

Geometric Phase through Spatial Potential Engineering

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We propose a spatial analog of the Berry's phase mechanism for the coherent manipulation of states of nonrelativistic massive particles moving in a two-dimensional landscape. In our construction the temporal modulation of the system Hamiltonian is replaced by a modulation of the confining potential along the transverse direction of the particle propagation. By properly tuning the model parameters the resulting scattering input-output relations exhibit a Wilczek-Zee non-Abelian phase shift contribution that is intrinsically geometrical, hence insensitive to the specific details of the potential landscape. A theoretical derivation of the effect is provided together with practical examples.

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In recent years a strong demand for developing quantum engineering [1–3] procedures has been fostered by the huge technological development requiring faster and more efficient circuits and transistors, but also by the first prototypes of quantum computers. As the main resource for quantum supremacy is ultimately embodied by the amount of quantum coherence one can store on a system, the ability to design control schemes that allow for its manipulation becomes of paramount importance [4]. A possibility in this direction is presented by applications of the non-Abelian generalization [5] of the Berry phase mechanism [6]. In these approaches [7–17] a target (state-independent) transformation is implemented by driving the system Hamiltonian along a closed path in the control parameter space either adiabatically, as in the original proposal [6], or nonadiabatically [18]. The resulting operation (typically referred to as *holonomy*) has an intrinsic geometrical character [19,20] that makes it resilient to local fluctuations [21,22], hence offering an attractive alternative to quantum error-correction techniques [23,24].

Inspired by the above approaches we present here a proposal for the coherent manipulation of a nonrelativistic massive particle A through holonomies obtained by properly engineering the potential landscape it experiences when traveling through a scattering region. Although the scheme can be in principle applied to arbitrary spatial configurations, we shall focus on 2D geometries (see Fig. 1) where desired potential profiles with a high degree of accuracy and low numbers of impurities can be easily achieved in semiconductor platforms, either by direct nanofabrication [25–29] or via external gate potential techniques. As a further simplification, the kinetic energy of the incoming particle will be taken to be the largest of the model. While not being essential, this assumption allows us to isolate in the solution of the Schrödinger equation the

geometric term (the holonomy) from an irrelevant dynamical phase.

Model.—Let A be a nonrelativistic particle of mass m , propagating in the xy plane, under the action of a scattering potential $V(\hat{x}, \hat{y})$, so that the resulting Hamiltonian is $\hat{H} := \hat{p}_x^2/2m + \hat{p}_y^2/2m + V(\hat{x}, \hat{y})$. As shown in Fig. 1, we assume A to enter the setup with assigned energy E corresponding to an input state that, far away from the scattering center in the negative y direction, is described by an impinging plane wave with assigned momentum $p_0 > 0$ which sets the largest energy scale in the system [i.e., $E_{\text{kin}} := p_0^2/(2m) \simeq E$]: adopting the scattering formalism, we analyze the dynamics of the particle by looking for solutions of the time-independent Schrödinger equation $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$ that are compatible with the chosen

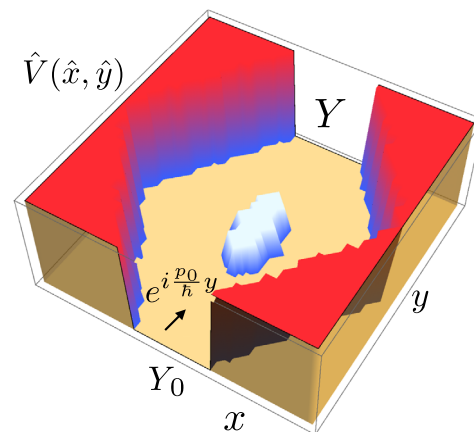


FIG. 1. Pictorial representation of a 2D potential landscape. As the particle A is moving forward along the longitudinal y axis, it sees a varying potential along the transverse axis x defined by the scattering potential $V(\hat{x}, \hat{y})$.

