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A model of magnetic impurities within the Josephson junction of a phase qubit

R P Erickson and D P Pappas

National Institute of Standards and Technology, Boulder, CO 80305, USA

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Abstract

We consider a superconducting phase qubit consisting of a monocrystalline sapphire Josephson junction with its symmetry axis perpendicular to the junction interfaces. Via the London gauge, we present a theoretical model of Fe³⁺ magnetic impurities within the junction that describes the effect of a low concentration of such impurities on the operation of the qubit. Specifically, we derive an interaction Hamiltonian expressed in terms of angular momentum states of magnetic impurities and low-lying oscillator states of a current-biased phase qubit. We discuss the coupling between the qubit and impurities within the model near resonance. When the junction is biased at an optimal point for acting as a phase qubit, with a phase difference of $\pi/2$ and impurity concentration no greater than 0.05%, we find only a slight decrease in the *Q* factor of less than 0.01%.

1. Introduction

Devices based on superconducting materials and tunnel junctions can interact strongly with their surrounding electromagnetic environment. For example, quantum bits (qubits) conceived to leverage the quantum state of a Josephson junction to provide computational operations [1], couple to a variety of sources ranging from two-level systems (TLSs) in surrounding amorphous insulating layers to quasiparticles in the superconducting electrodes. Mitigation of these interactions has been a primary concern in qubit design since they can lead to decoherence of the qubit state. In particular, spectroscopic studies of phase qubits have revealed discrete splittings, presumably due to imperfections in the tunnel junction. While these splittings can be modelled as separate TLSs that strongly couple to the superconducting phase qubit [2-6], the microscopic origin of the splittings has yet to be determined positively. Aside from their contribution to decoherence, based on predictions by Zagoskin et al [7], these TLSs can be exploited to construct a quantum memory device [8]. Also, strong coupling to extraneous TLSs is not limited to phase qubits, though the mechanisms involved may differ between devices. For example, in a recent experiment, Kim et al [9] observed anomalous avoided-level crossings in the spectrum of a Cooper-pair box (CPB). Interactions of superconducting flux qubits with extrinsic quantum fluctuators have also been observed [10, 11].

It is difficult to control the behaviour of TLSs in the above-mentioned devices due to their inherently random

occurrences within the amorphous constituents, such as barrier Typically, one is left to manipulate the and substrate. dimensions of the devices in order to control the number of TLSs that can interact with the superconductor. Alternatively one can employ epitaxially grown materials to reduce the number of TLSs. For example, a phase qubit can be fabricated using a Josephson junction composed of monocrystalline sapphire [12, 13]. In addition to significantly reducing the spectral density and overall number of spurious TLSs [14] this has the further advantage of allowing one to exert control over the concentration and type of magnetic impurities in the barrier by intentionally doping the junction during growth. In our laboratory we currently are engaged in such experiments. The focus of the present theoretical discussion is on the effect of magnetic impurities within specifically monocrystalline sapphire junctions.

Thus, via artificial means, magnetic impurities can be introduced into the sapphire crystal barrier that may couple coherently with the qubit at a specific frequency, either via nuclear or electronic impurity states, depending on the dopant. One implementation of this idea originates from the design of masers constructed from sapphire doped with Fe³⁺ ions substituted for Al [15, 16]. At cryogenic temperatures the Fe³⁺ ion maintains a zero-field splitting of the electron 3d states due to the crystal field of the hexagonal sapphire. The form and strength of coefficients of the corresponding model spin Hamiltonian, of spin length S = 5/2, have been well measured [17]. Indeed, there is a pumping frequency at 12.038 GHz, associated with $|5/2, \pm 3/2\rangle$ to $|5/2, \pm 1/2\rangle$ transitions, whose energy is comparable to $\hbar\omega_{10}$, the energy of transition between the $|0\rangle$ and $|1\rangle$ states of a typical phase qubit. In a recent experiment [18] involving whispering gallery modes of a single-crystal HEMEX-grade sapphire, with Fe³⁺ concentration of a few parts per billion, a high-*Q* resonance from the Fe³⁺ impurities was clearly visible.

