# Gate-induced ionization of single dopant atoms

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Gate-induced wave function manipulation of a single dopant atom is a possible basis of atomic scale electronics. From this perspective, we analyzed the effect of a small nearby gate on a single dopant atom in a semiconductor up to field ionization. The dopant is modeled as a hydrogenlike impurity and the Schrödinger equation is solved by a variational method. We find that—depending on the separation of the dopant and the gate—the electron transfer is either gradual or abrupt, defining two distinctive regimes for the gate-induced ionization process.

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The size regime where the discreteness of doping must be taken into account is brought within experimental reach by today's semiconductor lithography techniques. In this regime, single dopant atoms have been demonstrated to dominate the behavior of downscaled versions of conventional devices.[1] On the other hand, the promising opportunity is offered to study the physics of semiconductors on their ultimate length scale by addressing separate dopants. Putting a small gate close to a single impurity would, for example, allow for the manipulation of *individual* hydrogenlike wave functions. Furthermore, large electric fields (otherwise only achievable in astronomy) can be experimentally obtained in semiconductors due to the occurrence of large dielectric constants and small effective masses. Apart from the fundamental importance, an ultimate application is found in a Si-based solid state quantum computer,[2,3] in which the nuclear spins of single $^{31}$P dopants are envisioned as qubits. In this proposal, addressing a single qubit by nuclear magnetic resonance is achieved via the hyperfine interaction of the nuclear spin and its valence electron, which can be tuned by modifying the electron wave function with a nearby gate. In a recent variation of this design,[4] the ionization of single dopants by this gate is an essential ingredient.

Our aim is to quantitatively investigate the effect of the electric field generated by a local gate on a single neutral dopant atom in a semiconductor, ultimately leading to ionization. The response to small fields has been addressed before in the context of quantum computing.[5,6] In this paper, the complete ionization process is discussed. Our approach incorporates the computation of time independent ground state wave functions of the system and, subsequently, the estimation of transition probabilities. We conclude that the separation of the dopant and the gate determines the nature of the ionization process. When the dopant resides close to the gate, the electron is gradually pulled away from the dopant when the gate voltage is increased, while for a larger separation the dopant ionizes abruptly at a well-defined gate voltage.

Addressing a single dopant requires a small local gate. When a dopant would be ionized by a large gate (e.g., an infinite strip[6]), the electron would be delocalized along the gate. This would be undesirable in applications where (spin-)phase coherence must be kept under control, such as a quantum computer. Therefore, we chose to model the gate as a circular disc, having the additional advantage that the complete system (dopant plus gate) is radially symmetric. The layout of our model system is schematically depicted in the inset of Fig. 1. The disc-shaped metallic gate with radius $r_A$ is separated from the semiconductor bulk (relative dielectric constant $\varepsilon_s$) by a barrier (relative dielectric constant $\varepsilon_b$) of thickness $d_{\mathrm{bar}}$. A dopant is positioned at distance $d$ from the barrier-semiconductor interface and centered with respect to the gate.

At low temperatures, the semiconductor can be considered as a dielectric, due to the absence of free charges. Charges at the barrier-semiconductor interfaces and in the barrier will be neglected. In our calculations, we assume the barrier to be infinitely high and infinitely thin ($d_{\mathrm{bar}}=0$), which allows us to take advantage of the fact that the potential due to a charged metallic disc in a uniform dielectric medium can be expressed in closed form[7] (we will demonstrate the applicability of our results to a realistic layout). The total potential was obtained by adding a Coulomb potential well due to a positive unit charge in the semiconductor. A cross section of the total electron potential for some typical parameters is shown in Fig. 1. Image charge effects at

