdew–Barke–Ernzerhof generalized gradient approximation (PBE-GGA) [25]. Optimized structural parameters are from [26]. The muffin-tin radii are set to 2.44 and 2.10 a.u. for Mo and S atoms, respectively. The number of \( k \) points in the first Brillouin zone is at least 3000 for electronic self-consistent iterations. We have compared electronic structures of the cases with and without spin-orbital coupling (SOC) and find that for the former there is an obvious splitting of the valence band around \( K \) point. But in this work we focus on the bottom of the conduction band without any splitting. Thus, in the following model study we do not consider the SOC interaction.

Up to now, several groups have fitted the band structure using tight-binding models through considering different orbitals [27–30]. Our first-principles calculations show that the bands near the Fermi level are mainly contributed by Mo–4\( d_{x^2−y^2} \), \( d_{xy} \) and \( d_{z^2} \) orbitals, which are plotted in figure 1(b), and the latter two are degenerate. We choose these three orbitals to construct a tight-binding model

\[
H_{TB} = \sum_{i,\alpha,\sigma} \epsilon_\alpha \hat{d}_\alpha^{\dagger} \hat{d}_\alpha + \sum_{i,\alpha,\beta,\sigma} t_{R_{\alpha\beta}} \hat{d}_i^{\dagger} \hat{R}_{\alpha\beta\sigma} \hat{d}_{i+R_{\alpha\beta}}
\]

where \( \hat{d}_\alpha^{\dagger} (\hat{d}_{i\alpha\sigma}) \) is a creation (annihilation) operator with the orbital indices \( \alpha, \beta = 1, 2, 3 \) (corresponding to \( 3\vec{z}^2 − \vec{r}^2, \vec{x}\vec{y}, \text{ and } \vec{z}^2 \) respectively) and the spin index \( \sigma = \uparrow, \downarrow \) at site \( i \), and \( R = R_{\alpha\beta} \) is the nearest-neighbor (NN) Mo–Mo vector. \( \epsilon_\alpha \), and \( t_{R_{\alpha\beta}} \) are the energy level of orbital \( \alpha \) and the hopping integral from orbital \( \beta \) to \( \alpha \) along \( R \) direction, respectively. \( t_{R_{\alpha\beta}} \) is chosen as fitted parameters and the other hopping parameters can be found in appendix.

Then, we use the tight-bind model to fit the DFT band structure of the monolayer MoS₂. Since there is no definitive strategy to fit the bands, the values of the fitted parameters (see table 1) are a little different from those given in [30], in order to fit the bottom of the conduction band better. The corresponding band structures are

| \( t_1 \) | \( t_2 \) | \( t_{R_{11}} \) | \( t_{R_{12}} \) | \( t_{R_{13}} \) | \( t_{R_{22}} \) | \( t_{R_{23}} \) | \( t_{R_{33}} \) |
|------|------|------|------|------|------|------|------|
| 1.090 | 2.139 | -0.182 | 0.366 | 0.529 | 0.222 | 0.337 | 0.052 |

Figure 1. (a) Top view of monolayer MoS₂. Big blue and small green spheres are Mo and S atoms, respectively. \( R_{x, y} \) vectors show six Mo–Mo nearest neighbors. (b) Sketch of Mo–4\( d_{x^2−y^2} \) (red), \( d_{xy} \) (green), and \( d_{z^2} \) (white) orbitals.
plotted in figure 2(a). By comparing band structures and orbital weights between the tight-binding model and DFT calculations, we find that they agree well with each other in the bottom of the conduction band. Figure 2(b) shows the energy contours around the conduction band minimum (K point) for the monolayer MoS2. Again, we observe excellent agreement in the shape of the energy contours from DFT-PBE-GGA and tight-binding fitting.