Because of the existence of a 12.038 GHz frequency at zero field, incorporation of Fe3+ impurities into a monocrystalline sapphire tunnel barrier provides a resonance between impurity and qubit states that might be leveraged for quantum memory transfer, in a manner similar to that described in [7]. However, one first needs to understand the nature of the interaction of junction magnetic impurity with low-lying states of the phase qubit, as well as the potential for degradation of qubit performance by the presence of these impurities, as measured via the quality factor, or Q, metric. In this paper we derive a model for this coupling mechanism by calculating the gauge-invariant shift in phase difference across the Josephson junction due to the magnetic impurities within the junction. The shift in phase difference is a consequence of the interaction between magnetic impurities and tunnelling Cooper pairs. While other interactions, between impurities and between impurities and quasiparticles, may play a role, our focus here is on the basic nature of the interaction between impurity and qubit, at sufficiently low concentrations that other types of interactions may be neglected, to first approximation. From these assumptions, we predict the concentration of dopant needed to observe the coupling of magnetic impurities to the phase qubit, and we calculate the resulting Q factor.

2. The model

2.1. Derivation of the model

In the present analysis we develop a model from which we can study the effect of a low concentration of magnetic impurities contained within a Josephson junction on the operation of a phase qubit. We have in mind a cylindrical junction of radius R and thickness $d \ll R$ with superconductor interfaces at planes z = 0 and d, as illustrated in figure 1. We assume the axis of symmetry of the hexagonal crystal to be orientated perpendicular to the junction interfaces. The London equations describing the magnetic induction $\vec{B}(\vec{r})$ can be written as

$$\lambda^2 \nabla^2 \vec{B}(\vec{r}) = \vec{B}(\vec{r}); \qquad z < 0, \quad z > d$$

$$\nabla^2 \vec{B}(\vec{r}) = \vec{V}(\vec{r}); \qquad 0 < z < d,$$
(1)

where λ is the London penetration depth. Here, $\vec{V}(\vec{r}) = -\mu_0 \nabla \times \vec{j}(\vec{r})$ represents a localized source of bound current within the junction that we may express in the divergenceless form $\vec{j}(\vec{r}) = \nabla \times \vec{M}(\vec{r})$, where μ_0 is the permeability of free space. In our model, the magnetization $\vec{M}(\vec{r})$ is the result of a collection of N magnetic dipole moments $\vec{m}^{(n)}$, such that $\vec{M}(\vec{r}) = \sum_{n=1}^{N} \vec{m}^{(n)} \delta(\vec{r} - \vec{r}_n)$. For boundary conditions in (1), we take the z component of magnetic induction and its derivative in z to be continuous across both junction interfaces,



Figure 1. Illustration of a cylindrical single-crystal Josephson junction of radius *R* and thickness $d \ll R$. The *z* direction is normal to the junction interfaces, which reside at z = 0 and *d*.

and we assume the magnetic induction must vanish infinitely far in |z| from the junction.

The differential equation of (1) inside the junction can be integrated using Green's theorem [19]. In particular, the z component of the magnetic induction is

$$B_{z}(\vec{r}) = -\frac{1}{4\pi} \int_{V} d^{3}r' \frac{V_{z}(\vec{r}')}{|\vec{r} - \vec{r}'|} + \frac{1}{4\pi} \\ \times \int d^{2}\rho' \left[\frac{1}{|\vec{r} - \vec{r}'|} \frac{\partial}{\partial z'} B_{z}(\vec{r}') - B_{z}(\vec{r}') \frac{\partial}{\partial z'} \frac{1}{|\vec{r} - \vec{r}'|} \right]_{z'=d} \\ - \frac{1}{4\pi} \int d^{2}\rho' \left[\frac{1}{|\vec{r} - \vec{r}'|} \frac{\partial}{\partial z'} B_{z}(\vec{r}') - B_{z}(\vec{r}') \frac{\partial}{\partial z'} \frac{1}{|\vec{r} - \vec{r}'|} \right]_{z'=0}$$
(2)