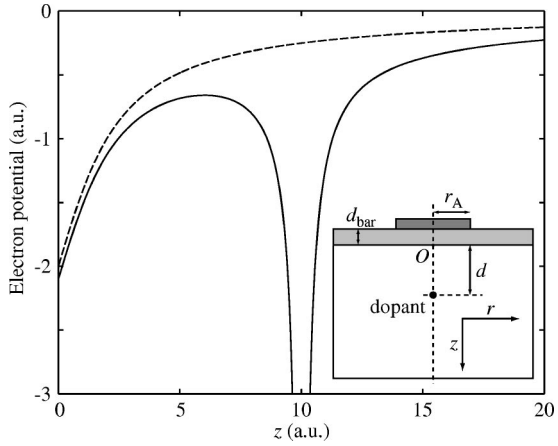


FIG. 1. The dashed line represents the calculated potential due to the gate at the symmetry axis of the device for $r_A=2$ a.u. and a gate voltage of 2 a.u. The solid line includes the dopant potential for $d=10$ a.u. (Note that, e.g., in silicon 1 a.u.$\approx$3 nm for lengths and 1 a.u.$\approx$90 mV for voltages.) The inset shows a schematic of the device layout, indicating the important parameters.

 

the semiconductor-barrier and the barrier-gate interfaces were neglected.

In our calculations, the dopant atom is described within an effective mass approach: the contribution of the semiconductor bandstructure is accounted for by considering it as an uniform dielectric medium and using an isotropic effective mass. Such a hydrogenlike model is known to provide a good first order description of a dopant atom (although it fails to accurately describe the energy levels[8] and interactions[9]). It is sufficient for our purpose and allows us to capture crucial phenomena and obtain estimates of important parameters. To keep our results general and transparent, physical quantities will be expressed in (effective) atomic units (a.u.). To simplify the conversion to conventional units, some values for silicon are given as an example in the caption of Fig. 1.

The time-independent Hamiltonian of the problem reads (in atomic units)

$$\mathcal{H}=-\frac{1}{2}\nabla^2-\frac{1}{\sqrt{r^2+(z-d)^2}}+V_g(r,z),$$

where $V_g(r,z)$ describes the potential landscape in the semiconductor due to the gate and $(r,z)$ are cylinder coordinates as defined in Fig. 1 (inset). Approximate ground state wave functions are found by a variational method. As trial wave function we use a linear combination of functions from a fixed and finite set $\mathcal{S}$, where the weights are used as variational parameters. To this end, we choose $\mathcal{S}$ to contain functions of the form

$$\varphi(r,z)=\exp(-\alpha r^2)z\exp[-\beta(z-d)^2] \tag{1}$$

and

$$\tilde{\varphi}(r,z)=\exp(-\gamma r^2)z\exp(-\delta z^2), \tag{2}$$

where $\alpha$, $\beta$, $\gamma$, and $\delta$ are constants that will be chosen later. The functions are cylinder symmetric, motivated by the radial symmetry of the potential and the fact that the ground state is expected to be *s*-like. To allow for a full description of the ionization process, it is important that $\mathcal{S}$ includes both wave functions of the form (1), having large electron density at the dopant site, and of the form (2), where the electron resides close to the gate.

The functional form of Eq. (1) is motivated by the fact that the (exponential) ground state wave function of hydrogenlike atoms can be quite well approximated as a linear combination of Gaussians,[11] which are much easier to work with numerically. To make sure that the wave functions vanish at the interface $(z=0)$, it is multiplied by $z$. The $\varphi(r,z)$ are allowed to become aspherical due to the gate action by choosing different values for $\alpha$ and $\beta$. Concerning the form of Eq. (2), we note that the potential well caused by the gate can in the radial direction be approximated by a parabola. Consequently, a ground state wave function similar to that of a linear harmonic oscillator is expected and therefore the $r$-dependent part of $\tilde{\varphi}(r,z)$ is chosen as a Gaussian. The ground state wave function of the triangular shaped well in the $z$ direction can be approximated as $ze^{-\zeta z}$ (Ref. 12). Again, we will approximate the exponential by a linear combination of Gaussians.

