Thermal electron spin flip in quantum dots

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We study a thermally induced spin flip of an electron spin located in a semiconductor quantum dot. This interesting effect arises from an intriguing interplay between the Zeeman coupling to an external magnetic field and the hyperfine interaction with the surrounding nuclear spins. By considering a minimal model, we explain the main mechanism driving this spin flip and analyze its dependence on the strength of the external magnetic field, the number of nuclear spins and the ratio of the electron and nuclear Zeeman energies, respectively. Finally we show, that this minimal model can be applied to experimentally relevant QDs in III-V heterostructures, where we explicitly predict the temperature at which the spin flip occurs.

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I. INTRODUCTION

The physics of an electron spin confined to a quantum dot (QD) has been in the focus of condensed matter research for many years due to its possible applications in quantum information processing. Following the seminal work\cite{Loss98} of Loss and DiVincenzo, the two eigenstates of the electron spin can be used to define a quantum bit (qubit). However, in the host nanostructures, the electron spin is subject to a variety of different interactions\cite{Loss03} leading to a loss of the stored information and decoherence. Important examples for these interactions are the hyperfine interaction (HI) with surrounding nuclear spins or the coupling of the electron spin to electrical fields via spin orbit interaction. The dynamics of the electron spin influenced by these effects - alone or combined - have been studied in great detail\cite{loss03,diVincenzo01,loss04,DiVincenzo98,DiVincenzo99} in the last years enhancing our knowledge about spin physics in QDs\cite{Loss03,diVincenzo01,loss04}. Along with these insights also strategies were developed to reduce the loss of information\cite{loss04,DiVincenzo98}. However, while electrical noise seems fairly controllable, the HI with the nuclear spins remains nonetheless as a major source of decoherence, since nuclear spins are intrinsic to most QD host materials such as the widely used III-V heterostructures. Yet recently, also a change of paradigm can be observed, where the unavoidable interaction with the nuclear spins is considered rather as a resource for interesting physics than an obstacle\cite{loss04}.

In this notion, we want to present our findings on a thermally induced flip of the electron spin. These results were obtained by applying standard statistical physics to a minimal model for spin dynamics in a QD consisting of an external magnetic field to which the electron and the nuclear spins couple and the HI which links the electron spin to all nuclear spins. The effect of an external magnetic field on the electron is described by the Zeeman Hamiltonian

\[ \hat{H}^S_{ZE} = g^* \mu_B B_z \hat{S}_z, \]  

where \( g^* \) is the effective g-factor\cite{Loss04} of the electron, \( \mu_B \) is the Bohr magneton, and \( \hat{S}_z \) is the electron spin component parallel to the external magnetic field \( B_z \). Likewise, nuclear spins also align with respect to the external magnetic field by means of another Zeeman term

\[ \hat{H}^I_{ZE} = \sum_{k=1}^{K} \hat{I}^k_{ZE} = - \sum_{k=1}^{K} g_N \mu_N B_z \hat{I}^k_{z}, \]  

where \( g_N \) is the nuclear g-factor, \( \mu_N \) is the nuclear magneton and the sum is running over all nuclear spin z components \( \hat{I}^k_{z} \). Note the relative sign difference between Eq. (1) and Eq. (2), which resembles the negative sign of the electron charge.

By writing the nuclear Zeeman Hamiltonian in the form of Eq. (2), we already assume that there is only one spin species present in the dot. This assumption will simplify our reasoning and, thus, allows us to better identify the main physics being relevant for our results. Distinguishing different spin species would not change our findings significantly as we discuss in the end of this article. This specific choice also simplifies the HI Hamiltonian

\[ \hat{H}_{HI} = A_{HI} \sum_{k=1}^{K} |\phi(\vec{r}_k)|^2 \left[ \hat{S}_z \hat{I}_k^z + \frac{1}{2} (\hat{S}_+ \hat{I}_{k,-} + \hat{S}_- \hat{I}_{k,+}) \right], \]  

where \( |\phi(\vec{r}_k)|^2 \) is the probability to find the electron at the site of the \( k \)-th spin-carrying nucleus. The energy of the HI is given by a constant

\[ A_{HI} = g \cdot g_N \cdot C \]  

with \( C > 0 \) being a material dependent energy scale. Since the HI interaction is strongly localized around the respective nucleus, the bare electron g-factor \( g \approx 2 \) enters here\cite{loss04}. Thus, the sign of the HI is determined by the sign of the nuclear g-factor \( g_N \). This sign, however, plays an important role, since it determines the form of the ground state of the HI.

