Temperature Dependence of the Energy-Band Structure for the Holstein Molecular-Crystal Model*

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Abstract: We study the influences of the temperature on the energy-band structure for the Holstein molecular-crystal model. We show that the energy-band width and the energy-gap width of a solid are relevant to both the interaction between an electron and thermal phonons and to thermal expansion. For a one-dimensional Li atom lattice chain, under the chosen parameters, the width of the 1s and 2s energy bands narrows as the temperature increases and the energy-gap width between the two bands widens. These results agree qualitatively with those observed experimentally. Studying temperature dependence of the energy-band structure is of great importance for understanding optical and transporting characteristics of a solid.

Key words: temperature dependence; energy-band structure; thermal phonon; thermal expansion
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1 Introduction

Electron-phonon interaction has been a major subject in condensed matter physics. Almost seven decades ago, Landau first introduced the concept of a polaron, a quasiparticle formed by an electron and phonons. Due to Coulomb interaction, the electron will be accompanied by the lattice deformation. Meanwhile, the deformation potential induced by the lattice deformation will affect the electron and the state of motion of an electron depends largely on the interaction between the electron and phonons. The study of the electron-phonon interaction is important in understanding dynamic properties of an electron in a solid.

In the past several decades, the study of electron-phonon interactions has been fruitful[1~18]. In 1957, Bardeen, Cooper and Schrieffer[1] established the BCS theory of superconductivity based on phonon-mediated Cooper pairs. The electron-phonon interaction plays an important role in forming Cooper pairs. Recently, a large amount of experimental results, ranging from infrared spectroscopy to transport properties involving the colossal magnetoresistance and high-Tc superconductivity, has revealed the importance of the electron-phonon interaction[10] and renewed interest in studying models of the electron-phonon coupled system.

In the study of electron-phonon coupled system, the relatively simple Holstein model is mostly considered for the interaction of a single tight-binding electron coupled to phonons. Various theoretical methods, such as the Global-Local variational method[5], the coherent-state expansion method[6], and variational approaches[7,10], have been developed to study the physical characteristics of the Holstein polaron including the ground-state energy, polaron energy band, and effective mass. However, so far, no work examining the influences of the temperature on the energy-band structure of the Holstein model has been reported.

The main aim of this paper is to investigate the influences of the temperature on the energy gap and the energy-band width of the Holstein molecular-crystal model. In the early period, the influence of the temperature on the energy-gap width of semiconductors was observed experimentally[19]. While the energy-gap width of most semiconductors narrows, a few widen as well. However, some experimental results have not yet been adequately explained. In this paper, we consider the influences of the temperature on the energy-band structure of the Holstein molecular-crystal model from two aspects: the interaction between the electron and thermal phonons, and thermal expansion.

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2 Model and the canonical transformation

The Hamiltonian for the Holstein molecular-crystal model is[6,7,10]

$$H = H^{\mathrm{ex}} + H^{\mathrm{ph}} + H^{\mathrm{ex\text{-}ph}} \tag{1}$$

with

$$H^{\mathrm{ex}} = \sum_n \varepsilon c_n^+ c_n - J\sum_n c_n^+ (c_{n+1} + c_{n-1}) \tag{2}$$

$$H^{\mathrm{ph}} = \hbar\omega \sum_n b_n^+ b_n \tag{3}$$

$$H^{\mathrm{ex\text{-}ph}} = -g\sum_n c_n^+ c_n (b_n^+ + b_n) \tag{4}$$

in which H^{ex} describes an electron in the tight binding approximation, c_n^+ (c_n) is the electron creation (annihilation) operation at site n, and J is the electron transfer integral between nearest-neighbor sites. H^{ph} is the Hamiltonian of N identical Einstein oscillators, b_n^+ creates a quantum of vibrational energy in the Einstein oscillator at site n, and ω is the Einstein frequency. $H^{\mathrm{ex\text{-}ph}}$ is the term of the electron-phonon interaction, and g is the electron-phonon coupling constant.