In order to choose concrete values for the constants $\alpha$, $\beta$, $\gamma$, and $\delta$, we note that for each positive integer $N$ it is possible to find a set of $N$ real numbers $\{\lambda_i\}_{i=1}^{N}$, such that a linear combination of $\exp(-\lambda_i r^2)$ optimally approximates the ground state wave function of hydrogen.[11] We will use the values given in Ref. 10, which are, for example, $\{0.101,0.321,1.15,5.06,33.6\}$ for $N=5$. In our calculation, we created functions of type (1) by taking values for $\alpha$ and $\beta$ from such a set in all possible $N^2$ combinations. Functions of type (2) were created by choosing values for $\gamma$ and $\delta$ from the same set, after multiplying all elements by the scaling constant $r_A^{-1/2}$ to account for the size of the gate. Proceeding like this, $\mathcal{S}$ contains a total of $2N^2$ functions. It was found that taking $N>5$ hardly improved the accuracy. Therefore, $N=5$ was used in all presented results.

Denoting the elements of $\mathcal{S}$ by $\psi_n$, the variational procedure is now performed by forming the trial wave function

$$\psi(r,z)=\sum_{\psi_n\in\mathcal{S}} c_n\psi_n(r,z)$$

as a linear combination of the $\psi_n$ and minimizing the functional

$$\frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

with respect to the variational parameters $c_n$. This minimum is an upper bound to the ground state energy of $\mathcal{H}$. This variational problem is equivalent to finding the smallest eigenvalue of the generalized matrix eigenvalue problem

$$(\mathbf{H}-E\mathbf{M})\cdot\mathbf{c}=0, \tag{3}$$

where $\mathbf{H}$ is the Hamiltonian matrix expanded on the $\psi_n$ with elements $H_{ij}=\langle\psi_i|\mathcal{H}|\psi_j\rangle$ and $\mathbf{M}$ is the overlap matrix of the $\psi_n$ defined as $M_{ij}=\langle\psi_i|\psi_j\rangle$. Furthermore, $\mathbf{c}=(c_1,c_2,\ldots,c_m)$ and the inner product $\langle\cdot|\cdot\rangle$ is (as usual) defined as

$$\langle\psi_i|\psi_j\rangle=\int_0^\infty\int_0^\infty\psi_i^*(r,z)\psi_j(r,z)2\pi r\,dr\,dz.$$

Note that $\mathbf{M}$ would be the unit matrix if $\mathcal{S}$ would be an orthonormal set with respect to $\langle\cdot|\cdot\rangle$. In that case, Eq. (3) would reduce to an ordinary eigenvalue problem.

The smallest eigenvalue $E_0$ of Eq. (3) is an upper bound to the ground state energy of the system. When $\mathcal{S}$ is chosen properly, $E_0$ is a good approximation to the real ground state energy of $\mathcal{H}$ and the corresponding eigenvector $\mathbf{c}$ defines a wave function that is a good approximation of the real ground state wave function.

Once this wave function is known for several values of the dopant depth $d$, gate voltage $V_g$, and gate radius $r_A$, we will use it to study the ionization process of the dopant. As an example, the radially integrated probability density of the calculated electron wave function (i.e., $\int_0^\infty|\psi(r,z)|^2 2\pi r\,dr$)

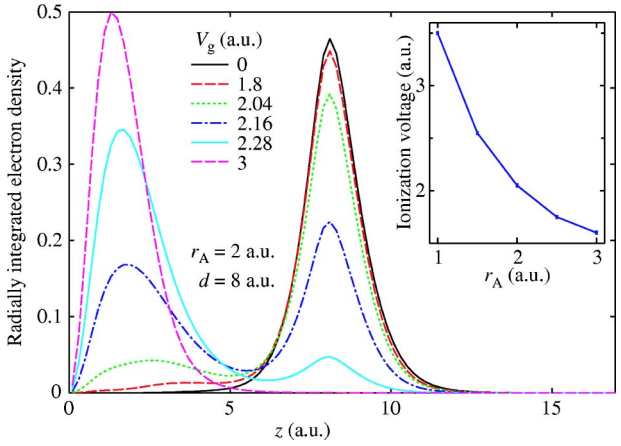


FIG. 2. (Color online) The radially integrated probability density of the electron wave function as a function of $z$ for various gate voltages. The inset shows the ionization voltage versus gate radius $r_A$. (In silicon: 1 a.u.≈3 nm and 90 mV, respectively.)

