

13 Quantum Computing – Quo Vadis?

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1 Quantum computing science is everywhere

In this small lecture, I will first comment on the generalities of quantum computing, and then plunge into some particulars.

Quantum computing continues to evolve as a science. It is now entering a phase where some concrete applications are seriously anticipated. Highly technological projects are underway in various companies and large organizations, and very ambitious efforts to assemble the unique and complex hardware required have borne some fruit. The 53-qubit device of the Google laboratory, and now the 56-qubit device of the Chinese Academy of Sciences, has executed a few algorithms that, to a very limited extent, were difficult for conventional computers. Tentative plans are drawn up for executing some additional algorithms, for example from quantum chemistry, for which these new machines may be capable of some modest successes.

We have, however, not reached the stage where truly society-changing computations are performable on any existing quantum computer. One issue is sheer size: estimates can be made of the size of quantum computer that would be transformative, and these estimates are generally in the millions of qubits. This is still far short of the bit-counts in even modest conventional computers of today, but it is a big, and expensive, leap from the unique Google and CAS processors. The optimistic timelines (I draw from IBM's projections here) for getting there involve many, many years of additional work.

Much of this work is a clearly engineering effort, required to make a unique, high precision piece of hardware at 10,000 times the present scale. Work on quantum computers have reached such a highly technological stage.

But, looking at IBM and others, we see reasons for the field cannot be purely one involving systems engineering. No qubit in use today meets the precision requirements needed to make the 10,000-fold leap. To tell the story for the superconducting qubits of the Google/CAS/IBM machines, they have in about 20 years improved in the quality of operation by about 6 orders of magnitude. However, the consensus is that about another 2 orders of magnitude are needed.

The improvements that I have just referred to require pure quantum physics insights. This is connected with a realization that we had 20 years ago, and that remains the focal point of our struggle: quantum physics has the property that it can, under the right circumstances, predict physical properties to fantastically high precision. But these circumstances are also fantastically difficult to bring into being.

One can see this as related to the struggle that we have had in crystal physics in the last 100 years. We have a wonderfully complete understanding of band theory, Fermi surfaces, van-Hove singularities, thermal conductivity, and a host of other properties. But the things we predict were quite hard to realize: materials are no perfect crystals, it takes a lot of work to make them so.

On the quantum computer side, the big stumbling block has been the many manifestations of decoherence. Quantum mechanics predicts in wonderful detail what happens to a two-level system when you apply forces to it, if it is isolated from everything else. We can tell less well what happens when you take account of the environment. But we know enough about this to

say that it creates a no-go condition for quantum computing.

So, quantum theorists have been forced to tell the growers (or better synthesizers, because it is both the materials and the devices that you make from them) to achieve conditions that are unquestionably very hard, and to not even be able to tell them what the exact target is. It is a fortunate thing that progress has been possible under these conditions. It has been iterative and slow, but at least it has been steady.

In the area of superconducting qubits, we might have been persuaded to say that 30 years ago there was already not really that much more to learn about the physics of superconductivity in Aluminium. The trouble was, this physics knowledge said that it would be possible to make ideal quantum two-level systems with Aluminium, with its superconductivity and with the Josephson effect made possible by tunnel junctions of AlO_x . All derivations could have been confidently done on the basis of material given in lectures at the time.

It initially didn't work at all. The things left out about the actual state of these devices made reality completely different from the model. It exposed our ignorance of the physics that really went on when you put an Aluminium junction into a circuit.

But over the last 20 years, we have gradually learned. Our models have been extended, experiments have become more sophisticated. Interestingly, this didn't require much new work from the crystal grower, the important sources of imperfections were not so much in her domain.

2 My main thesis

The thesis that I announce based on these observations is that progress on quantum computers, including from the pure engineering point of view, requires all the physics knowledge that we've got and that we know how to make. In short, quantum computing science is all of physics theory. Let me take as examples the other lectures of this school. In most cases, I can see an application for these efforts that have a chance to impact the efforts to build a quantum computer. Let me go through them:

- The Hubbard model. This is the fundamental model on which we base our thinking about spin qubits. It is also a good model to think about in working on algorithms for quantum simulation.
- Frustrated magnetism. This topic connects with ideas of topological order in eigenstates, and therefore with problems in quantum error correcting codes.
- Quantum chemistry. This is a topic for devising quantum algorithms and quantum simulations.
- Calculating with Green functions. This has been taken up in other work on quantum simulation, notably in the work of Jim Freericks, who has lectured in several of these schools in years past. See his article [1].
- Second quantization. The language used throughout quantum information science.

- Superconductivity. This is one of the most basic topological states of matter. Protection from dissipation and decoherence is very fundamental here.
- Entanglement. It goes without saying that this is the cornerstone of most thinking in quantum information science.

My premise for the rest of these lecture notes is that since quantum information science needs all of theoretical physics, I will just proceed to give a few living examples of how we need all details of our understanding to make progress on the problems of quantum computing, including those in the most engineering directions.

My examples will be in the area of semiconductor physics.

3 Electron theory for qubits

I will go through a small case study of a “correlation” effect in electronic qubits that has many consequences, some good and some bad, for the quality of the qubits. The qubit I have in mind is that defined by the electron spin of extra carriers in semiconductors. The “correlation” effect is that which arises from spin-orbit interaction.

One should immediately object that I have a strange definition of “correlation” here, since spin-orbit is a single-electron term in the Hamiltonian. This is a good objection: in the right basis, the electron problem with spin-orbit but without electron-electron interaction still has eigenstates that are single Slater determinants, so there is always a way in which the computational problem for this setting is “easy”. On the other hand, there is an important new correlation: with spin-orbit interaction, the spin and orbital degrees of freedom are *entangled*, while they occur in an unentangled product state in the absence of spin-orbit coupling. This entanglement already occurs at the single-particle level: the single-particle states from which the single Slater determinant eigensolutions are constructed are already entangled between spin and orbit. This entanglement varies dramatically from one part of the single-particle spectrum to another, which is very consequential for electron-qubit physics.

