Preparation of two-particle total hyperfine spin singlet states via spin-changing dynamics

Chao-Chun Huang\textsuperscript{1}, M.-S. Chang\textsuperscript{2} and S.-K. Yip\textsuperscript{1,2}

\textit{Institute of Physics}, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan

We present our proposals for generating total hyperfine spin zero state for two \( f = 1 \) or two \( f = 2 \) particles, starting from initial unentangled states. We show that our goal can be achieved by exploiting spin changing dynamics and quadratic Zeeman shifts with realistic choices of external magnetic fields and evolution time intervals.

PACS numbers: 37.10.Jk, 67.85.-d, 75.10.Jm

I. INTRODUCTION

State preparation for many-particle systems is gaining increasing attention recently. States with desired quantum entanglement properties find important applications in quantum information processing, cryptography, and computation\cite{1}. Indeed efforts in this direction can be found in areas as diverse as quantum dots\cite{2}, trapped ions\cite{3}, and cold atoms\cite{4,5}, to name a few. It has also been recognized recently that similar ideas can be used to create exotic many-body states in cold atoms. Many of these states are of particular interest in the condensed matter context. Examples of such proposals include the Haldane state for a spin-1 lattice\cite{6}, resonant valence bond states\cite{7}, antiferromagnetic states\cite{8,9}, d-wave "superconductivity"\cite{10,11}, Luttinger liquids\cite{12}, and even states that correspond to highest energy (instead of ground) state for a given Hamiltonian\cite{6,12}.

In this paper, we would like to discuss our proposal to generate a total hyperfine spin-zero singlet pair, starting from two particles that each has hyperfine spin-1 or 2. Our primary motivation is that the ground states of certain one (spatial) dimensional lattice of Bosons with one atom per site and with suitable interaction between the Bosons are expected to be in the dimerized state\cite{13,14}. In this state, the lattice translational symmetry is spontaneously broken so that the spin-correlation between neighboring sites alternate between strong and weak. Furthermore, it can be shown that this dimerized state is smoothly connected to the ground state of a new Hamiltonian where alternate bonds are weakened\cite{14,15}. In the limit where the alternate bonds are weakened completely to zero, we have a collection of isolated singlet pairs. The system remains gapped throughout this process. Reversing the argument, once singlet pairs can be prepared, in principle one can then obtain the many-body dimerized state of the original Hamiltonian by gradually turning on the coupling between the pairs. A similar argument can also be applied generally to valence bond states. Thus preparing the singlets would be a useful first step in generating these unconventional magnetic states.

Irrespective of whether we can ultimately obtain the dimerized states experimentally using this method, we believe that our proposals of generating singlet pairs of hyperfine spin-1 and spin-2 particles are of interest in their own right. While most literature on quantum information and cryptography deals with particles with only two internal states (e.g. spin-up versus down for spin-1/2 particles or horizontal versus vertical polarization for photons), it is known that higher dimensional quantum systems (i.e., systems with more than two internal states) offer many advantages such as higher tolerance in noise in quantum key distribution\cite{16} or tests of Bell inequalities\cite{17}. A spin-singlet state of two spin-1 (2) particles is (one of) the most entangled two-particle state in a dimension 3 (5) quantum system. It is therefore of high interest to know how to generate them, and here we offer a scheme starting from completely unentangled initial states\cite{18}.

We shall discuss two schemes. The first is simply to vary an external magnetic field adiabatically. This scheme is simple, but would work only in very special cases. The second, the central work of this paper, is a dynamical scheme. The main idea is to exploit the spin changing dynamics of two interacting particles in the presence of a (generally time-dependent) quadratic Zeeman field. This dynamics has been studied experimentally by Widera et al\cite{19}. However, their focus was to extract the spin dependent interaction parameters (the spin dependent s-wave scattering lengths). We shall show that, for proper choice of parameters, one can prepare pure spin-singlet pairs using this spin changing dynamics.

We introduce our proposal for hyperfine spin-1 particles in section\cite{11}. The case for hyperfine spin-2 particles is discussed in section\cite{11}. In these two sections, we emphasize the basic ideas and simplify our analysis by putting the magnetic field to be zero during some time intervals. The generalization to the cases where the magnetic fields are always finite are discussed in section\cite{11}. The conclusions are in section\cite{11}. In appendix A we provide some details of our estimate on the fidelity of our scheme. For simplicity, we shall occasionally use "spins" for hyperfine spins when there is no danger of confusion.
II. HYPERFINE SPIN-1 SYSTEMS

We assume that one can initially prepare two particles in a potential well (or a double well, the detailed shape of the potential does not matter), each with hyperfine state \(|f, m_f\rangle = |f, 0\rangle\). In this (next) section \(f = 1\) (\(f = 2\)). This initial state has also been obtained by Widera et al.\[19, 20\]. We shall assume that these particles reside and stay in the lowest motional ground state throughout the dynamics, thus their spins are the only degrees of freedom. A quantum mechanical state can therefore be indicated only by the quantum numbers \(m_f\)'s of the two particles. For simplicity we shall suppress the \(f\) labels. Thus \(|0, 0\rangle_m\) would indicate that both particles have \(m_f = 0\), whereas \(\frac{1}{\sqrt{2}}(|1, -1\rangle_m + | -1, 1\rangle_m\) indicates that there is one particle each in the \(m_f = \pm 1\) state. Since we are dealing with Bosons, only symmetric states need to be kept. The subscripts \(m\) remind us that we are using the \(m_f\) basis.