where $V = \pi R^2 d$ is the volume of the junction. Introducing Fourier transform pairs of the x-y plane of the form $\vec{f}(\vec{r}) = (1/2\pi) \int \vec{f}(\vec{k}_{\parallel}, z) e^{i\vec{k}_{\parallel}\cdot\vec{\rho}} d^2k_{\parallel}$ and $\vec{f}(\vec{k}_{\parallel}, z) = (1/2\pi) \int \vec{f}(\vec{r}) e^{-i\vec{k}_{\parallel}\cdot\vec{\rho}} d^2\rho$, where $\vec{r} = \vec{\rho} + z\hat{z}$ and $\vec{\rho} = x\hat{x} + y\hat{y}$, the transformation of (2) yields a Fourier coefficient

$$B_{z}(\vec{k}_{\parallel}, z) = -\frac{1}{2k_{\parallel}} \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{-k_{\parallel}|z-z'|} dz' + \frac{1}{2} \bigg[B_{z}(\vec{k}_{\parallel}, d) + \frac{1}{k_{\parallel}} \frac{\partial}{\partial z'} B_{z}(\vec{k}_{\parallel}, z') \bigg|_{z'=d} \bigg] e^{-k_{\parallel}(d-z)} + \frac{1}{2} \bigg[B_{z}(\vec{k}_{\parallel}, 0) - \frac{1}{k_{\parallel}} \frac{\partial}{\partial z'} B_{z}(\vec{k}_{\parallel}, z') \bigg|_{z'=0} \bigg] e^{-k_{\parallel}z}.$$
(3)

Similarly transforming the differential equation of (1) outside the junction gives $[\partial^2/\partial z^2 - \gamma (k_{\parallel})^2]B_z(\vec{k}_{\parallel}, z) = 0$, with $\gamma (k_{\parallel})^2 = k_{\parallel}^2 + \lambda^{-2}$, which suggests a solution

$$B_{z}(\vec{k}_{\parallel}, z) = \begin{cases} c_{1}(\vec{k}_{\parallel})e^{-\gamma(k_{\parallel})(z-d)}; & z > d\\ c_{2}(\vec{k}_{\parallel})e^{\gamma(k_{\parallel})z}; & z < 0. \end{cases}$$
(4)

So substituting (4) into (3), we have

$$B_{z}(\vec{k}_{\parallel}, z) = -\frac{1}{2k_{\parallel}} \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{-k_{\parallel}|z-z'|} dz' + \frac{1}{2} \left[1 - \frac{\gamma(k_{\parallel})}{k_{\parallel}} \right] [c_{1}(\vec{k}_{\parallel}) e^{-k_{\parallel}(d-z)} + c_{2}(\vec{k}_{\parallel}) e^{-k_{\parallel}z}], \quad (5)$$

such that matching the solutions of (4) and (5) at the interfaces yields

$$c_{1}(k) = -\left\{ [k_{\parallel} + \gamma(k_{\parallel})] \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{k_{\parallel}z'} dz' + [k_{\parallel} - \gamma(k_{\parallel})] \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{-k_{\parallel}z'} dz' \right\} \\ \times \left\{ [k_{\parallel} + \gamma(k_{\parallel})]^{2} e^{k_{\parallel}d} - [k_{\parallel} - \gamma(k_{\parallel})]^{2} e^{-k_{\parallel}d} \right\}^{-1}, \quad (6a)$$

$$c_{2}(k) = -\left\{ [k_{\parallel} + \gamma(k_{\parallel})] \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{k_{\parallel}(d-z')} dz' + [k_{\parallel} - \gamma(k_{\parallel})] \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{-k_{\parallel}(d-z')} dz' \right\} \\ \times \left\{ [k_{\parallel} + \gamma(k_{\parallel})]^{2} e^{k_{\parallel}d} - [k_{\parallel} - \gamma(k_{\parallel})]^{2} e^{-k_{\parallel}d} \right\}^{-1}. \quad (6b)$$

