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Supplementary Materials for

Entanglement classifier in chemical reactions

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Supplementary Material

Section SA. Bell's inequality for continuous measurement results

In this appendix we show how to build the auxiliary function $V(r,t,\mathbf{x_1},\mathbf{x_2})$ to calculate the correlation function $E(r,t)$ from the continuous measurement results r and t. For the continuous variables, we can define the correlation function as

$$E(r,t)=\sum_{i=1}^{m}p_i|c_i(r,t,++)|^2+\sum_{i=1}^{m}p_i|c_i(r,t,--)|^2-\sum_{i=1}^{m}p_i|c_i(r,t,+-)|^2-\sum_{i=1}^{m}p_i|c_i(r,t,-+)|^2 \tag{S1}$$

Generally, $\{S(|\phi_r^{j_1}\rangle\langle\phi_r^{j_1}|,r,\mathbf{x_1})S(|\phi_t^{j_2}\rangle\langle\phi_t^{j_2}|,t,\mathbf{x_2})\}$ are linearly independent, which makes it possible to calculate $\sum_{i=1}^{m}p_i|c_i(r,t,j_1,j_2)|^2,(j_1,j_2=+,-)$. For arbitrary measurement r, we have

$$\int S(|\phi_r^{\pm}\rangle\langle\phi_r^{\pm}|,r,\mathbf{x})d\mathbf{x}=1$$

To simplify the analysis, we defined the following functions

$$v(r,+,\mathbf{x_1})=\frac{S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})-\int S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})d\mathbf{x_1}}{\int S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})d\mathbf{x_1}-\int S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})d\mathbf{x_1}} \tag{S2}$$

$$v(r,-,\mathbf{x_1})=\frac{S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})-\int S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})d\mathbf{x_1}}{\int S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})d\mathbf{x_1}-\int S(|\phi_r^{+}\rangle\langle\phi_r^{+}|,r,\mathbf{x_1})S(|\phi_r^{-}\rangle\langle\phi_r^{-}|,r,\mathbf{x_1})d\mathbf{x_1}} \tag{S3}$$

$$v(t,+,\mathbf{x_2})=\frac{S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,t,\mathbf{x_2})-\int S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,t,\mathbf{x_2})S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,t,\mathbf{x_2})d\mathbf{x_2}}{\int S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,t,\mathbf{x_2})S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,t,\mathbf{x_2})d\mathbf{x_2}-\int S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,r,\mathbf{x_2})S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,r,\mathbf{x_2})d\mathbf{x_2}} \tag{S4}$$

$$v(t,-,\mathbf{x_2})=\frac{S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,t,\mathbf{x_2})-\int S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,t,\mathbf{x_2})S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,t,\mathbf{x_2})d\mathbf{x_2}}{\int S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,t,\mathbf{x_2})S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,t,\mathbf{x_2})d\mathbf{x_2}-\int S(|\phi_t^{+}\rangle\langle\phi_t^{+}|,t,\mathbf{x_2})S(|\phi_t^{-}\rangle\langle\phi_t^{-}|,t,\mathbf{x_2})d\mathbf{x_2}} \tag{S5}$$

with

$$\int v(r,\pm,\mathbf{x_1})S(|\phi_r^{\pm}\rangle\langle\phi_r^{\pm}|,r,\mathbf{x_1})d\mathbf{x_1}=1 \tag{S6}$$

and

$$\int v(r,\pm,\mathbf{x_1})S(|\phi_r^{\mp}\rangle\langle\phi_r^{\mp}|,r,\mathbf{x_1})d\mathbf{x_1}=0 \tag{S7}$$

Then, the correlation function is given by

$$E(r,t) = \int S(\rho, r, t, \mathbf{x_1}, \mathbf{x_2})[v(r,+,\mathbf{x_1}) - v(r,-,\mathbf{x_1})][v(t,+,\mathbf{x_2}) - v(t,-,\mathbf{x_2})]d\mathbf{x_1}d\mathbf{x_2} \tag{S8}$$