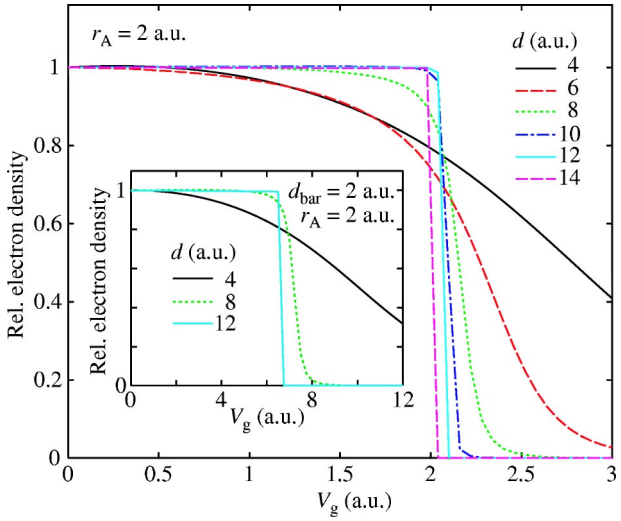


FIG. 3. (Color online) The electron density at the dopant site as a function of gate voltage for various dopant depths, showing the process of ionization. All curves are normalized to their value at $V_g=0$. The transition from a smooth to a steplike behavior is clearly visible at $d\approx 8a_0^*$. The inset shows the corresponding data with a 2 a.u. thick oxide barrier present. The behavior is similar, but occurs at higher gate voltage.

is plotted versus $z$ in Fig. 2. At zero gate voltage, the electron occupies the dopant site.[13] For increasing gate voltage, the electron is gradually pulled away from the donor site. Finally, for large enough gate voltage, it resides completely in the newly created potential well at the gate.

An interesting physical quantity is the electron density $|\psi_0(0,d)|^2$ at the dopant site, as derived from the approximated ground state wave function $\psi_0(r,z)$. We will use it as an indication of the position of the electron: when the electron is pulled away from the dopant site, this number decreases. Moreover, it is of physical importance because the hyperfine interaction is proportional to this number.[14]

The characteristics of the electron transfer from the dopant to the gate with increasing gate voltage depend on the distance $d$ of the dopant under the gate. In Fig. 3, the electron density at the dopant site $|\psi_0(0,d)|^2$ (normalized to the value at zero gate voltage) is plotted as a function of gate voltage for several values of $d$. It can be seen that for small $d$ the electron is transferred gradually from the dopant to the gate, while for larger $d$ an abrupt electron jump occurs, defining an ionization voltage. This can be explained from the fact that for large $d$, a sufficiently large barrier separates the two potential wells. For small $d$, the two wells are so strongly coupled that they can be considered as a single well, the position of which is pulled towards the gate with increasing gate voltage.

The calculations were repeated for several gate radii $r_A$. The inset of Fig. 2 shows the ionization voltage for $d=15$ versus $r_A$. From the figure it is clear that the voltage gets smaller for larger $r_A$. The reason for this is that the transfer roughly takes place when the ground state energy of the gate well drops below that of the dopant well. When the gate well is larger, the ground state energy is closer to the bottom of the well and the transfer takes place at lower gate voltage.

In a realistic device, the barrier between the gate and the semiconductor will have a finite thickness (in the most common material systems this will be at least 1 to 2 a.u.). Usually, this barrier does not have the same dielectric constant as the semiconductor and hence it can modify the gate potential considerably. Moreover, the gate must be connected to the outside world by some kind of interconnect. Such an interconnect must be separated from the semiconductor by a much thicker barrier in order to sufficiently screen its potential.[15] Therefore, in a realistic device, the gate must be buried in a thick layer of barrier material.