Since we are interested in obtaining a total spin singlet, we would also like to keep track of the total hyperfine spin \(F\) of the two particles. It is therefore also convenient to use the basis \(|FM_F\rangle_F\) where \(M_F\) is the projection of \(F\). We only need to consider even \(F\)'s) and can be written in this basis. It is simple to rewrite \(E\) we have simply a two-level system.

The conservation of total \(m\) implies that we only need to consider the two states \(|00\rangle_F\) and \(|20\rangle_F\).

We consider the time evolution of these particles under the presence of a (in general time-dependent) quadratic Zeeman field. The linear Zeeman field need not be considered due to the conservation of total \(m\) and hence \(M\) within our proposed schemes.

The Hamiltonian consists of simply two terms: the quadratic Zeeman energy and the interaction energy. The first contribution is a single particle term. It represents a \(m_f\) dependent energy quadratic in magnetic field \(B\) (for not too large \(B\)'s) and can be written in the form \(H_Q = q \left(\sum_{m_1,m_2} (m_1^2 + m_2^2)|m_1,m_2\rangle (m_1,m_2)\langle m_1,m_2|\right)\) where \(q = \hat{q}B^2\) with \(\hat{q}\) a coefficient depending on the atom under consideration. The interaction energy is diagonal in the total hyperfine spin basis \(|00\rangle_F\) and \(|20\rangle_F\). We shall denote these interaction energies by \(E_0\) and \(E_2\) respectively.

We first discuss the adiabatic scheme. The singlet state can be generated by adiabatically varying the external field \(B\) hence \(q\) if both the initial and final states are either the highest or the lowest energy states when \(q\) varies. Suppose \(q\) is positive. Then the initial state \(|0, 0\rangle_m\) is the lowest energy state for large \(q\). If \(E_2 > E_0\), then the singlet state is also the ground state at \(q = 0\). Hence, if the initial \(|0, 0\rangle_m\) state was produced at sufficiently large \(q\), then decreasing the magnetic field to zero would automatically generate the singlet \(|00\rangle_F\) state. Such a scheme would not work of \(E_2 < E_0\) [21], or their difference is too small for adiabaticity to be satisfied for \(q\) to be varied in time.

Below we turn to our dynamical scheme which works for both \(E_2 > (\langle E_0\rangle\) Let us first set up the Hamiltonian. In the \(|00\rangle_F\) and \(|20\rangle_F\) basis, the interaction part of the energy is simply a diagonal matrix,

\[
H_I = \begin{pmatrix} E_0 & 0 \\ 0 & E_2 \end{pmatrix}.
\]

Since we are targeting the state \(|00\rangle_F\) as the final state, we shall work in this basis. It is simple to rewrite \(H_Q\) in this \(|FM_F\rangle\) basis since, from the Clebsch-Gordan coefficients, we know that

\[
|00\rangle_F = \frac{1}{\sqrt{3}} (|1, -1\rangle_m + | -1, 1\rangle_m - |0, 0\rangle_m)
\]

\[
|20\rangle_F = \frac{1}{\sqrt{6}} (|1, -1\rangle_m + | -1, 1\rangle_m + 2|0, 0\rangle_m),
\]

From which we find

\[
H_Q = \frac{2q}{3} \left(\frac{2}{\sqrt{2}} \sqrt{2} \right).
\]

Hence the total Hamiltonian is

\[
H = \left( E_0 \ 0 \\ 0 \ E_2 \right) + \frac{2q}{3} \left(\frac{2}{\sqrt{2}} \sqrt{2} \right) . \tag{2}
\]

In this basis, our initial state \(|00\rangle_m\) is simply \((u(0), v(0))^T = (-1/\sqrt{3}, \sqrt{2/3})^T\) where \(T\) denotes the transpose.

Let us consider the evolution of the state vector \((u(t), v(t))^T\) in time \(t\). Its value can be easily found since we have simply a two-level system. \(H\) can be rewritten as \((\vec{E}_z + \vec{E}_x + q) + \vec{H}_{eff} \cdot \vec{\tau}\) where \(\vec{\tau}\) are the Pauli matrices and \(H_{eff,x} = \frac{2\sqrt{q}}{3}\) and \(H_{eff,z} = \frac{E_0 - E_2}{2} + \frac{q}{3}\). The scalar term only gives an overall phase and will be dropped below. The state vector at time \(t\) is then given by

\[
\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = \left( \cos \Omega - i \frac{\vec{H}_{eff} \cdot \vec{\tau}}{\Omega} \sin \Omega \right) \begin{pmatrix} u(0) \\ v(0) \end{pmatrix}, \tag{3}
\]

where

\[
\Omega \equiv |\vec{H}_{eff}| = \left[\left(\frac{E_0 - E_2}{2} + \frac{q}{3}\right)^2 + \frac{8}{9} q^2\right]^{1/2}. \tag{4}
\]

Here \(2\Omega\) is the Rabi frequency. The condition that we have a singlet at time \(t = t^*\) is \(v(t^*) = 0\). Given that \((u(0) = -1/\sqrt{3}\) and \(v(0) = \sqrt{2/3}\) we need

\[
\left( \frac{i\vec{H}_{eff,x} \sin \Omega t^*}{\Omega} + \sqrt{2} \left( \cos \Omega t^* + \frac{i\vec{H}_{eff,z} \sin \Omega t^*}{\Omega} \right) \right) = 0,
\]

and hence

\[
\cos \Omega t^* = 0 \tag{6}
\]

and

\[
H_{eff,x} + \sqrt{2} H_{eff,z} = 0. \tag{7}
\]
These require, respectively,
\[ t^* = \left( n + \frac{1}{2} \right) \pi / \Omega \]  
(8)

and
\[ q = \frac{E_2 - E_0}{2}. \]  
(9)