For convenience, we transform the local phonon operators in site n into the operators in the phonon momentum space, making the following substitution

$$b_n^+ = \frac{1}{\sqrt{N}}\sum_q \mathrm{e}^{iq\cdot n} b_q^+, \quad b_n = \frac{1}{\sqrt{N}}\sum_q \mathrm{e}^{iq\cdot n} b_q \tag{5}$$

Substituting Eq. (5) into Eq. (1), and noting $\frac{1}{N}\sum_n \mathrm{e}^{\mathrm{i}(q-q')\cdot n} = \delta_{qq'}$, $\frac{1}{N}\sum_q \mathrm{e}^{\mathrm{i}q\cdot(n-n')} = \delta_{nn'}$, we have

$$H = \sum_n \varepsilon c_n^+ c_n - J\sum_n \sum_\rho c_{n+\rho}^+ c_n + \hbar\omega\sum_q b_q^+ b_q - \frac{g}{\sqrt{N}}\sum_n \mathrm{e}^{-iq\cdot n} c_n^+ c_n (b_{-q}^+ + b_q) \tag{6}$$

In Eq. (6), there is still the electron-phonon coupling term, which causes complexity in the treatment of the polaron energy band. In order to pave the way for the following sections, we introduce the following canonical transformation

$$\overline{H} = e^{-S} H e^{S} \tag{7}$$

The chosen transformation S is

$$S = (g/\hbar\omega)\sum_{q,n} \frac{1}{\sqrt{N}} \mathrm{e}^{-iq\cdot n} c_n^+ c_n (b_{-q}^+ - b_q) \tag{8}$$

The transformations of phonon and electron operators are

$$e^{-S} b_q e^{S} = b_q + \frac{g}{\hbar\omega}\sum_n \frac{1}{\sqrt{N}} \mathrm{e}^{iq\cdot n} c_n^+ c_n \tag{9}$$

$$e^{-S} b_q^+ e^{S} = b_q^+ + \frac{g}{\hbar\omega}\sum_n \frac{1}{\sqrt{N}} \mathrm{e}^{-iq\cdot n} c_n^+ c_n \tag{10}$$

$$e^{-S} c_n e^{S} = c_n X_n \tag{11}$$

$$e^{-S} c_n^+ e^{S} = c_n^+ X_n^{-1} \tag{12}$$

with

$$X_n = \exp\left[\frac{g}{\hbar\omega}\sum_q \frac{1}{\sqrt{N}} \mathrm{e}^{-iq\cdot n}(b_{-q}^+ - b_q)\right] \tag{13}$$

$$X_n^{-1} = \exp\left[-\frac{g}{\hbar\omega}\sum_q \frac{1}{\sqrt{N}} \mathrm{e}^{-iq\cdot n}(b_{-q}^+ - b_q)\right] \tag{14}$$

$$X_n X_n^{-1} = X_n^{-1} X_n = 1 \tag{15}$$

From Eqs. (7) and (9)～(12), the Hamiltonian after the canonical transformation becomes

$$\overline{H} = \sum_n \varepsilon c_n^+ c_n - J\sum_n c_{n+\rho}^+ c_n f(\boldsymbol{\rho}) + \hbar\omega\sum_q b_q^+ b_q + \frac{g^2}{\hbar\omega}\sum_n c_n^+ c_n c_n^+ c_n \tag{16}$$

with

$$f(\boldsymbol{\rho}) = \exp\left[\sum_q (\lambda_q^* b_q^+ - \lambda_q b_q)\right] \tag{17}$$

$$\lambda_q = \frac{g}{\hbar\omega\sqrt{N}} \mathrm{e}^{-iq\cdot n}(1 - \mathrm{e}^{-iq\cdot\rho}) \tag{18}$$

In Eq. (16), phonon operators are included in the second term, which shows the electron-phonon interaction will influence the transfer of electrons from one site to another. In addition, $\overline{H}$ contains the quartic term of the electron operators. Therefore, the Holstein model is a complex nonlinear system.