Recall the general situation from relativistic quantum mechanics: Foldy and Wouthuijsen derived a series in $1/c$ for the effective Hamiltonian. The terms to be added to the Pauli-Schrödinger Hamiltonian are

$$-\frac{p^4}{8m^3c^2}, \text{ mass-velocity term} \quad (1)$$

$$-\frac{e\hbar}{8m^2c^2} \nabla \cdot \mathbf{E}, \text{ Darwin term} \quad (2)$$

$$-\frac{e\hbar}{8m^2c^2} \boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p} - \mathbf{p} \times \mathbf{E}), \text{ spin-orbit term.} \quad (3)$$

The first two terms are quantitatively important but do not change the entanglement structure of the electron state, while the last term does, so we will continue with this term in the following. First, we slightly rewrite the spin-orbit term in the conventional way

$$H_{so} = -\frac{\hbar}{4m^2c^2} \boldsymbol{\sigma} \cdot \nabla V(\mathbf{r}) \times \mathbf{p}. \quad (4)$$

Three things to note: 1) $V(\mathbf{r})$ is now a potential energy, not a voltage; 2) The form here given doesn't look hermitian, since in general p_i doesn't commute with $\partial_j V$, but the situation is saved because $\nabla \times \nabla V = 0$; 3) the replacement is not correct if \mathbf{E} is time dependent, but the effect of this error is negligible at ordinary frequencies.

I always find it informative to analyze how big a term is for atomic matter. Given that the characteristic scale of p_i is \hbar/a_0 and the characteristic scale of ∇V is E_h/a_0 , we rewrite Eq. (4) as

$$H_{so} = \frac{E_h}{4} \left(\frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c} \right)^2 \boldsymbol{\sigma} \cdot \frac{\nabla V(\mathbf{r})}{E_h/a_0} \times \frac{\mathbf{p}}{\hbar/a_0} = \frac{E_h}{4} \alpha^2 \boldsymbol{\sigma} \cdot \frac{\nabla V(\mathbf{r})}{E_h/a_0} \times \frac{\mathbf{p}}{\hbar/a_0}. \quad (5)$$

Here the Rydberg constant $E_h = \hbar^2/ma_0^2$, the Bohr radius $a_0 = 4\pi\epsilon_0\hbar^2/me^2$, and the fine structure constant $\alpha = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c} \approx 1/137$. The appearance of the square of the fine structure constant signals the smallness of the term for atomic matter. However, we will see that under some circumstances, this term is nevertheless fully entangling.

3.1 Other spin-orbit terms

I referred to Eq. (4) as *the* spin-orbit term. But there are in fact many others that could occur. In this generous way of looking at things, we will call any Hamiltonian term a spin-orbit term if it involves both the electron coordinate, or momentum, and its spin. An example would be

$$i\alpha^{18} E_h \sigma_x e^{y/y_0} \tanh\left(\frac{p_z}{p_0}\right) \left(\frac{x}{x_0}\right)^7 \sigma_z + h.c. \quad (6)$$

Very few such expressions will pass muster as being physically interesting. There are two major exceptions, that is, two other spin-orbit terms are worth our attention:

1. First is the ‘‘micromagnet’’ term:

$$-g\mu_B \boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{r}) \quad (7)$$

There is nothing fundamental one can say about the size or importance of this term, since it requires engineering a spatial dependence to the applied magnetic field. With the use of micromagnets, its effect can indeed be significant in laboratory experiments on spin qubits.

2. Next is the magnetic dipole-dipole interaction:

$$\frac{\mu_0 g^2 \mu_B^2}{16\pi|\mathbf{r}|^3} \left(3(\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}})(\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right), \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad (8)$$

This can indeed lead to spin-orbit entanglement – the barely-bound p states of $^{129}\text{Xe}_2$ is the cleanest example that I know of. While we often use Eq. (8) in the case where one or the other of the spins are nuclear, it is also a perfectly good Hamiltonian for the pure electron problem. In this setting, it is not to be confused with the Heisenberg exchange Hamiltonian $J\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$, which is merely an effective Hamiltonian that describes electrons

in particular orbital configurations. The dipole-dipole interaction Eq. (8), by contrast, is “fundamental” – at least as fundamental as the normal spin-orbit interaction. Like that, it has the status of a leading relativistic correction. To see this, we “de-dimensionalize” Eq. (8) using atomic units. The new replacement we must employ is Maxwell’s relation $\mu_0 = \frac{1}{\epsilon_0 c^2}$. With this, the de-dimensionalized form of the overall factor in the electronic dipole-dipole interaction is

$$\frac{\mu_0 g^2 \mu_B^2}{16\pi |\mathbf{r}|^3} = \frac{g^2}{16} \frac{E_h}{(r/a_0)^3} \frac{4}{4\pi\epsilon_0 c^2} \frac{\mu_b^2}{E_h a_0^3} = \frac{g^2}{16} \frac{E_h}{(r/a_0)^3} \alpha^2. \quad (9)$$

Thus, just like the normal spin-orbit term, the dipolar term is second order in the fine structure constant.

Given that it is of the same order, why does it not emerge as a term in the Foldy-Wouthuysen series? The answer is that is a *two-electron* spin-orbit term, which can never emerge from the one-particle Dirac equation. It is understood that it emerges from the same sort of analysis (as a series in α) applied to the two-particle relativistic wave equation, the Bethe-Salpeter equation. The dipolar term, along with another novel orbit-orbit term, emerges from this. The derivation via the Breit equation is also informative, but less rigorous.

Now let’s turn to the consequences of spin-orbit coupling in a semiconductor that hosts a spin qubit. The relevant semiconductors, the various group-IV and III-V compound semiconductors like GaAs, have a rather universal structure near the Fermi energy. All these semiconductors have full cubic symmetry, so that the electron states at the center of the Brillouin zone have high symmetry. The relevant irreducible representations at the Gamma point are isomorphic to those for full spherical symmetry.