Note that ρ in Eq.(S8) represents density matrix of bipartite systems. We define the auxiliary function as

$$V(r,t,\mathbf{x_1},\mathbf{x_2}) = [v(r,+,\mathbf{x_1}) - v(r,-,\mathbf{x_1})][v(t,+,\mathbf{x_2}) - v(t,-,\mathbf{x_2})] \tag{S9}$$

Section SB. Details of the simulation method

For simplicity, the density matrix of the two particles discussed in the text, Eq. (5) and Eq. (6) can be written as

$$\rho_{r,t} = \begin{bmatrix} A_{rt}^{++} & B_{rt}^{1,2} & B_{rt}^{1,3} & B_{rt}^{1,4} \\ B_{rt}^{2,1} & A_{rt}^{+-} & B_{rt}^{2,3} & B_{rt}^{2,4} \\ B_{rt}^{3,1} & B_{rt}^{3,2} & A_{rt}^{-+} & B_{rt}^{3,4} \\ B_{rt}^{4,1} & B_{rt}^{4,2} & B_{rt}^{4,3} & A_{rt}^{--} \end{bmatrix} \tag{S10}$$

where the diagonal elements A are real and the off diagonal elements B are complex

$$A_{rt}^{j_1,j_2} = \sum_{i=1}^{m} p_i |c_i(r,t,j_1 j_2)|^2 \qquad j_i, j_2 = +,- \tag{S11}$$

$$\begin{gathered} B_{rt}^{n_1,n_2} = \sum_{i=1}^{m} p_i c_i(r,t,J(n_1)) c_i(r,t,J(n_2))^* \\ where \quad n_1,n_2 = 1,2,3,4,\ n_1 \neq n_2 \\ and \quad J(1) = ++,\ J(2) = +-,\ J(3) = -+,\ J(4) = -- \end{gathered} \tag{S12}$$

with $B_{rt}^{n_1,n_2} = B_{rt}^{n_2,n_1 *}$. All A components in Eq.(S10) can be obtained by analyzing the spectrum $S(\rho, r, t, \mathbf{x_1}, \mathbf{x_2})$. One possible method is to find the set $A_{rt}^{j_1,j_2}$, with which the function $D(\mathbf{A_{rt}})$ would be minimum, where

$$D(\mathbf{A_{rt}}) = \int d\mathbf{x_1} \int d\mathbf{x_2} \left[S(\rho, r, t, \mathbf{x_1}, \mathbf{x_2}) - \sum_{j_1,j_2} A_{rt}^{j_1 j_2} S(|\phi_r^{j_1}\rangle, r, \mathbf{x_1}) S(|\phi_t^{j_2}\rangle, t, \mathbf{x_2}) \right]^2 \tag{S13}$$

To obtain the off-diagonal components in the density matrix, other measurements are needed. For particles going through channel I, the $r-$ and $q-$measurements are used, while $s-$ and $t-$measurement are used for particles from channel II. The relationship between eigenstates of the two different measurements can be written as

$$\begin{bmatrix} |\phi_{k_1}^{+}\rangle \\ |\phi_{k_1}^{+}\rangle \end{bmatrix} = \begin{bmatrix} a_{k_1,k_2}^{++} & a_{k_1,k_2}^{+-} \\ a_{k_1,k_2}^{-+} & a_{k_1,k_2}^{--} \end{bmatrix} \begin{bmatrix} |\phi_{k_2}^{+}\rangle \\ |\phi_{k_2}^{+}\rangle \end{bmatrix} \tag{S14}$$

For simplicity, we can write

$$\mathbf{C_i}(r,t) = \begin{bmatrix} c_i(r,t,++) & c_i(r,t,+-) \\ c_i(r,t,-+) & c_i(r,t,--) \end{bmatrix}$$