This last expression and Eq. (4) together give
\[ \Omega = \frac{|E_2 - E_0|}{\sqrt{3}}. \]  
(10)

Hence if \( q \) (hence \( \hat{q} \)) has the same sign as \( E_2 - E_0 \), we obtain a singlet at times \( t^* = \frac{\pi}{2\Omega} \), \( \frac{3\pi}{2\Omega} \), ..., As an example, consider \(^{23}\)Na atoms in its \( f = 1 \) hyperfine state, where \( \hat{q} > 0 \). The s-wave scattering lengths satisfy \( a_2 > a_0 \), hence \( E_2 > E_0 \). Hence it is possible to obtain a pure singlet at time \( t^* \) when we choose the magnetic field to be \( B = \left( \frac{E_2 - E_0}{2q} \right)^{1/2} \). If the spatial wavefunction is \( \psi(\vec{r}) \), then \( E_F = \frac{4\pi}{m_a} \int d^3r |\psi(\vec{r})|^2 = a_F \hat{U} \), where \( \hat{U} \) is defined by this expression as in [19], and \( m_a \) is the mass of the atoms. Immediately following that \( E_2 - E_0 = \hat{U}(a_2 - a_0) \), and for \(^{23}\)Na \( a_2 - a_0 \) is approximately \( 3.5a_B \) [22], where \( a_B \) is the Bohr radius. Given that \( \hat{q} = 278 \) Hz/G² and if we choose \( \hat{U}a_B = (2\pi)30 \) Hz, then the required magnetic field and the time to obtain a singlet are calculated to be \( B = 1.08G \) and \( t = 4.1 \) ms, respectively.

As mentioned above this dynamical scheme is directly applicable to \(^{23}\)Na, where \( \hat{q} \) and \( E_2 - E_0 \) are of the same sign. With simple modifications, this scheme can be generalized to cases where \( \hat{q} \) and \( E_2 - E_0 \) are of the opposite sign, such as \(^{87}\)Rb. This is done by simply letting the state first evolves under zero field till time \( t_1 \), so that the wavefunction at \( t_1 \) is
\[ \frac{-\frac{1}{2} e^{-iE_0 \epsilon t_1}}{\sqrt{\frac{3}{4} e^{-iE_2 \epsilon t_1}}} = \frac{e^{-iE_0 \epsilon t_1}}{\sqrt{3}} \left( e^{-i\phi} \right), \]
where \( \phi = (E_2 - E_0)t_1 \) is the phase difference between the \( F = 0 \) and \( F = 2 \) states due to the interparticle interaction during the interval \( 0 < t < t_1 \). Then a magnetic field and hence the quadratic Zeeman energy is turned on at \( t_1 \), and the condition for obtaining a singlet after a further time \( t^* \) (thus at total time \( t = t_1 + t^* \)) is simply the same as Eq. (5), except an extra factor \( e^{i\phi} \) multiplying the first term. In this case condition (7) is now replaced by
\[ H_{e_{\text{eff},z}} e^{i\phi} + \sqrt{2} H_{e_{\text{eff},z}} = 0, \]  
(11)
which requires
\[ q \left( 1 + 2\cos \phi \right) = \frac{E_2 - E_0}{2}. \]  
(12)

With suitable choice of \( \phi \) (i.e., \( t_1 \)), this condition can be satisfied even if \( q \) and \( E_2 - E_0 \) are of opposite signs. For this \( q \), the frequency \( \Omega \) is given by
\[ \Omega = \frac{|E_2 - E_0|}{\left( 1 + 2\cos \phi \right)^{1/2}}, \]  
(13)
and the required time \( t^* \) is given by
\[ \cot \Omega t^* = \frac{H_{e_{\text{eff},x}} \sin \phi}{\sqrt{2} \Omega} = \frac{(\sgn q)\sin \phi}{(2 + \cos^2 \phi)^{1/2}}. \]  
(14)

It follows that for a solution \((\phi(t_1), t^*)\) solved by Eq. (12, 14), \((\phi + n2\pi, t^* + m\pi/\Omega)\) and \((-\phi + n2\pi, -t^* + m\pi/\Omega)\) are also solutions, where \( n \) and \( m \) are integers, and \( \Omega \) is an implicit function of \( \phi \). Of the solutions above only positive \( t_1 \) and \( t^* \)’s are realistic, and Eq. (12) implies that there is no solution when \(-1.5 < \frac{q}{E_2 - E_0} < 0.5 \) which holds for arbitrary signs of \( q \) and \( E_2 - E_0 \). Fig. (a)(b) show two possible sets of \((t_1, t^*)\), where \( E_2 < E_0 \) and \( q > 0 \). In Fig. (c) the value of \( \pi/\Omega \) is shown. It is note that the solutions in Fig. (a) are also applicable for cases where \( q < 0 \) and \( E_2 > E_0 \), due to the symmetry properties of equations (12) and (14). When the signs of \( q \) and \( E_2 - E_0 \) are both reversed, it is observed that \( H \rightarrow -H \), up to a constant, and \( \phi \rightarrow -\phi \) in Eq. (12).