Thus, the states at the Gamma point, in the absence of spin-orbit, have a conserved orbital angular momentum L . It happens that the states near the Fermi energy always have $L = 1$, in \hbar units, at the top of the valence band (which can host hole qubits), and the first state of the conduction band is always $L = 0$. Around an origin of high symmetry, we can rewrite the spin-orbit Hamiltonian as in atomic physics

$$V(\mathbf{r}) \approx V(|r|) \quad (10)$$

$$\nabla V \approx \hat{r} \frac{\partial V}{\partial r} \quad (11)$$

$$H_{so} \propto \frac{1}{r} \frac{\partial V}{\partial r} \boldsymbol{\sigma} \cdot (\mathbf{r} \times \mathbf{p}) = \frac{1}{r} \frac{\partial V}{\partial r} \boldsymbol{\sigma} \cdot \mathbf{L}. \quad (12)$$

An aside: it is sometimes said that the atomic spin-orbit operator is $\boldsymbol{\sigma} \cdot \mathbf{L}$. This is misleading; $\frac{1}{r} \frac{\partial V}{\partial r}$ is an operator too, on the position Hilbert space! When this is replaced by a “spin-orbit constant”, it should rather be understood as a matrix element between specific radial orbital pairs.

Thus, the situation with the top of the valence band is the same as with the p -state in an atom: the total angular momentum, $\mathbf{J} = \mathbf{S} + \mathbf{L} = \frac{1}{2} \boldsymbol{\sigma} + \mathbf{L}$ is conserved. The angular momentum addition

rules say that the angular momentum states are $J = 3/2$ and $J = 1/2$, due to the composition rule for irreducible representations $\frac{1}{2} \otimes 1 = \frac{1}{2} \oplus \frac{3}{2}$. This also means that the p -states, which would be 6-fold degenerate (3 orbital times 2 spin), split up into a 4-fold degenerate set of states $J = \frac{3}{2}$, and a two-fold pair $J = \frac{1}{2}$.

In semiconductors of interest the $J = \frac{3}{2}$ states are always the higher ones, and thus define the valence-band edge. The $J = \frac{1}{2}$ states are, rather prosaically, referred to as the “split-off band”. the spin-orbit splitting between these multiplets, Δ , is one of the important band parameters in semiconductors. We will see below the crucial role that it plays in the behavior of electron [sic] spin qubits.

Note that this lifting of valence-band degeneracy comes along with there being strong spin-orbit entanglement in these states. For example, one of the eigenstates in the $J = \frac{3}{2}$ space, made non-degenerate by a magnetic field in the (100) crystal direction, is

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle = \frac{1}{\sqrt{3}} \left(\psi_{p_+}(\mathbf{r})\chi_{\downarrow} + \sqrt{2}\psi_{p_z}(\mathbf{r})\chi_{\uparrow} \right). \quad (13)$$

Here $\psi_{p_+}(\mathbf{r})$ is the $k = 0$ Bloch state constructed from the orbital $p_x + ip_y$, $\psi_{p_z}(\mathbf{r})$ is the different orbital Bloch state constructed from the p_z orbital, and χ_{\downarrow} and χ_{\uparrow} are the orthogonal spin wavefunctions that can also be denoted $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Thus, the “weak” spin-orbit interaction can, in this circumstance, result in an almost maximally entangled wavefunction.

We will pursue this interesting topic much further, but note that the $J = \frac{3}{2}$ states come with two different effective masses, so that away from the Gamma point they disperse into two pairs of states. A remaining two-fold degeneracy is guaranteed by Kramers’ theorem plus the inversion symmetry in the point group. Because of these two different masses, the top of the valence band is further split if the crystal is strained, as happens in the formation of heterostructures.

The bottom of the conduction band, the place where we normally put electrons in order to make spin qubits, is at first glance immune from the large effect of spin-orbit interaction. The state is essentially of the simple form

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle \approx \psi_s(\mathbf{r})\chi_{\downarrow}, \quad (14)$$

with basically no spin-orbit entanglement. But I say “basically” because the spin-orbit Hamiltonian still couples this state perturbatively to other eigenstates.

This, in some cases, produces a significant physical effect. This is very evident in the effective g -factor of these states, in other words, the splitting between the $|1/2, 1/2\rangle$ and $|1/2, -1/2\rangle$ due to a magnetic field, Without spin-orbit interaction this splitting is $g\mu_B B$, with a g factor always equal to $g = 2 + \alpha/2\pi$ (that is, a fraction of a percent above 2, with additional, even smaller terms of higher order in α). The fine structure constant α appears here due to a distinct vacuum relativistic effect, the coupling of the electron to the quantized electromagnetic field.

But spin-orbit effects in crystalline matter modify this dependence dramatically. First, the Zeeman splitting is no longer rigorously linear in B , there are B^2 , etc. terms. But more dramatic and significant is the departure of g far from 2. This can be analyzed by perturbation theory. The most significant contributors are couplings to the six valence band states. A beautiful formula

emerges from this, due to Laura Roth in 1959 [2]

$$g = 2 - \frac{2\Delta}{3E_g + 2\Delta} \left(\frac{m}{m_{eff}} - 1 \right). \quad (15)$$

(This is ignoring the Schwinger correction $\alpha/2\pi$, which is almost always far smaller.) Here Δ is the valence band spin-orbit splitting discussed above, E_g is the band gap of the semiconductor, and m_{eff} is the effective mass of the conduction band electrons. These latter two parameters are not primarily determined by spin-orbit interaction, while Δ is only non-zero when spin-orbit is included.

The parameters on the right-hand side of the Roth formula are all accurately known from experiment. For example, $\Delta = 44, 295, 341, 380, 930$ (in meV) for Si, Ge, GaAs, InAs, and ZnTe, respectively. Plugging these in gives for GaAs $g_{GaAs}^R = 0.09$, and for InAs $g_{InAs}^R = -14.9$. The Zeeman splittings are also readily measured, and the experimental values are $g_{GaAs} = -0.44$, and for $g_{InAs} = -15$. While not being precisely accurate, Roth's analysis correctly predicts the dramatic departures of the Zeeman splitting from its non-relativistic value, and the trend of increasing departure when going to heavier elements.

The important message of this formula is that the g factor depends, potentially strongly, on details of the orbital electronic structure. One can imagine, based on the kind of perturbation theory involved, that the result will depend on where we are in \mathbf{k} -space. To get ahead of our story somewhat, this tells us something of what will happen when we form a quantum dot: depending on the size of the dot, the resulting wavefunction will sample a greater or lesser part of this \mathbf{k} space – thus, the g factor will depend on the degree of confinement. This variation, while not particularly large in, e.g., Si, has been observed recently and is definitely a source of concern for applications as qubits.