First-principles results show that the electronic states at the bottom of the conduction band are mainly contributed by the Mo-4d orbital. So we only consider the BCS superconducting pairing of 4d_{z^2-r^2} electrons and ignore other pairings. The interaction term for the superconducting pairing is given as

$$H_I = U \sum_i n_{i1\uparrow} n_{i1\downarrow}$$

with $n_{i1\sigma} = \dagger d_{i1\sigma} d_{i1\sigma}$. $U$ is a local effective interaction for BCS superconducting pairing. Furthermore, we perform a mean-field decoupling with respect to the superconducting order parameter $\Delta = U \langle d_{i1\uparrow} d_{i1\downarrow} \rangle$ and a Fourier transformation

$$H_I = \frac{1}{2} \sum_k (\Delta_{d_{k1\uparrow} d_{k1\downarrow}}^{\dagger} + \Delta_{d_{-k1\downarrow} d_{k1\uparrow}}),$$

These particles at each site satisfy the constraint $n_0 = \sum_{\alpha, \sigma} n_{i0\alpha\sigma}$. The Hamiltonian of the local constraint at every site is replaced by a global one

$$H_{\mu} = \mu \sum_{i, \alpha, \sigma} n_{i0\alpha\sigma}.$$  

Then the total Hamiltonian can be written as

$$H_{tot} = H_{TB} + H_I - H_{\mu}.$$  

3. Effective interactions and self-consistent solutions

3.1. Effective interactions based on BCS theory

As well known, in conventional BCS superconductors the formation of Cooper pairs is attributed to the electron–phonon coupling. With increasing electron concentration, the coupling will be screened gradually, causing that the effective attractive interaction between electrons near the Fermi level decays [31–34]. To explain the superconducting dome phenomenon, it is critically important to find what relationship the effective attractive interaction and doping concentration satisfy. Here, we start from the BCS theory and give a qualitative analysis.

Following the BCS theory, we can write the Hamiltonian of the effective attractive interaction from the virtual exchange of phonons in the form [31, 33]:

$$H_{attr} = \frac{1}{2} \sum_{k, q, \sigma} V_{kq}^{\text{attr}} \dagger d_{k+q, \sigma} d_{-k-q, -\sigma} d_{-k, -\sigma} d_{k, \sigma},$$

Figure 2. (a) Band structures of monolayer MoS2 and (b) contour plots of the energies around the conduction band minimum (K point) from DFT (red dashed lines) and tight-binding (blue solid lines) calculations. Contour lines are placed at $E = 1.64, 1.71, 1.78, 1.92$, and $2.05$ eV. They are plotted through examining the energy value at each $k$ point with an accuracy of 0.01 eV, leading to uneven curves. (c) Sketch of the intervalley phonon scattering in the first Brillouin zone.
where \( V_{\text{attr}}^{k-q} = \left( \frac{N_0}{2M\omega_0} \right) \left( \frac{4\pi e^2}{q^4} \right) (\hbar^2 q^2)^2 \frac{2\omega_0}{\hbar k_{\text{eq}} - \hbar k^r - \hbar k_0^r}. \) The index of orbital \( 3z^2-r^2 \) is ignored and the vacuum dielectric constant \( \varepsilon_0 \) has been set to 1. \( \lambda^2 = \frac{6\pi e^2}{k_{\text{eq}} m} \) is a screening factor. \( \hat{q} \) is the polarization vector of phonons. For simplicity, we assume the polarization direction is parallel to the scattering direction.

When \( |E_{k+q} - E_k| < \hbar\omega_0 \), there is an effective attractive interaction between each pair of electrons and a larger difference of energy levels will lead to a stronger attractive interaction. In order to guarantee all of electrons in this region to be paired, we only qualitatively consider the smallest attractive interaction with \( E_{k+q} = E_k \). Then we can obtain

\[
V_{k-q}^{\text{attr}} = -\frac{4\pi e^2 (q^2 + \lambda^2)}{q^4}.
\]