boundary conditions. Moving to a representation with respect to the y coordinate, we hence cast this equation in the form

$$-\frac{\hbar^2}{2m}\partial_y^2|\psi_E(y)\rangle + \hat{h}_y(\hat{x})|\psi_E(y)\rangle = E|\psi_E(y)\rangle, \quad (1)$$

with $|\psi_E(y)\rangle := \langle y|\psi_E\rangle$ being the transverse wave vector component for fixed longitudinal position ($|y\rangle$ being the eigenstate of the position operator \hat{y}). In Eq. (1) the self-adjoint operator $\hat{h}_y(\hat{x}) := \hat{p}_x^2/2m + V_y(\hat{x})$ is the transverse Hamiltonian, where $V_y(\hat{x}) := V(\hat{x}, y)$ is obtained by replacing in $V(\hat{x}, \hat{y})$ the operator \hat{y} with its eigenvalue y . Therefore, from now on y will be treated as a real variable, while \hat{x} is still an operator. Without loss of generality, in what follows we shall assume the parametric dependence upon y of $V_y(\hat{x})$ to be mediated via a collection of (real) *control* functions, which we represent collectively as components of the vector $\vec{R}_y := (R_y^{(1)}, R_y^{(2)}, \dots)$, i.e.,

$$V_y(\hat{x}) = V_0(\hat{x}; \vec{R}_y). \quad (2)$$

For the sake of simplicity, we shall then assume $\hat{h}_y(\hat{x})$ to have discrete spectrum, for instance, forcing the potential $V_y(\hat{x})$ to induce local transverse confinement for all values of y . Thus, for fixed y , we identify the eigenvectors of $\hat{h}_y(\hat{x})$ with the discrete orthonormal set $\{|\phi_y^{(\ell)}\rangle; \ell = 0, 1, 2, \dots\}$, the associated eigenvalues being the quantities $E_y^{(\ell)} := (\hbar^2/2m)\epsilon_y^{(\ell)}$, which we assume to be in increasing order with respect to the index ℓ . Decomposing hence $|\psi_E(y)\rangle$ as $|\psi_E(y)\rangle = \sum_{\ell} C_y^{(\ell)}|\phi_y^{(\ell)}\rangle$ with $C_y^{(\ell)}$ being complex amplitudes, and introducing the rescaled energy $\epsilon := (2m/\hbar^2)E$, without any approximations, as shown in Sec. II of Supplemental Material (SM) [30], we can recast Eq. (1) as

$$(\partial_y + K_y)^2 \mathbf{C}_y + (\epsilon - \Omega_y) \mathbf{C}_y = 0, \quad (3)$$

where \mathbf{C}_y is the column vector of components $(C_y^{(0)}, C_y^{(1)}, C_y^{(2)}, \dots)$ and Ω_y is a Hermitian matrix with elements $[\Omega_y]_{\ell\ell'} := \epsilon_y^{(\ell)}\delta_{\ell\ell'}, \delta_{\ell\ell'}$ being the Kronecker delta. In the above expression $K_y = -K_y^\dagger$ is a real anti-Hermitian matrix which ultimately triggers the coupling among the various components of \mathbf{C}_y with an intensity that scales with the inverse of the gaps of the associated local energies $E_y^{(\ell)}$, i.e.,

$$[K_y]_{\ell\ell'} = \langle \phi_y^{(\ell)} | \partial_y \phi_y^{(\ell')} \rangle = \frac{\langle \phi_y^{(\ell)} | (\partial_y V_y(\hat{x})) | \phi_y^{(\ell')} \rangle}{E_y^{(\ell')} - E_y^{(\ell)}} (1 - \delta_{\ell\ell'}); \quad (4)$$

see Secs. I and II of the SM for details [30]. As in Refs. [31–34], the presence of K_y can be thought as arising via

minimal coupling from a non-Abelian vector potential: accordingly it can be gauged away through the action of the unitary mapping induced by the path-ordered exponential $\mathcal{U}_{Y_0 \rightarrow y} := P \exp[-\int_{Y_0}^y K_{y'} dy']$, Y_0 being the longitudinal coordinate defining the beginning of the scattering region. Specifically, by setting $\mathbf{C}_y = \mathcal{U}_{Y_0 \rightarrow y} \tilde{\mathbf{C}}_y$ we can rewrite Eq. (3) as the following spinor 1D Schrödinger equation,

$$\partial_y^2 \tilde{\mathbf{C}}_y + (\epsilon - \tilde{\Omega}_y) \tilde{\mathbf{C}}_y = 0, \quad (5)$$

