Cancellation of Spin-Orbit Effects in Quantum Gates Based on the Exchange Coupling in Quantum Dots

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We study the effect of the spin-orbit interaction on quantum gate operations based on the spin exchange coupling where the qubit is represented by the electron spin in a quantum dot or a similar nanostructure. Our main result is the exact cancellation of the spin-orbit effects in the sequence producing the quantum XOR gate for the ideal case where the pulse shapes of the exchange and spin-orbit interactions are identical. For the nonideal case, the two pulse shapes can be made almost identical and the gate error is strongly suppressed by two small parameters, the spin-orbit constant and the deviation of the two pulse shapes. We show that the dipole-dipole interaction leads only to very small errors in the XOR gate.

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The spin $1/2$ of an electron is a "natural" representation of a quantum bit (qubit) since it comprises exactly two levels; there are no additional degrees of freedom into which the system could "leak" and thereby cause errors in a quantum computation. In addition to this, magneto-optical experiments have revealed unusually long spin coherence times in doped semiconductors, exceeding 100 μs [1], thus making electron spins in semiconductors suitable candidates for a scalable quantum computer architecture. These advantages have motivated the idea of spin-based solid-state quantum computation using electron spins in coupled quantum dots [2], where the required two-spin coupling is provided by the Heisenberg exchange interaction between the two spins in adjacent quantum dots. The microscopic origin of the exchange coupling lies in the virtual tunneling of electrons from one quantum dot to the other and back, and there are several external physical parameters (gate voltages, magnetic field, etc.) which can in principle be used for controlled quantum gate operation [3]. Subsequent schemes [4–8] for solid-state quantum computation rely also on the exchange interaction between spins, and it has been pointed out that the exchange interaction alone (without single-spin manipulation) is in principle sufficient for universal quantum computation [9,10].

However, the two-level structure of the *spin* of the electron is only approximate if one includes relativistic effects which lead to spin-orbit coupling [11]. The exchange Hamiltonian can acquire anisotropic terms due to spin-orbit coupling [12,13]. For conduction band electrons in single GaAs dots, the spin-orbit energy is typically small [3]; however, it was recently pointed out by Kavokin [14] that the spin-orbit coupling can be relevant for tunneling between two dots, leading to an anisotropy in the resulting spin Hamiltonian, and it was suggested that it may lead to additional spin decoherence. Subsequently, Bonesteel *et al.* [15] have demonstrated that the first-order effect of the spin-orbit coupling during quantum gate operations can be eliminated by using time-symmetric pulse shapes for the coupling between the spins.

In this paper, we present a different method for dealing with the spin-orbit interaction. Our main result is that the spin-orbit effects *exactly* cancel in the gate sequence [Eq. (2)] required to produce the quantum XOR (CNOT) gate, provided that the pulse form for the spin-orbit and the exchange couplings are the same. Since XOR is sufficient to assemble any quantum computation together with single-qubit operations, this result has far-reaching consequences for spin-based quantum computation with the exchange interaction; it ascertains that the spin-orbit coupling can be dealt with in any quantum computation. In reality, the pulse shapes for the exchange and the spin-orbit coupling cannot be chosen completely identical. Typically, however, we can choose two pulse shapes which are very similar and show that our result still holds to a very good approximation, i.e., the effect of the spin-orbit coupling is still strongly suppressed. Finally, we discuss the effect of the dipole coupling between adjacent spins, providing another anisotropic coupling. The anisotropy due to an inhomogeneous magnetic field was studied in [16].

The spin-orbit coupling for a conduction-band electron (momentum $\mathbf{k}$, spin $\mathbf{S}$) can be written as $H_{\rm so} = \mathbf{h}(\mathbf{k}) \cdot \mathbf{S}$. In two dimensions, the Rashba term [17] $\mathbf{h}_1(\mathbf{k}) = a_1(k_y, -k_x, 0)$ arises from an asymmetric quantum well or from an external field. The absence of the inversion symmetry, e.g., in GaAs, causes a term [18] $\mathbf{h}_2(\mathbf{k}) = a_2(-k_x, k_y, 0)$. Such a term was already shown to exist in [19]. The isotropic Heisenberg coupling with exchange energy J and the anisotropic exchange between two localized spins $\mathbf{S}_1$ and $\mathbf{S}_2$ ($s = 1/2$) are combined in the Hamiltonian [15] $H(t) = J(t)[\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathcal{A}(t)]$. We divide $\mathcal{A}(t)$ into asymmetric and symmetric parts [14],