While the derivation of the Roth formula is a bit time consuming, I will give a flavor of this kind of band perturbation for the simpler problem of the band effective masses that appear in her formula. This formula has nothing to do with spin-orbit, so we revert to the regular Schrödinger equation.

When we substitute the Bloch function

$$\Phi_{nk}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{nk}(\mathbf{r}) \quad (16)$$

in the Schrödinger equation

$$\left(\frac{p^2}{2m} + V(\mathbf{r}) \right) \Phi_{nk}(\mathbf{r}) = E_{nk}(r) \Phi_{nk}(\mathbf{r}), \quad (17)$$

we get the wave equation for the periodic part of the Bloch function,

$$\left(\frac{p^2}{2m} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} + V(\mathbf{r}) \right) u_{nk}(\mathbf{r}) = E_{nk}(r) u_{nk}(\mathbf{r}). \quad (18)$$

The new term here is referred to as the “cay-dot-pee” perturbation; although it is not really a perturbation, Eq. (18) is just an exact rewriting of Eq. (17).

The procedure is as follows: one obtains solutions for $\mathbf{k} = 0$, $u_{n0}(\mathbf{r})$ and E_{n0} . Then one treats the $\mathbf{k} \cdot \mathbf{p}$ term (together with the simple k^2 term) using perturbation theory to get the dispersion. Around $\mathbf{k} = 0$ the lowest order perturbation result is quadratic in $|k|$. The band curvature gives the effective mass. The simple formula for this is

$$\frac{1}{m_{\text{eff}}} = \frac{1}{m} + \frac{2}{m^2} \sum_{n' \neq n} \frac{|\hat{\mathbf{k}} \cdot \langle u_{n0} | \mathbf{p} | u_{n'0} \rangle|^2}{E_{n0} - E_{n'0}}. \quad (19)$$

In our high symmetry situation, m_{eff} is independent of the direction of the unit vector $\hat{\mathbf{k}}$.

We can note that, generically, large contributions to $1/m_{\text{eff}}$ will occur (so that m_{eff} will have a small magnitude) if the energy gap is small.

With spin-orbit interaction, our Schrödinger equation Eq. (17) becomes

$$\left(\frac{p^2}{2m} + V(\mathbf{r}) + \frac{\hbar}{4m^2 c^2} \mathbf{p} \cdot (\boldsymbol{\sigma} \times \nabla V) \right) e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk\sigma}(\mathbf{r}) = E_{nk\sigma}(r) e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk\sigma}(\mathbf{r}). \quad (20)$$

The band energies E and the periodic part of the Bloch wavefunction u have acquired spin labels σ . As above, one obtains a $\mathbf{k} \cdot \mathbf{p}$ -style Schrödinger equation for the u function

$$\left(H_0 + \frac{\hbar^2 k^2}{2m} + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2}{4m^2 c^2} \mathbf{k} \cdot (\boldsymbol{\sigma} \times \nabla V) \right) u_{nk\sigma}(\mathbf{r}) = E_{nk\sigma}(r) u_{nk\sigma}(\mathbf{r}). \quad (21)$$

Here H_0 is the whole Hamiltonian for the $\mathbf{k} = 0$ states, including the spin-orbit contributions; often this is left as a separate term to be treated, along with the \mathbf{k} -dependent terms, with perturbation theory. We will again look at what happens to the conduction band in, e.g., GaAs. The approach is as for the effective mass: take into account the effect of other bands perturbatively. Since the conduction band is two spin states, we get not a single corrected dispersion, but an effective 2×2 Hamiltonian

$$H_{\text{eff}} = \frac{\hbar^2 k^2}{2m_*} + \gamma \hbar^2 \left(\sigma_x k_x (k_y^2 - k_z^2) + \text{cyclic permutation } x \rightarrow y \rightarrow z \rightarrow x \right). \quad (22)$$

The form here is universal for s -bands in crystals with a form of cubic symmetry, with only γ depending on details of the perturbation matrix elements; but for full cubic symmetry (i.e., including inversion symmetry, e.g., in Si and Ge) $\gamma = 0$. This set of terms is called ‘‘Dresselhaus spin-orbit coupling’’.

A few interesting notes about this term: 1) While it respects cubic symmetry, it does not have full rotational symmetry, so the band dispersion is not isotropic. 2) Except along high-symmetry directions, the energy splitting of the two spin states is nonzero with a quantization axis that is a function of \mathbf{k} . 3) There is a superficially similar term, called the Rashba spin-orbit coupling, that is *not* intrinsic to the crystal structure, but is activated by additional applied magnetic fields. This Rashba coupling produces a variety of interesting effects, but in the interests of space will not go into them here.

We are now going to see how this affects the electrons that are confined to quantum dots, for the purpose of making spin qubits. I will state without proof the use of effective Hamiltonians like

Eq. (22) when we consider the envelope function approximation. When we describe an electron as being confined to a quantum dot, we have in mind that the Bloch function is modulated by a slowly varying envelope wavefunction

$$\psi_{env,n\sigma}(\mathbf{r})e^{i\mathbf{k}_0\cdot\mathbf{r}}u_{nk_0\sigma}(\mathbf{r}). \quad (23)$$

Here \mathbf{k}_0 is the extremum of the band, i.e., $\mathbf{k}_0 = 0$ for the examples we have been discussing. The envelope-function theory shows that to apply the effective Hamiltonian to ψ_{env} alone to get an eigenvalue equation, the prescription is to elevate \mathbf{k} to operator status with the replacement $\mathbf{k} \rightarrow i\nabla$. You are probably very familiar with this in the case of the simple effective mass term, where we say that the kinetic energy operator in the effective mass approximation is just

$$-\frac{\hbar^2\nabla^2}{2m_{eff}}. \quad (24)$$

With spin-orbit interaction, we just make this replacement everywhere in Eq. (22).

We will now explore what consequences this has for the control of two spin-qubits. We will follow the derivation of Kavokin [3]. We will assume the Hamiltonian consists of Eq. (22), along with a spatial confining potential. This potential is assumed smooth on the scale of the lattice constant. Notationally we will write this double quantum dot Hamiltonian as

$$H(\mathbf{r}, \mathbf{k}) = H_{eff}(\mathbf{k}) + V_{conf}(\mathbf{r}). \quad (25)$$

This notation indicates, as suggested above, that the envelope coordinate \mathbf{r} and the crystal momentum \mathbf{k} will function as conjugate variables. “conf” refers to “confinement”.