3 Electron energy-band function

In this section, we derive the electron energy-band function of the Holstein model and investigate the effect of the thermal phonons. We assume that motion of an electron is not accompanied by the creation and annihilation of phonons. In this approximate condition, the wave function of the electron-phonon system takes the form

$$|1_\ell, \{n_q\}\rangle = \frac{1}{\sqrt{N}}\sum_\ell \mathrm{e}^{\mathrm{i}k\cdot\ell} |1_\ell\rangle \prod_q |n_q\rangle \tag{19}$$

The electron energy band of the phonon combination state $\{n_q\}$ is the expectation value of the Hamiltonian (16) to the quantum state (19), that is to say

$$E_{\mathrm{k}}(\{n_q\}) = \langle 1_\ell, \{n_q\} | \overline{H} | 1_\ell, \{n_q\}\rangle = \left(\varepsilon + \frac{g^2}{\hbar\omega}\right) - J\sum_\rho \mathrm{e}^{-ik\cdot\rho}\langle\{n_q\}|f(\boldsymbol{\rho})|\{n_q\}\rangle + \hbar\omega\sum_q n_q \tag{20}$$

with

$$\langle\{n_q\}|f(\boldsymbol{\rho})|\{n_q\}\rangle = \prod_q \langle n_q | \left(\exp\left(\sum_q (\lambda_q^* b_q^+ - \lambda_p b_q)\right)\prod_q |n_q\rangle = \prod_q \langle n_q | \exp(\lambda_q^* b_q^+ - \lambda_p b_q) | n_q\rangle \tag{21}$$

When temperature changes, the thermal excitation of phonons influences the electron energy band. By finding the statistical average of phonon combination states, the electron energy-band function of finite temperature can be obtained

$$E_{\mathrm{k}}(T) = \varepsilon + \frac{g^2}{\hbar\omega} -$$

$$J\sum_{\rho}e^{ik\cdot\rho}\prod_{q}\langle\exp(\lambda_q^* b_q^+ - \lambda_p b_q)\rangle_T + \hbar\omega\sum_q\langle n_q\rangle_T \tag{22}$$

in which $\langle n_q\rangle_T$ is the mean phonon number at temperature T and is

$$\langle n_q\rangle_T = 1/[\exp(\hbar\omega/kT) - 1] \tag{23}$$

$\prod_q\langle\exp(\lambda_q^* b_q^+ - \lambda_p b_q)\rangle_T$ can be calculated by using a method similar to that in Ref.[20], and the result is

$$\prod_q\langle\exp(\lambda_q^* b_q^+ - \lambda_p b_q)\rangle_T = e^{-D_T} \tag{24}$$

with

$$D_T = \sum_q|\lambda|^2\left(\langle n_q\rangle_T + \frac{1}{2}\right) \tag{25}$$

$$|\lambda|^2 = \left(\frac{g}{\hbar\omega}\right)^2\times\frac{2}{N}(1-\cos(\boldsymbol{q}\cdot\boldsymbol{\rho})) \tag{26}$$

Using Eqs.(25) and (26), we have

$$D_T = \left(\frac{g}{\hbar\omega}\right)^2\times\left(\langle n_q\rangle_T + \frac{1}{2}\right)\times\frac{2}{N}\sum_q(1-\cos(\boldsymbol{q}\cdot\boldsymbol{\rho})) \tag{27}$$

For the 1D system and in the case of considering the nearest-neighbor approximation, we have

$$\frac{2}{N}\sum_q(1-\cos(\boldsymbol{q}\cdot\boldsymbol{\rho})) = \frac{2}{N}\times\frac{L}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}}(1-\cos qa)\,dq = 2 \tag{28}$$

From Eqs.(22), (24), (27), and (28), the electron energy-band function of a 1D lattice chain is

$$E_k(T) = \varepsilon + \frac{g^2}{\hbar\omega} - 2J\cos ka\,e^{-D_T(a)} + \hbar\omega\sum_q\langle n_q\rangle_T \tag{29}$$

with

$$D_T(a) = 2\left(\frac{g}{\hbar\omega}\right)^2\left(\langle n_q\rangle_T + \frac{1}{2}\right) \tag{30}$$

Similarly, the electron energy-band function of a 2D square lattice is

$$E_k(T) = \varepsilon + \frac{g^2}{\hbar\omega} - 2J(\cos k_x a + \cos k_y a)e^{-D_T} + \hbar\omega\sum_q\langle n_q\rangle_T \tag{31}$$