$$\mathcal{A}(t) = \boldsymbol{\beta}(t) \cdot (\mathbf{S}_1 \times \mathbf{S}_2) + \gamma(t)[\boldsymbol{\beta}(t) \cdot \mathbf{S}_1][\boldsymbol{\beta}(t) \cdot \mathbf{S}_2], \tag{1}$$

where $\boldsymbol{\beta} = \langle \psi_1 | i\mathbf{h}(\mathbf{k}) | \psi_2 \rangle$ is the spin-orbit field, $|\psi_i\rangle$ the ground state in dot $i = 1, 2$, and $\gamma \approx O(\beta^0)$. For $\mathcal{A} = 0$,

the quantum XOR gate can be obtained by applying $H(t)$ twice, together with single-spin rotations [2,20],

$$U_g = e^{i\pi S_1^z/2} e^{-i\pi S_2^z/2} U e^{i\pi S_2^z} U\,, \tag{2}$$

where U is the (unitary) time-ordered exponential $U = T\exp[-i\int_{-\tau_s/2}^{\tau_s/2} H(t)\,dt]$. Here τ_s denotes the switching time, during which the spin interactions via tunneling are turned on. In the case $\mathcal{A} = 0$, the Hamiltonian commutes with itself at different times and thus U is only a function of the integrated interaction strength,

$$\varphi = \int_{-\tau_s/2}^{\tau_s/2} J(t)\,dt\,, \tag{3}$$

with $\varphi \neq 0$. In particular, we obtain the desired quantum gate (up to a trivial change of basis) $U_g = U_{\mathrm{CPF}} = e^{i\pi S_2^y/2} U_{\mathrm{XOR}}\, e^{-i\pi S_2^y/2}$ if we choose $\varphi = \pi/2$ (in this case, U is the "square-root of swap" gate [2]).

First, we study the case $\mathcal{A} \neq 0$, retaining the property that $H(t)$ commutes with itself at different times. This is the case if β and γ (and thus $\mathcal{A}$) are time independent, i.e., if the anisotropic part of the Hamiltonian H is proportional to the isotropic exchange term. This allows us to fix a coordinate system in which β points along the z axis, and in which the anisotropy can be written as

$$\mathcal{A} = \beta(S_1^x S_2^y - S_1^y S_2^x) + \delta S_1^z S_2^z\,, \tag{4}$$

with $\delta = \gamma\beta^2$. In this basis H commutes with the z component $S^z = S_1^z + S_2^z$ of the total spin, $[H, S^z] = 0$, and thus $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, being nondegenerate eigenstates of S^z, are also eigenstates of H. Note that in their energy eigenvalue $J(1+\delta)/4$ there is no contribution from the first term in Eq. (4). In the $S^z = 0$ subspace we choose a basis consisting of the spin singlet $|s\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ and the triplet $|t\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ because this choice makes the isotropic part $J\mathbf{S}_1\cdot\mathbf{S}_2$ of the Hamiltonian diagonal. The complete Hamiltonian in the basis $\{|\uparrow\uparrow\rangle, |s\rangle, |t\rangle, |\downarrow\downarrow\rangle\}$ is

$$H(t) = \frac{J(t)}{2}\begin{pmatrix} 1+\delta & 0 & 0 & 0 \\ 0 & -1 & i\beta & 0 \\ 0 & -i\beta & 1 & 0 \\ 0 & 0 & 0 & 1+\delta \end{pmatrix}, \tag{5}$$

where we have added an irrelevant term $J(1+\delta)/4$ proportional to the unity matrix.