To allow for comparison with the idealized situation in which our calculations were carried out, several calculations were repeated with a realistic barrier present. To that end, we obtained the potential landscape due to the gate by solving the Poisson equation with a finite element method (FEM).[16] It was found that for typical realistic parameters (e.g., a $SiO_2$ Si system with $\varepsilon_s=12$, $\varepsilon_b=4$, and $d_{\mathrm{bar}}=2$ a.u.), the potential landscape in the semiconductor is qualitatively similar to the situation where the gate is put directly on the semiconductor. As demonstrated in the inset of Fig. 3, the same phenomena are observed, but they occur at a higher voltage than in the absence of a barrier. The voltage drop over the barrier can roughly be accounted for by a linear scaling factor that depends on $\varepsilon_b$ and $d_{\mathrm{bar}}$. Indeed, we find from the FEM calculations that for the given parameters about 31% of the gate voltage drops in the semiconductor. This number is similar to the observed ratio between the ionization voltages with and without a finite barrier thickness. This justifies the presentation of mainly results obtained with an idealized barrier.

As a final remark in our discussion of the barrier, we note that for any application or measurement of a single dopant device, it is crucial that there are no charge traps present near the dopant. Therefore it is highly desirable to have the barrier epitaxially grown on the semiconductor. A promising candidate is a $Si_{1-x}Ge_x$ layer as barrier on a Si substrate,[3] although the maximum achievable barrier height in this system is only about 100 meV.[17]

The presented time-independent calculations are not suf-

ficient to predict whether the dopant atom will indeed be ionized when the ground state wave function has a low electron density at the dopant site. In order to complete our analysis, an estimate of the tunnel probability is needed. This is obtained by comparison with the resonance lifetime of a hydrogen atom in an electric field. The typical field strengths considered in the region between the gate and the dopant site are very large (e.g., 0.05–0.5 a.u. for $r_A=2$, $d=10$, $V_g=2$, see Fig. 1). Using a calculation of the Stark effect in hydrogen[18] while taking the value of Ry* for silicon, it is found that the electron lifetime at the dopant site ranges roughly from 0.1 ps to 1 ns. This can be interpreted as the time it takes for the dopant to be ionized when the gate voltage is switched on and justifies our interpretation of Fig. 3 as the representation of an ionization process.

Our general analysis can be readily applied, as we performed the calculations with parameters that are consistent with the quantum computer design mentioned. First, controlled tuning of the hyperfine interaction by the gate, which is required in Ref. 2, is possible only when $d$ is small enough: from Fig. 3 we estimate $d \lesssim 6$ a.u. Switching off the hyperfine interaction, as required in the "digital approach,"[4] can only be achieved for large separation between dopant and gate ($d \gtrsim 10$ a.u.). Hence, the dimensions of the device determine in which of both regimes operation takes place. Second, our analysis can be used to estimate the required gate voltage to tune the hyperfine interaction to a certain value (Fig. 3). Third, it is found that the required voltage to fully ionize the dopant depends on $r_A$, but it is nearly independent of $d$ (Fig. 3).

In conclusion, we analyzed the wave function manipulation of a semiconductor dopant atom by a small electrostatic gate. We find that two regimes can be distinguished for the ionization process of the dopant. For a dopant-gate separation smaller than $\sim 8a_0^*$ (e.g., $\sim 24$ nm for P in Si), the electron is gradually pulled out of the Coulomb potential of the dopant. When the dopant resides further away from the gate, the transfer takes place abruptly at a well-defined threshold field. Both regimes are accessible, since, e.g., epitaxial growth techniques allow for sufficiently accurate positioning of the dopant under the gate.

*Note added in proof.* We learned that similar results have been obtained independently with different methods by A.S. Martins *et al.*[19] and L.M. Kettle *et al.*[20]

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