If the coupling constant \( A_{HI} \) is positive (negative), the ground state of the bare HI will favor an anti-parallel (parallel) alignment of the electron spin with respect to
all nuclear spins. Both ground states are twice degenerate, since a flip of all spins results in the same energy. Similarly, the two Zeeman terms also show the same two types of spin ordering depending on the signs of the respective g-factors $g^*$ and $g_N$. In contrast to the HI, these ground states are unique. If, for instance, $g^* < 0$ and $g_N > 0$, the Zeeman terms would force both the electron spin and all nuclear spins to be parallel to the external magnetic field at zero temperature. Thus, when both the HI and the Zeeman interaction are present, there can arise an interesting competition of spin ordering with the electron spin being parallel or anti-parallel with respect to the nuclear spins. In particular, if the external magnetic field is sufficiently small, the HI is still strong enough to maintain the anti-parallel alignment of the electron spin with respect to the nuclear spins. If then additionally the sign of the g-factors are given by $g^* < 0$ and $g_N > 0$, the electron spin will be anti-parallel to the external magnetic field, whenever its Zeeman energy is below the total Zeeman energy of all nuclear spins. Starting from this particular ground state, we will show that a sudden flip of all spins can happen at a finite temperature $T_0 > 0$.

The article is organized as follows: In Sec. II.A, we will argue how the HI Hamiltonian can be simplified based on physical arguments. In Sec. II.B, we will then apply standard statistical physics to the total Hamiltonian $\hat{H} = \hat{H}^{ZE}_{I} + \hat{H}^{ZE}_{N} + \hat{H}_{HI}$ in order to calculate the thermal expectation value of the electron spin. Its properties are studied both analytically and numerically in Secs. II.C and II.C, respectively. After this mathematical analysis, we will then explain the physical mechanism being responsible for this spin flip in Sec. II.E. In Sec. III, we finally review our initial simplifications of the HI and discuss in which real systems our findings should be observable.

II. MAIN PART

A. Simplified Hamiltonian

As mentioned above, we will first introduce certain simplifications to the HI Hamiltonian, which allow for an analytical calculation of thermal expectation values:

1. We assume that all nuclear spins are spin one-half, where the number of nuclear spins is $K$.

2. We will use the so-called box-model, where the probabilities $|\phi(\vec{r}_k)|^2 = 1/K$ are all the same. By this, we assume that every nucleus in the dot carries a spin and that the envelope function $\phi(\vec{r}_k)$ of the electron does not change much inside the QD.

3. We will neglect the flip-flop terms $\hat{S}_+ \hat{I}_{k,-} + \hat{S}_- \hat{I}_{k,+}$. The last approximation is justified for sufficiently strong external magnetic fields. The reason for this is the fact that the energy gained by the HI spin flip is not enough to compensate the Zeeman splitting of the electron spin, which is large compared to the Zeeman splitting of a nuclear spin. With these assumptions and $g^* < 0$ as explained in the introduction, the total Hamiltonian

$$\hat{H} = \hat{H}^{ZE}_{I} + \hat{H}^{ZE}_{N} + \hat{H}_{HI} =$$

$$-|g^*|\mu_B B_z \hat{S}_z + \sum_{k=1}^{K} \left( -g_N \mu_B B_z \hat{I}_{k,z} + \frac{A_{HI}}{K} \hat{S}_z \hat{I}_{k,z} \right)$$

is already diagonal in the product basis $|n\rangle = |m^0_n\rangle \otimes \bigotimes_{k=1}^{K} |m^0_k\rangle$, where $|m^0_n\rangle$ is an eigenstate of $\hat{S}_z$ with $m^0_n \in \{-1/2, 1/2\}$. Similarly, the state $|m^0_k\rangle$ is an eigenstate of the $k$-th nuclear spin operator $\hat{I}_{k,z}$ with $m^0_k \in \{-1/2, 1/2\}$.