We will solve the two-electron problem. Importantly, we will proceed with first quantization, which flexibly deals with undetermined and non-orthogonal space orbitals. In first quantization the two electron Hamiltonian is

$$H_{tot} = \sum_{i=1}^2 H(\mathbf{r}_i, \mathbf{k}_i) + C(\mathbf{r}_1 - \mathbf{r}_2). \quad (26)$$

C is some screened electron-electron interaction whose details will not be important here.

One can proceed with a Heitler-London (two-orbital) calculation which, in the absence of spin-orbit, gives the familiar Heisenberg exchange expression for the effective qubit-qubit interaction (calculated in [4])

$$H_{2qu} = J\mathbf{S}_A \cdot \mathbf{S}_B. \quad (27)$$

Here we specialize to a double-well confinement potential, with distinct wells A and B . We expect that with two electrons, electron one will occupy the A well, and electron two will occupy the B well, and vice versa. Note we are again using the first quantized language. In second quantization we should just say that the state is obtained from the vacuum (i.e., filled semiconductor bands) by applying a creation operator for spatial orbital A , and a creation operator for spatial orbital B , with the spin content of the orbital left for the present unspecified.

Kavokin begins by specializing the Dresselhaus contribution Eq. (22). We consider quantum dots that are strongly confined in one direction (z direction). This means that we will only

consider dynamics in the xy plane. It also means that, if we think in terms of expectation values, we expect that the strong confinement will mean that $\langle k_z^2 \rangle \gg \langle k_x^2 \rangle, \langle k_y^2 \rangle$. Thus, we approximate Eq. (22) by

$$\begin{aligned} H &= \frac{\hbar^2 k^2}{2m_*} + V_{conf}(\mathbf{r}) + \gamma \hbar^2 \left(-\sigma_x k_x \langle k_z^2 \rangle + \sigma_y k_y \langle k_z^2 \rangle \right) \\ &= -\frac{\hbar^2 \nabla^2}{2m_*} + V_{conf}(\mathbf{r}) + ia \left(-\sigma_x \nabla_x + \sigma_y \nabla_y \right), \end{aligned} \quad (28)$$

where $a = \gamma \hbar^2 \langle k_z^2 \rangle$.

I now proceed, following closely Sec. IV of [3]. Again with our mindset of first-quantization, we write a wavefunction basis states involving “electron 1” and “electron 2”, providing for the possibility of antisymmetrization

$$\Psi_A(1)\Psi_B(2)\chi_1^{\sigma_1}\chi_2^{\sigma_2} \text{ and } \Psi_A(2)\Psi_B(1)\chi_1^{\sigma'_1}\chi_2^{\sigma'_2}. \quad (29)$$

Note that unlike in second quantization, the spin functions χ are associated with electron number 1, 2 and not with spatial orbital A, B . Also, $(1, 2)$ is shorthand for $(\mathbf{r}_{1,2})$. The σ 's are indices for the spin basis states \uparrow and \downarrow , and are not to be confused with Pauli matrices. Observe that these are 8 basis functions overall, but we will come back to a 4D space due to antisymmetrization.

We now proceed with Heitler-London. The sleight of hand here involves recognizing that orbitals A and B are almost, but not quite, orthogonal, so that where their non-orthogonality is crucial for the leading-order term, it is accounted for; but other parts of the calculation are done as if the orbitals are orthogonal.

We will get matrix elements for the basis above. The two-electron Hamiltonian is split into two parts

$$H_{tot} = H_0 + H_1 \quad (30)$$

$$H_0 = \sum_{i=1}^2 \left(-\frac{\hbar^2 \nabla^2(i)}{2m_*} + V_{conf}(\mathbf{r}_i) \right) + C(\mathbf{r}_1 - \mathbf{r}_2). \quad (31)$$

$$H_1 = i \frac{2a}{\hbar} \sum_{i=1}^2 \left(-S_x(i) \nabla_x(i) + S_y(i) \nabla_y(i) \right). \quad (32)$$

In Heitler London the key matrix element is the off-diagonal one

$$\langle \Psi_A(1)\Psi_B(2)\chi_1^{\sigma_1}\chi_2^{\sigma_2} | H_0 | \Psi_A(2)\Psi_B(1)\chi_1^{\sigma'_1}\chi_2^{\sigma'_2} \rangle = J \delta_{\sigma_1, \sigma'_1} \delta_{\sigma_2, \sigma'_2}. \quad (33)$$

This gives the usual exchange constant J of the Heisenberg model Eq. (27). Note that it is only nonzero if orbitals A and B are *nonorthogonal*.

The interesting new spin-orbit contribution is

$$\begin{aligned} & \langle \Psi_A(1)\Psi_B(2)\chi_1^{\sigma_1}\chi_2^{\sigma_2} | H_1 | \Psi_A(2)\Psi_B(1)\chi_1^{\sigma'_1}\chi_2^{\sigma'_2} \rangle \\ & = i\langle \Psi_A | \Psi_B \rangle \langle \sigma_2 | \mathbf{b} \cdot \mathbf{S}_2 | \sigma'_2 \rangle \delta_{\sigma_1, \sigma'_1} - i\langle \Psi_B | \Psi_A \rangle \langle \sigma_1 | \mathbf{b} \cdot \mathbf{S}_1 | \sigma'_1 \rangle \delta_{\sigma_2, \sigma'_2}, \end{aligned} \quad (34)$$

$$\mathbf{b} \equiv \frac{2a}{\hbar} \begin{pmatrix} -\langle \Psi_A | \nabla_x | \Psi_B \rangle \\ \langle \Psi_A | \nabla_y | \Psi_B \rangle \\ 0 \end{pmatrix}. \quad (35)$$

The minus sign in Eq. (34) comes from the fact that the matrix elements comprising the vector \mathbf{b} are real and antisymmetric (Anti-Hermitian) in A, B . We give a 3D version of the vector \mathbf{b} because there are other spin-orbit terms, e.g., the ‘Rashba’ spin-orbit coupling, for which z -components of this vector are recovered.

