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Citation (APA)
Ventura Meinersen, C., Valvo, E., Bosco, S., & Rimbach-Russ, M. (2026). Multilevel spectral navigation with geometric diabatic-adiabatic control. *Physical Review Research*, *8*(3), Article L032034. https://doi.org/10.1103/hfv7-3pxt

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Letter

Multilevel spectral navigation with geometric diabatic-adiabatic control

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(Received 18 March 2026; accepted 14 July 2026; published 28 August 2026)

We introduce a geometric framework for efficient few-parameter pulse optimization in multilevel quantum systems, enabling high-fidelity state transfer beyond the adiabatic limit. Our method interpolates smoothly between adiabatic and diabatic dynamics to minimize unwanted excitations and maximize desired transitions even within a multilevel structure. Crucially, for single-parameter pulse control, the optimization reduces to solving a first-order ordinary differential equation. We showcase the flexibility of our diabatic-adiabatic protocols through two examples in spin-based quantum information processing: state initialization and qubit state transfer.

DOI: 10.1103/hfv7-3pxt

Introduction. A universal challenge for the control of any multilevel quantum system is the efficient navigation of quantum states through complex parameter space landscapes [1]. Dense spectra occur in various material platforms from superconducting circuits [2,3], trapped ions [4], photonic circuits [5], and many more [6–10]. A wide range of approaches have been developed to improve performance and control. These include mathematical control theory [11–20], implementing advanced numerical methods [21–25], spectral approaches [26–29], and employing techniques designed to accelerate adiabatic processes, dubbed shortcut to adiabaticity [30–59].

An approach to gain operational performance with enhanced interpretability exploits the geometry of quantum dynamics, as those based on geometric space curves [60–63] and the quantum metric tensor [64–66]. A key requirement to efficiently manipulating quantum states is to perform targeted excitations, beyond the adiabatic limit with minimal overhead. Employing piecewise-constant sudden-switch methods, which locally approximate the energy spectrum by a two-level Landau-Zener model, one can engineer transitions at the cost of a discontinuous pulse [67,68]. With the rise of larger quantum systems, there is a need to find a framework that smoothly interpolates between adiabatic and diabatic dynamics during the time evolution, to allow for experimental feasibility with finite bandwidth, without requiring approximations or constraints to the energy spectrum.

In this Letter, we present a versatile approach to perform efficient single-parameter pulse shaping of experimentally accessible parameters of the system's Hamiltonian, making it ideal for any multilevel quantum system. The single-parameter pulse shaping efficiency is granted because the resulting optimization task maps to a simple first-order ordinary differential equation. Our resulting framework provides various diabatic-adiabatic (di-ad) protocols (see Fig. 1), which are described by a continuous family of Riemannian geometries. The di-ad protocols allow for enhanced experimental flexibility, as one can adjust the pulse smoothness to the experimental hardware constraints by continuously deforming the resulting Riemannian geometry to one that is experimentally achievable. Henceforth, our di-ad protocol presents a geometric framework for high-fidelity quantum state transfer of adiabatic and diabatic evolution that requires only experimentally accessible control parameters.

We illustrate the applicability of the di-ad protocol by studying two exemplary open problems in spin-based quantum information processing: quantum state initialization and quantum state shuttling.

Optimal control with di-ad tensor. The task of quantum information transfer can be stated as a dynamical problem, where a given initial state $|\psi(0)\rangle$ is mapped to a target state $|\psi_{\text{target}}\rangle = |\psi(t_f)\rangle$, with t_f being the pulse time, via engineered time evolution. Here, we resort to a geometric formulation using the quantum metric tensor [64–66], where the above task is framed as the geodesic evolution on the space of experimentally accessible parameters. Given a set of control parameters x^μ of the system Hamiltonian $\hat{H}[x^\mu]$, we want to map an initial state $|\psi(0)\rangle = |\psi[x^\mu(0)]\rangle$ to the final target state $|\psi_{\text{target}}\rangle = |\psi[x^\mu(t_f)]\rangle$ through the geodesic evolution of $x^\mu(\tau)$, where $\tau = t/t_f$ is the rescaled time parameter. The infinitesimal state overlap of the evolved state can be expressed by the quantum metric tensor $g_{\mu\nu}(x)$ [66]:

$$1 - |\langle\psi(x)|\psi(x+dx)\rangle|^2 \approx g_{\mu\nu}(x) dx^\mu dx^\nu. \tag{1}$$

