Dressed Qubits in Nuclear Spin Baths

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We present a method to encode a dressed qubit into the product state of an electron spin localized in quantum dot and its surrounding nuclear spins via a dressing transformation. In this scheme, the hyperfine coupling and a portion of nuclear dipole dipole interaction become logic gates, while they are the sources of decoherence in electron spin qubit proposals. We discuss errors and corrections for the dressed qubits. Interestingly, the effective Hamiltonian of nuclear spins is equivalent to a pairing Hamiltonian, which provides the microscopic mechanism to protect dressed qubits against decoherence.

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Introduction.— The building blocks of quantum information processors are controllable quantum bits. Electron spins in quantum dots are promising candidates for these basic units [1, 2, 3, 4]. The control of electron spins in quantum dots has been investigated extensively in areas such as quantum information. However, the decoherence, dominantly originating from the hyperfine coupling between an electron spin and its surrounding nuclear spins in the host material, may ruin the quantum process of the electron spin [5, 6]. Distinct from random noise, the hyperfine coupling causes inherent error with non-Markovian feature [5] and can be manipulated to some extent [7]. This nature has been utilized to create long-lived quantum memory of electron spin qubits via the surrounding nuclear spins and to implement optical pumping [7, 8, 9, 10, 11]. Theoretical motivations along this line have lead to interesting experimental results [13, 14, 15, 16]. Alternatively, this inherent error may be corrected by the dressed qubit method [17]. The essential ingredient to use this method is to find a unitary dressing transformation between the basis of electron spin and the product basis of electronic and nuclear spins, such that the matrix representations of operators on the electron spin Hilbert space are the same as those on the corresponding product space. This paper demonstrates the feasibility of applying the dressed qubit method to the electronic-nuclear spin system. Different from a bare electron spin interacting with nuclear spins, the corresponding dressed qubit is only subject to leakage, which may be suppressed by the Bang-Bang method in terms of a universal leakage elimination operator [17]. Engineering of nuclear spin distribution in the host material may also be an option in dealing with these leakages. It is interesting to note that the effective Hamiltonian of nuclear spins is equivalent to a pairing Hamiltonian, which helps the dressed qubit to protect against decoherence.

Invariant subspaces spanned by electronic spin and nuclear spins.— Consider a single electron confined in quantum dot. The Hamiltonian for the electron spin and its surrounding $K$ ($\approx 10^5$) nuclei with spin $I$ is

$$H = H_B + H_I + H_{nuc},$$

where $H_B = g_s \mu_B BS_z + g_n \mu_n BI_z$ is the Zeeman energy of the electron spin and nuclear spins in a magnetic field $B$ along the $z$ axis. Here $S_z$ ($I_z = \sum_i I_z^i$) is the $z$-component of the electronic (total nuclear) spin operator. The $z$-component of the total angular momentum, $J_z = S_z + I_z$, is conserved in the system. We can write the hyperfine coupling between nuclear spins and the electron spin

$$H_I = A\sqrt{2I}(A_s S_z + V_f),$$

where $A$ is an average hyperfine coupling constant. Operators $A_{\mu} = \sum_i \alpha_i I_{\mu}^i/\sqrt{2I}$ are expressed in terms of the nuclear spin $I_{\mu}^i$ ($\mu = z, +, -$), where the real numbers $\alpha_i$’s correspond to values of the electronic wave function at the point $R_i$ and are normalized such that $\sum_i \alpha_i^2 = 1$ (slightly different from the normalization in Ref. [17]). The dominant contribution of $A_s S_z$ is an effective magnetic field for the electron spin, known as Overhauser shift [7]. We will show later that the effective magnetic field on the electron spin, including Overhauser shift characterized by $\alpha_i$’s and $A$, can be written

$$B_{eff} = B - A \sum \alpha_i (I + \alpha_i^2/2)/g_s \mu_B.$$

The spin exchange $V_f = 1/2 A_s S_+ + 1/2 A_s S_-$ plays crucial roles in creating long-lived quantum memory [7] and implementing optical pumping [8]. Significantly, this term will also act as a logic gate in our scheme. The nuclear dipole dipole interaction $H_{nuc}$ reads as

$$H_{nuc} = \sum_{i=1;i<j}^K b_{ij} (I_{+i} I_{-j}^* + I_{+j} I_{-i}^* - 4I_{+i} I_{+j}^*),$$

where $b_{ij} \propto (3 \cos^2 \theta_{ij} - 1)/r_{ij}^3$, $r_{ij}$ is the distance between nuclei $i$ and $j$, $\theta_{ij}$ is the zenith angle of the relative vector pointing from nucleus $i$ to $j$.