Before we proceed with the calculation of thermal expectation values, we will introduce dimensionless units by measuring all energies in units of $\frac{\mu_B B_z}{2K}$. The simplified total Hamiltonian then reads

$$\hat{H} = -\sigma \hat{S}_z + \sum_{k=1}^{K} (- \nu \hat{I}_{k,z} + 2 \hat{S}_z \hat{I}_{k,z}),$$

where the dimensionless parameters are given by $\sigma = |g^*|\mu_B B_z/\frac{\mu_B B_z}{2K}$ and $\nu = g_N \mu_B B_z/\frac{\mu_B B_z}{2K}$. These two quantities are obviously not independent of each other since both are proportional to the external magnetic field $B_z$. Thus we choose $\sigma = K \nu$, where $\rho = \sigma \mu_B B_z/(K g_N \mu_B B_z)$ is the ratio of the Zeeman energies of the electron and all nuclear spins, respectively. In other words, if the number of nuclear spins $K$ is above the critical number $\kappa = \rho K$, i.e. $\rho < 1$, the competition mentioned at the end of the introduction is apparent in our model. This situation will be further analyzed in subsequent sections.

B. Thermal expectation values

Introducing the dimensionless temperature $\tau = k_B T/\frac{\mu_B B_z}{2K}$, the partition function for this Hamiltonian is easily calculated in the product basis

$$Z = \text{Tr} \left[ e^{-\hat{H}/k_B T} \right] = \sum_n e^{-\langle n | \hat{H} | n \rangle / k_B T},$$

where the diagonal matrix elements are given by

$$-\frac{\langle n | \hat{H} | n \rangle}{k_B T} = \frac{2}{\tau} [\rho \nu K m^0_n + \sum_{k=1}^{K} (\nu m^0_k - 2 m^0_n m^0_k)].$$

Exploiting the fact that sums in the exponential functions factorize finally yields

$$Z = \sum_{m_S} \prod_{k=1}^{K} \sum_{m_k} e_{m_S, m_k}$$

$$= (e^{+1} + e^{-1})^K + (e^{-1} + e^{+1})^K,$$
FIG. 1: (Color online) \(\Pi(\tau, \nu, \rho, K)\) (black, solid) as a function of temperature \(\tau\) for \(\nu = 2, \rho = 0.09\) and \(K = 10^4\). As we show in the text and in Fig. 2, this choice of parameters fulfills the necessary conditions for the spin flip. At a temperature \(\tau_0\), the function suddenly drops from very large values to zero. At temperatures \(\tau \gtrsim \tau_1\) the function surprisingly rises again and saturates at \(\Pi = 1\) for large temperatures. The thermal expectation value of the electron spin \(\langle S_z \rangle_{\tau}\) (red, dashed) exhibits a sudden drop at \(\tau_0\). For temperatures above \(\tau_1\) the electron spin is thermally equilibrated.

where

\[ e_{m_S,m_k} = \exp\left[\frac{2}{\tau} (\rho \nu m_S + \nu m_k - 2 m_S m_k)\right]. \tag{10} \]

With the partition function at hand, the calculation of the thermal expectation value of the electron spin is readily obtained

\[ \langle S_z \rangle_{\tau} = \frac{\tau}{2} \frac{\partial}{\partial \sigma} \ln[Z] = \frac{\tau}{2K\nu} \frac{\partial}{\partial \rho} \ln[Z] \]

\[ = \frac{1}{2} \left( \frac{1}{1 - \Pi} - \frac{1}{1 - \Pi^{-1}} \right), \tag{11} \]

where the function

\[ \Pi = \Pi(\tau, \nu, \rho, K) = \left[ \frac{\exp\left[\frac{1}{2} \left\{-\nu - 1\right\}\right] + \exp\left[\frac{1}{2} \left\{\nu + 1\right\}\right]}{\exp\left[\frac{1}{2} \left\{-\nu + 1\right\}\right] + \exp\left[\frac{1}{2} \left\{-\nu - 1\right\}\right]} \right]^K \tag{12} \]

controls the behavior of \(\langle S_z \rangle_{\tau}\). If \(\Pi \to \infty\), we find \(\langle S_z \rangle_{\tau} \to -1/2\), \(\Pi = 0\) results in \(\langle S_z \rangle_{\tau} = 1/2\) and, finally, \(\Pi = 1\) yields \(\langle S_z \rangle_{\tau} = 0\). As it turns out, the electron spin has to go through exactly these steps for the thermal spin flip to occur as illustrated in Fig. 1. In the following, we will first explore the parameter space of \(\Pi(\tau, \nu, \rho, K)\) to find mathematically the conditions necessary for the spin flip to occur. Afterwards we calculate at which temperatures \(\Pi\) and, consequently, \(\langle S_z \rangle_{\tau}\) undergo their characteristic changes. To this end, we will analyze \(\Pi\) analytically and compare the findings with numerical calculations of \(\langle S_z \rangle_{\tau}\). Finally, we will interpret these results in order to understand when and why this effect appears in a physical system.

