Gauge field in ultra-cold bipartite atoms

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(Dated: November 21, 2018)

The effects of entanglement and spin-spin collision on the gauge field in ultracold atoms are presented in this paper. Two gauge fields are calculated and discussed. One of the fields comes from space dependent spin-spin collisions in ultra-cold atoms, while another results from the usual Born-Oppenheimer method, which separates the center-of-mass motion from the relative motion in the two-body problem. Adiabatic conditions that lead to the key results of this paper are also presented and discussed. Entanglement shared between the two atoms is shown to affect the atomic motion. In the presence of entanglement, the additional scalar potential disappears, this is different from the case of atoms in separable states.

PACS numbers: 03.75Ss, 42.50Gy, 32.50.Fx

Gauge potentials have been found to appear very naturally in the description of quantum mechanical systems, which depend upon slowly varying external parameters. Beside the central role the gauge fields play in the theory of fundamental interactions, gauge fields are of interest in a variety of single- and many-body quantum systems, leading to a variety of phenomena, for example quantum Hall effect [1, 2]. In recent years ultracold atomic gases[3] have become an ideal playground for studies on the gauge field for ultra-cold atoms with spin-dependent collisions[4, 5] well below the Fermi temperature. This is fascinating as it provides us an interface between ultra-cold atoms and fermions in solid state systems. Fermi systems are well known from the study of electron properties in materials, however trapped atomic fermions are electrically neutral and each atom has internal structure, hence directly mapping from the electron properties into the atomic one is not necessarily straightforward.

Combining the ultra-cold atoms and gauge field, a interesting study is to create an effective magnetic field for ultra-cold atoms[6, 7], the method is based on light-induced gauge potentials for atom with a space-dependent dark state[8]. The dark state is created in three-level Λ-type atoms interacting with two laser fields under conditions of electromagnetically induced transparency[8]. A vector gauge potentials arises for the adiabatic center-of-mass motion, as the dark state is space dependent. From the side of trapped atoms, the strength of the atomic pair interaction can be strongly relying on the magnetically tuned Feshbach resonance[9]. These give rise to a question of how the gauge fields depend on the inter-couplings between the two Fermi atoms. Alternatively, it is believed that intersubsystem couplings would lead to entanglement, then how the entanglement affects the gauge field?

In this paper, we will try to answer these questions by studying the gauge field for ultra-cold atoms with spin-dependent collisions and investigating the effect of entanglement on the gauge field. This is of relevance to the recent study on BCS-BEC crossover in ultra-cold $^{40}K$ gases[10], where the inter-atomic interaction is specified by a two-body potential that depends only on the electron spin

$$V(\vec{r}_1 - \vec{r}_2) = V_\text{c}(\vec{r}_1 - \vec{r}_2) + V_\text{s}(\vec{r}_1 - \vec{r}_2)\vec{S}_1 \cdot \vec{S}_2.$$  (1)

Here the spin states are $|F, m_F\rangle = \{|\frac{7}{2}, \frac{7}{2}\}$ for $^{40}K$. This collision preserves the total spin projection of the two-body system, and then any scattering process between atomic states that conserves the total spin projection is allowed. Taking the atomic motion $\vec{p}^{2i}/2m_i(i=1, 2)$ and trapping potentials $V_i(\vec{r}_i)$ into account, the total Hamiltonian of the system reads,

$$H = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + V_1(\vec{r}_1) + V_2(\vec{r}_2) + V(\vec{r}_1 - \vec{r}_2) + H_0,$$

$$H_0 = \frac{\hbar \omega_1}{2}\sigma_{1z} + \frac{\hbar \omega_2}{2}\sigma_{2z},$$  (2)

where $\sigma_{1z}(i=1, 2)$ stand for the Pauli matrix, and $\omega_i$ is the Rabi frequencies. As you will see, the spin-dependent collision $V_\text{s}(\vec{r}_1 - \vec{r}_2)\vec{S}_1 \cdot \vec{S}_2$ together with the energy difference $(\hbar \omega_2 - \hbar \omega_1)$ lead to a gauge field $\vec{A}$, which would affect the relative motion of the two atoms. This is different from the earlier study in diatom[11]. For fixed $(\vec{r}_1 - \vec{r}_2)$ the Hamiltonian $H_s = H_0 + V_s(\vec{r}_1 - \vec{r}_2)\vec{S}_1 \cdot \vec{S}_2$ can be diagonalized to give a set of eigenvectors $|E_i\rangle$ and corresponding eigenvalues $E_i$ as follows,