The nuclear spin operators may be represented in terms of fermionic pairs. To each index $i$, we define a pair of “imaginary state” $(i, \bar{i})$, where $\bar{i}$ is the time reversal of the imaginary state $i$. The nuclear spin operators $I_{-i}$ and $I_{+i}$ are then rewritten by fermionic pairs,

$$I_{-i} = \sum_{s=1}^{2I} \epsilon_i^s \epsilon_i^{s*}, \quad I_{+i} = \sum_{s=1}^{2I} \epsilon_i^{s*} \epsilon_i^s,$$
which satisfy the restrictions $(I^+_{\lambda})^{2J+1} = 0$. The commutator $[I^+_\lambda, I^+_\lambda'] = 2\delta_{\lambda\lambda'}(I - \hat{n}_\lambda)$ is represented by a nuclear pair operator $\hat{n}_\lambda = \sum_{i=1}^{2J} (c^+_i c^+_i + c_i c_i)/2$. When $I = 1/2$, the sums (4) are simplified $I^+_\lambda = c^+_0 c_i$, $I^+_\lambda' = c_i c^+_0$ and $\hat{n}_\lambda = (c^+_i c_i + c_i c^+_i)/2$. A total nuclear pair operator can be defined as $\hat{n} = \sum_{\lambda} \hat{n}_\lambda$. Likewise, electron spin can be faithfully represented by pair operators on a imaginary pair $(0, 0)$, $S_- = c^*_0 c_0$, $S_+ = c^*_0 c^+_0$ and $S_z = \hat{n}_0 - 1/2$. The total pair operator of the electron and nuclei is $\hat{N} = \hat{n} + \hat{n}_0$.

In recently proposed techniques of long-lived memory and optical pumping [8], it has been suggested that the dominant part of the Hamiltonian (1)

$$H_D = F(t) S_z + A \sqrt{2} T V_f,$$  

where $F(t) = g^* \mu_B B_{eff} - g_n \mu_n B$ includes contributions from electronic and nuclear spins as well as Overhauser shift. We have neglected the constant $g_n \mu_n B J_z$, where $J_z = N - K - 1/2$ is conserved. There exist two-dimensional invariant subspaces of the Hamiltonian $H_D$ for each given value of $N \in (0, 2K + 1)$. In order to show this explicitly, we consider a Hermitian operator $\hat{h} = \hat{A} \hat{A}^\dagger$, which commutes with the total nuclear pair operator $\hat{n}$. Let $| m \rangle$ be common eigenstates of the operators $\hat{h}$ and $\hat{n}$ such that $\hat{h} | m \rangle = h_m | m \rangle$. It is clear that the eigenvalues $h_m = \langle m | \hat{A} \hat{A}^\dagger | m \rangle$ are positive numbers. The two-dimensional subspaces, spanned by states

$$|0\rangle_d = |\uparrow\rangle \langle \uparrow| |m\rangle, \quad |1\rangle_d = |\downarrow\rangle \langle \downarrow| \Phi_{m+1},$$  

are invariant under the Hamiltonian $H_D$. Here $|\uparrow\rangle$ ($|\downarrow\rangle$) is the electron spin-up (down) state, and $\Phi_{m+1} = \hat{A}^\dagger |m\rangle / \sqrt{h_m}$ are nuclear spin states but usually are not eigenstates of $\hat{h}$. $V_f$ exchanges the two states,

$$V_f |0\rangle_d = \sqrt{h_m / 4} |1\rangle_d,$$

$$V_f |1\rangle_d = \sqrt{h_m / 4} |0\rangle_d.$$  

Note that we have excluded two one-dimensional subspaces, where both electronic and nuclear spins are completely polarized, with $N = 0$ and $N = 2K + 1$.