Exponentiation of Eq. (5) in the $S^z = 0$ subspace yields

$$U|_{S^z=0} = \begin{pmatrix} c + is/x & \beta s \\ -\beta s & c - is/x \end{pmatrix}, \tag{6}$$

where $c = \cos(x\varphi/2)$, $s = \sin(x\varphi/2)$, $x = \sqrt{1+\beta^2}$, and where φ is defined in Eq. (3). Since $\exp(i\pi S_2^z) = -i\sigma_x$ in the $S^z = 0$ subspace, we find $Ue^{i\pi S_2^z}U|_{S^z=0} = -i\sigma_x$, i.e., the dependence of $U|_{S^z=0}$ on the phase φ as well as on the spin-orbit parameter β as shown in Eq. (6) cancels exactly in the sequence Eq. (2). In other words, when we construct the XOR gate there will be no effect of the time-independent anisotropic terms $\mathcal{A}$ in the $S^z = 0$ subspace. By a proper choice of φ, we can also eliminate the effect of the anisotropy for the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$. This can be seen by writing down the full unitary operator Eq. (2) using the Hamiltonian Eq. (5),

$$U_g = \mathrm{diag}\big(ie^{-i\varphi(1+\delta)}, 1, 1, -ie^{-i\varphi(1+\delta)}\big)\,, \tag{7}$$

where $\mathrm{diag}(x_1,\ldots,x_4)$ denotes the diagonal matrix with diagonal entries $x_1,\ldots,x_4$. The pulse strength φ and the spin-orbit parameters only enter U in the $S^z = \pm 1$ subspaces. We would like U_g to be the conditional phase flip operation $U_{\mathrm{CPF}} = \mathrm{diag}(1,1,1,-1)$, being equivalent to the XOR operation up to a basis change. Indeed, the condition $U_g = U_{\mathrm{CPF}}$ can be fulfilled for $\varphi = \pi/2(1+\delta)$.

We have shown that in the case where the anisotropic term in the Hamiltonian is proportional to the isotropic term (i.e., $\mathcal{A} = \mathrm{const}$), we can completely eliminate the effect of the anisotropy by a proper choice of the pulse strength φ. In real systems, however, the anisotropic terms in the Hamiltonian H cannot be expected to be exactly proportional to $J(t)$, i.e., $\mathcal{A}(t)$ is time dependent. In general, both β and γ depend on time. Under these circumstances, we cannot exactly eliminate the effect of the anisotropy because of the time ordering in the definition of U and since the Hamiltonian does, in general, not commute with itself at different times, $[H(t), H(t')] \neq 0$.

In the following, we estimate the errors due to the anisotropy in the Hamiltonian in the case where $\mathcal{A}(t)$ is only weakly time dependent. Subsequently, we present a procedure which allows us to achieve exactly this situation (i.e., a weakly time-dependent $\mathcal{A}$). We write $\mathcal{A}(t) = \mathcal{A}_0 + \Delta\mathcal{A}(t)$, where $\mathcal{A}_0$ is constant, as in Eq. (4), and $\Delta\mathcal{A}(t)$ is the small time-dependent deviation from $\mathcal{A}_0$. The Hamiltonian is written as the sum $H(t) = H_0(t) + H'(t)$ where $H_0(t)$ is given by Eq. (5) and

$$H'(t) = J(t)\Delta\mathcal{A}(t) = J(t)[\Delta\boldsymbol{\beta}(t)\cdot(\mathbf{S}_1\times\mathbf{S}_2) + \Delta\boldsymbol{\gamma}(t)\,(\boldsymbol{\beta}\cdot\mathbf{S}_1)\,(\boldsymbol{\beta}\cdot\mathbf{S}_2)]\,. \tag{8}$$

Note that in the symmetric part we have already omitted terms which are of the order of $\Delta\beta\Delta\gamma$. This Hamiltonian generates a unitary time evolution $U = U_0 + \Delta U$, where $U_0 = T\exp[-i\int_{-\tau_s/2}^{\tau_s/2} H_0(t)\,dt]$ is the contribution due to H_0. The explicit form of ΔU is rather complicated; however, we are only interested in estimating the gate error $\Delta U_g = U_g - U_{\mathrm{CPF}}$ caused by $H'(t)$ (note that ΔU_g is not unitary). For this purpose we work in the interaction picture with respect to $H_0(t)$, where $U_I = U_0^\dagger U = T\exp[-i\int_{-\tau_s/2}^{\tau_s/2} H_I'(t)\,dt]$ and $H_I' = U_0^\dagger H' U_0$. In this representation, the deviation ΔU from the "ideal" time evolution U becomes $\Delta U_I = U_I - 1 = -i\int_{-\tau_s/2}^{\tau_s/2} H_I'(t)\,dt + O(H_I'^2)$. The norm of the gate error $\|\Delta U_g\| = \max_{\langle\psi\,|\,\psi\rangle=1}\sqrt{\langle\psi|\Delta U_g^\dagger\Delta U_g|\psi\rangle}$ (to lowest order in H') can now be estimated as follows,