C. Analytical analysis of the spin flip

By inserting the definition of the exponential functions in Eq. (10) into Eq. (12) and rearranging factors, we find

\[ \pi^K = \Pi(\tau, \nu, \rho, K) = \left[ \exp\left[-\frac{2\rho\nu}{\tau} \frac{1}{2} \left\{-\nu - 1\right\}\right] + \exp\left[\frac{1}{2} \left\{\nu + 1\right\}\right]\right]^K. \tag{13} \]

By further rearrangements of factors in Eq. (13), we identify that \(\rho < 1\) and \(0 < \nu < \rho^{-1}\) are necessary conditions for \(\Pi\) to diverge at \(\tau \to 0\) and, consequently, for the spin flip to occur. Within this parameter regime, we want to identify the temperature \(\tau_0\), at which \(\Pi\) drops from infinity to zero, and the temperature \(\tau_1\) at which \(\Pi\) rises to 1 as indicated in Fig. 1.

The latter temperature can be readily read off from Eq. (13), since \(\Pi = 1\) for all temperatures \(\tau\) well above

\[ \tau_1 = 2\rho\nu K = 2k\nu \quad \text{if} \quad \nu \gg \frac{1}{2K}. \tag{14} \]

At a specific temperature \(\tau\) the function \(\pi\) defined in Eq. (12) changes from \(\pi > 1\) to \(\pi < 1\). Since one has to take it to the power of \(K \gg 1\), this marks the temperature, at which the sudden drop from \(\Pi \gg 1\) to \(\Pi \ll 1\) and, hence, the spin flip occurs. Thus, the transcendental equation defining \(\tau_0\) reads

\[ \rho = -\frac{\tau_0}{2\nu} \ln \left[ \frac{\exp\left[\frac{1}{2\tau_0} \left\{-\nu - 1\right\}\right] + \exp\left[\frac{1}{2\tau_0} \left\{\nu + 1\right\}\right]}{\exp\left[\frac{1}{2\tau_0} \left\{-\nu + 1\right\}\right] + \exp\left[\frac{1}{2\tau_0} \left\{-\nu - 1\right\}\right]} \right]. \tag{15} \]

This equation can be expanded in powers of \(\frac{1}{\tau_0} \ll 1\),

\[ \rho \approx \frac{1}{\tau_0} + O\left(\frac{1}{\tau_0^2}\right). \tag{16} \]

As a consequence, the temperature \(\tau_0 \approx \rho^{-1}\) is independent of \(\nu\) for \(\rho \ll 1\). Since \(\rho = \kappa/K\) is a material constant for a given QD, this is a rather intriguing result. This constant being \(\rho \ll 1\) corresponds to a situation, where the total nuclear Zeeman energy is much larger than the electron Zeeman energy. Before we give a detailed physical interpretation of our results, let us compare the analytical results with a numerical analysis of Eqs. (11) and (12), respectively.

D. Numerical analysis of the spin flip

In order to verify our analytical results, we show density plots of \(\langle S_z \rangle_{\tau} = \langle S_z \rangle_{\tau}(\tau, \nu, \rho, K)\), where we choose the number of nuclear spins to be \(K = 10^4\). With \(K\) being fixed, \(\tau, \rho,\) and \(\nu\) remain as parameters. In Fig. 2 (a), we show \(\langle S_z \rangle_{\tau}\) as a function of \(\tau\) and \(\rho\) with \(\nu = 2\). As we will show below, for this choice of \(\nu\), the electron Zeeman energy competes with the total HI energy. If \(\rho\nu > 1\) the
Zeeman energy exceeds the HI energy and the electron spin is up for all $\tau$, which is clearly shown in Fig. 2 a). Additionally, we plotted Eqs. (14) and (15) in order to demonstrate the behavior of $\tau_1$ and $\tau_0$, respectively. Both analytical results show a remarkable agreement with the numerical findings. In Fig. 2 b), we show the same plot for $\nu = 0.09$. For this choice of $\nu$, the electron Zeeman energy is always smaller than the total HI energy. However, if $\rho > 1$, the electron Zeeman energy is larger than the total nuclear Zeeman energy and, consequently, the electron spin flip is absent up for all $\tau$ as can be seen from Fig. 2 b).