While there are many two-dimensional invariant subspaces characterized by the total pair number $N$, we now concentrate on the $N = 1$ invariant subspace $\mathcal{H}_2$, which has been studied extensively. The eigenstate $|m\rangle$ in this subspace is $|0\rangle = |\uparrow\rangle - |\downarrow\rangle$ with eigenvalue $h_m = 1$, where nuclear spins are perfectly polarized. The state $\Phi_{m+1} = \hat{A}^\dagger |0\rangle$, denoted as $|1\rangle$, is orthogonal to the state $|0\rangle$ and becomes an eigenstate of $\hat{h}$ in this particular case. In general, given numbers $N$ and $I$, there are $\Omega(I, N)$ states in the combined system of the electron spin and nuclear spins, for instance, when $I = 1/2$, $\Omega(1/2, N) = \frac{(K+1)!}{(K-1)!}$. The $N = 1$ Hilbert space, denoted by $\mathcal{H}_{K+1}$, is $K + 1$-dimensional (i. e., $\Omega(K, 1) = K + 1$). This means that there are additional $K - 1$ states in the space, which can be made orthogonal against the two states in eq. (6). The $K - 1$ states are all in the electron spin-down state and can be written $|1_k\rangle = |\downarrow\rangle_c |1\rangle$, where $|1\rangle = A_{k+} |0\rangle$ and $A_{k+} = \sum_i \alpha_i I^+_1 / \sqrt{2I}$. We identify the “collective” mode $k = 0$, i. e., $A_+ = A_{0+}$ and $\alpha_0 = \alpha^0$. The set $\{\alpha_k\}$ corresponds to a $K \times K$ matrix $[\alpha]$ and can, as usual, be made as a unitary matrix by using Gram-Schmit orthogonalization such that $|1_k\rangle \langle 1_k| = \delta_{kk} [I]$. These operators obey the commutation relations

$$[A_{k-}, A_{k'+}] = \delta_{kk'} - \sum_i \alpha_i^k \alpha^k_i \hat{n}_i / I.$$  

The Hilbert space $\mathcal{H}_{K+1}$ can be spanned by the orthogonal bases $|0\rangle_d, |1\rangle_d$ and $|1_k\rangle$, where $k = 1, ..., K - 1$. Note that with equation (8) we have $V_f |1\rangle_d = 0$, for all $k \neq 0$.

The bosonization of the nuclear spin operators has been used to discuss the electron spin qubit protection against decoherence [10]. Consider the bosonic form $V_f = \frac{1}{2} A^\dagger S_- + \frac{1}{2} A S_+$ of the hyperfine coupling, where $A = \sum_i \alpha_i b_i$ corresponds to the collective mode and $b_i$’s are bosons. The additional modes $A^k_i = \sum_i \alpha_k^i b_i^\dagger$ are defined by using the same matrix $[\alpha]$ as above. $A_k$ and $A^k_i$ obey the bosonic commutation relations

$$[A_k, A^k_i] = \sum_i \alpha_i^k \alpha^k_i = \delta_{kk'}.$$  

By comparison with Eq. (8), it is clear that the nuclear spin ensemble behaves like that of collective bosons when nuclear spins are in well polarized states or $\sum_i \alpha_i^k b_i^\dagger b_i < I$.

Dressing transformation and single dressed qubit operations.— Here we introduce a dressing transformation between the electron spin space and the subspace $\mathcal{H}_2$,

$$W = |\uparrow\rangle \langle \uparrow| |0\rangle + |\downarrow\rangle \langle \downarrow| |1\rangle,$$

which satisfies the unitary condition $WW^\dagger = W^\dagger W = 1$ since $|0\rangle_d |0\rangle + |1\rangle_d |1\rangle = 1$ - the completeness in the invariant subspace $\mathcal{H}_2$. Under this transformation $V_f$ acts as $S_x$ :

$$W^\dagger S_x W = \frac{1}{2} (|\uparrow\rangle \langle \uparrow| + |\downarrow\rangle \langle \downarrow|) = \frac{1}{2} (|0\rangle_d \langle 0| + |1\rangle_d \langle 1|) = |V_f\rangle.$$  