Therefore, using (6a) and (6b) we see that (5) becomes

$$B_{z}(\vec{k}_{\parallel}, z) = -\frac{1}{2k_{\parallel}} \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') e^{-k_{\parallel}|z-z'|} dz' - \frac{1}{k_{\parallel}} \int_{0}^{d} V_{z}(\vec{k}_{\parallel}, z') \{\{[k_{\parallel}^{2} - \gamma(k_{\parallel})^{2}] \cosh k_{\parallel}(d - z - z') + [k_{\parallel} - \gamma(k_{\parallel})]^{2} e^{-k_{\parallel}d} \cosh k_{\parallel}(z - z')\} \{[k_{\parallel} + \gamma(k_{\parallel})]^{2} e^{k_{\parallel}d} - [k_{\parallel} - \gamma(k_{\parallel})]^{2} e^{-k_{\parallel}d}\}^{-1}\} dz',$$
(7)

which gives the *z* component of magnetic induction for an arbitrary source of bound current. In the limit *d* goes to infinity, (7) recovers the result of Coffey [20] for the semi-infinite superconductor. The tangential components of magnetic induction, continuous and differentiable across the junction interfaces when λ is not equal to 0, follow in the same manner.

In the limit of a very thin junction, where $d \ll R$ and $k_{\parallel}d \ll 1$, the integrals over z' in (7) have dependence on z' from $V_z(\vec{k}_{\parallel}, z')$ alone, and the remaining factor in the second term of the right side of (7), taken outside the integral in z', becomes

$$\frac{k_{\parallel}^{2} - \gamma(k_{\parallel})^{2} + [k_{\parallel} - \gamma(k_{\parallel})]^{2} e^{-k_{\parallel}d}}{[k_{\parallel} + \gamma(k_{\parallel})]^{2} e^{k_{\parallel}d} - [k_{\parallel} - \gamma(k_{\parallel})]^{2} e^{-k_{\parallel}d}} \\
\approx \frac{k_{\parallel} - \gamma(k_{\parallel}) - \frac{1}{2} [k_{\parallel}^{2} - 2k_{\parallel}\gamma(k_{\parallel}) + \gamma(k_{\parallel})^{2}]d}{2\gamma(k_{\parallel}) + [k_{\parallel}^{2} + \gamma(k_{\parallel})^{2}]d} \\
\approx \frac{k_{\parallel} - \frac{1}{2} [k_{\parallel}^{2} + \gamma(k_{\parallel})^{2}]d}{[k_{\parallel}^{2} + \gamma(k_{\parallel})^{2}]d}]d; \qquad k_{\parallel}d \ll 1.$$
(8)

In the last step of (8) we discard terms linear in $\gamma(k_{\parallel})$ since they do not contribute in the physically import limit of $\lambda = 0$, and their absence for small finite values $\lambda \ll R$ should not lead to gross error in approximation. Thus, applying our thin-junction approximations to (7), noting the subsequent cancellation of the first term on the right of (7), and transforming back to real space, we find

$$B_{z}(\vec{\rho}) \cong -\frac{\lambda^{2}}{2\pi d} \int \mathrm{d}^{2}k_{\parallel} \frac{\mathrm{e}^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{1+2\lambda^{2}k_{\parallel}^{2}} \int_{0}^{d} V_{z}(\vec{k}_{\parallel},z')\,\mathrm{d}z', \quad (9)$$

which is constant in z and necessarily vanishing in the full Meissner limit of $\lambda = 0$.

Since $V_z(\vec{k}_{\parallel}, z) = -i\mu_0(k_x + k_y)\partial/\partial z M_z(\vec{k}_{\parallel}, z) - \mu_0 k_{\parallel}^2 M_z(\vec{k}_{\parallel}, z)$, such that over the thickness of the junction $\int V_z(\vec{k}_{\parallel}, z) dz = -\mu_0 k_{\parallel}^2 \int M_z(\vec{k}_{\parallel}, z) dz$, we find for a collection of N impurities that we can write (9) as

$$B_{z}(\vec{\rho}) \cong \frac{\mu_{0}\lambda^{2}}{4\pi^{2}d} \sum_{n=1}^{N} m_{z}^{(n)} \int d^{2}k_{\parallel} \frac{k_{\parallel}^{2} \exp i\vec{k}_{\parallel} \cdot (\vec{\rho} - \vec{\rho}_{n})}{1 + 2\lambda^{2}k_{\parallel}^{2}}, \quad (10)$$