In the eigenbasis of the Hamiltonian and in the adiabatic limit, the quantum metric tensor is related to the energy fluctuations [69]:

$$\sigma_E^2 = \langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2 = g_{\mu\nu}(x)\frac{dx^\mu}{d\tau}\frac{dx^\nu}{d\tau}, \tag{2}$$

where $g^{(m)}_{\mu\nu}$, with respect to a given state $|\psi_m\rangle$, can then be conveniently written in terms of the Hamiltonian $\hat{H}$, and its

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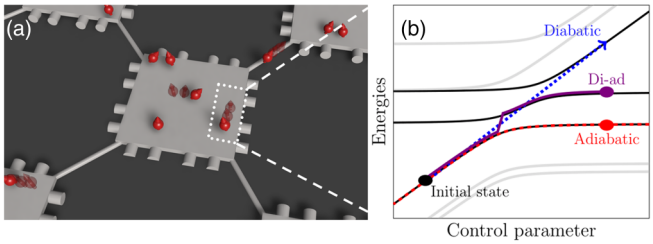


FIG. 1. Application of the di-ad protocol [panel (a)], here, spin qubit shuttling, and the emergent dense energy spectrum as a function of some control parameter [panel (b)]. The di-ad protocols allow for flexible and high-fidelity state transfer beyond the extrema of adiabatic (red, dashed) and diabatic (blue, dashed) limits by selectively operating between both regimes (purple).

eigenvalues and eigenvectors $\{E_n, |\psi_n\rangle\}$:

$$g_{\mu\nu}^{(m)} = \mathrm{Re}\sum_{n\neq m} \frac{\langle\psi_m|\partial_\mu \hat{H}|\psi_n\rangle\langle\psi_n|\partial_\nu \hat{H}|\psi_m\rangle}{(E_n - E_m)^2}, \tag{3}$$

where $\partial_\mu = \partial/\partial x^\mu$ is the derivative with respect to the parameters of the Hamiltonian. If we assume that the energy fluctuations are constant, we can minimize the infinitesimal state overlap by minimizing Eq. (2) [64]. Finding the control pulse that minimizes the energy fluctuations is equivalent to solving the geodesic equations. The quantum metric depends on two fundamental aspects of the control Hamiltonian: the overlap matrix elements of its gradients $\langle\psi_m|\partial_\mu \hat{H}|\psi_n\rangle$, with respect to the control parameter x^μ, and the corresponding energy splittings $(E_n - E_m)$ of the coupled eigenstates. Together, these factors determine the resulting pulse shape and the associated state-transfer infidelity. For adiabatic state transfer, this protocol achieves high fidelities [64], yet it is not well suited for diabatic evolution. Deducing from the adiabatic impulse approximation [70,71], we now locally maximize the components of the quantum metric to achieve diabatic state transfer [72]. Despite the nonperturbative nature of diabatic evolution, we make a phenomenological ansatz by defining a generalized quantum metric tensor

$$\begin{aligned}\mathcal{G}_{\text{di-ad}} &\equiv (\mathcal{G}_{\text{di-ad}})_{\mu\nu}^{(\alpha,\beta;\,\hat{\alpha},\hat{\beta})} \\ &= \mathcal{A}_{\mu\nu}^{(\alpha,\beta)} + \mathcal{D}_{\mu\nu}^{(\hat{\alpha},\hat{\beta})} \\ &= \sum_m \sum_{n\neq m} \left([1-\xi_{mn}]\,\mathcal{G}_{\mu\nu}^{nm,(\alpha,\beta)} + \xi_{mn}\,\mathcal{G}_{\mu\nu}^{nm,(\hat{\alpha},\hat{\beta})}\right),\end{aligned} \tag{4}$$

which we call the di-ad tensor. The di-ad tensor is comprised of an adiabatic component $\mathcal{A}$ and a potentially diabatic component $\mathcal{D}$. The individual components read identically, but may include different exponents,

$$\mathcal{G}_{\mu\nu}^{nm,(\alpha,\beta)} = \mathrm{Re}\frac{\langle\psi_m|\partial_\mu \hat{H}|\psi_n\rangle^{\beta/2}\langle\psi_n|\partial_\nu \hat{H}|\psi_m\rangle^{\beta/2}}{|E_n - E_m|^\alpha}, \tag{5}$$

and the components of the di-ad transition matrix $\xi_{mn} \in \{0, 1\}$ are defined in the eigenbasis of the Hamiltonian as

$$\xi_{mn} = \begin{cases} 0, & \text{adiabatic: } |\psi_m\rangle \to |\psi_m\rangle \text{ and } |\psi_m\rangle \not\to |\psi_n\rangle, \\ 1, & \text{diabatic: } |\psi_m\rangle \to |\psi_n\rangle. \end{cases} \tag{6}$$