If we choose a different measurement in one channel, the matrix $\mathbf{C_i}(r,t)$ becomes

$$\mathbf{C_i}(r,s) = \mathbf{C_i}(r,t) \cdot \begin{bmatrix} a_{t,s}^{++} & a_{t,s}^{+-} \\ a_{t,s}^{-+} & a_{t,s}^{--} \end{bmatrix} \tag{S15}$$

and similarly

$$\mathbf{C_i}(q,t) = \begin{bmatrix} a_{r,q}^{++} & a_{r,q}^{+-} \\ a_{r,q}^{-+} & a_{r,q}^{--} \end{bmatrix} \cdot \mathbf{C_i}(r,t) \tag{S16}$$

When $a_{st}^{+-} + a_{st}^{-+} = 0$, some off-diagonal components in density matrix can be calculated

$$\begin{aligned} B_{rt}^{1,2} &= \sum_{i=1}^{m} p_i c_i(r,t,++) c_i(r,t,--)^* \\ &= \sum_{i=1}^{m} p_i |c_i(r,s,++)|^2 \cdot |a_{st}^{++}|^2 + \sum_{i=1}^{m} p_i |c_i(r,s,--)|^2 \cdot |a_{st}^{--}|^2 \end{aligned} \tag{S17}$$

and by the same method one can calculate $B_{rt}^{1,3}, B_{rt}^{2,4}, B_{rt}^{3,4}$.

From Eq.(5) and Eq.(S15), we can write the connection between the descriptions of the density matrix with different eigenstate basis (under different measurement) as

$$\rho_{q,s} = \begin{bmatrix} a_{r,q}^{++} & a_{r,q}^{+-} \\ a_{r,q}^{-+} & a_{r,q}^{--} \end{bmatrix} \otimes \begin{bmatrix} a_{t,s}^{++} & a_{t,s}^{+-} \\ a_{t,s}^{-+} & a_{t,s}^{--} \end{bmatrix} \cdot \rho_{r,t} \cdot \begin{bmatrix} a_{r,q}^{++} & a_{r,q}^{+-} \\ a_{r,q}^{-+} & a_{r,q}^{--} \end{bmatrix}^{\dagger} \otimes \begin{bmatrix} a_{t,s}^{++} & a_{t,s}^{+-} \\ a_{t,s}^{-+} & a_{t,s}^{--} \end{bmatrix}^{\dagger} \tag{S18}$$

If we could know every component of the density matrix, there would be more choice to classify entanglement. According to the PPT criterion[1][2], if ρ^{T_B} has any negative eigenvalue, then these particles are entangled.

Section SC. An example of spin $\frac{1}{2}$ particles

Here, we will give an example to show how the simulation method works for spin $\frac{1}{2}$ particles. Although the simulation method designed mainly for continuous measurement results, it will also show a good performance for discrete measurement results.

When spin $\frac{1}{2}$ particles go through Stern-Gerlach (SG) apparatus whose magnetic field is along the z-axis, they will split into two beams along z-axis corresponding to eigenstate $|\uparrow\rangle$ and $|\downarrow\rangle$. When these particles go through SG apparatus with magnetic field along the x-axis, they will split into two beams along the x-axis corresponding to eigenstate $|+\rangle$ and $|-\rangle$. Assume that there is a machine that could produce particle pairs at some certain quantum states propagating along the y-axis. Each pair are separated and sent to two channels as shown in Fig.(S1). Particles would then go through SG apparatus with magnetic field along x or z-axis randomly, by which four spectrum measurements could be collected.

At the initial stage, we can prepare the spin-$\frac{1}{2}$ particle pairs in superposition, entangled, or mixed states as follow:

Case I Superposition state: Particle pairs produced in equal superposition

$$|\Psi_s\rangle = \frac{1}{2}[\,|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\,] \tag{S19}$$

Case II Entangled state: Particle pairs are all at Bell state

$$|\Psi_e\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \tag{S20}$$

Case III Mixed state: Every pair produced consists of one particle at state $|\uparrow\rangle$, and another one at state $|\uparrow\rangle$. These particles could be describe by using the density matrix

$$\rho_m = \frac{1}{2}[\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\,] \tag{S21}$$