Consider \(^{87}\)Rb atoms in its \( f = 1 \) hyperfine state, where the value of \( a_2 - a_0 \) is approximately \(-1.4a_B \) [19]. By choosing \( \hat{U}a_B = (2\pi)30 \) Hz, then \( E_0 - E_2 = 264 \) Hz. If we further choose \( q = 1.5(E_0 - E_2) \), then the required magnetic field is \( B = 2.35G \). Here we have used \( \hat{q} = 71.7 \) Hz/G² for \(^{87}\)Rb. For this particular choice of \( q \) the solutions in Fig. (a) and (b) are same and for the times are \( t_1 = 11.90 \) ms and \( t^* = 3.435 \) ms.

We shall estimate the error in producing the singlet state due to inaccuracies \( \Delta t_1 \) and \( \Delta t^* \) for \( t_1 \) and \( t^* \), respectively. Let \( t_1 \) and \( t^* \) be the times needed to generate the singlet state so that \(|u(t)| = 1 \) and \(|u(t)| = 0 \), then the expected value of \(|u(\Delta t_1, \Delta t^*)| = \sqrt{1 - |v(\Delta t_1, \Delta t^*)|^2} \approx 1 - \frac{|v|^2}{2} \). Here the approximation holds as long as \( \Delta t_1 \) and
\(\Delta t^*\) are not too large, and the analytical expression of \(v(\Delta t_1, \Delta t^*)\) is shown in Appendix A. Take for instance, if \(|\Delta t_1| + |\Delta t^*| < 0.31\) ms for \(^{87}\text{Rb}\), then \(|v|^2 < 0.02\) and \(|u| > 0.99\). Similarly for the \(^{23}\text{Na}\), if the total inaccuracies of time \(|\Delta t_1| + |\Delta t^*| < 0.36\) ms, the same fidelity is achieved. We also note that from Appendix A and Fig. 1(c), the value of \(|u(t)|\) is closer to 1 for the same inaccuracies in time if a smaller value of \(|q|\) is used.

In the above, we have illustrated our scheme where zero magnetic field is utilized. In real experiments, zero magnetic field is not easily attainable, and undesirable effects may occur in low fields. To avoid those practical issues, our scheme can be readily generalized to the case of finite field, by adjusting slightly the second applied field, provided that the first field is not too large. Before we address this issue in section IV, we shall discuss generalization of this dynamical scheme to \(f = 2\) systems.

III. HYPERFINE SPIN-2 SYSTEMS

The considerations here are direct generalization of those in the last section, and let us first consider the adiabatic scheme. Suppose \(q < 0\), as in the case of \(f = 2\) hyperfine states of \(^{23}\text{Na}\) and \(^{87}\text{Rb}\), then the initial state \(|0, 0 >_m\) is the highest energy level for large magnetic fields. In cases where \(E_0 > E_{2,4}\), then adiabatically switching off the external field would generate the desired singlet state. Conversely, if \(q > 0\), the singlet state can be obtained if \(E_{2,4} > E_0\). This scheme however is limited in its applicability, and in particular it neither works for \(^{23}\text{Na}\) nor \(^{87}\text{Rb}\), where \(q < 0\) and \(a_{2,4} > a_0\).

Let us proceed to consider the dynamical scheme. Similar to \(f = 1\) spinors, we can write down the Hamiltonian for \(f = 2\) spinors in the \(|00\>_F\), \(|20\>_F\) and \(|40\>_F\) basis, where

\[
|00\>_F = \frac{1}{\sqrt{5}}[(0, 0) - [(1, -1) + | - 1, 1) \\
+ (|2, -2| + |2, 2)|]\_m,
\]

\[
|20\>_F = \frac{1}{\sqrt{32}}[2(0, 0) + [(1, -1) + | - 1, 1) \\
+ 2(|2, -2| + |2, 2)|]\_m,
\]

\[
|40\>_F = \frac{1}{\sqrt{8}}[(\sqrt{18}(0, 0) + \sqrt{8}(1, -1) + | - 1, 1) \\
+ |2, -2| + |2, 2)|]\_m.
\]

The Hamiltonian is

\[
H = \begin{pmatrix}
E_0 & 0 & 0 \\
0 & E_2 & 0 \\
0 & 0 & E_4
\end{pmatrix}
+ 2q \begin{pmatrix}
\frac{2}{12} & \frac{14}{19} & 0 \\
\frac{2}{12} & \frac{14}{19} & 0 \\
0 & 0 & \frac{19}{14}
\end{pmatrix},
\]

where the two terms represent the interaction energy and the quadratic Zeeman effect, respectively. In this basis, our initial state \(|00\>_m\) is simply \(|\Psi_0\> = (1/\sqrt{5}, -\sqrt{2}/7, \sqrt{18}/35)\_T\), and the desired final state is the singlet state \(|00\>_F = (1, 0, 0)\_T\). In other words with

Here we need to solve for two complex equations, instead of just one \((v(t) = 0)\) for \(f = 1\) spinors. In the last section, we showed that our goal is achieved by evolving the system in two time intervals with a chosen \(q\) in each interval. Following this line, we attempt our goal with the following sequence: we first let the system evolve at \(q = 0\) for \(t_1\), and then at \(q \neq 0\) for \(t_2\), followed by \(q = 0\) for \(t_3\), then finally at \(q \neq 0\) again for \(t_4\). Thus the time-evolution operator is

\[
\hat{U}(t_1, t_2, t_3, t_4) = e^{-iHt_4}e^{-iHt_3}e^{-iHt_2}e^{-iHt_1}
\equiv \hat{U}_4\hat{U}_3\hat{U}_2\hat{U}_1.
\]

Here \(H_0\) represents the Hamiltonian in Eq. (10) with no quadratic Zeeman effect \((q = 0)\).