$$|E_1\rangle = |\downarrow\rangle, E_1 = -\frac{\hbar \omega_1 - \hbar \omega_2}{2} + V_s,$$

$$|E_2\rangle = |\uparrow\rangle, E_2 = -V_s + \sqrt{\left(\frac{\hbar \delta}{2}\right)^2 + V_s^2},$$

$$|E_3\rangle = |\lessdot\rangle, E_3 = -V_s - \sqrt{\left(\frac{\hbar \delta}{2}\right)^2 + V_s^2},$$

$$|E_4\rangle = |\rangle\rangle, E_4 = \frac{\hbar \omega_1 + \hbar \omega_2}{2} + V_s.$$  (3)

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By introducing \( \vec{R} \), relative and translational motion of the two atoms in the internal degrees of the atoms. Thus \( V \) affects both the relative and translational motion of \( \vec{R} \), \( \vec{r} \). Clearly, matrix analysis leads to an effective equation for the atomic motion in the internal state \( |E_n(\vec{r})\rangle \). Substituting equation Eq.(6) into Schrödinger equation, we get a set of coupled equations for the components \( \psi_i(\vec{R}, \vec{r}) \). These equations can be written in a simple form by introducing column matrices \( \vec{A} \) and \( V \) as

\[
\psi = (\psi_1, \psi_2, \psi_3, \psi_4)^T
\]

where \( A \) and \( V \) are 4 by 4 matrices given by

\[
A_{mn} = i\hbar \langle E_m(\vec{r})|\nabla E_n(\vec{r})\rangle,
\]

and

\[
V_{mn}(\vec{R}, \vec{r}) = E_m(\vec{r})\delta_{mn} + \langle E_m(\vec{r})|V(\vec{R}, \vec{r})|E_n(\vec{r})\rangle.
\]

Clearly, matrix \( A \) includes contributions only from internal atomic degrees, while \( V \) includes contributions from both the internal and external degrees of atoms. Thus \( A \) changes the relative motion of the two atoms, whereas \( V \) affects both the relative and translational motion of the system. Let us now calculate and discuss the vector gauge field \( \vec{A} \) in detail. By the expression of the matrix \( \vec{A} \), it is easy to show that the elements of \( \vec{A} \) take the following form,

\[
A_{22} = A_{33} = 0,
\]

\[
A_{23} = i\hbar \langle +|\nabla|- \rangle = \frac{1}{2}i\hbar \nabla \theta,
\]

\[
A_{32} = i\hbar \langle -|\nabla|+ \rangle = -\frac{1}{2}i\hbar \nabla \theta,
\]

\[
\text{others} = 0.
\]

This leads to \( \vec{B} = \nabla \times \vec{A} = 0 \), i.e., the vector gauge field yields a vanishing magnetic field. Consider two limiting cases \( |\hbar\delta| \gg 2|V_4| \) and \( |\hbar\delta| \ll 2|V_4| \), the first corresponds to a very small internal energy difference between the atoms, with respect to the collision strength \( V_4 \). In this situation \( \cos \theta \simeq 1 - V_4/(\hbar\delta) \) and \( \sin \theta \simeq 2V_4/(\hbar\delta) \) up to first order in \( |V_4/\hbar\delta| \). It yields \( \nabla \theta \simeq \frac{h\delta}{\hbar\delta} \nabla V_4 \). Similar analysis leads to \( \nabla \theta \simeq \frac{h\delta}{\hbar\delta} \nabla V_4 \). With all these together one arrives at

\[
\vec{A}_{23} = \frac{i\hbar V_4}{\delta}, \quad \text{for } |\hbar\delta| \gg 2|V_4|,
\]

\[
\vec{A}_{23} = \frac{i\hbar^2 \delta V_4}{4V_4^2}, \quad \text{for } |\hbar\delta| \ll 2|V_4|.
\]

Eq.(11) shows that, the non-zero elements of matrix \( \vec{A} \) are proportional to \( \nabla V_4 \), the gradient of the collision strength. Suppose \( V_4 \sim -1/r^n \), one gets \( \vec{A}_{23} \sim 1/r^{n+1} \) in the limit of \( |\hbar\delta| \gg 2|V_4| \), whereas \( \vec{A}_{23} \sim r^{n-1} \) in \( |\hbar\delta| \ll 2|V_4| \) limit. The dependence of the imaginary part of \( \vec{A}_{23} \) on the energy difference \( \delta \) as well as \( r \) was shown in figure 1. For plotting figure 1, we chose \( V_4 = -c_6/r^6 \), which is the leading part of atom-atom collisions in ultracold Alkali atoms [12].

