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ARTICLE

Calculation of the Energy Levels for a Quantum Dot Coupled to a Fixed Spin Impurity

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Abstract: Quantum dots are considered the cornerstone for the future of quantum computing, and understanding their properties and theories is essential for advancements in this vast field. The physical model is introduced for studying the spin-polarized electron currents through a quantum dot connected to a fixed spin impurity. This quantum dot is made of semiconductor material. The quantum dot features three energy levels, the fixed impurity has one energy level that exhibits different Zeeman splittings under an external magnetic field. A specific MATLAB program is used to solve the Schrödinger equation and calculate the energy levels of the quantum dot and the fixed spin impurity. The values of energy levels are used to calculate the spin-polarized current and polarization. Furthermore, the MATLAB program is utilized to plot the relationship between energy levels and magnetic field strength to explain the effect of the magnetic field produced by the connection between the single quantum dot and the fixed spin.
Keywords: Quantum dots, Spin-orbit interaction, E Spin-polarized electron current.

1. Introduction

Quantum dots are nanoparticles with diameters ranging from 2 to 10 nm, composed of hundreds to thousands of atoms within a single dot [1]. Typically made of semiconductor materials, quantum dots can also be constructed from metals such as gold, silver, copper, and cobalt. Quantum dots have the ability to confine charge carriers in three spatial dimensions due to the confinement force acting in all directions, as well as many allowed states (energy levels) in the quantum dot separately, implying that the quantum dot acts like a single atom rather than a group of atoms. Many known atomic properties, such as shell modeling, selection rules, and optical properties, have a counterpart in quantum dots, earning them the nickname “artificial atoms” [2-6].

The spin-orbit interaction is one of the effects of relative movement. When an electron moves in an electric field, this field generates a magnetic field along the electron’s fixed axis. This magnetic field is paired with the spin of the moving electron. From the electron's perspective, as it orbits the positively charged nucleus, the nucleus appears to revolve around the electron, generating a magnetic field. This field exerts a torque on the spin of the electron, causing its magnetic moment to align with the field [7-10].

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In this paper, we explore the spin-polarized current related to the tunneling through a fixed spin and single quantum dot system attached to leads. This study examines the effects of coherent tunneling t_c, spin-orbit interaction t_{so}, and Zeeman splitting. Our investigation builds upon previous research [12].

Suppose a quantum dot is connected to an impurity with a fixed spin of ½ through tunneling via a twisting tunnel t_c, a spin connection, and a non-twisting orbital t_{so}. As shown in Fig. 1, the quantum dot is also connected to two metal electrodes via a tunneling force at a transmission rate Γ [11].