with $\tilde{\Omega}_y := \mathcal{U}_{Y_0 \rightarrow y}^\dagger \Omega_y \mathcal{U}_{Y_0 \rightarrow y}$ holding the same spectrum of Ω_y and playing the role of an effective potential. For sufficiently smooth potential modulations and assuming ϵ (hence the rescaled kinetic component of the incoming particle E_{kin}) to be the largest energy scale in the system, Eq. (5) admits solutions which, according to the Wentzel-Kramers-Brillouin (WKB) approximation method [35], read $\tilde{\mathbf{C}}_y = \mathcal{W}_y^{(+)} \mathbf{A} + \mathcal{W}_y^{(-)} \mathbf{B}$, with the vectors \mathbf{A}, \mathbf{B} being determined by the boundary conditions of the problem and with the matrices $\mathcal{W}_y^{(\pm)}$ describing, respectively, the left-to-right and right-to-left propagations of the particle in the sample; see Sec. III of the SM for details [30]. In particular, in the very large ϵ limit, i.e., $\epsilon \gg \epsilon_y^{(\ell)}$ for all y and for all the energy levels $\epsilon_y^{(\ell)}$ involved in the process, we can safely conclude that all $\epsilon_y^{(\ell)}$ will yield approximately the same phase whose leading contribution can be expressed as $\mathcal{W}_y^{(\pm)} \simeq e^{\pm i\sqrt{\epsilon}(y-Y_0)}$. In other words, $\mathcal{W}_y^{(\pm)}$ will explicitly depend upon the length of the integration domain, and as it will be clarified in the next section, contribute to the final solution with an irrelevant global phase [see Eq. (6)].

Holonomy.—Consider now the case where the particle A propagates from left to right in a scattering region located in the spatial domain $\mathcal{I} := [Y_0, Y]$. Setting $\mathbf{A} = \mathbf{C}_{Y_0}$, $\mathbf{B} = 0$ we can then express the solution of Eq. (3) at $y = Y$ as

$$\mathbf{C}_Y = \mathcal{U}_{Y_0 \rightarrow Y} \mathcal{W}_Y^{(+)} \mathbf{C}_{Y_0}, \quad (6)$$

which, excluding the presence of the counterpropagating contribution $\mathcal{W}_Y^{(-)}$, formally accounts for neglecting reflection effects induced by the scattering region (a regime we can always achieve for large enough values of ϵ). The term $\mathcal{U}_{Y_0 \rightarrow Y}$ has a purely holonomic character, introducing a geometrical non-Abelian phase shift in the model. To see this explicitly, notice that from Eq. (2) it follows that the y functional dependence of the vectors $|\phi_y^{(\ell)}\rangle$ is fully mediated by the vector \vec{R}_y , i.e.,

$$|\phi_y^{(\ell)}\rangle = |\phi_{\vec{R}_y}^{(\ell)}\rangle. \quad (7)$$

Hence the matrix K_y can be equivalently expressed as

$$K_y = \vec{K}(\vec{R}_y) \cdot \partial_y \vec{R}_y, \quad [\vec{K}(\vec{R})]_{\ell\ell'} := \langle \phi_{\vec{R}}^{(\ell)} | \vec{\nabla}_{\vec{R}} \phi_{\vec{R}}^{(\ell')} \rangle, \quad (8)$$

which formally represents the Berry connection of the model [6]. Assume hence that the trajectory $\mathcal{R} := \{\vec{R}_y\}_{y \in [Y_0, Y]}$ followed by the vector \vec{R}_y in the control parameter's space forms a closed curve (i.e., $\vec{R}_Y = \vec{R}_{Y_0}$). We can then use Eq. (8) to write $\mathcal{U}_{Y_0 \rightarrow Y}$ as a path-ordered integral of the vector field $\vec{K}(\vec{R})$ along \mathcal{R} , i.e.,

$$\mathcal{U}_{Y_0 \rightarrow Y} = \mathcal{U}(\mathcal{R}) := P \exp \left[- \oint_{\mathcal{R}} d\vec{R} \cdot \vec{K}(\vec{R}) \right], \quad (9)$$

which no longer depends upon the ‘‘speed’’ $\partial_y \vec{R}$ of the longitudinal variation of the potential, making manifest the geometrical nature of the resulting operation. Notice that invoking the non-Abelian version of the Stokes theorem [36], the above expression can also be cast into a surface integral associated with the curvature tensor of $\vec{K}(\vec{R})$; see Ref. [37], and references therein. The resulting formula, while being more evocative, is possibly less informative, and we report it only in Sec. IV of the SM [30].