with $\vec{\rho_n} = \rho_n \cos \phi_n \hat{x} + \rho_n \sin \phi_n \hat{y}$. Similar expressions can be derived for the tangential components of magnetic induction. Also, the vector potential $\vec{A}(\vec{r})$ can be obtained by integrating $\vec{B}(\vec{r}) = \nabla \times \vec{A}(\vec{r})$; inside a very thin junction we find

$$\vec{A}(\vec{\rho}) \cong i \frac{\mu_0 \lambda^2}{4\pi^2 d} \sum_{n=1}^N \int d^2 k_{\parallel} \frac{\vec{k}_{\parallel} \times \vec{m}^{(n)}}{1 + 2\lambda^2 k_{\parallel}^2} \exp i \vec{k}_{\parallel} \cdot (\vec{\rho} - \vec{\rho}_n).$$
(11)

Cooper pairs tunnelling through a junction containing magnetic impurities will experience a shift in phase difference $\Delta\delta(\lambda) = -(2e/\hbar) \int A_z dz$, integrated over the thickness of the junction. However, magnetic impurities break the transverse symmetry of the junction. For simplicity, we assume tunnelling Cooper pairs most strongly experience the spatial average of the resultant magnetic field of the impurities¹. Thus, we approximate A_z over the cross-sectional area $S_0 = \pi R^2$ of the junction as $A_z = (1/S_0) \int A_z(\vec{\rho}) dS_0$. In this way, utilizing (11), our approximation of the shift in phase difference is

$$\Delta\delta(\lambda) = 2\pi \frac{\Phi_{\rm mi}(\lambda)}{\Phi_0}, \qquad (12a)$$
$$\Phi_{\rm mi}(\lambda) \cong \frac{\mu_0}{2\pi R} K_1\left(\frac{R}{\lambda\sqrt{2}}\right) \cdot \sum_{n=1}^N I_1\left(\frac{\rho_n}{\lambda\sqrt{2}}\right) \times [m_x^{(n)} \sin\phi_n - m_y^{(n)} \cos\phi_n], \qquad (12b)$$

where $\Phi_0 = h/2e$ is the flux quantum, and $K_1(x)$ and $I_1(x)$ are modified Bessel functions.

2.2. Phase qubit and magnetic impurity interaction Hamiltonian

From the resultant shift in phase difference of (12a) we can ascertain a Hamiltonian of interaction between individual qubit states and individual magnetic impurity states. Specifically, consider the Hamiltonian of the current-biased phase qubit represented by oscillator states and a washboard potential [21, 22], namely

$$H_{\rm qb} = \frac{q^2}{2C} - \frac{\Phi_0 I_0}{2\pi} \cos \delta - \frac{\Phi_0 I_{\rm bias}}{2\pi} \delta, \qquad (13)$$

where q is the charge, C is the capacitance, I_0 is the junction critical current, I_{bias} is the bias current, and δ is the phase. For $\Delta\delta(\lambda) \ll 1$, we have $\cos[\delta + \Delta\delta(\lambda)] \cong [1 - \frac{1}{2}\Delta\delta(\lambda)^2] \cos \delta - \delta(\lambda)$

¹ Specifically, our approximation is equivalent to neglecting all terms $A_z(\vec{k}_{\parallel}, z)$ except $A_z(\vec{k}_{\parallel} = 0, z)$. Thus, in real space, $A_z(\vec{r})$ is effectively replaced by the average value $\overline{A_z}(\vec{r}) = (1/4\pi^2) \int A_z(\vec{r}) d^2\rho$. Or, normalizing with respect to the cross-sectional area $S_0 = \pi R^2$, we have $\overline{A_z}(\vec{r}) = (1/S_0) \int A_z(\vec{r}) dS_0$. These averages are independent of z in the very-thin-junction limit.