It is convenient to define \(\varepsilon(> 0)\) and \(\theta\) by the relationships \(E_2 - E_0 \equiv \varepsilon \cos \theta\) and \(E_4 - E_0 \equiv \varepsilon \sin \theta\). The amplitude \(\varepsilon\) thus defines our energy scale and its inverse defines the time scale of the dynamics. The angle \(\theta\) then characterizes the element under consideration. For each (normalized) \(q\) and \(\theta\), we search for the times \(t_{1-4}\) so that Eq. (17) is satisfied. We have limited ourselves to total time \(t_1 + t_2 + t_3 + t_4\) smaller than 200 in unit of \(1/\varepsilon\), so that the total experimental time scales remain reasonably short (see below). There is a symmetry property: the solutions are the same for \(q = q^*\), \(\theta = -\pi + \theta^*\) and \(q = -q^*\), \(\theta = \theta^* + \pi\) (i.e., \(H \rightarrow -H\), up to a constant).

Fig. 2(a) shows the region where no solution is found (which may be due to the limits of our computational effort). Similar to the case of \(f = 1\), when \(|q|\) is small no solution is found. Here the values of \(\theta\) are limited to between 0 and \(\pi\), given the symmetry property mentioned above. We can not find a solution at \(\theta = \pi/2\) \((3\pi/2)\) for \(q < 0\) \((> 0)\). We note that for these special cases we allowed a longer search time with smaller stepsize, but no solution was found. When \(q\) approaches these values, \(t_{1-4}\) seem to diverge unfoundedly [23]. From the experimental point of view, if the value of \(\theta\) is very close to
these special cases, the system must have relatively long lifetime in order to achieve the singlet state using our scheme. However away from these values the singlet state can always be achieved with a reasonably short time. In Fig. 2(a), there also exist sharp spikes of \( q \) at \( \theta = 0, \pi/4, \pi/2, \pi \) and \( 3\pi/4 \). For general \( q \)'s and \( \theta \)'s (excluding those discussed in the last paragraph), there exist many sets of solutions for \( t_{4-1} \), and no obvious relationship is found between different sets since the time evolution is not periodic (c.f. Sec. III).

Let us consider \(^{23}\text{Na}\) and \(^{87}\text{Rb}\) in the \( f = 2 \) hyperfine state. For \( \text{Na} \) the differences of s-wave scattering lengths \((a_2 - a_0, a_4 - a_0)\) are approximately \((11, 30) a_B \) \(^{23}\), and its quadrature Zeeman energy \( q = -278 \times B \) Hz. For \(^{87}\text{Rb}\) their values are \((3.5, 11) a_B \) \(^{23}\) and \(-71.7 \times B \) Hz. Even though \((a_2 - a_0, a_4 - a_0)\) are different for \(^{23}\text{Na}\) and \(^{87}\text{Rb}\), it happens that their \( \theta \)'s are similar, which are approximately 0.39\( \pi \) and 0.40\( \pi \), respectively. As solutions \( t_i \)'s are not unique, we only present one set of \( t_{i-1} \) as functions of \( q \) for both atoms in Fig. 2(b). Take \( q/\varepsilon = -0.5 \), then \( \varepsilon \cdot t_{i=1-4} = (2.645, 2.571, 5.555, 3.350) \) for \(^{23}\text{Na}\) and \((2.781, 2.442, 5.533, 3.349) \) for \(^{87}\text{Rb}\). Note that the differences in \( \theta \) results in differences in \( t_i \)'s of up to 5\%. In real experiments if we further choose \( U a_B = (2\pi)30 \) Hz, then \( \varepsilon = (2\pi)959 \) Hz for \( \text{Na} \) and \((2\pi)346.5 \) Hz for \(^{87}\text{Rb}\). The controlled variables in laboratory units are \( B = 3.26 \) G and \( t_{i=1-4} = (0.450, 0.437, 0.944, 0.570) \) ms for \( \text{Na} \) and \( 3.90 \) G and \((1.307, 1.148, 2.601, 1.571) \) ms for \(^{87}\text{Rb}\).

Let us also estimate the impact of inaccuracies in the time intervals used. With our estimation in Appendix A the expected amplitude in singlet state is more than 0.99 if the total inaccuracies of time, \( |\Delta t_1| + |\Delta t_2| + |\Delta t_3| + |\Delta t_4| \), is less than 0.011 ms for \(^{23}\text{Na}\) and 0.030 ms for \(^{87}\text{Rb}\). Similar to \( f = 1 \) cases, to increase the tolerance in the time inaccuracies, we should use smaller value of \( |q| \), with a caution that when \( |q|/\varepsilon \lesssim 0.18 \) for both \(^{23}\text{Na}\) and \(^{87}\text{Rb}\), no solution may be found. In other words the \( B \) must be larger than 1.95 G \((^{23}\text{Na})\) and 2.33 G \((^{87}\text{Rb})\) in order to arrive the singlet state.

It is also possible to find solutions by restricting to three free time intervals, such as by letting \( t_1 = 0 \), \( t_2 = t_4 \), or \( t_1 = t_3 \), in the expense of fixing \( q \) to some special values. This is equivalent to the case in \( f = 1 \) systems, in which \( q = (E_2 - E_0)/2 \) when we set \( t_1 = 0 \).