Eq.(7) is analytically exact, which describes the joint dynamics of the relative and translational degrees of freedom. Suppose that the atomic state \( |+\rangle \) is well separated from the remaining atomic states \( |E_1\rangle, |E_3\rangle \) and \( |E_4\rangle \). Neglecting transitions from \( |E_2\rangle \) to the others, we get an effective equation for the atomic motion in the internal state \( |E_2\rangle \).

\[
\frac{i\hbar}{\delta} \frac{\partial}{\partial t} \psi_2 = \left[ \frac{1}{2\mu}(-i\hbar \nabla)^2 + U + \frac{\vec{F}_2^2}{2M} \right] \psi_2,
\]

where \( U = V_{22} + \frac{1}{2\mu} \vec{A}_{23} \cdot \vec{A}_{32} \). An additional scalar potential \( 1/(2\mu) \vec{A}_{23} \cdot \vec{A}_{32} \) appears due to the exclusion of the internal states \( |E_1\rangle, |E_3\rangle \) and \( |E_4\rangle \) in the effective equation of motion Eq.(12). The physics behind this may be understood as adiabatic eliminations of the internal states \( |E_1\rangle, |E_3\rangle \) and \( |E_4\rangle \), resulting in an effective potential like stark shifts. This result is interesting because
it provides us another way to test the effect of the vector potential, which yields zero magnetic fields $\vec{B}$. The Schrödinger equation which governs the adiabatic evolution of atoms in state $|\downarrow\rangle$ is similar to that for atoms in state $|\uparrow\rangle$. The difference is only in the effective potential $U$, in this case it is $U = V_{33} + \frac{1}{2m}\vec{A}_{33} \cdot \vec{A}_{32}$. In the Born-Oppenheimer method, the Born-Oppenheimer method[13], eigenfunction $\psi_2$ is decomposed into relative components $\psi^\alpha_2(\vec{R}, \vec{r})$ and components of center-of-motion $\Phi^\alpha(\vec{R})$.

$$\psi_2(\vec{R}, \vec{r}) = \sum_\alpha \Phi^\alpha(\vec{R}) \psi^\alpha_2(\vec{R}, \vec{r}), \quad (13)$$

The $\psi^\alpha_2$ form a basis of eigenfunctions for the relative motion Hamiltonian $\frac{1}{2m}(-i\hbar \nabla)^2 + U(\vec{R}, r)$ for fixed $\vec{R}$ when the translational kinetic energy term $\vec{P}^2/2M$ is ignored, namely

$$[\frac{1}{2\mu}(-i\hbar \nabla)^2 + U(\vec{R}, r)]\psi^\alpha_2(\vec{R}, \vec{r}) = \varepsilon^\alpha(\vec{R}) \psi^\alpha_2(\vec{R}, \vec{r}). \quad (14)$$

The vector wave functions $\Phi^\alpha(\vec{R}) = (\Phi^\alpha_1(\vec{R}), ..., \Phi^\alpha_N(\vec{R}))^T$ then satisfy

$$[-\frac{\hbar^2}{2M}(\nabla_R - i\vec{A})^2 + E^\alpha(\vec{R})] \Phi^\alpha(\vec{R}) = E\Phi^\alpha(\vec{R}), \quad (15)$$

where

$$\vec{A}_\alpha = i(\psi^\alpha_2(\vec{R})|\nabla_R|\psi^\alpha_2(\vec{R})), \quad (16)$$

with $(\vec{R}, \vec{r})\psi^\alpha_2 = \psi^\alpha_2$. To write Eq. (16), we assume that the two atoms remain in the $\alpha$ level, requiring that the translational motion vary very slowly with respect to the relative motion. In the case when this term could not be ignored, the Hamiltonian which governs the evolution of the vector wave functions $\Phi(\vec{R})$ is

$$H_{\alpha\beta} = -\frac{\hbar^2}{2M} \sum_\gamma \left[ \nabla_R + (\psi^\alpha_2)\nabla_R|\psi^\beta_2,\gamma \right] \cdot$$

$$\left[ \nabla_R + (\psi^\beta_2,\gamma)\nabla_R|\psi^\alpha_2,\beta \right] + E^\alpha(\vec{R}) \delta_{\alpha\beta}, \quad (17)$$