Using the di-ad transition matrix ξ_{mn}, you only need to define the initial and final target states, even if there is not a direct adiabatic path between them. By summing over all possible transitions, we can achieve direct state transfer between any eigenstate without occupying any intermediate state. The parameters $(\alpha, \beta; \hat{\alpha}, \hat{\beta})$ determine the degree of adiabaticity and diabaticity, respectively, as we will now see. For sufficiently separated level crossings, one can approximate a two-level crossing by a local Landau-Zener model [73] $\hat{H}_{\text{LZ}}/x = z(t)/x\,\sigma_z + \sigma_x$, with control parameter $z(t)$; one finds that the di-ad tensor simplifies to

$$\mathcal{G}_{\text{di-ad}} = [1-\xi_{01}]\,\mathcal{G}_{zz}^{01,(\alpha,\beta)} + \xi_{01}\,\mathcal{G}_{zz}^{01,(\hat{\alpha},\hat{\beta})}, \tag{7}$$

where the di-ad transition matrix is now determined, whether we want to have adiabatic ($|\psi_0\rangle \mapsto |\psi_0\rangle$, $\xi_{01}{=}0$) or diabatic ($|\psi_0\rangle \mapsto |\psi_1\rangle$, $\xi_{01}{=}1$) evolution, respectively. The di-ad tensor for the Landau-Zener model can be computed analytically and reads $\mathcal{G}_{\text{di-ad}} \simeq (1 + z(t)/x)^{-n_+}$, where $n_+{=}(\alpha{+}\beta)/2$ ($n_+{=}(\hat{\alpha}{+}\hat{\beta})/2$) labels all the different adiabatic (diabatic) pulses. In this simple case, the di-ad tensors for both evolutions are identical and only depend on n_+. In more complex systems, each parameter $(\alpha, \beta; \hat{\alpha}, \hat{\beta})$ will provide a unique contribution. Using the di-ad tensor, we can extend the geometric-adiabatic condition in Eq. (2) by substituting the standard quantum metric tensor with the di-ad tensor $g_{\mu\nu} \mapsto \mathcal{G}_{\text{di-ad}}$. The pulse shape is then given by solving for the appropriate differential equation [72] labeled by n_+.

In Fig. 2, we illustrate the possible state-transfer protocols for the Landau-Zener problem and find that pulses with $n_+ > 0$ ($n_+ < 0$) are well suited for adiabatic (diabatic) evolution. Concretely, we plot as solid (dashed) lines the diabatic (adiabatic) evolution in terms of the energy diagram [Fig. 2(a)]; the di-ad metric [Fig. 2(c)] yields the corresponding pulse shapes [Fig. 2(b)] and infidelities [Fig. 2(d)].

The highest diabatic state-transfer ($|\psi_0\rangle \mapsto |\psi_1\rangle$) fidelities are acquired for $x\,t_f \to 0$ [72]. In essence, the resulting state-transfer fidelity can be maximized by maximizing the energy fluctuations around the smallest energy gap, which in our protocol corresponds to choosing $\hat{\alpha}, \hat{\beta} < 0$. In contrast, and also in light of the quantum metric tensor and Eq. (2), pulses with $\alpha, \beta > 0$ allow for possibly reduced energy uncertainty around the energy gap. Due to the flexibility of adjusting the adiabatic and diabatic parameters $(\alpha, \beta; \hat{\alpha}, \hat{\beta})$ simultaneously, we can not only allow for purely diabatic or adiabatic transfer protocols (by maximizing or minimizing the energy fluctuations), but also generate pulses that interpolate between these two, providing the ability to maintain adiabatic evolution for some level crossings while being diabatic for others.