As indicated above, in a real system $\rho$ is rather a fixed parameter than a real variable. Hence, we also calculated $\langle \hat{S}_z \rangle_\tau$ as a function of temperature $\tau$ and the Zeeman energy of a single nucleus $\nu$, which is proportional to the magnetic field $B_z$. The result is shown in Fig. 2 c), where we chose $\rho = 0.09$. In this figure, the behavior of $\tau_0 = \rho^{-1}$ is most prominent. Moreover, it is obvious that $\rho \nu < 1$ is indeed a necessary condition for the spin flip.

E. Physical interpretation of the results

So far, we have mathematically clarified for which parameters one finds the spin flip. In the following, we want to explain why this spin flip occurs and how the conditions found above can be interpreted physically. Therefore, we will have a closer look on the energies of the Hamiltonian given in Eq. 6. In order to study the quantum mechanical expectation values of $\hat{H}$ for different states, another labeling of the states is useful: $|m_S, q, i\rangle = |m_S\rangle \otimes |q, i\rangle$, where state $|q, 1\rangle$ is defined by

$$|q, 1\rangle = \left| \begin{array}{c} 1 \quad 1 \quad \cdots \quad 1 \\ \frac{q}{K-q} \quad \frac{q}{K-q} \quad \cdots \quad \frac{q}{K-q} \end{array} \right|$$

(17)

All other states $|q, i\rangle$ with the same number $q$ of nuclear spins pointing up are given by all possible permutations of $|q, 1\rangle$ resulting in $n(K, q) = \binom{K}{q}$ different states labeled by $i$. Since the simplified total Hamiltonian is invariant under exchanging one nuclear spin with another one, all energy eigenvalues

$$E^\nu_{m_S} = \langle m_S, q, 1|\hat{H}|m_S, q, 1\rangle = \langle m_S, q, i|\hat{H}|m_S, q, i\rangle$$

$$= K \left[ -\nu m_S - \frac{1}{2} \left( g \frac{q}{K} - 1 \right) \nu + m_S \left( 2 \frac{q}{K} - 1 \right) \right]$$

(18)

are $n(K, q)$ times degenerate. A plot of $E^\nu_{1/2}$ and $E^\nu_{-1/2}$ as a function of the number of flipped nuclear spins $q$ is presented in Fig. 3. From this, the physics of the spin flip becomes clear. The ground state is given by $|{-1/2}, K, 1\rangle$, whose energy eigenvalue $E^\nu_{-1/2}$ is not degenerate. If one follows the energies $E^\nu_{-1/2}$ and $E^\nu_{1/2}$ starting from $q = K$, one finds that $E^\nu_{-1/2}$ increases much faster than $E^\nu_{1/2}$ for less spins pointing up, which is also obvious from Eq. (15). Since the degeneracy of the corresponding energy levels $n(K, K-q)$ is strongly increasing, many states with $m_S = 1/2$ become thermally available for finite temperatures. Once the temperature reaches $\tau_0$, there is a strong imbalance between the number of states with $m_S = -1/2$ and the number of states with $m_S = 1/2$, which finally causes the sudden spin flip. If the temperature is further increased above $\tau_1$ almost all states are reached and, hence, one finds $\langle \hat{S}_z \rangle_\tau = 0$.

Finally, we would like to interpret the mathematical conditions on the parameters physically. Let us start with the constraints on $\rho$ and $\rho \nu$. Since the $\rho = \kappa / K = |g^*|\mu_B B_z / (g_N \mu_N B_z K)$ is given by the ratio of the electron spin and the total nuclear Zeeman energy, the ratio being $\rho < 1$ implies that the Zeeman energy of all spins exceeds the electron Zeeman energy. Similarly the product $\rho \nu = \kappa \nu / K = 2|g^*|\mu_B B_z / A_{\text{HH}}$ tells us that the Zeeman energy of the electron has to be smaller than the total HI energy. This imposes an upper bound on the external magnetic field

$$B_z < B_{\text{max}} = \frac{A_{\text{HI}}}{2|g^*|\mu_B}.$$  

But the magnetic field has additionally to be large enough in order to separate the two temperatures $\tau_0$ and $\tau_1$. For small magnetic fields, the former temperature is given by $\tau_0 = \rho^{-1}$, which corresponds to an absolute temperature