The off-diagonal terms in $H_{\alpha\beta}$ would result in transitions between states $|\psi^\alpha_2,\alpha\rangle$ with different $\alpha$. Eq. (16) holds when the adiabatic condition satisfied. Mathematically, this condition may be expressed as $(\alpha \neq \beta)$,

$$\left| \frac{\langle \psi^\alpha_2|H_{\alpha\beta}|\psi^\beta_2 \rangle}{E^\alpha - E^\beta} \right| \ll 1, \quad (18)$$

i.e., the transition induced by the off-diagonal terms in $H_{\alpha\beta}$ may be ignored.

Now we turn to study the effect of entanglement on the gauge fields in ultracold atoms. Suppose that the bipartite atoms are in entangled states

$$|\psi\rangle = \sum_n \Phi_n(\vec{R}, \vec{r})|\alpha_n(\vec{R})\rangle_a \otimes |\beta_n(\vec{r})\rangle_b, \quad (19)$$

where $|\alpha_n(\vec{R})\rangle_a$, $(|\beta_n(\vec{r})\rangle_b)(n = 1, 2, ..., N)$ represent internal states of atom a (atom b). The entanglement shared between the atoms may be measured by the quantum entropy as $s = -\sum_n |\Phi_n(\vec{R}, \vec{r})|^2 \ln |\Phi_n(\vec{R}, \vec{r})|^2$, which would remain unchanged if there are no couplings between them. Consider a Hamiltonian

$$H = \frac{\vec{P}_a^2}{2M} + \frac{\vec{P}_b^2}{2m} + H_a(\vec{R}) + H_b(\vec{r}), \quad (20)$$

which governs the evolution of the bipartite atoms without couplings between them. Here, $H_a(\vec{R})$ ($H_b(\vec{r})$) denotes the Hamiltonian of the electronic degrees of freedom of atom a (atom b), and satisfies

$$H_a(\vec{R})|\alpha_n(\vec{R})\rangle_a = \varepsilon_n(\vec{R})|\alpha_n(\vec{R})\rangle_a. \quad (21)$$

Similarly, we require that

$$H_b(\vec{r})|\beta_n(\vec{r})\rangle_b = \varepsilon_n(\vec{r})|\beta_n(\vec{r})\rangle_b. \quad (22)$$

These restrictions can be relieved and we will show later that they do not change the results. Substituting Eq. (19) and $H$ into the Schrödinger equation, we arrive at (setting $\Phi(\vec{R}, \vec{r}, t) = (\Phi_1(\vec{R}, \vec{r}, t), ..., \Phi_N(\vec{R}, \vec{r}, t))^T$)

$$i\hbar \frac{\partial}{\partial t} \Phi = H_{eff} \Phi, \quad (23)$$

$$H_{eff} = \left[ \frac{1}{2m}(-i\hbar \nabla - \vec{a})^2 + \frac{1}{2M}(-i\hbar \nabla_R - \vec{A})^2 + \epsilon + \varepsilon \right].$$

It is readily to show that $\vec{A}$ and $\vec{a}$ are diagonal matrices, the elements can be expressed as $\vec{A}_{nn} = i\hbar(\langle \alpha_n|\nabla_R|\alpha_n(\vec{R})\rangle)$, and $\vec{a}_{nn} = i\hbar(\langle \beta_n|\nabla_R|\beta_n(\vec{r})\rangle)$. $\epsilon$ and $\varepsilon$ are also $N \times N$ diagonal matrices, composed by the eigenvalues of $H_b$ and $H_a$, respectively. In contrast with the results presented in Eq. (12), there is no any additional scalar potential resulting from $\vec{A}$ or $\vec{a}$, even if one of the atomic states is well separated from the remaining atomic states. This is due to the vanishing of the off-diagonal elements of the vector potentials $\vec{A}$ and $\vec{a}$. The physics behind this result is the entanglement. To show this point clearly, we suppose that the bipartite atoms are in separable states, for example,