After certain measurements, the spectrum for these cases could be simulated based on Eq.(8). For the case I, the superposition state could be transformed to a different basis

$$\begin{aligned} |\Psi_s\rangle &= \frac{1}{2}[\,|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\,] \\ &= \frac{1}{\sqrt{2}}[\,|\uparrow +\rangle + |\downarrow +\rangle\,] \\ &= \frac{1}{\sqrt{2}}[\,|+\uparrow\rangle + |+\downarrow\rangle\,] \\ &= |++\rangle \end{aligned} \tag{S22}$$

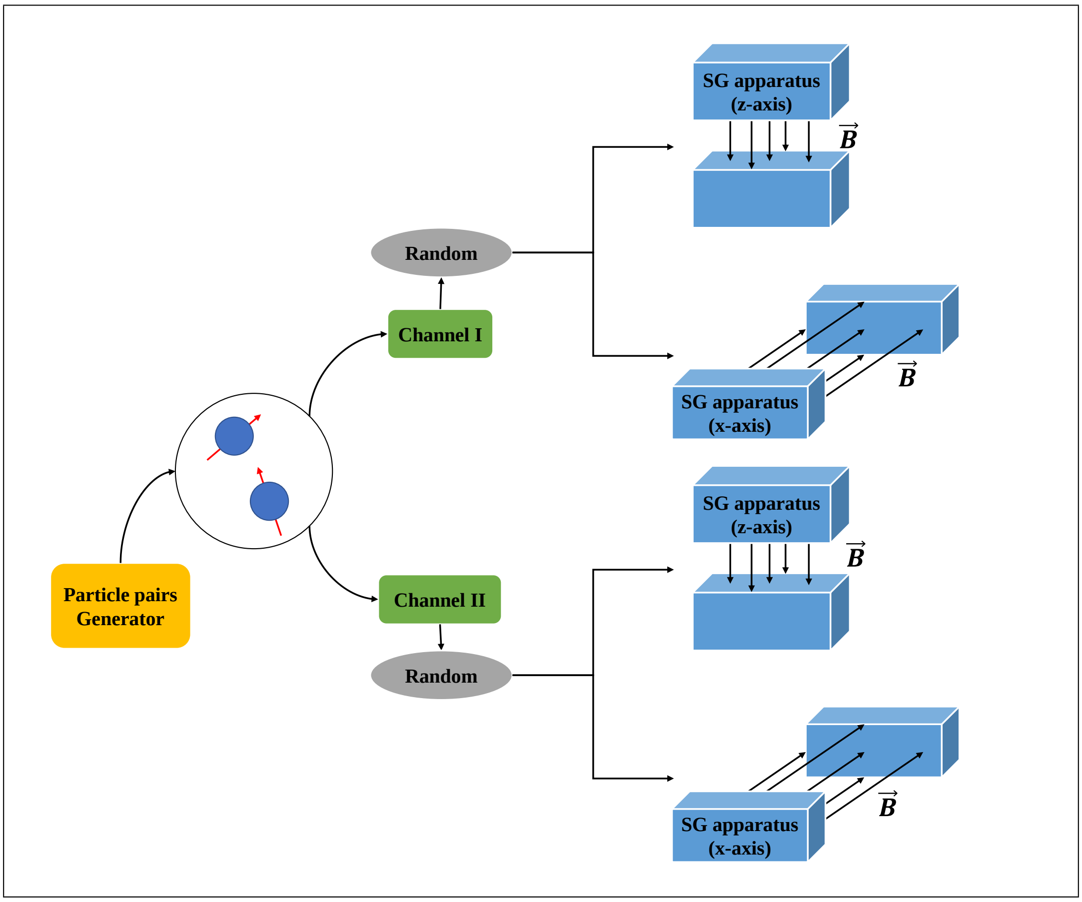

Fig. S1. Sketch of Bell's experiment of spin $\frac{1}{2}$ particles. The prepared spin-$\frac{1}{2}$ particles are divided into two channels, in each one they will go through SG-apparatus with magnetic field along the z-axis or the x-axis randomly. Then the count numbers of particle pairs are related to different measurement results.