Two-dimensional models.—To be more quantitative we now focus on the case where the dynamics can be reduced to a twofold Hilbert subspace spanned, say, only by the eigenstates $|\phi_y^{(0)}\rangle$, $|\phi_y^{(1)}\rangle$ of the transverse Hamiltonian $\hat{h}_y(\hat{x})$. From Eqs. (3) and (4) this is guaranteed provided that two conditions are satisfied: (i) $\Delta_y := \epsilon_y^{(1)} - \epsilon_y^{(0)}$ is the smallest energy gap for all y , such that $[K_y]_{\ell\ell'}$ results negligible for all the other choices of ℓ, ℓ' , and (ii) $V_y(\hat{x})$ is a sufficiently slowly varying function of y so as to avoid unwanted couplings with other energy levels (a condition which is in agreement with the WKB approximation we already assumed). Accordingly, we can now write $\Omega_y := \omega_y I - \Delta_y \sigma_3 / 2$, where I is the 2×2 identity matrix while

$$\sigma_3 := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

and where $\omega_y := (\epsilon_y^{(1)} + \epsilon_y^{(0)})/2$. Most importantly, K_y reduces to a 2×2 matrix proportional to the second Pauli matrix

$$\sigma_2 := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},$$

i.e.,

$$K_y = i\lambda_y \sigma_2, \quad \lambda_y = \lambda_y^* := \langle \phi_y^{(0)} | \partial_y \phi_y^{(1)} \rangle, \quad (10)$$

which produces trivial autocommutators $[K_y, K_{y'}] = 0$ for all y, y' . Accordingly, the expression for $\mathcal{U}_{Y_0 \rightarrow Y}$ simplifies to the following SU(2) rotation, $\mathcal{U}_{Y_0 \rightarrow Y} = \exp[-i\alpha_y \sigma_2]$, where

$\alpha_y := \int_{Y_0}^y dy' \lambda_{y'}$. In particular, for $y = Y$, this allows us to write Eq. (9) as

$$\mathcal{U}(\mathcal{R}) = e^{-i\alpha \sigma_2}, \quad (11)$$

with

$$\alpha := \oint_{\mathcal{R}} d\vec{R} \cdot \vec{\lambda}(\vec{R}) = \int_S d\vec{S} \cdot [\vec{\nabla}_{\vec{R}} \times \vec{\lambda}(\vec{R})], \quad (12)$$

where exploiting Eq. (7) we write $\vec{\lambda}(\vec{R}) := \langle \phi_{\vec{R}}^{(\ell_0)} | \vec{\nabla}_{\vec{R}} | \phi_{\vec{R}}^{(\ell_1)} \rangle$, and where in the second identity, following from the standard (Abelian) version of the Stokes theorem [37,38], the integration is performed on a regular surface S of the control parameter space which admits \mathcal{R} as bounding curve. Inserting this into Eq. (5) finally gives

$$\partial_y^2 \tilde{\mathbf{C}}_y + [(\epsilon - \omega_y)I + \Delta_y \tilde{\sigma}_3 / 2] \tilde{\mathbf{C}}_y = 0, \quad (13)$$

with $\tilde{\sigma}_3 = e^{i\alpha_y \sigma_2} \sigma_3 e^{-i\alpha_y \sigma_2}$. Assuming now, as for the general case discussed in the previous section, ϵ to be the largest energy scale in the system, i.e., imposing $\epsilon \gg |\omega_y|, |\Delta_y|$, the above equation can be integrated under