 $\Delta\delta(\lambda) \sin \delta$, such that substituting $\delta + \Delta\delta(\lambda)$ for δ in (13), and collecting the new terms that result, we identify the interaction Hamiltonian as

$$H_{\rm qb-mi} = -\frac{\Phi_0 I_{\rm bias}}{2\pi} \Delta \delta(\lambda) + \frac{\Phi_0 I_0}{2\pi} \Delta \delta(\lambda) \sin \delta + \frac{\Phi_0 I_0}{4\pi} \Delta \delta(\lambda)^2 \cos \delta.$$
(14)

Introducing quantization of magnetic dipole moments, we may replace $\vec{m}^{(n)}$ with $-g\mu_{\rm B}S^{(n)}$ in (12*b*), where *g* is the Landé factor, $\mu_{\rm B}$ is the Bohr magneton, and $S^{(n)}$ is the total spin operator of the *n*th ion. The 3d electron states of Fe³⁺ give rise to its moment, with spin length S = 5/2 and measured g = 2.00, as reported in [17]. Substituting (12*a*) and (12*b*) into (14), with $\delta \otimes S^{(n)}$ denoting the tensor product of operators δ and $S^{(n)}$, we obtain the expression

$$H_{qb-mi} = -\Delta_{mi}(\lambda) \frac{\Phi_0}{2\pi} (I_{bias} - I_0 \sin \delta)$$

$$\otimes \sum_{n=1}^N I_1 \left(\frac{\rho_n}{\lambda\sqrt{2}}\right) e^{-i\phi_n S_z^{(n)}} S_y^{(n)} e^{i\phi_n S_z^{(n)}} + \frac{1}{2} \Delta_{mi}(\lambda)^2$$

$$\times \frac{\Phi_0}{2\pi} I_0 \cos \delta \otimes \sum_{m,n=1}^N I_1 \left(\frac{\rho_m}{\lambda\sqrt{2}}\right) I_1 \left(\frac{\rho_n}{\lambda\sqrt{2}}\right)$$

$$\times e^{-i\phi_m S_z^{(m)}} S_y^{(m)} e^{i\phi_m S_z^{(m)}} e^{-i\phi_n S_z^{(n)}} S_y^{(n)} e^{i\phi_n S_z^{(n)}}$$
(15)

with coefficient

$$\Delta_{\rm mi}(\lambda) = \frac{g\mu_{\rm B}\mu_0}{R\Phi_0} K_1\left(\frac{R}{\lambda\sqrt{2}}\right),\tag{16}$$

which describes the interaction of oscillator states with the spin degrees of freedom of N magnetic impurities.

3. Results and discussion

Estimating the size of terms in (15), we take $K_1(x)$ the order of unity and set $\pi R^2 = 10^{-12} \text{ m}^2$ such that $\Delta_{\text{mi}}(\lambda) \sim$ 10^{-8} . Then, for example, with critical current $I_0 = 10^{-5}$ A, within the first term of (15) we have an energy contribution $\Delta_{\rm mi}(\lambda) \Phi_0 I_0 / 2\pi \sim 10^{-4} \,\mu {\rm eV}$ (24 kHz) per magnetic impurity. With respect to a phase qubit immersed in a bath of magnetic impurities, this contribution corresponds to a total of about 0.1 meV (24 GHz) at 0.05% impurity concentration, i.e., multiply by $N \sim 10^6$. Also, the second term of (15) expresses a non-local interaction between spins, mediated by the state of the phase qubit, where the ratio of the amplitude of this term to that of the first is $\sim N\Delta_{\rm mi}(\lambda) \sim 10^{-2}$. Furthermore, with regard to phase dependency, by virtue of the secondorder approximation in $\Delta\delta(\lambda)$ that results in (14), the coupling of (15) is zero when the phase qubit is precisely biased at $\delta = \pi/2, I_{\text{bias}} = I_0.$

As mentioned earlier, the pumping transition of Fe³⁺ at 12 GHz is comparable to $\hbar\omega_{10}$ of typical phase qubits. This suggests near-resonance behaviour may be exhibited between the qubit and Fe³⁺ electron states. However, the situation is somewhat more complicated than the resonance between a phase qubit and a TLS since the $|5/2, \pm 1/2\rangle$ and $|5/2, \pm 3/2\rangle$ states are each degenerate Kramers doublets that are slightly split (and mixed with $|5/2, \pm 5/2\rangle$ in the case of $|5/2, \pm 1/2\rangle$) due to the local crystal field, as quantified in [15]. We consider the effect of hexagonal crystal symmetry on the near-resonance behaviour of our model a topic for future study.