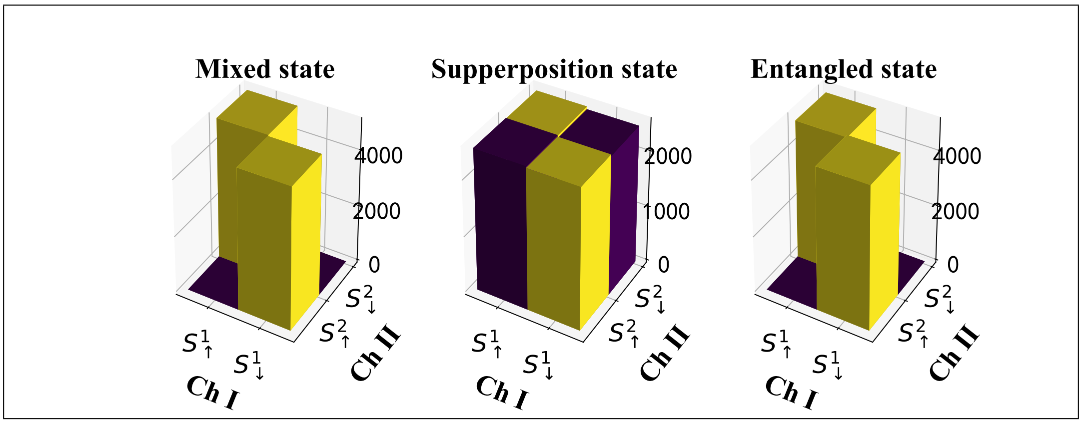

Fig. S2. Simulation result (1z2z).
We simulate the count number along Channel I and Channel II under the same measurement, where the magnetic field in SG apparatus of channel I and II are both along the z-axis (1z2z). $S^{1,2}_{\uparrow,\downarrow}$ represent particles that show state $|\uparrow\rangle$ or $\downarrow\rangle$ in channel I or channel II. Three figures represents simulation results of the three cases mentioned (Left: Mixed state; Middle: Superposition state; Right: Entangled state).

Then it is convenient to calculate its spectrum under different measurement. If both of the SG apparatus in channel I and II have magnetic field along z-axis, then we obtain

$$\begin{aligned} S(|\Psi_s\rangle\langle\Psi_s|, z, z, \mathbf{x_1}, \mathbf{x_2}) = & \frac{1}{4}S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_1})S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_2}) \\ & +\frac{1}{4}S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_1})S(|\downarrow\rangle\langle\downarrow|, z, \mathbf{x_2}) \\ & +\frac{1}{4}S(|\downarrow\rangle\langle\downarrow|, z, \mathbf{x_1})S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_2}) \\ & +\frac{1}{4}S(|\downarrow\rangle\langle\downarrow|, z, \mathbf{x_1})S(|\downarrow\rangle\langle\downarrow|, z, \mathbf{x_2}) \end{aligned} \tag{S23}$$

Eq.(S23) explains the nearly same results in the spectrum measurements of $|\Psi_s\rangle$ in Fig.(S3). And from Eq.(8), we could calculate its spectrum under other measurements as

$$\begin{aligned} S(|\Psi_s\rangle\langle\Psi_s|, z, x, \mathbf{x_1}, \mathbf{x_2}) = & \frac{1}{2}S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_1})S(|+\rangle\langle+|, x, \mathbf{x_2}) \\ & +\frac{1}{2}S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_1})S(|-\rangle\langle-|, x, \mathbf{x_2}) \end{aligned} \tag{S24}$$

$$\begin{aligned} S(|\Psi_s\rangle\langle\Psi_s|, x, z, \mathbf{x_1}, \mathbf{x_2}) = & \frac{1}{2}S(|+\rangle\langle+|, x, \mathbf{x_1})S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_2}) \\ & +\frac{1}{2}S(|-\rangle\langle-|, x, \mathbf{x_1})S(|\uparrow\rangle\langle\uparrow|, z, \mathbf{x_2}) \end{aligned} \tag{S25}$$

These equations explain why there are only two columns (histogram) left in spectrum of $|\Psi_s\rangle$ in Fig.(S3) and Fig.(S4). Since that $|\Psi_s\rangle = |++\rangle$ is already an eigenstate under the measurement $1x2x$ in which both of the magnetic field in channel I and II are along x-axis, we can directly get its spectrum $S(|\Psi_s\rangle\langle\Psi_s|, x, x, \mathbf{x_1}, \mathbf{x_2}) = S(|+\rangle\langle+|, x, \mathbf{x_1})S(|+\rangle\langle+|, x, \mathbf{x_2})$, as shown in $Fig.(S2)$.