$$\|\Delta U_g\| \lesssim 2\|\Delta U\| = 2\|U_0\Delta U_I\| = 2\|\Delta U_I\| \lesssim 2\tau_s \max_{|t|\le\tau_s/2}\|H'(t)\| \equiv 2\Delta\,, \tag{9}$$

where the first equality comes from Eq. (2) and the unitarity of the involved quantum gates. Using $\beta \ll 1$, we approximate $\|H'(t)\| \lesssim |J(t)\Delta\beta(t)|/2$, since the second term in H' is $O(\beta^2)$. We use $\Delta\beta(t) = \beta(t) - \beta_0$ to write

$$\Delta = \frac{|\varphi|\beta_0}{2} \max_{|t|\le\tau_s/2} \left| \frac{J(t)}{J_0} \left[\frac{\beta(t)}{\beta_0} - 1 \right] \right|, \qquad (10)$$

where J_0 denotes the average exchange coupling $J_0 = \varphi/\tau_s \neq 0$. Note that the position of the dots is fixed during the switching process, thus $\boldsymbol{\beta}(t)/|\boldsymbol{\beta}(t)| = \text{const}$ [14]. For the XOR gate, $\varphi \approx \pi/2$. The error probability for the described gate operation can now be estimated as $\epsilon \equiv \|\Delta\Psi_{\text{out}}\|^2 \le \|\Delta U_g \Psi_{\text{in}}\|^2 \le \|\Delta U_g\|^2 \lesssim 4\Delta^2$.

In order to obtain an estimate for Δ, we consider the case of coupled quantum dots in a 2DEG. For parabolic confinement potential $V(r) = m\omega r^2/2$, the ground-state orbitals are $\psi(r) = (\pi a_B^2)^{-1} \exp(-r^2/2a_B^2)$, where $a_B = \sqrt{\hbar/m\omega}$ is the effective Bohr radius of the electronic orbitals and m is the effective electron mass. If two such quantum dots containing one electron each are separated by a distance $2a$, the exchange coupling between the spins of the electrons at zero magnetic field is given by [3]

$$J(d,q) = \frac{\hbar\omega_0}{\sinh(2qd^2)} \left\{ c[e^{-qd^2} I_0(qd^2) - 1] + \frac{3q}{4}(1 + qd^2) \right\}, \qquad (11)$$

where I_0 is the zeroth order Bessel function, $d = a/a_B^0$ the dimensionless ratio between the half-distance a and the effective Bohr radius $a_B^0 = \sqrt{\hbar/m\omega_0}$, c characterizes the strength of the (bare) Coulomb interaction ($\hbar\omega_0 = 6$ meV and $c = 1.71$ in our numerical example), and $q = \omega/\omega_0$ is the strength of the confinement ω in units of its minimum value ω_0. Following [14], we find for both $\mathbf{h}_1$ and $\mathbf{h}_2$ that $b(d,q) \equiv |J(d,q)\beta(d,q)| = b_0\sqrt{q}\, d \exp(-2qd^2)$, where $b_0 = a_i/a_B^0$, $i = 1,2$. For $\mathbf{h}_2$ in a 5 nm wide [100] GaAs quantum well $a_2 \approx 2$ meV nm, or $\beta \approx 0.02$ at $d = q = 1$. In Fig. 1, we plot $J(d,q)$ and $b(d,q)$.