2. Model and Hamiltonian

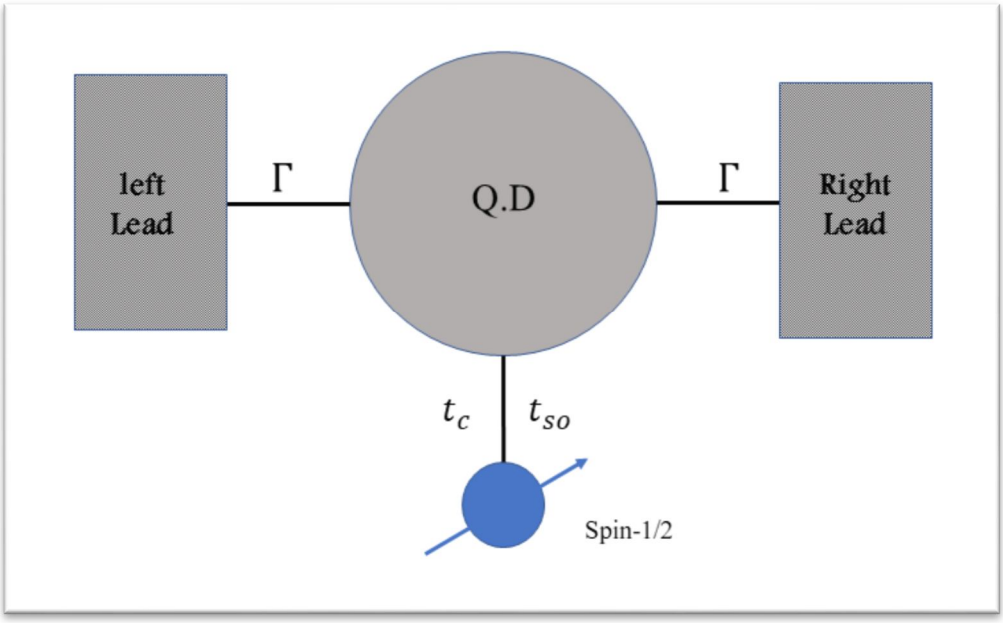

FIG. 1. Schematic diagram of the described system.

Based on Fig. 1, the Hamiltonian system can be written as follows:

$$\widehat{H} = H_{DS} + H_I + H_L + H_T \quad (1)$$

The first term of Eq. (1) represents the Hamiltonian for the quantum point H_{DS} [4] and is given by:

$$H_{DS} = \sum_{i=1}^{2}(\epsilon_i n_i + U_i n_{i\uparrow} n_{i\downarrow} + ½ g\mu_B B\sigma_i^z) \quad (2)$$

where $i = 1, 2$ represents the positions $i = 1$ of the quantum dot and $i = 2$ of the impurity, while n_i is the number of electrons given by:

$$n_i = \sum_\sigma n_{i\sigma} = c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow} \quad (3)$$

Here, $(c_{i\uparrow})\, c_{i\uparrow}^\dagger$ represents the creation and demolition effects of electrons at $i = 1, 2$ and $\sigma = (\uparrow, \downarrow)$ is the electron spin up and down. ϵ_i is the energy of the orbital, U_i is the charge energy, B is the fixed magnetic field, μ_B is the Bohr magnet, g is the g-factor of the electron, and the Pauli spin effect σ_i^z is given by:

$$\sigma_i^z = c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \quad (4)$$

The second term of Eq. (1), H_I Hamiltonian represents the interaction between the quantum dot and the impurity and is given by:

$$H_I = H_c + H_{so} + H_V \quad (5)$$

Equation (5) contains three terms representing the coupling forces between the quantum dot and the impurity. The term H_c represents the Hamiltonian of the tunnel correlation between the point and the impurity and is given by:

$$H_c = -t_c\left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow}\right) + H.c. \quad (6)$$

Here, t_c represents the strength of the twisted tunnel coupling between the point and the impurity.

The H_{so} term in Eq. (5) represents the Hamiltonian relationship of the point and the impurity to the force resulting from the spin-orbit interaction (SOI) and is given by:

$$H_{so} = -t_{so}\left(c_{1\uparrow}^\dagger c_{2\downarrow} - c_{1\downarrow}^\dagger c_{2\uparrow}\right) + H.c. \quad (7)$$

where t_{so} represents the non-conserved spin-orbit coupling strength of the spin between the point and the impurity.

The last term H_V in Eq. (5) refers to the Coulomb repulsion and is given by:

$$H_V = V n_1 n_2 \tag{8}$$

where V represents the Coulomb force.

In this study, we focus on calculating the energy gap between the quantum dot and the impurity, so the Hamiltonian matrix formed by H_{DS} and H_I will be taken into consideration. Thus, the total Hamiltonian $\widehat{H} = H_{DS} + H_I$ can be written in the form of a matrix as follows:

$$H = \begin{pmatrix} \epsilon_1+\epsilon_2+V & -t_c\sqrt{2} & 0 & 0 & 0 \\ -t_c\sqrt{2} & -2(V_g-V_p)+U_2 & t_{so} & 0 & t_{so} \\ 0 & t_{so} & (\epsilon_1+\epsilon_2+V-g\mu_B B) & 0 & 0 \\ 0 & 0 & 0 & \epsilon_1+\epsilon_2+V & 0 \\ 0 & t_{so} & 0 & 0 & (\epsilon_1+\epsilon_2+V+g\mu_B B) \end{pmatrix} \tag{9}$$

Adopting the energy levels of the sampling is indicated in Eq. (9) on both the magnetic and harmonic fields. Here, ε is of particular relevance because it provides us with knowledge of the internal composition of the areas through which the current passes.