Versatile state initialization. To demonstrate our protocol, we enhance the initialization of a semiconductor spin qubit [74] within a double quantum dot (DQD) using spin-to-charge conversion [75–84]. A common bottleneck for high-fidelity initialization is the emergence of small gaps caused by small Zeeman vector differences [84]. The di-ad tensor enables a combination of adiabatic and diabatic dynamics through the transition matrix ξ_{mn}. This flexibility enables us to develop state-transfer protocols tailored to versatile spin-to-charge conversion [85,86]. The spin-to-charge conversion inside a DQD system is well

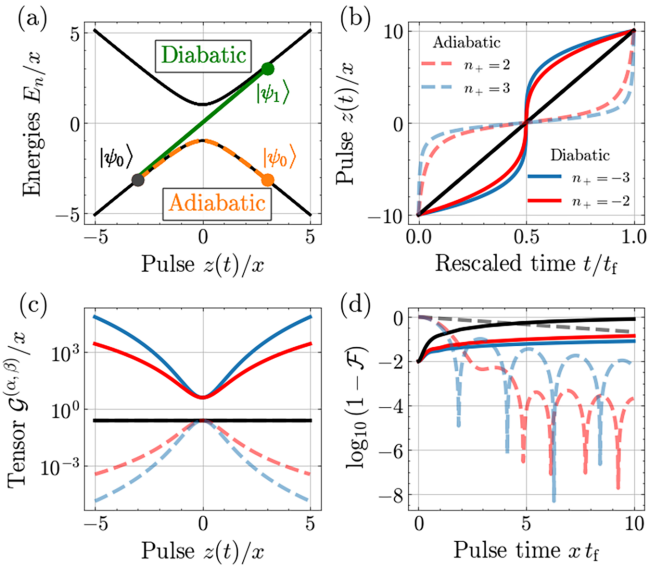


FIG. 2. Coherent state transfer for the adiabatic ($|\psi_0\rangle \mapsto |\psi_0\rangle$, dashed lines) and the diabatic ($|\psi_0\rangle \mapsto |\psi_1\rangle$, solid lines) evolution in the Landau-Zener model. We show the energy spectrum [panel (a)], the di-ad pulse [panel (b)], originating from the corresponding di-ad metric [panel (c)], and the resulting infidelities $1-\mathcal{F}$ [panel (d)] with $\mathcal{F}=|\langle\psi_0(t_f)|U(t_f)\psi_0(0)\rangle|^2$ for adiabatic and $\mathcal{F}=|\langle\psi_1(t_f)|U(t_f)\psi_0(0)\rangle|^2$ for diabatic evolution, where $U(t_f)$ describes the unitary evolution given the pulse $z(t)/x$. The Hamiltonian parameters used are $z(0)/x=-z(t_f)/x=-10$. The colored pulses refer to different n_+ with the appropriate sign for adiabatic (dashed) and diabatic (solid) protocols: $|n_+|=0,2,3$ corresponds to black, red, and blue, respectively.

described by an extended Fermi-Hubbard-Zeeman Hamiltonian [72]. Projecting the model to the relevant charge states $(n_L, n_R)=(2,0)$ and (1,1) with the associated spin basis states $\{|\uparrow\downarrow,\cdot\rangle, |\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$ results in the following matrix representation [86–88]:

$$\hat{H}_{\mathrm{DQD}} = \begin{pmatrix} \tilde{U}-\varepsilon(t) & 0 & -t_c & t_c & 0 \\ 0 & E_Z & \Delta E_X & -\Delta E_X & 0 \\ -t_c & \Delta E_X & \Delta E_Z & 0 & \Delta E_X \\ t_c & -\Delta E_X & 0 & -\Delta E_Z & -\Delta E_X \\ 0 & 0 & \Delta E_X & -\Delta E_X & -E_Z \end{pmatrix}. \tag{8}$$