**IV. NON-ZERO MAGNETIC FIELD RESULTS**

In the above sections we have shown the basic ideas of our proposal, exemplified with \( f = 1 \) and \( f = 2 \) spinors. However, zero \( B \) field environment may be difficult to prepare, and there could be undesirable effects in a zero field, such as spin-flips due to fluctuations of the magnetic field. Here we consider generalization of our scheme to the case where the magnetic field is always finite. For \( f = 1 \), we let the system evolve at \( q = q_1 \neq 0 \) for a time \( t_1 \) and then at \( q = q_2 \neq 0 \) for a time \( t_2 \). For \( f = 2 \), we first let the system evolve at \( q = q_1 \neq 0 \) for a time interval \( t_1 \), then at \( q = q_2 \neq 0 \) for \( t_2 \), followed by \( q = q_3 \neq 0 \) for another time \( t_3 \), and finally again \( q = q_2 \neq 0 \) for interval \( t_4 \). For realistic solutions, \( q_1 \) and \( q_2 \) must be of the same sign, dictated by the element under consideration.

**A. HYPERFINE SPIN-1**

Here we directly show the analytic solution for \( t_1 \) and \( t_2 \) as functions of \( q_1 \) and \( q_2 \) for \( f = 1 \). The state vector at time \( t = t_1 + t_2 \) is given by

\[
\begin{pmatrix}
  u(t) \\
  v(t)
\end{pmatrix} = \begin{pmatrix}
  \cos \Omega t_2 - \frac{H_{\text{eff},2} \cdot \vec{v}}{\Omega_2} \\
  \frac{\sin \Omega t_2}{\Omega_2}
\end{pmatrix}
\times
\begin{pmatrix}
  \cos \Omega t_1 - \frac{H_{\text{eff},1} \cdot \vec{v}}{\Omega_1} \\
  \frac{\sin \Omega t_1}{\Omega_1}
\end{pmatrix}
\begin{pmatrix}
  u(0) \\
  v(0)
\end{pmatrix},
\]

where \( H_{\text{eff},i} \) and \( \Omega_i \) are defined as Eq. (13). We obtain the solution of \( t_i \) for the equation \( u(t_1 + t_2) = 0 \) as

\[
t_1 = \pm \frac{1}{\Omega_1} \cot^{-1} \left( \frac{|E_0 - E_2|}{2\sqrt{3}\Omega_1} \right) \left( \frac{2q_1' + 1 + C(q_1', q_2')}{2q_2' + 1} \right)^{1/2},
\]

\[
t_2 = \mp \frac{1}{\Omega_2} \cot^{-1} \left( \frac{|E_0 - E_2|}{2\sqrt{3}\Omega_2} \right) \left( \frac{2q_1' + 1 + C(q_1', q_2')}{2q_2' + 1} \right)^{1/2},
\]

where \( C(q_1', q_2') = 2q_2' - 3 - 6q_1' - 12q_1'q_2' \). For convenience we have defined \( q_1' = q_1/(E_0 - E_2) \). From Eq. (20), given one solution \( (t_1', t_2') \), the other solutions can be obtained as \((t_1' + n\pi/\Omega_1, t_2' + m\pi/\Omega_2)\) and \((-t_1' + n\pi/\Omega_1, -t_2' + m\pi/\Omega_2)\), where \( n \) and \( m \) are integers.

Interestingly no solution is found when the condition \((2q_1' + 1)(2q_2' + 1)(2q_2' - 3 - 6q_1' - 12q_1'q_2') \geq 0\) does not hold. The conditions on \( q_1' \) for the existence of solutions can be classified into two cases according to signs of \( q_1' \); case(1) corresponds to \( q_1' \leq 0 \), and case(2) corresponds to \( q_1', q_2' \geq 0 \). The conditions for both cases are listed below in more details.

Case(1) : \[
q_1' \leq \frac{1}{2}, \quad \frac{1}{2} \leq q_2' \leq \frac{3 + 6q_1'}{2 - 12q_1'} \leq 0
\]

or \[
-\frac{1}{2} \leq q_1' \leq 0, \quad q_2' \leq -\frac{1}{2}.
\]

Case(2) : \[
0 \leq q_1' \leq \frac{1}{6}, \quad \frac{3}{2} \leq \frac{3 + 6q_1'}{2 - 12q_1'} \leq q_2'.
\]

Case(1) applies to \(^{23}\text{Na}\) and case(2) applies to \(^{87}\text{Rb}\). When \( q_1' = 0 \) the results reduce to that in Section III. In both cases either \( |q_1'| \) or \( |q_2'| \) can not be too large, otherwise no solution is found. In Fig. 3(a)(b) we show the solutions for \( t_1 \) with the choices \( q_1' = 1/96 \) and 1/12 respectively for case (2), and solutions exist only when \( q_2' \geq 49/30 \) and 7/2 accordingly.

For the \(^{87}\text{Rb}\) case, by choosing \( U a_B = (2\pi)30 \) Hz, we have \( E_0 - E_2 \approx 264 \) Hz. So the required magnetic fields for \( q_1' = 1/96 \) and 1/12 are \( B \approx 0.20 \) G and 0.55 G,
that when the absolute value of $q$
pared with the result of $-t$
obtained. Here we also have limited ourselves to
$q_0$, the time-evolution operator is just Eq. (18). By a
Here $H_{\text{tot}}$ represents the Hamiltonian in Eq. (16). If $q_1 = 0$,
the time-evolution operator is just Eq. (18). By a
similar method in section III the solutions $t_i$'s can be
obtained. Here we also have limited ourselves to $t_{\text{tot}} =
t_1+t_2+t_3+t_4 < 200$, in units of $1/\varepsilon$. There is a symmetry
property: the solutions are the same when $q_i = -q_i^*$ and
$\theta = \theta^*$ or $q_i = -q_i$ and $\theta = -\theta^*$.