One is now to infer the effective spin Hamiltonian that this leads to, and see how the effective interaction departs from the Heisenberg form. We simplify Eq. (35) further, by setting the coordinate system in spin space so that the z spin axis is parallel to the vector \mathbf{b} . Then we can write

$$\begin{aligned} \langle \Psi_A(1)\Psi_B(2)\chi_1^{\sigma_1}\chi_2^{\sigma_2} | H_{tot} | \Psi_A(2)\Psi_B(1)\chi_1^{\sigma'_1}\chi_2^{\sigma'_2} \rangle & = (J + i\Omega |\mathbf{b}| (S_{2z} - S_{1z})) \delta_{\sigma_1, \sigma'_1} \delta_{\sigma_2, \sigma'_2} \\ & \approx J' e^{i(\gamma/2)(S_{1z} - S_{2z})} \delta_{\sigma_1, \sigma'_1} \delta_{\sigma_2, \sigma'_2} \end{aligned} \quad (36)$$

Here Ω is the real number $\langle \Psi_A | \Psi_B \rangle$, $J' = \sqrt{J^2 + (\Omega |\mathbf{b}|)^2}$ and $\gamma = \arctan(\Omega |\mathbf{b}| / J)$. Typically $J' \approx J$ and $\gamma \ll \pi$, but I will review Kavokin’s estimates at the end, indicating that this will not be an entirely negligible effect.

Finding eigensolutions to the full Hamiltonian (all the interesting spin dependence comes from the ‘exchange integral’ Eq. (36)), we can write these down by requiring antisymmetry. These are constructed in precise analogy to the case of no spin-orbit ($\gamma = 0$), with the change of sign characterizing the antisymmetry appearing in one of two factors, according to the quantum number I

$$\Phi_{IM} = \frac{1}{2} (\Psi_A(1)\Psi_B(2) e^{i(\gamma/2)(S_{1z} - S_{2z})} + (-1)^I \Psi_A(2)\Psi_B(1) e^{-i(\gamma/2)(S_{1z} - S_{2z})}) \zeta_{IM} \quad (37)$$

Here ζ_{IM} are the usual spin eigenfunctions of the two-particle system, i.e., the triplets ($I = 1, M = -1, 0, 1$), and the singlet ($I = 0, M = 0$). Our last task is to understand what effective two-spin Hamiltonian will produce such states as eigenstates. To understand how this works, I show the singlet case of these states in a more explicit notation, in which the spin operators have been applied to the state

$$\Phi_{00} = \frac{1}{2} \left(\Psi_A(1)\Psi_B(2) (e^{i\gamma/2} | \uparrow_1 \downarrow_2 \rangle - e^{-i\gamma/2} | \downarrow_1 \uparrow_2 \rangle) + \Psi_A(2)\Psi_B(1) (e^{-i\gamma/2} | \uparrow_1 \downarrow_2 \rangle - e^{i\gamma/2} | \downarrow_1 \uparrow_2 \rangle) \right). \quad (38)$$

Note this does not factorize into a spin part and a space part, but the total is clearly antisymmetric with respect to $1 \leftrightarrow 2$.

We will take a next step that will give us an effective wavefunction for the spins alone. It is based on the following premise: we suppose that the A and B orbitals are disjoint in space (clearly

not exactly true in reality, since they have a finite inner product Ω), and that the wavefunction has no double-occupancy character. Then we see that the first term of wavefunction Eq. (38) is only nonzero if electron 1 is in the A quantum dot, and electron 2 is in the B quantum dot. Then, the spin state associated with this first term is

$$\Psi_{spin} = e^{i\gamma/2} |\uparrow_A \downarrow_B\rangle - e^{-i\gamma/2} |\downarrow_A \uparrow_B\rangle. \quad (39)$$

Note the crucial change of labeling $1, 2 \rightarrow A, B$ motivated by our argument. If we apply the same reasoning to the second term of Eq. (38), noting that it is only nonzero if electron 1 is in the B quantum dot, and electron 2 is in the A quantum dot (note the reversal from above). We then transcribe the spin wavefunction of this term as

$$e^{-i\gamma/2} |\uparrow_B \downarrow_A\rangle - e^{i\gamma/2} |\downarrow_B \uparrow_A\rangle, \quad (40)$$

which is in fact exactly the same (after rearranging) as Ψ_{spin} . The same observations go through for the triplet states. This encourages us to look for an effective Hamiltonian with only spin operators which has Eq. (39) as an eigenstate. The answer is

$$H_{spin} = \exp\left(i\frac{\gamma}{2}(S_{Az} - S_{Bz})\right) \mathbf{S}_A \cdot \mathbf{S}_B \exp\left(-i\frac{\gamma}{2}(S_{Az} - S_{Bz})\right) = \mathbf{S}'_A \cdot \mathbf{S}'_B. \quad (41)$$

So this is a kind of Heisenberg exchange, except that the coordinate system has been rotated, so there are two different frames of reference used at the A site and the B site. Let me comment that the line of argument just given is basically a switchover from first-quantized to second-quantized thinking, since it changed from “which electron is where?” to “where are the electrons?”. It has the limitation that it is only proper if the A and B orbitals are orthogonal; I note that Eq. (41) is not even Hermitian if A and B are non-orthogonal.

Finally, I mention Kavokin’s calculations for the size of this effect. He estimates:

1. quantum dots in GaAs, 10 nm heterostructure: $\gamma \approx 0.1$
2. shallow donors, bulk GaAs: $\gamma \approx 0.01$
3. donors near oxide interface in Si: $\gamma \approx 0.03$

This just serves to illustrate that this is not necessarily a very small effect.

4 A few thoughts about electron-electron interaction for spin qubits

I will here briefly discuss the electronic structure of the double quantum dot from another angle. We have taken into account electron-electron interaction in the calculation done above. More generally, how do interaction effects enter the electron problem for the quantum dot? Is there a basically one-electron picture that is close to the truth?

For this I explain some of the insights of [5]. In this work we retreat from the problem of spin-orbit interaction, considering only the electronic structure of few-electron dots in the non-relativistic limit.

Let me review some of the most basic facts about multi-electron eigenstates. I will state the facts in both first- and second-quantization.

If there are no e-e interactions, then eigenstates are single spin-orbital Slater determinants.