Similarly, we calculated the spectrum of case 2 and 3, whose spectrum under different measurements are shown in Fig.(S2,S3,S4,S5) together with spectrum of $|\Psi_s\rangle$.

As we can see from the simulation results, we can not distinguish these three states only from the spectrum $S(z, z, \mathbf{x_1}, \mathbf{x_2})$, yet when we take all the four spectrum measurements into account, it is possible to classify them.

Next we will discuss measurements starting from Warner state, which plays an important role in quantum teleportation[3][4]. Assume that a machine M could generate particles at Werner state of the

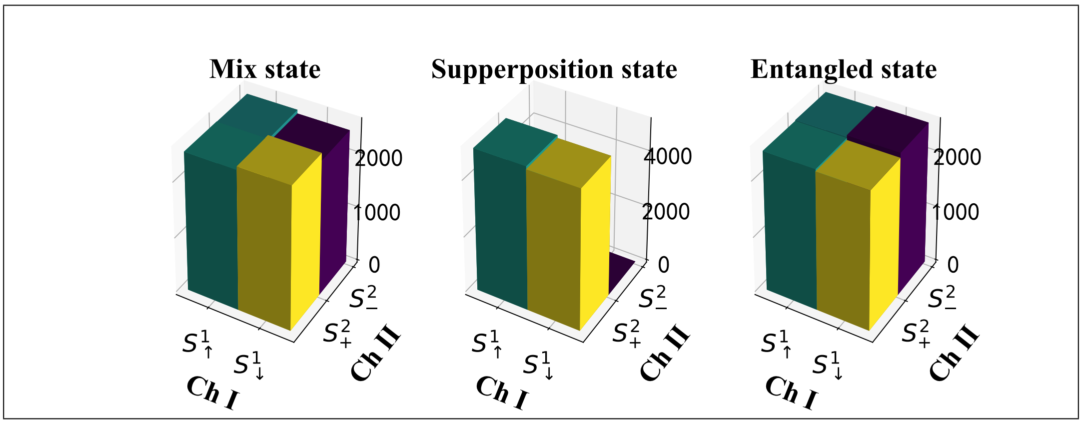

Fig. S3. Simulation result (1z2x).
We simulate the count number along Channel I and Channel II under the same measurement, where the magnetic field in SG apparatus of channel I is along z-axis, and II is along x-axis (1z2x). $S^1_{\uparrow,\downarrow}$ represent the particles that show state $|\uparrow\rangle$ or $|\downarrow\rangle$ in channel I, and $S^2_\pm$ represent the particles that show state $|+\rangle$ or $|-\rangle$ in channel I. Three figures represents simulation results of the three cases mentioned (Left: Mixed state; Middle: Superposition state; Right: Entangled state).