Besides the above indirect attractive interaction, there is a direct Coulomb interaction between electrons. For the electrons which participate in superconducting pairing, the corresponding Hamiltonian is given [31, 33]

\[
H_{\text{coal}} = \frac{1}{2} \sum_{k,\sigma} V_{k-q}^{\text{coal}} d_{k+q,\sigma}^\dagger d_{-k-q,\sigma} d_{-k,\sigma} d_{k,\sigma}
\]

with

\[
V_{k-q}^{\text{coal}} = \frac{4\pi e^2}{q^2 + \lambda^2}.
\]

Previous theoretical studies by Cohen have pointed out that the largest contribution to the attractive electron-electron interaction in many-valley semiconductors arises from the exchange of intervalley phonons [35]. For example, in SrTiO3 the intervalley phonon interaction is the dominant attractive interaction [12]. Thus, for the many-valley MoS2 monolayer, we only consider intervalley phonon scattering, as illustrated in figure 2(c). In the momentum space there are three kinds of intervalley scatterings, including NN, next NN and third NN intervalley scatterings. The scattering moment \( q \) is defined as

\[
q = 2(\beta K + \alpha k_0),
\]

where \( |K| \) and \( k_0 \) are two scalars and their corresponding vectors are marked in figure 2(c). \(-0.5 < \alpha < 0.5 \) and \( 0.5 < \beta < 1 \). Here, the two parameters are set as two global effective ones for all intervalley scatterings in following calculations.

The carrier concentration at the bottom of the conduction band is \( n = \frac{4\pi k^2}{\Omega} \), where \( \Omega \) is the area of the first Brillouin zone and \( n + 2 = n_0 \). Substitute \( E_F = \frac{m_0 q^2}{2} \) and \( \nu_F = \frac{\hbar v_F}{m} \) into the screening factor, then \( \lambda^2 = \frac{4\pi e^2 m}{\omega_0^2} \). One can find that it is a constant with respect to the doping concentration. The total effective interaction is given as

\[
U = V_{k-q}^{\text{attr}} + V_{k-q}^{\text{coal}} = -\frac{4\pi e^2 \lambda^2}{q^4 (q^2 + \lambda^2)}.
\]

Substitute the scattering momentum with equation (10) and \( k_0 = \frac{1}{2} \sqrt{\frac{n_0}{\pi}} \), and set \( A = \frac{2\beta |K|}{\alpha} \sqrt{\frac{\pi}{n_0}} \), \( B = \frac{\pi \lambda^2}{\alpha \lambda^2} \), and \( C = \frac{4\pi e^2 \beta^2}{\lambda^2} \). The total interaction can be rewritten as a function of doping concentration

\[
U = -\frac{2C(A + \sqrt{m})^2 + BC}{(A + \sqrt{m})^4},
\]

3.2. Results and discussion

In the experiment about the superconducting dome of MoS2 by Ye et al [5], the superconductivity sharply appears at the doping concentration \( n_{2D} = 6.8 \times 10^{13} \text{ cm}^{-2} \). For the non-superconducting behavior at low doping concentration, previous theoretical studies by Das et al have given a explanation that the Coulomb interaction is larger than the attractive interaction [21]. However, we think there may be another explanation. Look back to the experiment, where \( n_{2D} \) is measured by Hall effect at 20 K and is estimated from the Thomas Fermi screening length. It is assumed that the carriers are accumulated in a half of the top unit cell [5]. So it is also possible that the measured carriers are not all from the top monolayer. Part of them may be from the bulk.

To clarify this issue, we compare band structures between a bulk system and a monolayer one in figure 3. The deep level of Mo-4s electrons is chosen as a reference. We find that the conduction band bottom of the bulk system is about 0.25 eV lower than that of the monolayer system. The inset of figure 3 shows a constant-energy surface of the bulk system at \( E = 1.05 \text{ eV} \), which corresponds to the conduction bottom of the monolayer system. There are six approximate spheres with a diameter \( d = 0.233 |\Gamma K| \). We can calculate the corresponding carrier concentration of the experimental sample (~20 nm thick) with respect to a two-dimensional system,
$n_{2D} \approx 1.24 \times 10^{14} \text{ cm}^{-2}$. The carriers will not contribute to the surface superconductivity of the sample. When the HfO$_2$ back gate $V_{BG} = -4 \text{ V}$ is not applied, which has been applied in experiments [5], there are approximate $6.23 \times 10^{13} \text{ cm}^{-2}$ doped carriers entering into the bulk. This value is close to the critical carrier concentration, $6.8 \times 10^{13} \text{ cm}^{-2}$. Therefore, for the non-superconducting behavior at low doping concentration, we think the carriers are doped into the bulk of the sample. In the following we will shift the horizontal axis from $n_{2D} = 0$ to $6.8 \times 10^{13} \text{ cm}^{-2}$ and use the equation $\frac{2\Delta}{k_B T_c} = 3.53$ to estimate the superconducting transition temperature [36].