4 Influence of thermal expansion

In the preceding section, we only considered the interaction between the electron and the thermal phonons. In fact, the lattice constant of a solid changes as the temperature increases. Therefore, the thermal expansion also influences the energy band of a solid. According to tight-binding theory, the energy band function of index n for a solid is

$$E_{nk}(T) = E_n - A_n + \frac{g^2}{\hbar\omega} - J_n\sum_q e^{ik\cdot\rho}e^{-D_T} + \hbar\omega\sum_q\langle n_q\rangle_T \tag{32}$$

in which E_n is the energy level of an isolated atom, and A_n represents the energy level shift of the isolated atom caused by all other atoms except the atom in site ℓ. J_n represents the hopping integral between site ℓ and its nearest neighbors, which transfers the binding electron from one site to another and forms the energy band in a solid. A_n and J_n are calculated with

$$A_n = -\int\Phi_n^*(\boldsymbol{r}-\ell)\sum_{\ell'\neq\ell}V_a(\boldsymbol{r}-\ell')\Phi_n(\boldsymbol{r}-\ell)\,d\boldsymbol{r} \tag{33}$$

$$J_n = -\int\Phi_n^*(\boldsymbol{r})\sum_{\ell'\neq 0}V_a(\boldsymbol{r}-\ell')\Phi_n(\boldsymbol{r}-\boldsymbol{\rho})\,d\boldsymbol{r} \tag{34}$$

where A_n and J_n are the functions of the lattice constant and temperature, in other words, the thermal expansion influences the numerical values of A_n and J_n.

Next, we take the Li atom lattice chain as an example and discuss the temperature dependences of the 1s and 2s energy-band width and the energy-gap width between two energy bands. First, we calculate A_n and J_n. From Eqs.(33) and (34), A_n contains two-center integrals and J_n has two-center and three-center integrals. However, the three-center integrals have not been calculated exactly. Thus, we neglect three-center integrals and introduce a parameter as a remedy for errors. In addition, we employ hydrogen-like atom wave functions as atom-orbit wave functions and two-center integrals are evaluated using elliptic coordinates. After considering these approximations and performing complex calculations, we obtain

$$J_{1s} = M_{1s}Z'_{1s}Z_{1s}(e^2/a_o)(Z_{1s}R/a_o+1)\exp(-Z_{1s}R/a_o) \tag{35}$$

$$A_{1s} = GZ'_{1s}Z_{1s}(e^2/a_o)[1-(Z_{1s}R/a_o+1)\exp(-2Z_{1s}R/a_o)]/(Z_{1s}R/a_o) \tag{36}$$

$$J_{2s} = M_{2s}Z'_{2s}Z_{2s}(e^2/a_o)[(1/4)+(1/8)(Z_{2s}R/a_o)-(1/24)(Z_{2s}R/a_o)^2+(1/96)(Z_{2s}R/a_o)^3]\exp(-Z_{2s}R/2a_o) \tag{37}$$

$$A_{2s} = \frac{G}{2}Z'_{2s}Z_{2s}(e^2/a_o)\langle\{[1-(Z_{2s}R/2a_o+1)\exp(-Z_{2s}R/a_o)]/(Z_{2s}R/a_o)\}-\{3-[2(Z_{2s}R/2a_o)^2+4(Z_{2s}R/2a_o)+3]\exp(-Z_{2s}R/a_o)\}/(Z_{2s}R/2a_o)+3\{1-[(1/3)(Z_{2s}R/2a_o)^3+(Z_{2s}R/2a_o)^2 1.5(Z_{2s}R/2a_o)+1]\exp(-Z_{2s}R/a_o)\}/(Z_{2s}R/2a_o)\rangle \tag{38}$$

in which M_{1s} and M_{2s} are parameters introduced for remedying the neglect of the three-center integrals. Z'_{1s} and Z'_{2s} are the effective nuclear charge number of the nearest-neighbor atom potential of the 1s and 2s orbits, respectively. Z_{1s} and Z_{2s} represent the effective nuclear charge number of 1s and 2s orbital wave functions of the isolated atom, respectively. a_0 is the Bohr radius, G is the number of the nearest-neighbor atoms, and R is the distance between two nearest-neighbor atoms. From Eqs.(35)～(38), we conclude that A_n and J_n are functions of R. Furthermore, R is a function of temperature. Therefore, the thermal ex-