The Hamiltonian in Eq. (9) is a two-electron system with wavefunctions $|T_+\rangle$،$|T_-\rangle$،$|T_0\rangle$ ،$|S_{11}\rangle$،$|S_{02}\rangle$. The tunneling energy t_c connects the two singular cases $|S_{11}\rangle$،$|S_{02}\rangle$, and causes anti-cross in the energy spectrum. t_{so} led to spin-orbit interaction that allowed jumping processes between dot and impurity through the spin-flip.

If $t_{so} \neq 0$, this leads to mixing between the singular and triple cases, generating extra anti-cross in the energy spectrum.

The functions that are relevant to our work are only $|T_-\rangle$،$|T_0\rangle$،$|S\rangle$. If $|S\rangle = \alpha|S_{11}\rangle + \beta\,|S_{02}\rangle$, where α and β are constants.

If $t_{so} = 0$, the system is either singular or triple.

The following is an explanation of the singular and triple cases:

$$\begin{aligned} |T_+\rangle &= c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger}|0\rangle \\ |T_-\rangle &= c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger}|0\rangle \\ |T_0\rangle &= \tfrac{1}{\sqrt{2}}\left(c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} + c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger}\right)|0\rangle \\ |S_{11}\rangle &= \tfrac{1}{\sqrt{2}}\left(c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} - c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger}\right)|0\rangle \\ |S_{02}\rangle &= c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger}|0\rangle \end{aligned} \tag{10}$$

Here, $|T_+\rangle$،$|T_-\rangle$،$|T_0\rangle$ are the wavefunctions for the coupled electrons triple cases, and $|S_{11}\rangle$،$|S_{02}\rangle$ are the wavefunctions for singular cases in dot and impurity.

Triple and singular are produced by the interaction of two electrons, each of which has a different spin in the energy levels of the system. The symmetric and antisymmetric wavefunctions are formed as follows:

$$\Psi = \tfrac{1}{\sqrt{2}}\left[\Psi_a^1\Psi_b^2 - \Psi_a^2\Psi_b^1\right] \cdot \begin{cases} \chi_1^+\chi_2^+ \\ \tfrac{1}{\sqrt{2}}[\chi_1^+\chi_2^- + \chi_1^-\chi_2^+] \\ \chi_1^-\chi_2^- \end{cases} \tag{11}$$

Here, $\Psi_{a,b}^{2,1}$ and $\Psi_{a,b}^{1,2}$ are the electron positions, and $\chi_{1,2}^{\pm}\chi_{2,1}^{\pm}$ are the electron spins (up and down) for the first and second positions.

The singular state $|S_{11}\rangle$ can be represented by the following wavefunction:

$$\Psi = \tfrac{1}{\sqrt{2}}\left[\Psi_a^1\Psi_b^2 + \Psi_a^2\Psi_b^1\right] \cdot \tfrac{1}{\sqrt{2}}[\chi_1^+\chi_2^- - \chi_1^-\chi_2^+] \tag{12}$$

The orbital energies for quantum dot and impurity are given by:

$$\begin{aligned} \epsilon_1 &= -(V_g - V_p) + \varepsilon + U_2 - V \\ \epsilon_2 &= -(V_g - V_p) \end{aligned} \tag{13}$$

Where V_g is the gate potential, V_p is the constant potential, and U_2 is the charge energy for the impurity.

3. Results and Discussion

The energies of the quantum system consisting of a quantum dot coupled with an impurity are calculated to find the energy gap dependent on the spin-orbit interaction Δ_{so} using

the Schrödinger equation. The characteristic energies of the system are found by substituting the two Hamiltonians defined by the relationship (9) into the time-independent Schrödinger equation:

$$(\mathrm{H} - \varepsilon)\,\Psi = 0 \qquad (14)$$

Thus, the following energies were obtained:

$$E_{T_+} = \epsilon_1 + \epsilon_2 + V + g\mu_B B$$

$$E_{T_-} = \epsilon_1 + \epsilon_2 + V - g\mu_B B$$

$$E_{T_0} = \epsilon_1 + \epsilon_2 + V \qquad (15)$$

$$E_{S_{11}} = \epsilon_1 + \epsilon_2 + V - \frac{1}{2}\left(\sqrt{\varepsilon^2 + 8t_c^2} + \varepsilon\right)$$

$$E_{S_{02}} = \epsilon_1 + \epsilon_2 + V$$

Using a MATLAB program, the energies were calculated and drawn for constant values of $\mathrm{t_c} = 0.1$, $\mathrm{V} = 1$ meV, $\mathrm{V_g} = 0.14$ meV, $\mathrm{V_p} = 20$ meV, $\mathrm{U_2} = 20$ meV, $\varepsilon = -0.46$. For several values of $\mathrm{t_{so}}$ as in Fig. 2 below:

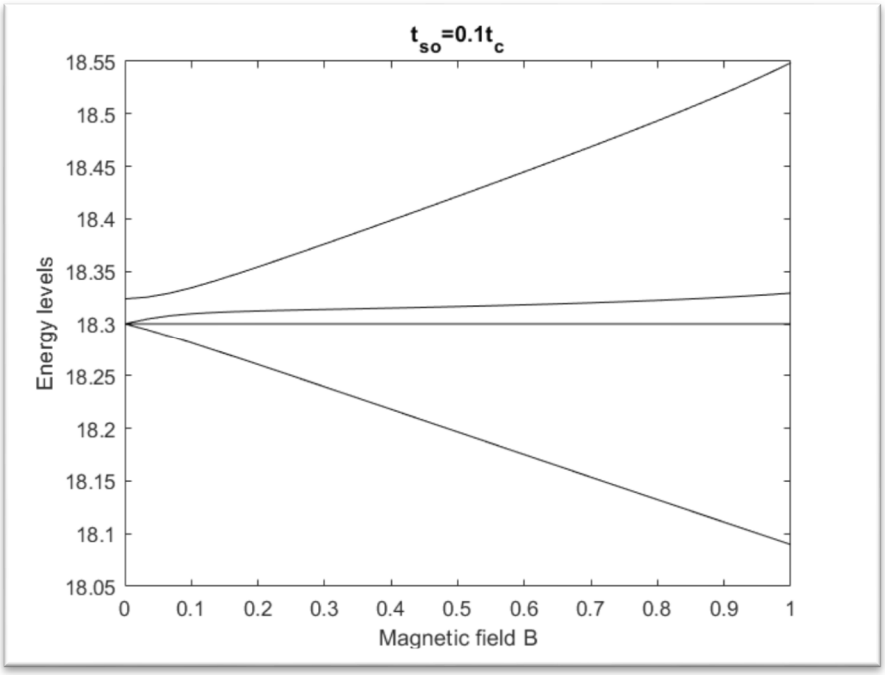

FIG. 2. Energy levels as a function of magnetic field B for $t_{so} = 0.1t_c$.

According to Fig. 2, energy is a function of the magnetic field, with the first three lines representing the energy of the triple levels. They all start from the same point $E = 0.2$, but each level behaves differently. The level E_{T_+} increases steadily, while the plane E_{T_0} remains constant, unaffected by the magnetic field. The spin rate here is zero, the plane E_{T_-} gradually decreases until it reaches a point of intersection with the single plane and then its value becomes constant. The singular plane remains constant until it reaches the point of intersection at $B \approx 0.35$ and then gradually decreases.

In Fig. 2, energy gap Δ_{so} between level E_{T_-} and the singular level depends on spin-orbit interaction. When $t_{so} = 1t_c$, the energy gap value increases between the two levels to $\Delta_{so} = 0.01$, indicating a relatively large difference compared to other values.

Spin-orbit Gap Calculation

The best approximation to calculate the energy of hybrid levels from a two-level system, E_{T_-}, E_S, is given by [3]:

$$E_i \approx \tfrac{1}{2}\left(E_{T_-} + E_S\right) \pm \tfrac{1}{2}\sqrt{\left(E_{T_-} - E_S\right) + \Delta_{so}^2} \qquad (16)$$

Where Δ_{so} represents the energy gap of spin-orbit coupling, and E_i denotes the hybrid energy.