Here, t_c is the tunnel coupling, and $E_a = E_{a,1} + E_{a,2}$ and $\Delta E_a = E_{a,1} - E_{a,2}$ are the total Zeeman energy and the Zeeman splitting difference (with $a = x, y, z$) arising from a spatially varying g factor [88–97] or a magnetic field gradient [98–100]. In addition, we define an effective Coulomb repulsion $\tilde{U}$ and the detuning $\varepsilon \in \mathbb{R}_{\geqslant 0}$ between the DQD chemical potentials. For spin-qubit initialization, we employ the spin-to-charge conversion method, which requires the pulse shaping of the detuning $\varepsilon(t)$ from a far-detuned position $\varepsilon(0) \gg |t_c|, |E_Z|$, where the ground state is given by two charges in one quantum dot (i.e., $|\uparrow\downarrow,\cdot\rangle$), to the symmetric point $\varepsilon(t_f)=0$, where we have transferred one charge to the other dot $(2,0)\to(1,1)$. Therefore, we initialize a computational state. Due to a finite spin-flipping term ΔE_X, which causes a small anticrossing between the ground and the first

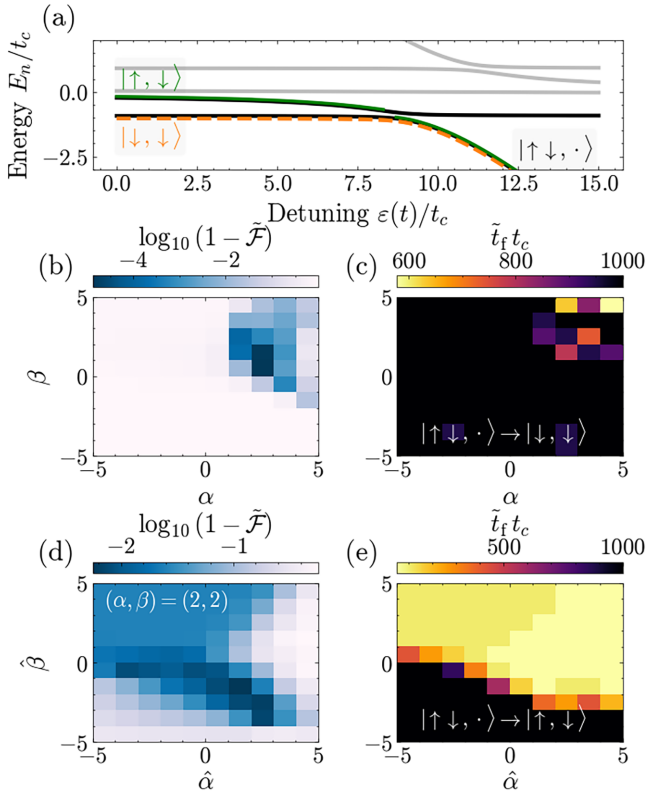


FIG. 3. Initialization of a spin qubit in a DQD. The energy spectrum is shown in panel (a). The optimal infidelity and corresponding pulse times for the adiabatic protocol ($|\uparrow\downarrow,\cdot\rangle \mapsto |\downarrow,\downarrow\rangle$) are illustrated in panels (b) and (c). Similarly, for the di-ad protocol ($|\uparrow\downarrow,\cdot\rangle \mapsto |\uparrow,\downarrow\rangle$), we showcase the infidelities and pulse times in panels (d) and (e). The DQD parameters read $\tilde{U}/t_c = 10$, $E_Z/t_c = 0.9$, $\Delta E_Z/t_c = 0.1$, $\Delta E_X/t_c = 0.01$, where we sweep the detuning $\varepsilon(0)/t_c = 15$ to $\varepsilon(t_f)/t_c = 0$. For the di-ad protocol, we fix the adiabatic parameters to $(\alpha,\beta)=(2,2)$. For the protocol, we sweep possible pulse times $t_f t_c \in [0, 1000]$.

excited state, a spin-flip event may occur during spin-to-charge conversion [see Fig. 3(a)]. We can make use of this hybridization to initialize two sets of computational states via our di-ad method. Starting from two charges in one dot, we have two initialization schemes, resulting in different parity sectors:

(1) Adiabatic evolution: $|\uparrow\downarrow,\cdot\rangle \mapsto |\downarrow,\downarrow\rangle$.
(2) Diabatic-adiabatic evolution: $|\uparrow\downarrow,\cdot\rangle \mapsto |\uparrow,\downarrow\rangle$.