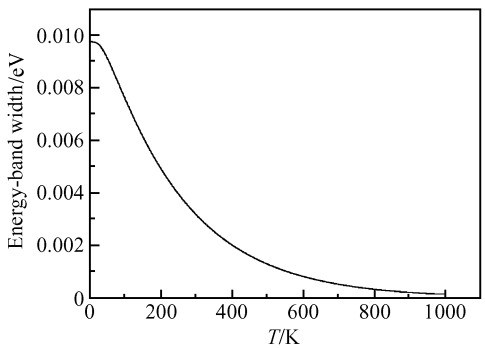

Fig. 1 1s energy-band width as a function of temperature

pansion also influences the energy-band structure of a solid.

Now, we investigate temperature dependence of the energy-band structure. For a one-dimensional Li atom lattice chain, the 1s and 2s energy-band widths are

$$D_{1s} = 4J_{1s}e^{-D_T(a)} \tag{39}$$

$$D_{2s} = 4J_{2s}e^{-D_T(a)} \tag{40}$$

The energy-gap width between the 1s and 2s energy bands is

$$E_f = (E_{2s} - E_{1s}) + (A_{1s} - A_{2s}) - 2(J_{1s} + J_{2s})e^{-D_T(a)} \tag{41}$$

where E_{1s} and E_{2s} are the energy level of the 1s and 2s quantum states for an isolated Li atom. For the numerical calculation, the selection of various parameters is as follows. $M_{1s} \approx 1.0$, $M_{2s} \approx 1.0$, $Z_{1s} \approx 2.1$, $Z'_{1s} \approx 0.2$, $Z_{2s} \approx 1.3$, $Z'_{2s} \approx 0.2$, $\hbar\omega = 0.01$eV, $g = 0.005$eV. Some of these parameters are based on the energy levels of an isolated Li atom, while others are determined by experimental data of the temperature relation of the energy gap obtained with other materials. However, without the experimental data of the Li atom chain, it is difficult to make these parameter values exact.

Using these parameter values, the temperature dependence of the energy-band structure is illustrated in Figs. 1～3. These figures show that, for very low temperatures of about $T < 25$K, the width of the 1s and 2s energy bands narrow slowly and the width of the energy-gap between the two bands rises slowly. When T is larger than 25K roughly, the width of the 1s and 2s energy bands narrow quickly as the temperature increases and the energy-gap width between the two bands widens quickly. When the temperature is high enough, the energy-band width becomes nearly zero, and the energy-gap width tends practically to a constant. In other words, when temperature is very high, the energy-band structure inclines almost to the energy levels of an isolated atom. This situation is in line with the actual physical features.

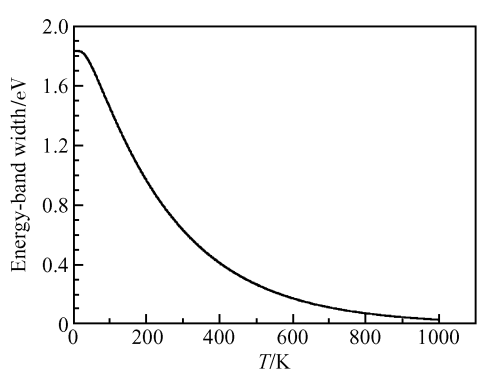

Fig. 2 2s energy-band width as a function of temperature

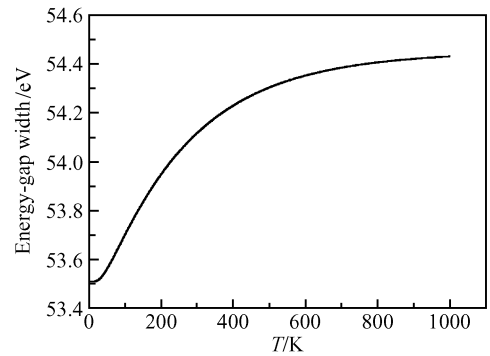

Fig. 3 Energy-gap width between 1s and 2s energy bands as a function of temperature

Figure 4 shows the temperature relation of the average thermal-phonon number and helps us understand the physical significance of the temperature characteristics of the curves in Figs. 1～3. In the low temperature range of about $T < 25$K, the average thermal-phonon number increases slowly as the temperature increases, and then the average thermal-phonon number rises quickly. This situation demonstrates that the temperature characteristics of curves in Figs. 1～3 come mainly from the interaction between the electron and the thermal phonons. The influence of thermal expansion on the energy-band structure of a Li atom chain is very small, giving the curves in Figs. 1～3 such temperature characteristics.