In another word, the matrix representation of $V_f$ in $\mathcal{H}_2$ is the same as that of $S_x$ in the electronic spin space, i. e.,

$$[V_f] = \frac{1}{2} \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) = X_d / 2,$$

denoted as $X_d / 2$. Another operator $S_z$ is transformed as

$$W^\dagger S_z W = \frac{1}{2} (|0\rangle_d \langle 0| - |1\rangle_d \langle 1|) = Z_d / 2,$$

where $S_z$ in $\mathcal{H}_2$ plays the same role as that in the electron spin space, denoted by $Z_d / 2$. The Hamiltonian $H_D$ is therefore rewritten

$$H_D = F(t) Z_d / 2 + A \sqrt{2} T X_d / 2.$$  


and the dressed qubit is supported by the two states in (6).

This form of the Hamiltonian, equivalent to that for the NMR quantum computer, can generate a universal logic gate set for the dressed qubit, even in cases when the hyperfine is not controllable. Single dressed qubit gates can also be performed by using a sequence of square pulses, whose evolution operators, in general, are

$$U(\phi, \theta) = e^{-i\phi(\cos \theta Z_d + \sin \theta X_d)} = e^{-i\phi Y_d/2} e^{-i\phi Z_d} e^{i\theta Y_d/2}.$$  

Here $\phi = t\sqrt{F^2 + 2IA^2} > 0$ and $\theta = \arctan(\sqrt{2IA}/F)$. By controlling parameter $F$, we can manipulate the angles $\phi$ and $\theta$. For instance, by setting $F = 0$ we obtain $U(\phi, \pi/2) = e^{-i\phi X_d}$ and $U(\phi + \pi, \pi/2) = e^{i\phi X_d}$. An effective gate $Y_d$ is $iZ_d X_d$ in $\mathcal{H}_2$ can be generated by the circuit $U(\pi/2, \theta) X_d = e^{-i(\theta + \pi/2)Y_d}$. We can effectively generate any logic single-qubit operation in the invariant subspace $\mathcal{H}_2$ with $e^{i\phi X_d}$ and $e^{-i\theta Y_d}$.

The same approach can be applied in the $N > 1$ cases, except that another nuclear spin eigenstate $|n\rangle$ of $\hat{h}$, other than the perfectly polarized state, has to be initially prepared. Since the perfectly polarized state usually is hard to be realized, it might be an encouraging option to initially prepare another eigenstate instead, for instance, a state with $I_z = 0$ being zero.

Effective logic gates and leakage.— Different from electron-spin qubits, the present dressed qubits only suffers from leakage from the dressed state $|1\rangle_d$ into the rest of the Hilbert space $\mathcal{H}_{K+1}$ spanned by $|1\rangle_k$. The leakage is caused by the residual effect of $A_z S_z$ (or $A_z$, for $S_z = -1/2$ in the leakage-related space) and the nuclear dipole dipole interaction, which preserve the total nuclear pair number $n$. However, it is interesting to note that, in the dressed qubit approach, the major portion of the hyperfine term $A_z S_z$ and the dipole dipole interaction only provide additional contributions to logic gates but do not result in leakage.

As discussed previously, Overhauser shift is the major effect of $A_z S_z$. While $|0\rangle_d$ is its eigenstate, i.e., $A_z |0\rangle = c_z |0\rangle$, the interaction $A_z S_z$ will ruin the state $|1\rangle_d$

$$A_z |1\rangle = (c_z + \sum_i \alpha_i^2/\sqrt{2I}) |1\rangle + |0\rangle,$$

where the constant $c_z = -\sqrt{I/2} \sum_{i=1} \alpha_i$. A part of the second coefficient of the state $|1\rangle$ contributes a constant in the subspace $\mathcal{H}_2$. The other part of second coefficient and the first coefficient correspond to an additional phase gate $-A \sum_i \alpha_i (I + \alpha_i^2/2)Z_d/2$. Overhauser shift. The magnitude of the leaked state $|0\rangle$ is much smaller than that of its orthogonal state $|1\rangle$, with the relative ratio being approximately $\sum_{i=1} \alpha_i \sim A^2 \tau_0 \sim 10^{-5}$. It is small but still in the order of the fault tolerance threshold estimates of quantum error correction theory [18].