WKB approximation yielding $\mathcal{W}_Y^{(\pm)} \simeq e^{\pm i \int_{Y_0}^Y \sqrt{\epsilon - \omega_{y'}} dy'}$, which, although constituting a refinement of the solution $\mathcal{W}_Y^{(\pm)} \simeq e^{\pm i \sqrt{\epsilon} (Y - Y_0)}$, still acts on \mathbf{C}_{Y_0} as an irrelevant global phase shift. Accordingly, from Eq. (6) we can conclude that when emerging from the scattering region the transverse component of the wave function of A gets modified via the holonomic rotation (11), resulting in the following one-qubit gate transformation:

$$\begin{aligned} |\psi_E(Y_0)\rangle &= a|\phi_y^{(0)}\rangle + b|\phi_y^{(1)}\rangle \\ \rightarrow |\psi_E(Y)\rangle &\simeq e^{i \int_{Y_0}^Y \sqrt{\epsilon - \omega_{y'}} dy'} [(a \cos \alpha - b \sin \alpha) |\phi_y^{(0)}\rangle \\ &\quad + (b \cos \alpha + a \sin \alpha) |\phi_y^{(1)}\rangle], \end{aligned} \quad (14)$$

a and b being arbitrary complex amplitudes. As a final remark, notice that, since α does not bear any functional dependence upon the input energy ϵ , the effect can be easily generalized to the cases where the longitudinal component of the incoming wave function of A is a wave packet given by the superposition of plane waves involving different kinetic energies, as long as the latter are much larger than the energy gap between the two levels on which the holonomy acts.

As already observed, having $[K_y, K_{y'}] = 0$ greatly simplifies the calculations. The drawback is that under this condition all the generated holonomy will commute, hence allowing us only to span an Abelian subgroup of all possible unitaries of the system. As discussed explicitly in Sec. V of the SM [30], this limitation however can be overcome by concatenating in series different modulation regions where the spatial potential selectively couples

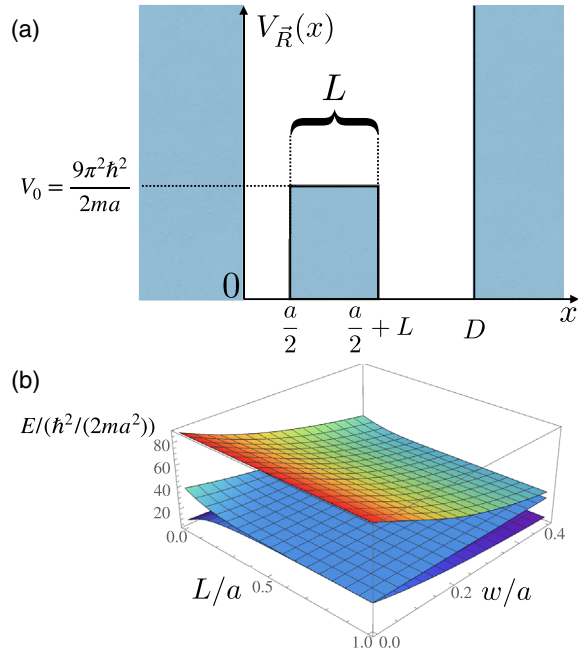


FIG. 2. (a) Sketch of the structured infinite well potential $V_y(x) = V_{\vec{R}_y}(x)$ discussed in the text. The model is characterized by a two-dimensional control vector $\vec{R}_y = (L(y), w(y))$ with the positive quantities $L(y)$ and $w(y)$ carrying the y dependence. For assigned \vec{R} , $V_{\vec{R}}(x)$ exhibit a potential step of constant height $V_0 = 9\pi^2\hbar^2/(2ma^2)$ and width L located at fixed distance $a/2$ from the left border of an infinite well that contains it. The total length of the infinite well is also variable and equal to $D = a + L + w$. (b) Plot of the first three energy levels E_0 , E_1 , and E_2 of the model [see Eq. (1)] as a function of L and w for fixed a . Here the energies are measured in unit of $\hbar^2/(2ma^2)$ while the controls are in units of a .

different pairs of energy levels, e.g., first $\epsilon_y^{(0)}$ and $\epsilon_y^{(1)}$ then $\epsilon_y^{(0)}$ and $\epsilon_y^{(2)}$ etc., introducing hence extra generators for the holonomy which do not commute.