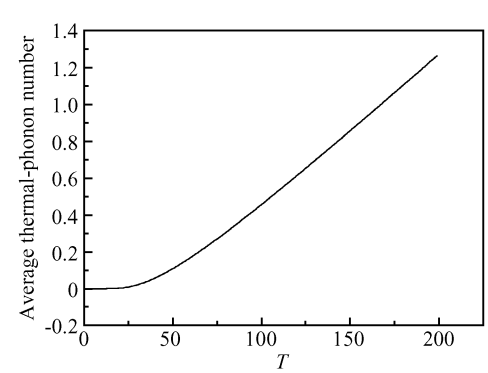

Fig. 4 Average thermal-phonon number as a function of temperature

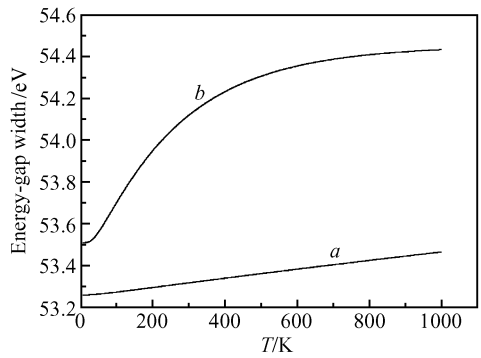

Fig. 5　Energy-gap width as a function of temperature for two different values of the coupling constant g　a: g = 1meV; b: g = 5meV

5 Conclusion

In summary, we studied temperature dependence of the energy-band structure for the Holstein lattice model. Our results indicate that both the interaction between an electron and thermal phonons and thermal expansion influence the energy-band structure of a solid. For a one-dimensional Li atom lattice chain, under the chosen parameters, the energy-band width narrows as the temperature increases, and the energy-gap width widens. These situations are illustrated in Figs. 1～3. In addition, as illustrated in Fig. 5, the temperature dependence of the energy-band structure is highly sensitive to the coupling constant g between an electron and thermal phonons. When the coupling constant g is very small, the energy gap between the 1s and 2s energy bands of a Li atom chain widens very slowly. When the coupling constant g is slightly larger, the energy gap width changes very quickly as the temperature increases. In not too large range of temperature, the energy-band structure tends nearly to the energy levels of an isolated atom. Therefore, when the coupling constant is large enough, the interaction between an electron and thermal phonons play a major role, and the influence of thermal expansion can be ignored.

As pointed out in the introduction, the influence of temperature on the energy-gap width of semiconductors was observed experimentally. However, for a one-dimensional Li atom chain, without experimental data, we can only compare our numerical results with those observed experimentally with other materials. From Ref. (19), the influence of temperature on the energy-gap width between the valence band and the conduction band of the semiconductor Ge is approximately -0.43×10^{-3} (eV/K), and PbTe is roughly 0.35×10^{-3} (eV/K). Our computed value for the one-dimensional Li atom lattice is about 1.0×10^{-3} (eV/K). This result is on the same order of magnitude as those observed experimentally. Therefore, we believe that our results agree qualitatively with experimental ones. By correctly choosing parameters, we might obtain better results.

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Holstein 分子晶体模型能带结构的温度依赖性*

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摘要：研究了温度对 Holstein 分子晶体模型能带结构的影响，结果表明固体的能带宽度和禁带宽度都与电子和热声子相互作用以及热膨胀密切相关.对一维 Li 原子晶格链，在所选定的参数下，1s 和 2s 的能带宽度随着温度的增加而变窄，两带之间的禁带宽度变宽，这些结果与实验结果在定性上是一致的.显然，研究能带结构的温度依赖性对于理解固体的光学和输运性质都是十分重要的.

关键词：温度依赖性；能带结构；热声子；热膨胀
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