Leakage also arises from the nuclear dipole dipole interaction. While $H_{nuc} |0\rangle = c_0 |0\rangle$, the interaction acting on the other state yields $H_{nuc} |1\rangle = (c_0 + c_1) |1\rangle + |O\rangle$, where $|O\rangle$ is a state orthogonal to $|1\rangle$. The dominant contribution to $\mathcal{H}_2$ is $c_0 = -16I^2 \sum_{n \neq m} b_{nm}$, which is a constant in this subspace. The second coefficient $c_1 = 4I \sum_{n \neq m} \alpha_i b_{ni} (\alpha_n + \alpha_i)$ of the state $|1\rangle$ indicates that the dipole dipole interaction also induces an additional phase gate $c_1 Z_d/2$ for the dressed qubit.

We now try to find a special form of the dipole dipole Hamiltonian that preserves the subspace $\mathcal{H}_2$. Since the coupling constants $b_{ni}$ represent the classical dipole dipole interaction, the sum $\sum_{n \neq m} b_{ni}$ should stand for an average field acting on the $i$th nuclear spin due to all the others. We can assume that each spin is subject to the same average field, i.e., $\sum_{n \neq m} b_{ni} = \tilde{b}$ being a constant. This assumption should be valid for homogeneous materials. We then consider a family of $\{b_{ni}\}$ satisfying the $K$ constraints $\sum_i b_{ni} \alpha_i = \tilde{b} \alpha_i$, where $\tilde{b}$ is a constant. Based on the two assumptions, we can show $\tilde{b} = \tilde{b}$ and the dipole dipole interaction acts as

$$(H_{nuc} - c_0) |1\rangle = 36\tilde{b} |1\rangle. \quad (11)$$

This special form of $H_{nuc}$ does not cause leakage but provides additional contribution to the phase gate. With this result, one may get rid of leakage by adjusting the $K (K - 1)/2$ coupling constants $b_{ij}$ towards the $K$ constraints, as intimate as possible, through engineering the angles $\theta_{ij}$ and the distances $r_{ij}$.

The deviation from the special form causes leakage from the subspace $\mathcal{H}_2$ into the Hilbert space $\mathcal{H}_{K+1}$. We symbolize the portion of Hamiltonian (1) causing leakage as $\mathcal{H}_L$, which contains the leakage due to both $A_z S_z$ and $H_{nuc}$.

Leakage elimination.— Leakage can be eliminated by making use of fast “bang-bang” pulses [19]. The key to this open-loop solution is to find a universal leakage-elimination operator $R_L$ such that $R_L H_L R_L = -H_L$. The leakage operator has the diagonal matrix representation in the space $\mathcal{H}_{K+1}$

$$[R_L] = \begin{pmatrix} [-I] & 0 \\ 0 & [I'] \end{pmatrix}, \quad (12)$$

where $-I$ is a $2 \times 2$ unit matrix in dressed bases $|0\rangle_d$ and $|1\rangle_d$, and $[I']$ is a $(K - 1) \times (K - 1)$ unit matrix in the rest of the space $\mathcal{H}_{K+1}$. It can be shown that the operator $R_L = \exp(-i\pi [A_z S_z + A_z S_+])$ has the matrix representation (12) and thus is a leakage elimination operator. Leakage can be eliminated by the standard bang-bang circuit $R_L \exp(-iH\tau/2) R_L \exp(-iH\tau/2)$ [19], where time $\tau$ is made very short compared to the bath correlation time. This circuit for the dressed qubit simplifies the error control technique in electron spin qubits [20].

Equivalent pairing Hamiltonian.— The hyperfine coupling induces interaction among nuclear spins via the electron spin. An effective correlation $V_{eff} = -\frac{4}{3} K A_z A_r$ can be introduced by the well-known Fröhlich transformation $e^{-3V_f e^S}$ with a generator $S = -\frac{4}{3} \sqrt{T} (A_r S_+ - A_z S_-)$. The correlation is determined by $A_r^2 / F$.