Based on the expression of the total effective interaction (equation (12)), we perform self-consistent calculations with different doping concentration. Through fitting the experimental superconducting transition temperature of the monolayer MoS$_2$ [5], we obtain $A = 10.466$, $B = 8.0$, $C = 5980.0$. We compare the calculated superconducting transition temperature to the experimental measurement by Ye et al [5] in figure 4. Our calculated result fits the $T_c$ dome quite well.

Note that our fitting result is based on the three-band tight-binding model, which can only fit bands near the Fermi level well, as shown in figure 2(a). With increasing electron concentration, when the chemical potential $\mu$ is greater than 1.9 eV, the tight-binding model will not reflect the real material. Hence, we only calculate the case with the doping concentration less than 0.115 electrons per unit cell.

The effective attractive interaction and the Coulomb interaction has been given in equations (7) and (9), respectively. According to the above assumption and analysis, we can further obtain

$$V_{\text{attr}} = -\frac{C[(A + \sqrt{n})^2 + B]}{B(A + \sqrt{n})^4}$$

and

$$V_{\text{coul}} = \frac{C/B}{(A + \sqrt{n})^2 + B}$$

with omitting the indices $k$ and $q$.

From the fitting result, we plot the two interactions and their sum as functions of the doping concentration $n$ in figures 5(a)–(c). The effective attractive interaction ($V_{\text{attr}}$) between electrons through intervalley phonon scattering decreases with increasing $n$. This is because the rising electron concentration make Fermi pockets become larger, leading to an increase of intervalley scattering momentum of part of electron states. At low temperature, the increase of scattering momentum will reduce the probability of the electron pairing and make the effective attractive potential decay. Similarly, the Coulomb interaction ($V_{\text{coul}}$) also decreases with doping due to the growing Fermi pocket. It should be noted that $V_{\text{coul}}$ is the Coulomb interaction between the electrons which participate in superconducting pairing. Within the considered doping concentration range, the effective attractive interaction is always greater than the Coulomb interaction. This guarantees the superconducting...
pairing between electrons. The decay rate of the effective attractive interaction is larger than that of the Coulomb interaction with increasing $n$. It leads to the decrease of total interaction.

We can further predict some physical quantities qualitatively from the fitting of parameters $A$, $B$, and $C$. For example, the global effective parameters $\alpha = 0.197$ and $\beta = 0.938$, both of which are in a reasonable range. In addition, for a degenerate semiconductor with equivalent valleys Cohen has given a Lindhard dielectric function\[35\], which can be used to estimate the relative dielectric function $\varepsilon_r$ of the monolayer MoS$_2$. Through substituting the scattering moment with equation (10), we can obtain $\varepsilon_r$ as a function of $n$,

$$\varepsilon_r = 1 + \frac{B}{(A + \sqrt{n})^2} \left[ \frac{1}{2} + \frac{n - \alpha^2(A + \sqrt{n})^2}{4\alpha\sqrt{n}(A + \sqrt{n})} \ln \left| \frac{\sqrt{n} + \alpha(A + \sqrt{n})}{\sqrt{n} - \alpha(A + \sqrt{n})} \right| \right]$$

(15)

The calculation results show that $\varepsilon_r$ is close to 1 in the doping range. It is a little different from that given by Molina-Sanchez and Wirtz ($\varepsilon_r = 1.63$ for the case of $n = 0$), which are obtained within density functional perturbation theory\[37\]. But both of them indicate that MoS$_2$ monolayer in the range of considered doping concentration is a non-polar system ($\varepsilon_r < 2.8$). The reasonability of these parameters indicates that our fitting result of the superconducting dome is also qualitatively reasonable.