The switching process can be modeled, e.g., by a time-dependent distance d between the dots or by a time-dependent confinement strength q. Here, we choose the latter possibility and use a pulse $q(t) = \omega(t)/\omega_0 = \cosh^2(\alpha t/\tau_s)$, where we choose $\alpha = 4$. This pulse shape is suited for adiabatic switching [3,21] and leads to a pulsed exchange interaction $J(t) = J(d, q(t))$ and spin-orbit field $b(t) = b(d, q(t))$, where $-\tau_s/2 \le t \le \tau_s/2$. The pulse shapes of the resulting exchange coupling $J(t)$ and spin-orbit field $b(t)$ are plotted in Fig. 2. In our example, the switching time amounts to $\tau_s = \pi/2J_0 \approx 140$ ps. Note that a pulsed switching by electrostatic lowering of the tunneling barrier between the dots or by applying a magnetic field results in a very similar time dependence of J and b and a similar analysis could also be done in these cases. If the pulse shapes of b and J were identical, then the effect of the spin-orbit coupling in the XOR gate could be eliminated exactly (as explained above).

The optimal choice of β_0 (i.e., the one which minimizes Δ) in our numerical example turns out to be $\beta_0 \simeq \beta(t = 0.1\tau_s)$ and from Eq. (10) we find $\Delta \approx 7 \times 10^{-3}$. Therefore, the gate errors occur at a rate $\epsilon \lesssim 4\Delta^2 \approx 2 \times 10^{-4}$ which is around the currently known threshold for fault tolerant quantum computation [22] and could therefore be corrected by quantum error correction. Note that in cases where the error ϵ is too large for quantum error correction, it can be further reduced at the cost of a slower gate operation. This can be achieved by designing pulses with smaller intensity, where there is a long period of constant $\mathcal{A}$ between the rise and fall of the pulse.

We finally include the dipole-dipole interaction $H_d = \eta[\mathbf{S}_1 \cdot \mathbf{S}_2 - 3(\mathbf{S}_1 \cdot \hat{\mathbf{a}})(\mathbf{S}_2 \cdot \hat{\mathbf{a}})]$, being another source for anisotropic coupling among the spins $\mathbf{S}_1$ and $\mathbf{S}_2$, into our discussion. Here $\hat{\mathbf{a}}$ denotes the unit vector pointing from the center of one to that of the other dot. The coupling parameter $\eta = \mu_0 g^2 \mu_B^2/4\pi(2a)^3$ is typically much smaller than the spin-orbit energy, for $g = 2$ and $a = 20$ nm we obtain $\eta \approx 3 \cdot 10^{-12}$ eV, corresponding to a dipole field of $B_d = \eta/\mu_B \approx 0.5$ mG. Nevertheless, we show here that in cases where the dipole interaction matters (e.g., if g is very large), it can again be dealt with by using the

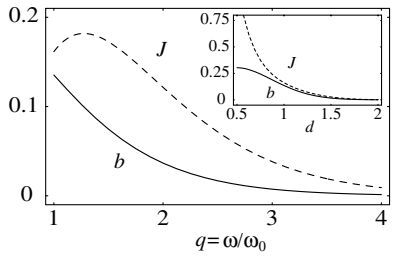

FIG. 1. The exchange coupling J (dashed line) in units of $\hbar\omega_0$ and the spin-orbit field $b = \beta J$ (solid line) in units of b_0 for two electron spins located in adjacent quantum dots as a function of the dimensionless parameter $q = \omega/\omega_0$ at fixed interdot distance $d = 1$ (inset: as a function of d at fixed $q = 1$), where $\hbar\omega$ is the (variable) single-dot confinement energy, ω_0 is the (fixed) minimum value of ω, and b_0 is the spin-orbit parameter. For this plot, $\hbar\omega_0 = 6$ meV and $c = 1.71$.