Example.—To test the construction described in the previous section, we consider the case of a structured infinite potential well $V_y(x) = V_{\vec{R}_y}(x)$ characterized by a two-dimensional control vector \vec{R}_y with Cartesian components $R_y^{(1)} := L(y)$ and $R_y^{(2)} := w(y)$ associated with two positive spatial parameters. Specifically, we assume the width of the infinite well to be variable and expressed as $D(y) = a + L(y) + w(y)$, with a being a fixed constant. Inside the well we also assume to add a finite potential barrier of width $L(y)$ having constant height $V_0 := (9\pi^2\hbar^2)/2ma^2$ and located at distance $a/2$ from the leftmost infinite wall; see Fig. 2(a). For $w(y) = 0$, $V_y(x)$ corresponds to a stretchable potential [39] exhibiting a third energy level eigenvalue constantly equal to V_0 which does not depend upon the selected value of $L(y)$. The energy landscape associated with the first three levels obtained by solving Eq. (1) is reported in Fig. 2(b) as a function of the

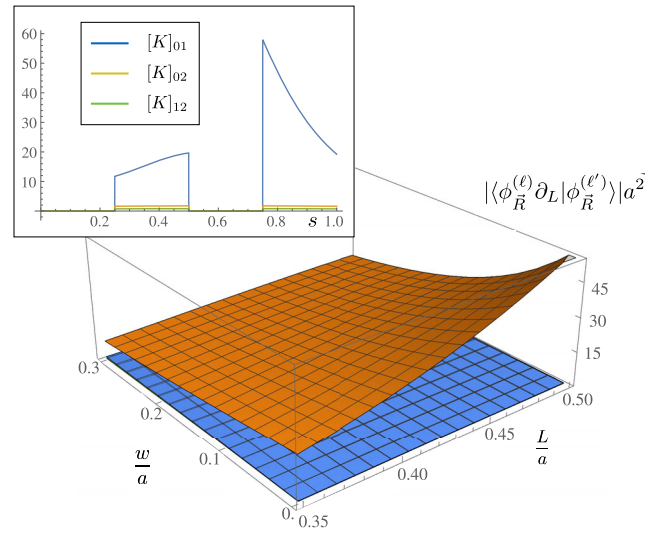


FIG. 3. Plot of $|\langle \phi_{\vec{R}}^{(\ell)} | \partial_L \phi_{\vec{R}}^{(\ell')} \rangle|^2 a^2$ in the control plane (L, w) : $(\ell, \ell') = (0, 1)$ (yellow surface) and $(1, 2), (0, 2)$ (blue surface, the differences between the two being not observable). Inset: Plot of the matrix elements $|K_{\ell\ell'}|$ when moving along a rectangular path \mathcal{R} with $\vec{R}_{\text{in}} = (0.35a, 0)$ and $\vec{R}_{\text{fin}} = (0.5a, 0.02a)$, see inset of Fig. 4, s being the length of the path along the trajectory expressed in unit of a . When w is changed, all the matrix elements are null, corresponding to the intervals $[0, 1/4]$ and $[1/2, 3/4]$, while as L is changed (corresponding to the intervals $[1/4, 1/2], [3/4, 1]$), we can observe how $[K]_{01}$ is always far larger than $[K]_{12}$ and $[K]_{02}$.

control parameters. We notice that as long as we prevent the ratio $w(y)/a$ to be above ~ 0.05 the energy gap between the first two levels is much smaller than the one between these levels and the third, so that we are ensured that the matrix elements $[K_y]_{\ell\ell'}$ are negligible for $\ell, \ell' > 2$; see Fig. 3. Moreover, in this region the energy gap between the ground state and the first excited level is also very small, ensuring that under WKB approximation the dynamical contribution to the system evolution will not add extra coupling terms that compete with the holonomy. Therefore, following the analysis of the previous section, we can safely consider the Hilbert space as twofold and compute the holonomy as in Eq. (14). We also observe that for the selected model, the second component of the vector $\vec{\lambda}(\vec{R})$ entering Eq. (12) is always identically null, yielding $\vec{\lambda}(\vec{R}) = (\langle \phi_{\vec{R}}^{(0)} | \partial_L \phi_{\vec{R}}^{(1)} \rangle, 0)$. Indeed we have $\langle \phi_{\vec{R}}^{(0)} | \partial_w \phi_{\vec{R}}^{(1)} \rangle = 0$ as it depends on the variation of the wave functions at the extremal point $x = a + L + w$ where the boundary conditions force both the wave functions to be exactly null. Moreover, in Sec. VI of SM [30] we have shown that the only nonzero component of $\vec{\lambda}(\vec{R})$ can be expressed as