For the diabatic-adiabatic case, we have the following di-ad transition matrix (in the eigenbasis of the Hamiltonian) that is fully determined by the initial and final states:

$$\xi_{mn}\big(|\uparrow\downarrow,\cdot\rangle \mapsto |\uparrow,\downarrow\rangle\big) = \begin{pmatrix} \cdot & 1 & 0 & 0 & 0 \\ 1 & \cdot & 0 & 0 & 0 \\ 0 & 0 & \cdot & 0 & 0 \\ 0 & 0 & 0 & \cdot & 0 \\ 0 & 0 & 0 & 0 & \cdot \end{pmatrix}. \tag{9}$$

The dots represent the excluded transitions. In Fig. 3, we simulate both initialization procedures, as shown in Fig. 3(a), and plot the minimum infidelity $1-\tilde{\mathcal{F}} \equiv 1-\mathcal{F}(\tilde{t}_f)$ [panels (b) and (d)] and the corresponding (rescaled) pulse time $\tilde{t}_f t_c$

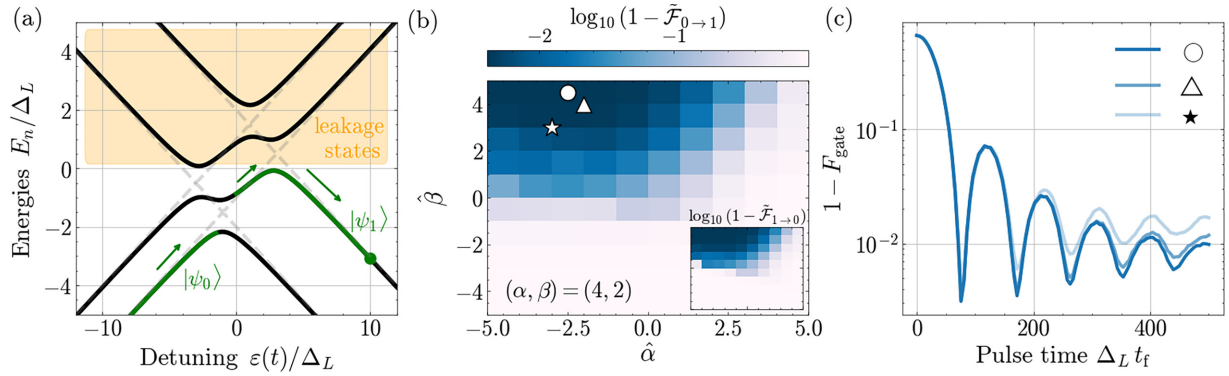


FIG. 4. On-the-go operations using coherent shuttling-induced excitations. The energy spectrum of the Hamiltonian (10), where we marked in orange the undesired leakage states, is plotted in panel (a). In addition, we plot the minimum infidelities $1-\tilde{\mathcal{F}}$ for the state transfers $|\psi_0\rangle \to |\psi_1\rangle$ [panel (b)] and $|\psi_1\rangle \to |\psi_0\rangle$ (inset), for possible pulse times $\Delta_L t_f \in [0, 500]$. Using the Horodecki identity, in panel (c), we analyze the effective X-gate average gate fidelity $F_{\text{gate}} = (1 + \sum_{j=0,1} |\langle\psi_j(0)|\psi_{1-j}(t_f)\rangle|^2)/3$ for the computational subspace spanned by the lower two eigenstates as a function of possible pulse times $\Delta_L t_f$ for the indicated circle, square, and star parameters in panel (b). The parameters used are $t_c/\Delta_L = 0.1$, $\Delta_R/\Delta_L = 5$, $\phi_L = 0.1$, $\phi_R = \pi/2$. The detuning is swept from $\varepsilon/\Delta_L \in [-10, 10]$.

[panels (c) and (e)]. For the purely adiabatic case [Figs. 3(b) and 3(c)], we only require sweeping the adiabatic parameters (α, β) as we aim to suppress excitations to any of the four possible excited states. For the diabatic-adiabatic initialization [Figs. 3(d), 3(e)], we fix the adiabatic parameters (α, β)=(2, 2) and sweep the diabatic ones $(\hat{\alpha}, \hat{\beta})$. Remarkably, both methods achieve fidelities exceeding 99% with short simulation times. Additionally, in the Supplemental Material [72], we consider the effects of charge and spin dephasing during the initialization processes. We can further enhance the efficiency of the di-ad protocol by using machine learning sampling methods to obtain the desired di-ad parameter configuration with even fewer infidelity simulations [72]. By allowing for the interpolation of diabatic and adiabatic dynamics, we unlock the ability to initialize different parity sectors, which, for instance, allows for flexible initial qubit configurations in a quantum circuit while reducing the circuit overhead for similar initial configurations or for analog simulation of many-body systems with limited individual qubit control [84,101].