Not to be confused with the spin-orbit interaction, spin-orbital functions are single-electron functions of both space and spin. In the nonrelativistic case there will be functions like the kind we have seen above, single products like $\Psi_{A\sigma} = \Psi_A(1)\chi_1$. (If we were doing spin-orbit coupling, these would be entangled spin and space functions.) Then a single Slater determinant of two electrons would have the form

$$\begin{vmatrix} \Psi_A(1)\chi_1 & \Psi_B(1)\chi'_1 \\ \Psi_A(2)\chi_2 & \Psi_B(2)\chi'_2 \end{vmatrix} \quad (42)$$

Here I use the convention that in a Slater determinant, the rows are indexed by electron number, and the columns are indexed by the distinct spin-orbital (which may involve a repetition of the spatial orbital). This seems to immediately contradict the observation that two electron systems have triplet eigenstates of the form

$$\begin{vmatrix} \Psi_A(1) & \Psi_B(1) \\ \Psi_A(2) & \Psi_B(2) \end{vmatrix} (|\uparrow_A\downarrow_B\rangle + |\downarrow_A\uparrow_B\rangle), \quad (43)$$

split off from the other triplets in the presence of a magnetic field. This appears to be, and indeed is, a sum of two spin-orbital Slater determinants. But there is no contradiction here, as this state is degenerate with the singlet state (even in a magnetic field), so each determinant is separately an eigenstate. It is only if we also insist that we have eigenstates that are labelled by total spin that superpositions become necessary.

Note that the equivalent statement in second quantization is that an eigenstate can be formed by applying, to the vacuum, two spin-orbital creation operators

$$a_{A\chi}^\dagger a_{B\chi'}^\dagger |0\rangle. \quad (44)$$

We will be considering two and four electron systems. We will not get further than the story of a single quantum dot. For this, the “vacuum” will be the filled valence band, and all calculations will be done at the level of the envelope function (“effective mass theory”). But the gigantic complication of many-electron theory is that the eigenstates are *not* single Slater determinants. But the Slater determinants form a complete, orthonormal basis for the many-electron Hilbert space. This means that the general form for these eigenstates is, using the second-quantized notation,

$$\sum_{i,j} c_{ij} a_i^\dagger a_j^\dagger |0\rangle. \quad (45)$$

Here the sums run over the orthogonal spin-orbitals i, j . The prime is a reminder that the $i = j$ term gives nothing, since $(a^\dagger)^2 = 0$.

In quantum chemistry the terms in Eq. (45) are called configurations, and using a set of basis functions like this is called the *configuration-interaction (CI) technique*. Convergence in this technique is difficult, the only useful calculations use a computer.

In [5] we have done a fairly large calculation for a harmonically confined quantum dot in a magnetic field, with two or four electrons. Here the number of single-particle eigenstates used is 50, meaning that the CI basis has $\binom{50}{2}$ or $\binom{50}{4}$ elements. Bases of these size were apparently necessary for good convergence.

We describe now a step which leads to a much more powerful starting basis. This is called the Natural Orbital (NO) method due to Löwdin.

Suppose we have chosen a spin sector to examine, e.g., the singlet; thus, we are left with just orbital determinants such as in Eq. (43). Löwdin's procedure involves first obtaining the first-order density matrix of the N -particle orbital wavefunction

$$\rho(\mathbf{r}', \mathbf{r}) = N \int d\mathbf{r}_2 \dots d\mathbf{r}_N \psi^*(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_N) \psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N). \quad (46)$$

He next notes that if there were no e-e interactions and the eigenstate was a single Slater determinant, the first-order density matrix would be given by a simple sum over the single-particle orbitals in that determinant

$$\rho(\mathbf{r}', \mathbf{r}) = \sum_{\alpha} \phi_{\alpha}^*(\mathbf{r}') \phi_{\alpha}(\mathbf{r}). \quad (47)$$

But very generally, as a symmetric, positive semi-definite function of \mathbf{r} and \mathbf{r}' , the first order density matrix has a spectral decomposition

$$\rho(\mathbf{r}', \mathbf{r}) = \sum_{\alpha} \rho_{\alpha} \phi_{(NO),\alpha}^*(\mathbf{r}') \phi_{(NO),\alpha}(\mathbf{r}). \quad (48)$$

This set of “natural orbitals” $\phi_{(NO)}$ is in general quite different from any approximate single particle orbital, and should provide a CI expansion that is more rapidly convergent. Note that the “NO occupation numbers” $\rho_{\alpha} \geq 0$, and obey the sum rule $\sum_{\alpha} \rho_{\alpha} = N$.

We find that a relatively small number of NOs (i.e., somewhat larger than N) capture most of the weight of Eq. (48). So, if we had been lucky enough to be given (say by some wizard Merlin) these NO functions, we could have done a very compact CI expansion with good convergence on the full many-body answer.

Our calculation in [5] is for a harmonically confined quantum dot for GaAs (in the sense of using the effective mass of the conduction band) in a heterostructure-confined structure, so it is a 2D calculation. A large CI basis is used for convergence. We do calculations for two electrons and for four electrons, fixing the spin state to be singlet and then triplet, as in Eq. (43). For the two electron case there is nothing more to be said about the spin state, but for four electrons there are several alternatives for making these spin states. We do it in shell-style, where the lowest two orbitals are “paired” (that is, in their own singlet), while the highest occupied orbitals have the freedom to be singlet or triplet.

Figure 1 just shows the Hartree-Fock one-particle spectrum for this dot, indicating the range of magnetic field of interest. The quantum numbers are those of the so-called “Fock-Darwin”

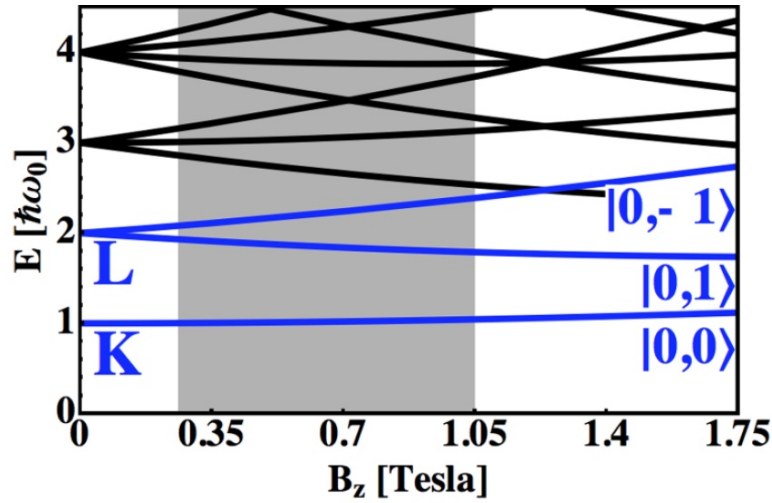


Fig. 1: Single-particle energy levels of the quantum dot, in the Hartree-Fock approximation.