The contribution of junction magnetic impurities to the quality factor Q can be approximated by noting that the shift in phase difference of (12a) implies a tunnelling current $I_0 \sin[\delta +$ $\Delta\delta(\lambda) \cong I_0 \sin\delta + I_0 \Delta\delta(\lambda) \cos\delta - \frac{1}{2} I_0 \Delta\delta(\lambda)^2 \sin\delta$. On average, at very low impurity concentration, particularly near $\delta = \pi/2$, the term first order in $\Delta\delta(\lambda)$ tends to vanish, and, within the second-order term, we can assume $\langle \Delta \delta(\lambda)^2 \sin \delta \rangle \cong$ $\langle \Delta \delta(\lambda)^2 \rangle \langle \sin \delta \rangle$. Here, the angle brackets $\langle \cdots \rangle$ imply that we evaluate these terms in the ground state, averaging over all orientations of the local magnetic moments, and averaging over an ensemble of spatial distributions of impurities within the junction. Thus, in this limit of approximation, the critical current is effectively reduced, i.e., $I_0 \rightarrow I_0(1 - \langle \Delta \delta(\lambda)^2 \rangle/2)$. If $Q_0 = \omega_p R_0 C$ is the Q factor in the absence of these impurities, where $\omega_{\rm p} = \sqrt{(2\pi I_0/\Phi_0 C)}$ is the plasma frequency (most closely associated with qubit transition frequency ω_{10}) and R_0 is the resistance of the junction, then the Q factor in the presence of junction magnetic impurities can be approximated, with the aid of (12a) and (12b), as

$$Q(\lambda) \cong Q_0 \left[1 - \frac{1}{4} \left(\frac{2\pi}{\Phi_0} \right)^2 \langle \Phi_{\rm mi}(\lambda)^2 \rangle \right].$$
(17)

We can estimate the size of $\langle \Phi_{\rm mi}(\lambda)^2 \rangle$ in the limit of a very low concentration of Fe³⁺ impurities by assuming a ground state consisting of products of independent impurity states, where S = 5/2 is still a good quantum number and the *n*th impurity state $|n\rangle$, neglecting crystal-field splitting, is two-fold degenerate, constructed from local angular momentum states $|5/2, \pm 1/2\rangle$. In this way, we find

$$\langle \Phi_{\rm mi}(\lambda)^2 \rangle \cong \left(\frac{g\mu_{\rm B}\mu_0}{2\pi R}\right)^2 K_1 (R/\lambda\sqrt{2})^2 \\ \times \left\langle \sum_{n=1}^N I_1 (\rho_n/\lambda\sqrt{2})^2 \langle n|S_y^{(n)\,2}|n\rangle \right\rangle_{\rm sp.avg.},$$
(18)

subject to a spatial average $\langle \cdots \rangle_{\text{sp.avg.}}$ over the ensemble of impurity distributions. Now, for any impurity we have $\langle 5/2, \pm 1/2 | S_y^{(n)2} | 5/2, \pm 1/2 \rangle = 17/4$; the two-fold degeneracy of the impurity state $|n\rangle$ introduces an overall multiplier of 2, i.e., $\langle n | S_y^{(n)2} | n \rangle = 17/2$; and, in performing the spatial average of (18), we assume magnetic impurities are uniformly distributed throughout the junction such that we may replace the sum $\sum_{n=1}^{N} I_1(\rho_n/\lambda\sqrt{2})^2$ by the average integral $(N/S_0) \int_0^R \rho I_1(\rho/\lambda\sqrt{2})^2 d\rho$, which evaluates to $(NR^2/2S_0)[I_0(R/\lambda\sqrt{2})^2 + I_1(R/\lambda\sqrt{2})^2]$. Thus, with the impurity concentration inferred from $n_{\text{mi}} = N/V$, where $V = S_0d$ is the volume of junction, (18) becomes

$$\langle \Phi_{\rm mi}(\lambda)^2 \rangle \cong \frac{17}{4} n_{\rm mi} d \left(\frac{g\mu_{\rm B}\mu_0}{2\pi} \right)^2 K_1 (R/\lambda\sqrt{2})^2$$