By using Eq. (4) and the induced nuclear interaction, we can generically write the nuclear effective Hamiltonian (1) as a pairing Hamiltonian. To simplify, we consider the $I = 1/2$
case, where the nuclear effective Hamiltonian is

$$H_{\text{eff}} = \sum_{i=1}^{K} \varepsilon_i \hat{n}_i - 2 \sum_{i \neq j=1}^{K} b_{ij} \hat{n}_i \hat{n}_j - \sum_{i \neq j=1}^{K} g_{ij} c_i^\dagger c_j c_j^\dagger,$$

where $\varepsilon_i = -A\alpha_i/2 - 2 \sum_{j \neq i} (b_{ij} + b_{ji})$ and $g_{ij} = \frac{\alpha_i^2}{4f} \alpha_j + b_{ij}$. The first term corresponds to a signal particle energy of imaginary states. The middle term stands for a on-site interaction and the last is a standard pair correlation, where the dominant contribution stems from the induced nuclear interaction $V_{\text{eff}}$. The ground state of the effective Hamiltonian can be expressed approximately by the BCS wave function,

$$|\text{BCS}\rangle \approx \exp \left( \sum_i \frac{\varepsilon_i \hat{n}_i}{\sqrt{N}} - A_+ \right) |0\rangle,$$

where $\varepsilon_i$ and $u_i$ are obtained by solving the set of BCS equations that can be found in textbooks (see, e. g., [22]). The gap parameters obey the self-consistent gap equations

$$\Delta_i = \frac{1}{2} \sum_j g_{ij} \Delta_j / \xi_j,$$

where $\xi_j = \sqrt{(\varepsilon_j - \lambda)^2 + \Delta_j^2}$ and $\lambda$ is the chemical potential determined by the nuclear pair number constraint $\langle \text{BCS} | \hat{n} | \text{BCS} \rangle = n$.

Ref. [10] proposes a phenomenological scheme to protect the nuclear spin memories by using the bosonization scheme [9]. The scheme demonstrates that there is an energy gap between the collective storage state, characterized by the collective boson $A$, and other states, which plays the critical key to protect the quantum memory against local spin-flip and spin-dephasing noise. Here the exact correspondence between the nuclear spin Hamiltonian and the pairing Hamiltonian [13] provides the microscopic mechanism of this energy gap and the scheme.

The set of BCS equations does not possess analytic solutions in the general case. We can estimate the solution by setting $\alpha_i = 1/\sqrt{K}$ and $b_{ij} = b$. In this case, all $\varepsilon_i$ are equal, $\varepsilon_i = \sqrt{n/K}$, $u_i = \sqrt{1 - n/K}$. The BCS wave function reads

$$|\text{BCS}\rangle \approx \exp \left( \sqrt{\frac{n}{K - n}} A_+ \right) |0\rangle,$$

where the nuclear dipole-dipole interaction does not contribute to the wave function under this level of approximation. However, it appears in the gap parameter

$$\Delta = \left( \frac{A^2}{4fK} + b \right) \sqrt{n(K - n)}.$$

The gap parameter keeps the BCS ground state away from other states. It also indicates that when $n = K/2$ ($I_z = 0$) the gap reaches its maximum and provides the most efficient protection for the BCS ground state against decoherence. The result is only valid for fermionic pairs but not for bosons.

In conclusion, we have introduced a method to encode a dressed qubit into an electron spin and nuclear spins. Unlike other treatments against decoherence, the dressed qubit method does not require extra overheads in gating, initialization and measurement. The hyperfine coupling and a part of nuclear dipole-dipole interaction now become logic gates in this scheme, while they are sources of decoherence in electron spin qubit proposals. The residual correlations from the hyperfine coupling $A_x S_x$ and dipole interaction are categorized as leakages which may be eliminated by the “Bang-Bang” method in a simple way. It is also interesting to note a passive strategy to reduce these leakages by engineering the distribution of nuclear spins in the host material.

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