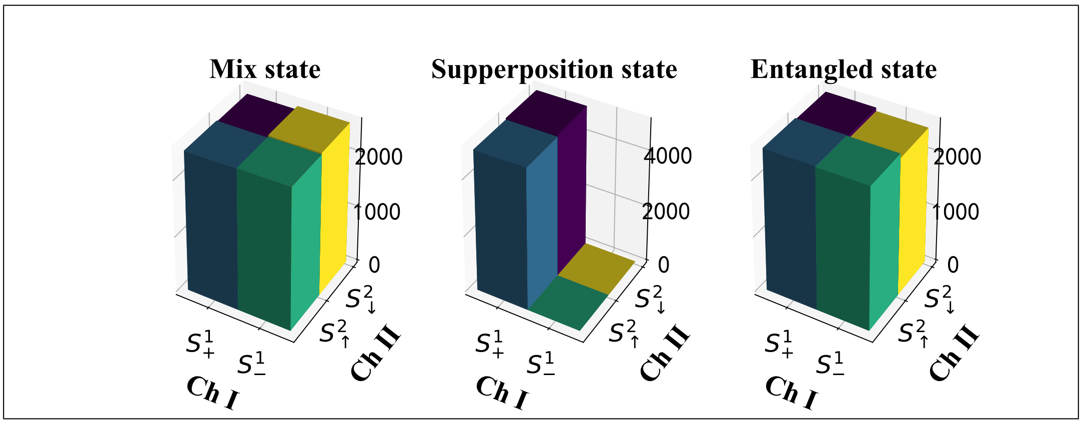

Fig. S4. Simulation result (1x2z).
We simulate the count number along Channel I and Channel II under the same measurement, where the magnetic field in SG apparatus of channel I is along x-axis, and II is along z-axis (1x2z). $S^1_\pm$ represent the particles that show state $|+\rangle$ or $|-\rangle$ in channel I, and $S^2_{\uparrow,\downarrow}$ represent the particles that show state $|\uparrow\rangle$ or $|\downarrow\rangle$ in channel II. Three figures represents simulation results of the three cases mentioned (Left: Mixed state; Middle: Superposition state; Right: Entangled state).

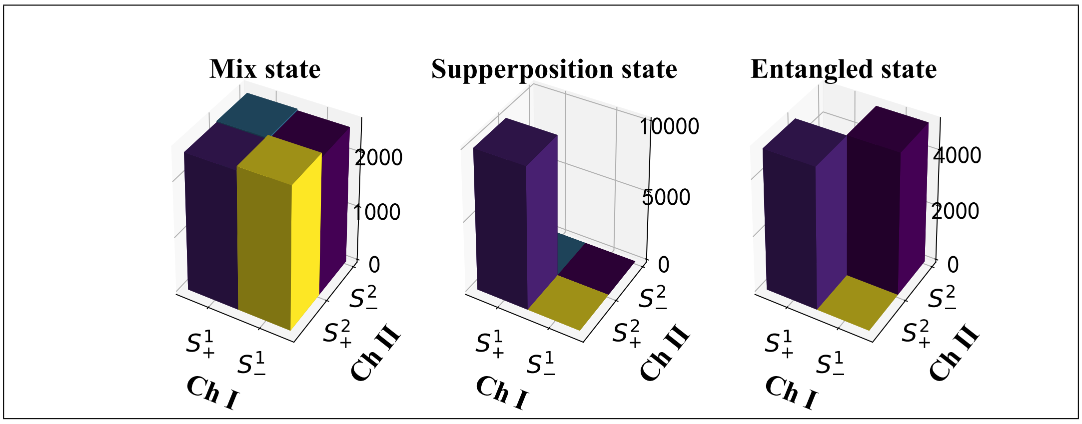

Fig. S5. Simulation result (1x2x).
We simulate the count number along Channel I and Channel II under the same measurement, where the both the magnetic field in SG apparatus of channel I and II are along x-axis (1x2x). $S_{\pm}^{1,2}$ represent the particles that show state $|+\rangle$ or $|-\rangle$ in channel I or channel II. Three figures represents simulation results of the three cases mentioned (Left: Mixed state; Middle: Superposition state; Right: Entangled state).

form:

$$\rho_w(p) = \frac{p}{2}(\,|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\,)(\,\langle\downarrow\uparrow| + \langle\uparrow\downarrow|\,) + \frac{1-p}{4}I \tag{S26}$$

According to PPT-criterion, when $p < \frac{1}{3}$, particles are in separated states; while when $p \geq \frac{1}{3}$ they are entangled. One can write the density matrix of such state in different basis according to various measurements. In the basis of $1z2z$ (both magnetic fields in channel I and II are along z-axis), we can rewrite the density matrix as

$$\rho = \begin{array}{c} \\ |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} \begin{array}{c} \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{pmatrix} \frac{1-p}{4} & 0 & 0 & 0 \\ 0 & \frac{1+p}{4} & \frac{p}{2} & 0 \\ 0 & \frac{p}{2} & \frac{1+p}{4} & 0 \\ 0 & 0 & 0 & \frac{1-p}{4} \end{pmatrix} \end{array} \tag{S27}$$