In Fig. 4 (a)(b) no solution is found in the shaded re-
regions, where the values of $q_1/\varepsilon$ are 0.002 and 0.02 for
the upper-half of the panels, and the values of $q_1/\varepsilon$ are
$-0.002$ and $-0.02$ for the lower-half of the panels. Com-
pared with the result of $q_1 = 0$ (see Fig. 2 (a)) we find that
when the absolute value of $q_1$ increases, the main
change occurs in the region for negative $q$, where the
total area with no solution found increases. Especially
the peaks near $\theta = \pi/4$ and $\pi/2$ grow quickly. Thus for
$0 \leq \theta \leq \pi$ and $q < 0$ (and similarly for $\pi \leq \theta \leq 2\pi$
and $q > 0$), $|q_1|$ cannot be too large in experiments. Besides
there are also some changes in the peak positions, and
some peaks are disappeared.

For $^{23}\text{Na}$ and $^{87}\text{Rb}$ in $f = 2$, if $q_1/\varepsilon = -0.002$ and
$\varepsilon t_i < 10$, then solutions exist when $q_2/\varepsilon \lesssim -0.21$.
For example with $(q_1/\varepsilon, q_2/\varepsilon) = (-0.002, -0.24)$ there
is one solution of $\varepsilon \cdot t_{i=1-4} = (3.76, 4.56, 3.72, 2.38)$ for
$^{23}\text{Na}$ and $(3.80, 4.38, 3.34, 2.49)$ for $^{87}\text{Rb}$. By choosing
$\hat{U}_{AB} = (2\pi)30$ Hz, the $B$ fields corresponding to
$(q_1, q_2)$ are $(0.20, 2.28)$ G and $(0.24, 2.7)$ G, and the solu-
tions for $t_{i=1-4}$ are $(0.624, 0.757, 0.618, 0.395)$ ms and
$(1.75, 2.01, 1.54, 1.14)$ ms for $\text{Na}$ and $^{87}\text{Rb}$, respectively.

V. CONCLUSION

In this paper we propose a method to dynamically gen-
erate a two-particle total hyperfine spin-singlet. For
hyperfine spin-1 systems, by allowing the system to evolve
in two time intervals, with a specific magnetic field in
each interval. For hyperfine spin-2 systems, a similar
scheme with four time intervals can also achieve our
goal. For some special cases, such as negative $q$ and
$E_2 \approx E_0 < E_4$, the singlet state is however hard to ob-
tain unless long evolution times are used. Except in these
very special circumstances, our proposed scheme should
be easy to implement in realistic experiments. Prepara-
tion of these singlet pairs would allow us to create some
exotic many-body states, and can also be useful in quan-
tum information applications.

ACKNOWLEDGMENTS

This research is supported by the National Science
Council of Taiwan.

Appendix A: Influence of inaccuracies in the time
intervals used in evolution

Here we provide some details on our error estimates on
the final wavefunction. First we consider $f = 1$. With
the condition $\nu(t_1, t_2) = 0$, we can get the analytic form
of $|v(t_1 + \Delta t_1, t_2 + \Delta t_2)|^2 \equiv |\Delta v|^2$ as

$$|\Delta v|^2 \approx \frac{2}{9} (E_{20} \Delta t_1)^2 + (2q_2 \Delta t_2)^2 \quad \text{(A1)}$$

$$+ \left( \Delta t_1 \Delta t_2 \right) (12q_1 q_2 + 3E_{20}^2 - 6q_1 E_{20} - 2q_2 E_{20})$$

where $E_{20} \equiv E_2 - E_0$. Here we have assumed that $\Delta t_1$
and $\Delta t_2$ are small enough. In addition, Eq. (A1) can also
be generalized to an inequality,

$$|\Delta v|^2 \leq |\Omega_1| |\Delta t_1| + |\Omega_2| |\Delta t_2|^2 \quad \text{(A2)}$$

$$\leq [\max(\Omega_1, \Omega_2)(|\Delta t_1| + |\Delta t_2|)]^2 \equiv \Lambda_1.$$
To get this inequality the condition, $(2q'_1 + 1)(2q'_2 + 1)(2q'_3 - 3 - 6q'_1 - 12q'_2q'_4) ≥ 0$, has been used. In a special case where $q_1 = 0$, $Ω_1$ reduces to $|E_{20}|/2$ seen in section [11].

This last formula for $A_1$ gives an upper limit on the error produced due to the inaccuracies of time intervals employed in an experiment. If $A_1 = 0.02$, then $|u|$(fidelity) would be higher than 0.99.

For $f = 2$ system we simply use the estimate $|∆v|^2 < A_2 ≡ [max(Δω_1, Δω_2)(|Δt_1| + |Δt_2| + |Δt_3| + |Δt_4|)]^2$, where $Δω_1$ and $Δω_2$ are defined as the maximum of $|ω_{1,i} - ω_{1,j}|/2$ and $|ω_{2,i} - ω_{2,j}|/2$, respectively. Here $ω_{1,i}$ and $ω_{2,j}$ represent the eigenvalues of the Hamiltonian in Eq. (10) at $q = q_1$ and $q = q_2$, respectively. Although we have not obtained the analytic form for the $f = 2$ systems, we verified numerically that this formula for $A_2$ works well in practice. The fidelities discussed in text were estimated using this formula for $A_2$.

[1] C. H. Bennett and D. P. DiVincenzo, Nature, 404, 247 (2000)

[2] R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. Vandersypen, Rev. Mod. Phys. 79, 1217 (2007).