In Fig. 3, the changes in Δ_{so} with detuning energy are observed.

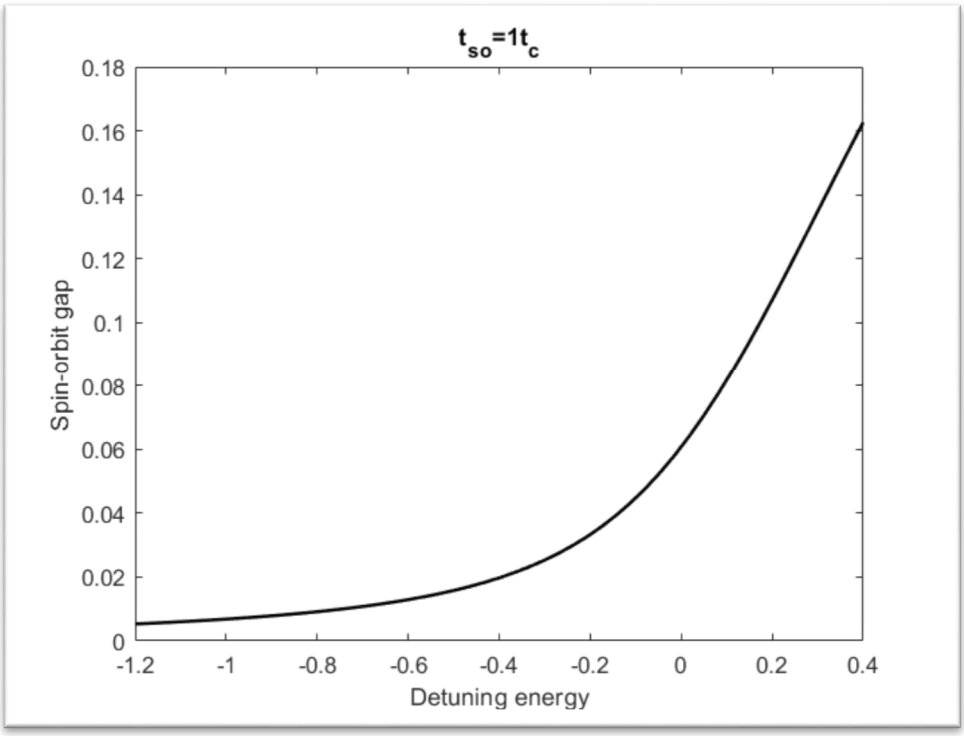

FIG .3. The energy gap of spin-orbit coupling, Δ_{so}, as a function of detuning energy.

In order to find out the behavior of the energy gap formed between the levels of the quantum dot, the MATLAB program was used to draw the relationship between Δ_{so} and spin-orbit interaction t_{so}. It is evident from Fig. 4 that there is a relationship between Δ_{so} and spin-orbit interaction t_{so}.