By Eq.(S18) we could transform it according to another measurement $1x2x$ (both magnetic field in channel I and II are along x-axis) as

$$\rho = \begin{array}{c} \\ |++\rangle \\ |+-\rangle \\ |-+\rangle \\ |--\rangle \end{array} \begin{array}{c} \begin{array}{cccc} |++\rangle & |+-\rangle & |-+\rangle & |--\rangle \end{array} \\ \begin{pmatrix} \frac{1+p}{4} & 0 & 0 & -\frac{p}{2} \\ 0 & \frac{1-p}{4} & 0 & 0 \\ 0 & 0 & \frac{1-p}{4} & 0 \\ -\frac{p}{2} & 0 & 0 & \frac{1+p}{4} \end{pmatrix} \end{array} \tag{S28}$$

Then we could predict its spectrum under measurement $1x2x$ as

$$\begin{aligned} S(|\Psi_s\rangle\langle\Psi_s|, z, z, \mathbf{x_1}, \mathbf{x_2}) = & \frac{1+p}{4} S(|+\rangle\langle+|, x, \mathbf{x_1}) S(|+\rangle\langle+|, x, \mathbf{x_2}) \\ & + \frac{1-p}{4} S(|+\rangle\langle+|, z, \mathbf{x_1}) S(|-\rangle\langle-|, z, \mathbf{x_2}) \\ & + \frac{1-p}{4} S(|-\rangle\langle-|, z, \mathbf{x_1}) S(|+\rangle\langle+|, z, \mathbf{x_2}) \\ & + \frac{1+p}{4} S(|-\rangle\langle-|, z, \mathbf{x_1}) S(|-\rangle\langle-|, z, \mathbf{x_2}) \end{aligned} \tag{S29}$$

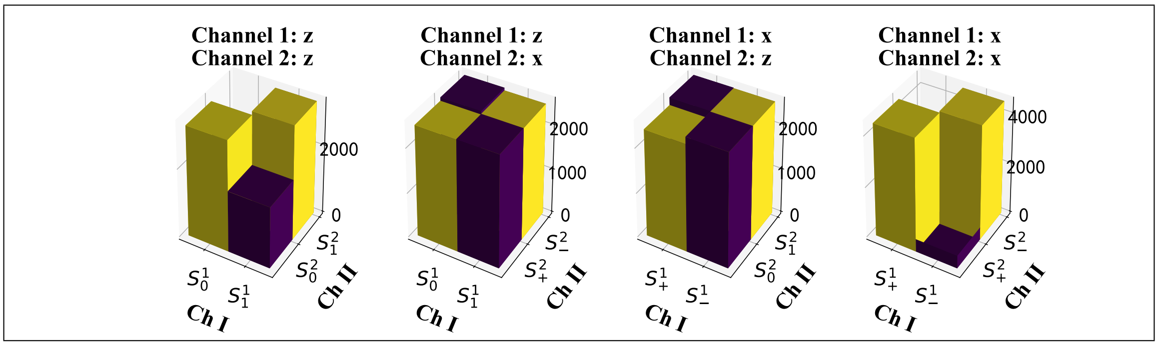

Fig. S6. Simulation result (Werner state,ρ = 0.6).
Left1 : Both the magnetic field in SG apparatus of channel 1 and 2 are along x-axis. Left2: Magnetic field in SG apparatus of channel 1 is along z-axis, and 2 is along x-axis. Right 2: Magnetic field in SG apparatus of channel 1 is along x-axis, and 2 is along z-axis. Right 1: Both the magnetic field in SG apparatus of channel 1 and 2 are along z-axis.).

Similarly, we would obtain the spectrum under other measurements. The simulation results of the Werner state are shown in Fig.(S6), where we set $p = 0.6$.