[3] K. Kim, M.-S. Chang, R. Islam, S. Korenblit, L.-M. Duan and C. Monroe, Phys. Rev. Lett. 103, 120502 (2009)

[4] Marco Anderlini, Patricia J. Lee, Benjamin L. Brown, Jennifer Seby-Strabley, William D. Phillips and J. V. Porto, Nature, 448, 452 (2007)

[5] Stefan Trotzky, Yu-Ao Chen, Ute Schnorrenberger, Patrick Cheinet, and Immanuel Bloch, Phys. Rev. Lett. 105, 265303 (2010)

[6] J. J. Garcia-Ripoll, M. A. Martin-Delgado, and J. I. Cirac, Phys. Rev. Lett. 93, 250405 (2004).

[7] S. Trebst, U. Schollwöck, M. Troyer, and P. Zoller, Phys. Rev. Lett. 96, 250402 (2006).

[8] A. M. Rey, V. Gritsev, I. Bloch, E. Demler and M. D. Lukin, Phys. Rev. Lett. 99, 140601 (2007)

[9] T. Barthel, C. Kasztelan, I. P. McCulloch, and U. Schollwöck Phys. Rev. A 79, 053627 (2009)

[10] A. M. Rey, R. Sensarma, S. Fölling, M. Greiner, E. Demler and M. D. Lukin, Euro Phys. Lett. 87, 60001 (2009)

[11] A. Rahmani and C. Chamon, Phys. Rev. Lett. 107, 016402 (2011)

[12] Anders S. Sorensen, Ehud Altman, Michael Gullans, J. V. Porto, Mikhail D. Lukin, and Eugene Demler, Phys. Rev. A 81, 061603(R) (2010)

[13] S.-K. Yip, Phys. Rev. Lett. 90, 250402 (2003); A. Imambekov, M. Lukin and E. Demler, Phys. Rev. A 68, 063602(2003); M. Rizzi, D. Rossini, G. De Chiara, S. Montangero and R. Fazio, Phys. Rev. Lett. 95, 240404 (2005)

[14] Pep Chung Chen, Zhi-Long Xue, I. P. McCulloch, Ming-Chiang Chung, and S.-K. Yip , Phys. Rev. A 85, 011601(R) (2012)

[15] Atsushi Kitazawa and Kiyohide Nomura, Phys. Rev. B 59, 11358 (1999)

[16] H. Bechmann-Pasquinucci and W. Tittel, Phys. Rev. A 61, 102306 (2000); M. Bourennane, A. Karlsson and G. Björk, Phys. Rev. A 64, 012306 (2001)

[17] Dagomir Kaszlikowski, Piotr Gnacinski, Marek Zukowski, Wieslaw Milakowski, and Anton Zeilinger, Phys. Rev. Lett. 85, 4418 (2000); Daniel Collins, Nicolas Gisin, Noah Linden, Serge Massar, and Sandu Popescu, Phys. Rev. Lett. 88, 040404 (2002)

[18] We note here that there are experimental implementations of quantum cryptography or tests of Bell inequalities using effective higher dimensional quantum states with photons (e.g. S. Gröblacher, T. Jennewein, A. Vaziri, G. Weihs and A. Zeilinger, New J. Phys. 8, 75 (2006); A. Dada, J. Leach, G. S. Buller, M. J. Padgett and E. Andersson, Nature Phys. 7, 677 (2011)), but we are not aware of any effort in this direction using finite mass particles.

[19] A. Widera, F. Gerber, S. Fölling, T. Gericke, O. Mandel and I. Bloch, New J. Phys. 8, 152 (2006)

[20] Though not all of the wells in their experiment are doubly occupied.

[21] We remark here that the sign of the quadratic Zeeman shift can be altered by off-resonant AC microwave fields coupling two hyperfine spin states (F. Gerber, A. Widera, S. Fölling, O. Mandel and I. Bloch, PRA 73, 041602(R) (2006)). By adopting this technique, the adiabatic scheme, as well as the dynamic scheme to be discussed below, to some extent, can be further generalized. This is however technically more involved, so we shall only focus on our proposed schemes and shall not investigate this degree of freedom in further detail here.

[22] J. Stenger, S. Inouye, D. M. Stamper-Kurn, H.-J. Miesner, A. P. Chikkatur and W. Ketterle, Nature, 396, 345 (1998)

[23] We understand this as follows. Consider $θ ≈ π/2$, where $E_f ≈ E_2 > E_4$. The state $|40⟩$ is well separated from the other two states at $q = 0$. At finite $q > 0$, the diagonal parts of the quadratic Zeeman energy satisfy $π/2 > 2 > π/4$, thus shifting the $|20⟩$ and $|00⟩$ states further up and away from the lowest $|40⟩$ level. The time evolution thus becomes inefficient to change the amplitude of our state in the $|40⟩$ component. Similar reasoning applies to $θ = π/4$ but $q < 0$.

[24] We understand this as follows. At $θ = π/4$, $E_2$ and $E_4$ are equal. The time evolution during the $q = 0$ time intervals therefore does not modify the relative phase between the $|20⟩$ and $|40⟩$ amplitudes, limiting the capability of the present scheme. The other cases can be understood in a similar manner.

[25] For $^{23}$Na, we use the scattering lengths in the paper (C. V. Ciobanu, S.-K. Yip, and T.-L. Ho, PRA 61, 033607(2000)), provided originally by J. Burke and C. Greene. For $^{87}$Rb, we use the results in Ref. [19].