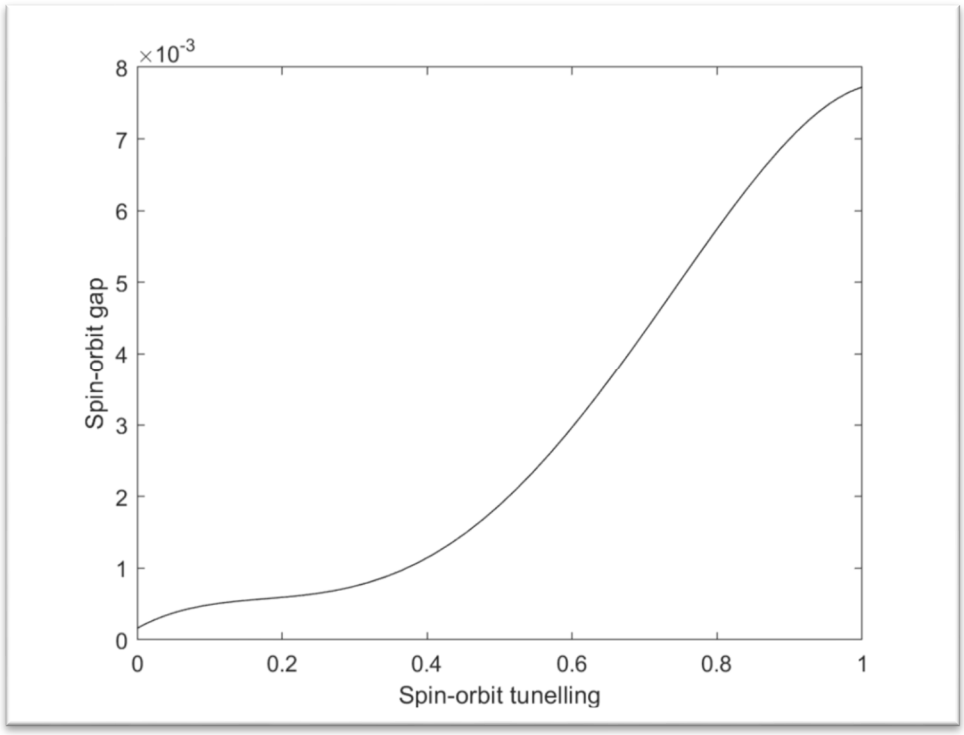

FIG.4. The relationship between the spin-orbit interaction energy gap Δ_{so} with the change in the energy of t_{so}.

4. Conclusion

In recent years, obtaining a polarized twist current through a system composed of two quantum coupled points has garnered significant interest, particularly in the context of using this system in quantum computers. Various effects, including spin-orbit coupling (SOC) and the Rashba spin-orbit coupling (RSOC), have been considered when calculating the spin-polarized current. In this work, a quantum system consisting of a quantum dot coupled with a fixed spin impurity is studied. The electron transfer process between the two leads is investigated, and the energies are calculated based on previous research [12].

Appendix (MATLAB code)

To calculate the energy levels for the Hamiltonian, MATLAB program can be used to find them:

```
clc
clear
na=51;
g=2;
mB=5.8e-2;
vp=20;
vg=0.14;
tc=0.1;
tso=0.8*tc;
U1=10;
U2=20;
V=1;
B=0.35;
e1=-1.2;
e2=0.4;
h=(e2-e1)./(na-1);
ep=e1;
A=0.33749578;
for j=1:na
D=g*mB*B;
ep1=-(vg-vp)+ep+U2-V;
ep2=-(vg-vp);
co=-2*(vg-vp)+U2;

syms E AA BB
BB    =    -(co-E+ep)*(D.^2*E.^2-
  2*D.^2*E*co-
  D.^2*E*ep+D.^2*co.^2+D.^2*co*e
  p-2*D.^2*tc.^2-
  E.^4+4*E.^3*co+3*E.^3*ep-
  6*E.^2*co.^2-9*E.^2*co*ep-
  3*E.^2*ep.^2+2*E.^2*tc.^2+2*E.
  ^2*tso.^2+4*E*co.^3+9*E*co.^2*
  ep+6*E*co*ep.^2-4*E*co*tc.^2-
  4*E*co*tso.^2+E*ep.^3-
  4*E*ep*tc.^2-4*E*ep*tso.^2-
  co.^4-3*co.^3*ep-
  3*co.^2*ep.^2+2*co.^2*tc.^2+2*
  co.^2*tso.^2-
  co*ep.^3+4*co*ep*tc.^2+4*co*ep
  *tso.^2+2*ep.^2*tc.^2+2*ep.^2*
  tso.^2);

r = abs(solve(BB));

R(j,1:6)=[ep r(1:5)'];

ep = ep + h;
end

ep=R(1:na,1);
E1=R(1:na,2)*A;
E2=R(1:na,3)*A;
E3=R(1:na,4)*A;
E4=R(1:na,5)*A;
E5=R(1:na,6)*A;
LL=1;
L3=LL*LL./((ep-B).^2+LL.^2);
Es=E5;
ET=E4;
Dso=(ET-Es).*L3;
plot(ep,E1,ep,E2,ep,E3,ep,E4,ep,E5)
```

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