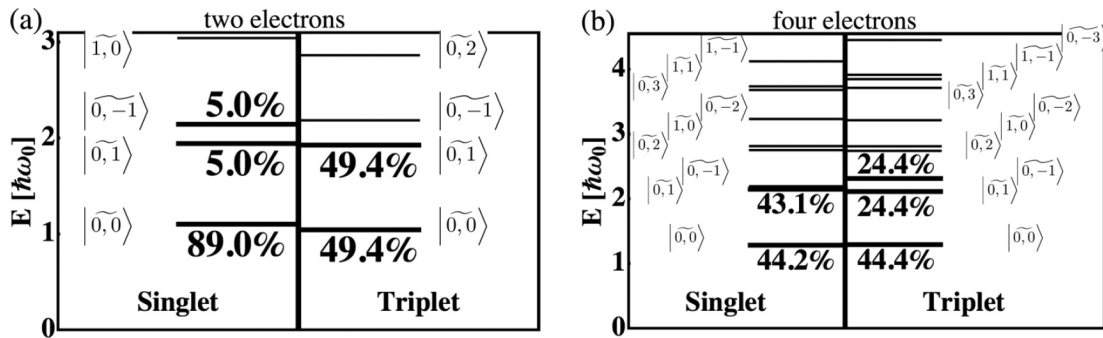


Fig. 2: Weights of natural orbitals for the four settings considered here.

states. In all four cases, the full CI calculation is done, and then the natural orbitals are extracted from the first-order density matrix as above. These give new orbitals which are indicated by a tilde; they can still be put in one-to-one correspondence with the Hartree-Fock orbitals. Figure 2 shows the results for these four cases. It shows percentages, we can multiply by the electron number N to talk about the number of electrons in different orbitals. The $N = 2$ singlet case shows that $2 \times 0.89 = 1.98$ of the electron weight is in the lowest orbital, doubled since both spin states can be occupied. In the $N = 2$ triplet case, 0.988 electrons are in each of the two first orbitals, as expected from the Pauli exclusion principle. The quality of the $N = 4$ case is only a bit less ideal: in the singlet case $4 \times 0.442 = 1.768$ electrons are a singlet in the first “shell”, with the second shell with 1.762 occupancy. This leaves 0.47 of an electron “unaccounted for”, in the sense that multiple Slater determinants are necessary to capture the effect of this much of the weight in the many-electron wavefunction. Finally, the story is similar for the $N = 4$ triplet: 1.776 electrons are in the core singlet, and 0.97 electrons each in the two next orbitals. 0.284 is “unaccounted for”. It is understandable that the single Slater determinant is a little better for the triplet cases, since the antisymmetric orbital wavefunction does a better job of keeping the electrons out of each other’s way and avoiding effects due to the Coulomb interaction.

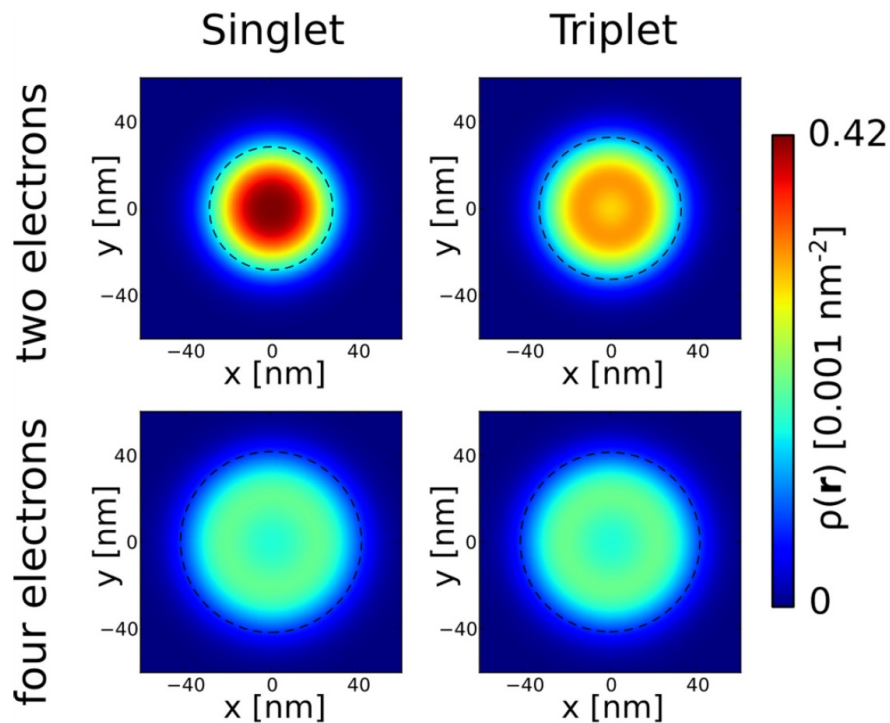


Fig. 3: Charge density of the four quantum-dot settings considered here, with full interaction effects.

Finally, this numerical study uncovered an important fact about the natural orbitals: to very good approximation, they are just the non-interacting Fock-Darwin orbitals with a simple rescaling of the radial coordinate. The natural orbital is in almost all cases blown-up compared with the Hartree-Fock orbitals – interactions push the electrons away from the center. This expansion is about 40% for the lowest-energy orbital, and is about half that for the next orbitals that participate in the $N = 2, 4$ states discussed above.

A concluding word about this study is that interaction effects are not so overwhelming, causing a definite renormalization of the Hartree-Fock picture but leaving it qualitatively intact. This is somewhat at odds with the general experience that very low-density electron systems have the largest departures from single electron physics (think of the Wigner crystal). But fortunately for our quantum-dot qubits, the mental picture of single-electron physics is shown to work quite well.

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