$$|\psi\rangle = \sum_n \Phi_n(\vec{R}, \vec{r}, t)|\alpha_n(\vec{R})\rangle_a \otimes |\beta(\vec{r})\rangle_b, \quad (24)$$

where $|\psi(\vec{r})\rangle_b$ represents a state of atom b. Clearly, for a specific $n$ that $|\alpha_n(\vec{R})\rangle_a$ is well separated from the others, $\Phi_n$ satisfies

$$i\hbar \frac{\partial}{\partial t} \Phi_n = \left[ \frac{1}{2M}(-i\hbar \nabla_R - \vec{A}_{nn})^2 + V(\vec{R}) \right] \Phi_n, \quad (25)$$

with $\vec{A}$ being $N$ by $N$ matrix given by $\vec{A}_{nn} = i\hbar(\langle \alpha_n|\nabla_R|\alpha_n(\vec{R})\rangle)$, and $V(\vec{R}) = \frac{1}{2m} \sum_{j\neq n} \vec{A}_{jn} \cdot \vec{A}_{jn}$. $\vec{A}_{nn}$ appears due to the nonzero off-diagonal elements of $\vec{A}$. The
restrictions Eqs.(21) and (22) can be removed, leading to no change of the conclusion, this can be understood as follows. Consider entangled states of the bipartite atoms,

$$|\psi\rangle = \sum_n \Phi_n(\vec{R}, \vec{r}, t) |\xi_n(\vec{R})\rangle_a \otimes |\gamma_n(\vec{r})\rangle_b,$$

(26)

where $|\xi_n(\vec{R})\rangle_a$ ($|\gamma_n(\vec{r})\rangle_b$) are not the eigenstates of $H_a$ ($H_b$). In terms of the eigenstates of $H_a$ and $H_b$, $|\xi_n(\vec{R})\rangle_a$ and $|\gamma_n(\vec{r})\rangle_b$ may be expressed as

$$|\xi_n(\vec{R})\rangle_a = \sum_j C^n_j(\vec{R}) |\alpha_j(\vec{R})\rangle_a,$$

$$|\gamma_n(\vec{r})\rangle_b = \sum_j c^n_j(\vec{r}) |\beta_j(\vec{r})\rangle_b.$$ 

(27)

The Schrödinger equation instead of Eq. (24) then takes,

$$i\hbar \frac{\partial}{\partial t} \Phi = \left[ \frac{1}{2m} (-i\hbar \nabla \vec{r} - \vec{a})^2 + \frac{1}{2M} (-i\hbar \nabla \vec{R} - \vec{A})^2 + e + E \right] \Phi,$$

(28)

where $\vec{c}$ and $\vec{E}$ are $N$ by $N$ matrices as follows. $e_{ij} = \langle \gamma_i | H_b | \gamma_j \rangle$, and $E_{ij} = \langle \xi_i | H_a | \xi_j \rangle$. $E_{ij}$ and $e_{ij}$ would induce population transfer, but these terms could not result in any scalar potential even if the population transfer induced may be ignored, because $\vec{A}$ and $\vec{a}$ are diagonal in this case, too. This means that the atoms experience no additional scalar potential when they evolve adiabatically in any internal states as long as they are entangled.

In conclusion, we have discussed the gauge fields in ultra-cold atoms with space dependent spin-spin collisions. The vector gauge field leads to zero magnetic fields, but gives rise to effective potentials to the relative motion of the atoms, this effective potential may be strong and results in escaping of the trapped atoms from the trapping potential. For the center-of-mass motion, the gauge field comes from relatively slow motion of the center-of-mass, the effects of the space dependent spin-spin collision on the center-of-mass motion take place through changing the eigenfunction of the relative motion. It is estimated to be large near the Feshbach resonance. The entanglement has been shown to eliminate the additional scalar potential, explanations and discussions are also given.

We acknowledge financial support from NCET of M.O.E, and NSF of China Project No. 10305002 and 60578014.

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