$$T_0 = k_B^{-1} \frac{A_{\text{HI}}}{2} \frac{g_N \mu_N}{|g^*|\mu_B}.$$  

The latter temperature $\tau_1$ corresponds to the Zeeman splitting of the electron since

$$T_1 = k_B^{-1} |g^*|\mu_B B_z.$$  

For $T_0 < T_1$ the spin flip is present, which is the case if the magnetic field obeys

$$B_z > B_{\text{min}} = \frac{g_N \mu_N}{|g^*|\mu_B} \frac{A_{\text{HI}}}{2|g^*|\mu_B} = \frac{1}{\kappa} B_{\text{max}}.$$  

III. DISCUSSION AND OUTLOOK

All of the above results were obtained applying certain approximations, which are in general not fulfilled by real systems. In the following, we will discuss all approximations one by one and analyze, how a more realistic model would change our results.

First off all, we assumed that all nuclear spins are of the same species. This is a commonly made approximation, where root-mean-square averages of the Zeeman and HI coupling constants can be used to mimic the situation of only one spin species being present. As long as the individual constants are not too different and if the sign
FIG. 2: (Color online) a): The thermal expectation value of the electron spin as a function of temperature $\tau$ and $\rho$ for $\nu = 2$. The green dashed line shows the defining Eq. (15) of $\tau_0$. For small $\rho$ one finds $\tau_0 = \rho^{-1}$ in agreement with the plot. The light blue line is given by $\tau_1$ in Eq. (14). For $\rho \nu \geq 1$ the spin flip is absent. For temperatures above $\tau_1$, the electron is thermally equilibrated and, hence, $\langle \mathbf{S}_z \rangle_\tau = 0$. b): The thermal expectation value of the electron spin as a function of temperature $\tau$ and $\rho$ for $\nu = 0.09$. Clearly, the spin flip is absent for $\nu = \rho^{-1}$ and the vertical green line to $\tau = \rho^{-1}$. For $\rho \nu \geq 1$ the spin flip is absent. For temperatures above $\tau_1$, the electron is again thermally equilibrated.

FIG. 3: (Color online) Energies of the Hamiltonian as a function of the number of nuclear spins being parallel to the magnetic field for electron spin up ($m_S = 1/2$, red) and down ($m_S = -1/2$, blue). The parameters used for this plot are $\nu = 2$, $\rho = 0.35$, and $K = 10$. The degeneracy of the energy levels is given by $n(K, q) = \binom{a}{b}$. The width of a column is proportional to the corresponding degeneracy. The green and light blue line show $\tau_0$ and $\tau_1$, respectively.

of the nuclear magnetic moment is the same for all nuclear spins, we do not expect qualitative changes of our findings. Additionally, we chose all nuclear spins to be one-half. If one allows for larger nuclear spin quantum numbers $I = 1/2, 3/2, \ldots$, the model can still be solved analytically. Since the thermal relaxation of the electron spin does only depend on its Zeeman energy, the temperature $\tau_1$ is unchanged. In contrast to this, the spin flip temperature $\tau_0 = \rho^{-1}4I(I + 1)/3$ increases by an $I$ dependent factor. Finally, we also implicitly assumed that all nuclei carry a spin. Yet, this is not the case for all materials. If there are $K$ of $N$ nuclei carrying a spin, the probability to find the electron at the site of a nuclear spin is $|\phi(\vec{r}_k)|^2 = N^{-1} = K^{-1} \cdot (K/N) \approx K^{-1} \cdot n_i$, where $0 \leq n_i \leq 1$ is the abundance of spin carrying nuclei. Hence, our results still hold if the HI constant $A_{\text{HI}}$ is replaced by $n_i A_{\text{HI}}$.

Beside approximations concerning the nuclear spins, we also simplified the physics of the electron spin by using the box model for its envelope function: $|\phi(\vec{r}_k)|^2 = K^{-1}$.