Operations during shuttling. Another state-transfer protocol important for quantum information processing is shuttling [100,102–108], where the qubit is physically moved around the quantum chip to enable sparse quantum architectures to minimize crosstalk and provide opportunities to include classical electronics on chip [109–111]. Furthermore, optimized bucket brigade shuttling is necessary for the operation of sparse, single-barrier control spin-qubit architectures [112]. For silicon quantum dots, we can model the Hilbert space by a tensor product structure $\mathcal{H} = \mathcal{H}_{\text{orbital}} \otimes \mathcal{H}_{\text{valley}}$, whose Hamiltonian, after a unitary transformation, is given by [104,113]

$$\hat{H}_{\text{BB}} = \begin{pmatrix} \varepsilon(t) + |\Delta_L| & 0 & t_{ee} & t_{eg} \\ 0 & \varepsilon(t) - |\Delta_L| & t_{ge} & t_{gg} \\ t_{ee}^* & t_{ge}^* & |\Delta_R| & 0 \\ t_{eg}^* & t_{gg}^* & 0 & -|\Delta_R| \end{pmatrix}, \tag{10}$$

where, as before, the detuning is given by $\varepsilon(t)$ and will constitute our control parameter, $\Delta_{L,R} \in \mathbb{C}$ are the valley terms resulting in the valley splitting $E_{\text{VS}} = 2|\Delta|$, and the bare tunnel coupling t_c is modified by the valley phases $\phi_{L/R}$:

$$t_{ee} = t_{gg}^* = \frac{t_c}{2}(1 + e^{i(\phi_L - \phi_R)}), \tag{11}$$

$$t_{eg} = -t_{ge}^* = \frac{t_c}{2}(e^{i\phi_L} - e^{i\phi_R}). \tag{12}$$

We note that a similar Hamiltonian emerges in the shuttling of holes in germanium quantum dots by changing to a different Hilbert space decomposition, namely, $\mathcal{H} = \mathcal{H}_{\text{orbital}} \otimes \mathcal{H}_{\text{spin}}$ [114]. The two lowest-energy eigenstates of the Hamiltonian (10) will constitute our computational subspace as seen in Fig. 4(a). Using our di-ad tensor, we can perform two relevant operations; namely, while shuttling or hopping, we can excite the ground state to the first excited state, while suppressing leakage [see Fig. 4(b)], and we can also force the first excited state to relax to the ground state [see inset of Fig. 4(b)]. Both shuttling operations achieve state-transfer fidelities of 99%, alongside an average effective X-gate fidelity with similar performance [see Fig. 4(c)], demonstrating the flexibility, scalability, and relevance for current quantum information processing.

Conclusion. We developed a general method for optimal state transfer that is capable of minimizing undesired transitions, while allowing for targeted excitations to allow for full navigation of any multilevel energy landscape. The resulting time evolution is not restricted to purely adiabatic dynamics, but can smoothly interpolate between adiabatic and targeted diabatic dynamics. In addition, the single-parameter di-ad protocols are efficiently computable, as the optimization task reduces to a first-order differential equation. Furthermore, the inclusion of the parameters $(\alpha, \beta; \hat{\alpha}, \hat{\beta})$ enables consideration of hardware limitations by design, making it highly adaptable to current experimental constraints.

Acknowledgments. We thank David Fernandez-Fernandez, Kristof Moors, George Simion, Yuta Matsumoto, Sander de Snoo, and all members of the Rimbach-Russ and Bosco group for providing valuable insights. M.R.-R., S.B., E.V., and C.V.M. acknowledge that the EU partly supported this research through the H2024 QLSI2 project and it was partly

sponsored by the Army Research Office under Award No. W911NF-23-1-0110. M.R.-R. and E.V. acknowledge support from the Dutch Research Council (NWO) under Award No. Vidi TTW 22204.

C.V.M. and E.V. performed the theoretical computations and numerical simulations with inputs from M.R.-R. and S.B. C.V.M. wrote the manuscript with inputs from all the authors. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Office or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes, notwithstanding any copyright notation herein.

Data availability. The data that support the findings of this article are openly available [115].

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