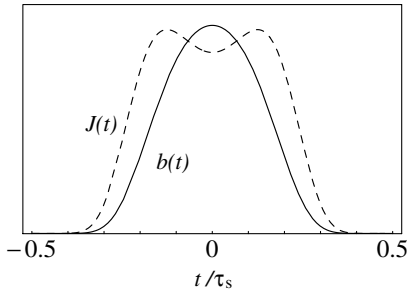

FIG. 2. Pulse form of the exchange coupling $J(t)$ (dashed line) and the spin-orbit field $b(t) = J(t)\beta(t)$ (solid line) for a simple model involving two coupled quantum dots which are coupled and decoupled with the time-dependent confinement strength $q(t) = \omega(t)/\omega_0$. For the distance between the dots we choose $d = 1$. The choice of the vertical scaling of the two pulses in this graph is such that the deviations of one pulse from the other are (approximately) minimal.

methods described above. An essential difference between the dipole and the spin-orbit interactions is that the dipole interaction between two spins located in adjacent quantum dots with fixed distance cannot be changed by applying gate voltages or static magnetic fields and therefore remains constant during the entire switching process and in the "idle" time between the switching. In the following, we assume for simplicity that $\mathcal{A}$ is independent of time, as in the first part of our discussion. In addition to this, we assume for the moment that J is also constant.

When investigating the combined effect of the spin-orbit and dipole couplings, we will restrict ourselves to the two cases $\mathbf{h}_1$ and $\mathbf{h}_2$. For $\mathbf{h}_2$, the spin-orbit field is parallel to the interdot coupling direction $\boldsymbol{\beta} \parallel \hat{\mathbf{a}}$ and thus the second term in H_d has the same form as the symmetric term in Eq. (4). We set $\xi = \eta/J$ and find

$$H = \frac{J}{2}\begin{pmatrix} 1+\delta-2\xi & 0 & 0 & 0 \\ 0 & -1-\xi & i\beta & 0 \\ 0 & -i\beta & 1+\xi & 0 \\ 0 & 0 & 0 & 1+\delta-2\xi \end{pmatrix}. \tag{12}$$

Using Eqs. (2) and (3) with $\varphi = \pi/2(1+\delta-2\xi)$, we exactly obtain $U_g = U_{\mathrm{CPF}}$, i.e., the combined effect of the spin-orbit and dipole coupling is eliminated. For $\mathbf{h}_1$, we find $\boldsymbol{\beta} \perp \hat{\mathbf{a}}$. Choosing $\hat{\mathbf{a}}$ along the x axis we obtain

$$H = \frac{J}{2}\begin{pmatrix} 1+\delta+\xi & 0 & 0 & -3\xi/2 \\ 0 & -1+\xi/2 & i\beta & 0 \\ 0 & -i\beta & 1-\xi/2 & 0 \\ -3\xi/2 & 0 & 0 & 1+\delta+\xi \end{pmatrix}. \tag{13}$$

Setting $\varphi = \pi/2(1+\delta+\xi)$, we obtain again $U_g = U_{\mathrm{CPF}}$, being related to U_{XOR} by a simple basis change (see above). Therefore it is possible to eliminate the spin-orbit and dipole coupling effects also in this case.

In principle, the analysis for time-dependent exchange and spin-orbit coupling can be repeated including the dipole interaction. However, the dipole interaction cannot easily be switched on and off, and therefore, the "pulse shape" of the dipole interaction is a constant, i.e., very different from those of the exchange and spin-orbit couplings (Fig. 2). Nevertheless, since the dipole interaction is usually very small, we can still use the estimate Eq. (9) to obtain a reasonable upper bound on the error by setting $H' = H_d$. We obtain $\Delta_d = \tau_s \eta = |\varphi|\eta/J_0$ which for typical numbers (as above, $J_0 \approx$ meV) is tiny, $\Delta_d \approx 10^{-9}$. The error $\epsilon_d = 4\Delta_d^2 = 4(\tau_s \eta)^2$ caused by the dipole interaction is therefore negligible in typical situations, and we have to take it into account only if for some reason (e.g., very large g) the dipole interaction becomes unusually large.

We conclude that while the spin-orbit interaction can cause weak decoherence in the combination with phonons [23], its direct effect on the quantum gate operation *nearly cancels* if the pulse shapes of the exchange and spin-orbit couplings are made as similar as possible. We have shown that in a typical case involving two tunnel-coupled quantum dots this is easily achievable. A simple estimate shows that the dipole interaction between the spins which also generates anisotropic terms in the Hamiltonian is usually much smaller than the spin-orbit interaction and can be neglected. Nevertheless, we have shown that in cases where the dipole effects are unusually large, the combined effect of spin-orbit and dipole coupling can be corrected with high precision.

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