 $\times [I_0 (R/\lambda\sqrt{2})^2 + I_1 (R/\lambda\sqrt{2})^2],$ (19)

which applied to (17), is the estimate of the Q factor near $\delta = \pi/2$. In the limit $\lambda \ll R$ the Bessel functions of (19)



Figure 2. Plot of the *Q* factor of a qubit biased near $\delta = \pi/2$, using the approximations of (17) and (19), as a function of λ/R . The magnetic impurity concentration of the junction is 0.05% and the junction thickness is d = 15 Å.

reduce to simple forms such that the Q factor of (17) can be approximated as

$$Q(\lambda) \cong Q_0 \left[1 - \frac{17}{16} n_{\rm mi} d \left(\frac{g \mu_{\rm B} \mu_0}{\Phi_0} \right)^2 \left(\frac{\lambda}{R} \right)^2 \right];$$

$$\lambda \ll R.$$
(20)

In figure 2 we plot the Q factor as a function of London penetration depth, with impurity concentration 0.05% and junction thickness d = 15 Å. The reduction in Q factor is less than 0.01% over the range of penetration depths that are physically meaningful. Again, our approximation of (17) and (19) assumes non-interacting impurity moments at low concentration. At higher concentration than 0.05%, where the average separation between impurities is much less than 100 Å, we expect interactions such as RKKY to play a more significant role.

4. Conclusion

In summary, we have derived a model of coupling between a phase qubit and the angular momentum degrees of freedom of a collection of Fe³⁺ ions contained within a single-crystal Josephson junction. The model predicts that coupling exists only for a non-zero London penetration depth. And when the phase qubit is fully biased at $\delta = \pi/2$, I_{bias} I_0 the coupling vanishes. Furthermore, predicted qubitto-impurity coupling strengths range from ~ 24 kHz (for a single impurity) to ~ 24 GHz (for coherent coupling to 10⁶ impurities). Assuming a minimum observable coupling strength of 50 MHz, we therefore expect an observable effect to require a strong coherent interaction involving $\sim 2 \times 10^3$ impurities, which corresponds to approximately 0.0001% impurity concentration. From our analysis at these concentrations, we expect a negligible reduction of the Qfactor of the qubit due to magnetic impurities.

The small effect of the magnetic impurity concentration on the Q value means that a 0.0001% concentration of magnetic ions should not alter the potential for adiabatic transfer of quantum state information between qubit and ion states, if such is possible. Hence, the possibility of an Fe³⁺ ion acting as a memory qubit is not unduly influenced by its location within the junction, at this concentration. However, if the impurity concentration is much higher than 0.0001% then we should expect RKKY interactions, with energies $\sim \mu_B^2/r^3$, to become more important. Thus, under these circumstances, our model would likely require amendment to account for the effects of strong correlations. Therefore we anticipate that a concentration of 0.0001% Fe³⁺ ions is a good starting point for experimental investigation since it is above the threshold of spectroscopic detection and affords near-adiabatic interaction of ions with qubit, within the regime of applicability of our model.

Lastly, we should point out that our model is not intended as a description of, or substitute for, other models of quantum fluctuators that have been described in the literature [2-5, 23, 24]. Nor do we envisage our model as explaining spectroscopic observations of recent experiments [2, 9–11]. Rather, we have proposed a mechanism for coupling a phase qubit to magnetic ions intentionally doped into an otherwise monocrystalline junction, with the purpose of establishing guidelines for conducting experiments. Our focus has been on Fe³⁺ because of the 12 GHz transition observed in this case. An ancillary result of our analysis, however, is that our model is applicable to the description of the coupling of other magnetic impurities (such as Fe²⁺, Cr³⁺ and Mn⁴⁺, which might be found naturally within dielectric junctions) to a qubit, regardless of resonance viability, within the range of parameter space we have outlined. We hope our work will stimulate further investigations in this area.

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