TABLE I: Relevant materials and their parameters. The values of $g^*$ are taken from Ref. [29]. The magnetic moment $g_N$ and the HI constant $A_{\text{HI}}$ are averaged by $g_N = \sum_i n_i g_N^i$ and $A_{\text{HI}} = \sum_i n_i A_{\text{HI}}^i$, where $n_i$ is the natural abundance of isotope $i$. The values are taken from Refs. [29,32]. The temperatures $T_1$ and $T_0$ are calculated at $B_z = 0.1 B_{\text{max}}$, at which $T_0 = k_B^{-1} \cdot [4I(I + 1)/3] \cdot \kappa^{-1} A_{\text{HI}}$ is valid. By this choice, we also take into account that larger nuclear spin quantum numbers $I$ increase $T_0$. For simplicity, we took the smallest quantum number $I_{\text{min}}$ of different isotopes present in the dot.

| Material  | $g^*$ | $g_N$ | $\kappa$ | $A_{\text{HI}}$ | $B_{\text{max}}$ | $I_{\text{min}}$ | $T_0$ | $T_1$ |
|-----------|-------|-------|----------|----------------|-----------------|----------------|------|------|
| GaAs      | -0.4  | 1.8   | 0.44     | 84             | 1700            | $\frac{3}{2}$  | 5.6  | 49   |
| CdTe      | -1.8  | -6.7  | 4.9      | -34            | 170             | $\frac{1}{2}$  | 0.04 | 20   |
| GaInAs$^a$| -4.4  | 3.1   | 2.6      | 93             | 180             | 1.0            | 54   |
| InAs      | -15   | 3.5   | 7.9      | 98             | 57              | $\frac{3}{2}$  | 0.36 | 57   |

$^a$Ga$_{4.47}$In$_{0.53}$As
In reality, the probability to find the electron, should strongly decrease with the distance from the center of the QD, which is often described by a Gaussian envelope function $|\phi(\vec{r}_e)|^2 \propto K^{-1} \exp[-r_e/R]$. Our results should be modified in this case by two aspects: Nuclear spins with $|\phi(\vec{r}_n)|^2 \ll K^{-1}$ couple only very weakly to the electron and can, thus, be neglected. Effectively, this reduces the number of involved nuclear spins from $K$ to $K_{\text{eff}} < K$. For nuclear spins in the center, one finds $\mathcal{O}(|\phi(\vec{r}_n)|^2) = K^{-1}$. As a consequence, the non-uniform HI will (slightly) lift the degeneracy of the energies in Eq. (18) and Fig. 3 but it will not change the energy spectrum in principle. Therefore, the main physical mechanism stays the same and our results still hold.

At last, we have to briefly comment on neglecting the flip-flop terms of the HI. As we explained already above, the physical reason allowing for this assumption is the large Zeeman energy of the electron spin, which can neither be compensated by the HI nor by the Zeeman splitting of a single nuclear spin. Formalizing this idea, one can apply time-independent perturbation theory to our model, where the small parameter is given by $\frac{A_{\text{HI}}}{\tau_1} \left| g^* \mu_B B_z \right| = \tau_1^{-1}$. By this, one can analytically show, that corrections on the product states $|n\rangle$ are in leading order of size $\tau_1^{-2}$, because first order terms vanish due to conservation of angular momentum. Since $\tau_1 \gg 1$ is anyway needed for the physics of the spin flip to be measurable, treating the full Hamiltonian should give mainly the same results as using the simplified model.

Having convinced ourselves, that the results obtained within the simplified model should be reasonable for real systems, we finally want to give several examples, where we expect the spin flip to occur. The most severe constraint is the negative sign of $g^*$. As can be seen from Tab. 1 this is realized, for instance, in III-V heterostructures, where the electron experiences a strong spin-orbit interaction. Most promising among the considered materials is GaAs, since its spin-flip temperature is on the order of mK. The other materials having a smaller $T_0$ suffer mostly from a large $g^*$ factor. Besides a small $g^*$ factor, potential materials would also benefit from a strong HI and from heavy nuclei with large $g^*N$ factors and large spin quantum numbers $I$. Among them, also systems with a negative $g_N$ such as CdTe can be considered, since this sign changes both the nuclear Zeeman coupling and the sign of the HI. Redefining the nuclear spin operator by $I_z \rightarrow -I_z$ then yields the same results.

Finally, we will briefly discuss the nature of the spin flip. If one leaves the equilibrium state while heating up the system (non-adiabatically), it will take some time for the system to reach the equilibrium at its new temperature. Especially for crossing $T_0$, the system is not only forced to flip the electron spin, but also approximately up to $\kappa \gg 1$ nuclear spins. Thus, depending, for instance, on the microscopic details of the coupling of the spins to one or several baths, the time needed to equilibrate could be comparably long.

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