There have been several theoretical studies to explain the dome-shaped dependence of the superconducting transition temperature on the electron doping concentration by using DFT and Eliashberg theory\[19–21\]. In particular, Das et al reported that both electronic correlation and electron–phonon coupling grows with doping in a bilayer MoS$_2$ system. Above some doping value the former becomes so large that it starts to reduce the quasiparticle–phonon coupling constant and $T_c$, creating a superconducting dome\[21\]. Although their calculation methods may be more advanced than ours (some approximations have been introduced for our effective interactions), we present a totally different physical picture, where it is the competition between the increase of carriers and the decrease of the effective attractive interaction to result in the superconducting dome.

Figure 4. A comparison between the calculated superconducting transition temperature (red curves) and the experimental measurement (green points). Experimental data points in the main figure and the inset are taken from the supplementary materials and the main text of \[5\], respectively. The horizontal axis is transformed into an exponential one in the inset. $n_{2D} = n/S$, where $S$ is the area of the unit cell.

Figure 5. (a) Effective attractive interaction $V^{\text{attr}}$, (b) Coulomb interaction $V^{\text{coul}}$, and (c) total interaction $U$ as functions of doping concentration $n$. A comparison between the calculated superconducting transition temperature (red curves) and the experimental measurement (green points). Experimental data points in the main figure and the inset are taken from the supplementary materials and the main text of \[5\], respectively. The horizontal axis is transformed into an exponential one in the inset. $n_{2D} = n/S$, where $S$ is the area of the unit cell.
4. Summary

In summary, we have performed first-principles calculations and employed a three-band tight-binding model to fit the band structure of MoSe₂ monolayer near the Fermi level. From the BCS theory, we find that the interaction which induces superconducting phases arises from the virtual exchange of intervalley phonons and the direct Coulomb repulsion between electrons. It depends sensitively on doping concentration. After introducing the interaction term into the tight-binding model, we solve the BCS superconducting order parameter self-consistently. Furthermore, through a fitting of the experimental data, the functional relationship between the interaction and doping concentration is obtained. Finally, we conclude that it is the competition between the growing Fermi pocket and the screened intervalley phonon scattering to lead to the dome-shaped dependence of the superconducting transition temperature on doping concentration. The former increases the number of intervalley phonon scatterings, while the latter decreases the probability of the scattering. This physical mechanism may also work for other BCS superconductors with a similar superconducting dome.

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Appendix. Hopping parameters in the tight-binding model

In section 2, we introduce a three-band tight-binding model involving Mo–4d_{z²−r²}, d_{xy}, and d_{x²−y²} orbitals and NN hoppings. The corresponding Hamiltonian is given in equation (1). We choose $t_{R_{ij};k}$ as fitted parameters to fit the DFT band structure of the monolayer MoSe₂. The hopping parameters along the other directions can be obtained according to the point-group symmetry ($D_{3h}$), as shown below:

$$
\{ t_{R_{ij};1} = t_{R_{ij};1} \}
$$

$\times$

$$
\{ t_{R_{ij};2} = \frac{1}{4} t_{R_{ij};2} - \frac{\sqrt{3}}{2} t_{R_{ij};32} - \frac{\sqrt{3}}{2} t_{R_{ij};23} + \frac{1}{2} t_{R_{ij};33} \}
$$

$\times$

$$
\{ t_{R_{ij};3} = -\frac{\sqrt{3}}{4} t_{R_{ij};2} - \frac{1}{4} t_{R_{ij};32} + \frac{1}{2} t_{R_{ij};23} - \frac{\sqrt{3}}{4} t_{R_{ij};33} \}
$$
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