$$\langle \phi_{\vec{R}}^{(0)} | \partial_L \phi_{\vec{R}}^{(1)} \rangle = -\frac{9\pi^2 \phi_{\vec{R}}^{*(0)}(\frac{a}{2} + L) \phi_{\vec{R}}^{(1)}(\frac{a}{2} + L)}{a^2 (\epsilon_{\vec{R}}^{(1)} - \epsilon_{\vec{R}}^{(0)})}, \quad (15)$$

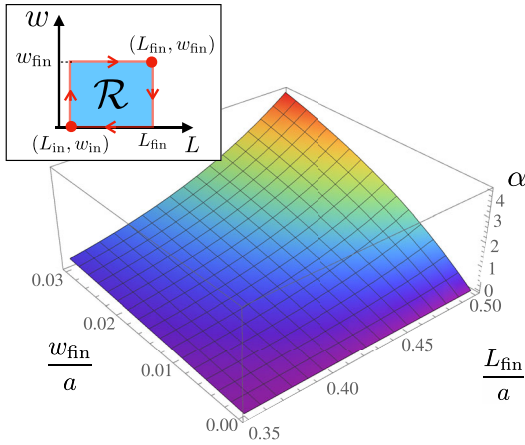


FIG. 4. Geometric phase (12) obtained following a rectangular closed path \mathcal{R} in the (L, w) plane specified by the extremal points $\vec{R}_{\text{in}} = (L_{\text{in}}, w_{\text{in}}) \rightarrow (L_{\text{in}}, w_{\text{fin}}) \rightarrow (L_{\text{fin}}, w_{\text{fin}}) \rightarrow (L_{\text{fin}}, w_{\text{in}}) \rightarrow \vec{R}_{\text{in}}$; see inset. The plot refers to the case where we keep fixed $L_{\text{in}} = 0.3a$ and $w_{\text{in}} = 0$, while spanning on L_{fin} and w_{fin} .

where for $\ell = 0, 1$, $\phi_{\vec{R}}^{(\ell)}(x)$ and $\epsilon_{\vec{R}}^{(\ell)}$ represent the ℓ th eigenfunction and the associated (rescaled) eigenenergy of the Hamiltonian $\hat{p}_x^2/2m + V_{\vec{R}}(\hat{x})$. Hence the geometric phase (12) computed along the rectangular paths shown in the inset of Fig. 4 can be expressed as $\alpha = \theta(w_{\text{fin}}) - \theta(w_{\text{in}})$, with $\theta(w)$ being the line integral defined as $\theta(w) := (9\pi^2/a^2) \int_{L_{\text{in}}}^{L_{\text{fin}}} dL \phi_{\vec{R}}^{*(0)}(a/2 + L) \phi_{\vec{R}}^{(1)}(a/2 + L) / (\epsilon_{\vec{R}}^{(1)} - \epsilon_{\vec{R}}^{(0)})$. As shown in Fig. 4, though moving in a small region of parameters space, we are able nonetheless to obtain a wide range of values of α .

Conclusions and outlook.—Exploiting the spatial analog of Berry phase we have shown how it is possible through spatial potential engineering to induce a geometrical phase on the internal state of a traveling particle. In our analysis we assume that the kinetic energy of the particle is much larger than the relevant energy levels of the system and the energy scale associated with the potential modulation. This allows us to separate two main contributions in the solution of the time-independent Schrödinger equation: one which has a purely holonomic character, and a dynamical one which amounts to an irrelevant global phase. The proposed scheme might be envisioned as a useful resource in the context of solid-state devices quantum computing, where potential profiles engineering has nowadays reached a sufficient level of precision needed for such applications. On the theoretical side it would be interesting to investigate how the presence of dissipation and particle interactions influence the appearance of a geometrical phase.

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