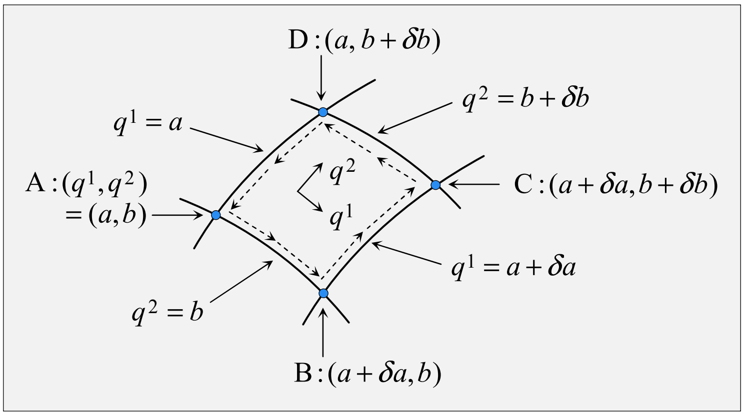
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material

Following Aitchison and Hey, parallel transport is carried out around the closed circuit indicated in the figure. Two examples are: a classical vector $\vec{V}$, and a wave function. We shall begin with $\vec{V}$. A natural setting for classical parallel transport is spacetime. Here, 3D is used to illustrate principles.



The change of the α^{th} component of $\vec{V}$ due to the curved nature of the surface upon which it is being transported is given by eqn (3.11):

$$dV^{\alpha} = -\Gamma^{\alpha}{}_{\gamma\mu} V^{\gamma} dq^{\mu} . \tag{3.11}$$

The right hand side is evaluated for each leg: A$\rightarrow$B, B$\rightarrow$C, C$\rightarrow$D, D$\rightarrow$A, and these contributions are combined to obtain the geometric phase for the infinitesimal closed circuit. The individual contributions to dV^{α} are given below.

$$dV^{\alpha}{}_{\mathrm{AB}} = -\int_{q^1=a,\ q^2=b}^{q^1=a+\delta a,\ q^2=b} dq^1\, \Gamma^{\alpha}{}_{\gamma 1} V^{\gamma} = -\Gamma^{\alpha}{}_{\gamma 1}(a,b) V^{\gamma}(a,b)\,\delta a \tag{1}$$

In evaluating the integral, the connection $\Gamma^{\alpha}{}_{\gamma\,1}$ times the vector component V^{γ} is taken at the starting point (a, b). The other terms are as follows:

$$dV^{\alpha}{}_{\mathrm{BC}} = -\Gamma^{\alpha}{}_{\gamma 2}(a+\delta a, b) V^{\gamma}(a+\delta a, b)\,\delta b \tag{2}$$

$$dV^{\alpha}{}_{\mathrm{CD}} = -\Gamma^{\alpha}{}_{\gamma 1}(a+\delta a,\, b+\delta b) V^{\gamma}(a+\delta a,\, b+\delta b)\left(-\delta a\right) \tag{3}$$

$$dV^{\alpha}{}_{\mathrm{DA}} = -\Gamma^{\alpha}{}_{\gamma 2}(a,\, b+\delta b) V^{\gamma}(a,\, b+\delta b)\left(-\delta b\right) \tag{4}$$

When combining the above contributions, it is necessary to reference each to (a, b). For example, the B$\rightarrow$C leg is expressed relative to (a, b) by expanding the connection $\Gamma^{\alpha}{}_{\gamma 2}(a,b)$ in powers of the displacement δa, and retaining the lowest order term, and using parallel transport to express $V^{\gamma}(a+\delta, b)$ in terms of $V^{\gamma}(a,b)$ plus a connection. Thus, the expression for $dV^{\alpha}{}_{\mathrm{BC}}$ becomes

$$dV^{\alpha}{}_{\mathrm{BC}} = -\left(\Gamma^{\alpha}{}_{\gamma 2}(a,b) + \frac{\partial \Gamma^{\alpha}{}_{\gamma 2}(a,b)}{\partial q^1}\delta a\right)\left(V^{\gamma}(a,b) - \Gamma^{\gamma}{}_{\delta 1}(a,b)V^{\delta}(a,b)\delta a\right)\delta b\ . \qquad (5)$$

The (a,b) parentheses are no longer necessary, as they are common to each term, so henceforth they are understood. Retaining the lowest order terms, $dV^{\alpha}{}_{\mathrm{BC}}$ becomes

$$dV^{\alpha}{}_{\mathrm{BC}} = -\Gamma^{\alpha}{}_{\gamma 2}V^{\gamma}\delta b - \left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 2}}{\partial q^1}V^{\gamma} - \Gamma^{\alpha}{}_{\gamma 2}\Gamma^{\gamma}{}_{\delta 1}V^{\delta}\right)\delta a \delta b \qquad (6)$$

$$= -\Gamma^{\alpha}{}_{\gamma 2}V^{\gamma}\delta b - \left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 2}}{\partial q^1} - \Gamma^{\alpha}{}_{\delta 2}\Gamma^{\delta}{}_{\gamma 1}\right)V^{\gamma}\delta a \delta b\ . \qquad (7)$$

The $\mathrm{C} \rightarrow \mathrm{D}$ leg is simplified by exchanging the integration limits and multiplying by -1. Thus, eqn (3) becomes

$$dV^{\alpha}{}_{\mathrm{CD}} = \int_{q^1=a,\ q^2=b+\delta b}^{q^1=a+\delta a,\ q^2=b+\delta b} dq^1\, \Gamma^{\alpha}{}_{\gamma 1}V^{\gamma} = \Gamma^{\alpha}{}_{\gamma 1}(a,\, b+\delta b)V^{\gamma}(a,\, b+\delta b)\delta a\ . \qquad (8)$$

As before, expanding the connection and vector component yields

$$dV^{\alpha}{}_{\mathrm{CD}} = \left(\Gamma^{\alpha}{}_{\gamma 1} + \frac{\partial \Gamma^{\alpha}{}_{\gamma 1}}{\partial q^2}\delta b\right)\left(V^{\gamma} - \Gamma^{\gamma}{}_{\delta 2}V^{\delta}\delta b\right)\delta a \qquad (9)$$

$$= \Gamma^{\alpha}{}_{\gamma 1}V^{\gamma}\delta a + \left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 1}}{\partial q^2}V^{\gamma} - \Gamma^{\alpha}{}_{\gamma 1}\Gamma^{\gamma}{}_{\delta 2}V^{\delta}\right)\delta a \delta b \qquad (10)$$

$$= \Gamma^{\alpha}{}_{\gamma 1}V^{\gamma}\delta a + \left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 1}}{\partial q^2} - \Gamma^{\alpha}{}_{\delta 1}\Gamma^{\delta}{}_{\gamma 2}\right)V^{\gamma}\delta a \delta b\ . \qquad (11)$$

Combining the $dV^{\alpha}{}_{\mathrm{AB}}$ and $dV^{\alpha}{}_{\mathrm{CD}}$ contributions gives

$$dV^{\alpha}{}_{\mathrm{AB}} + dV^{\alpha}{}_{\mathrm{CD}} = \left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 1}}{\partial q^2} - \Gamma^{\alpha}{}_{\delta 1}\Gamma^{\delta}{}_{\gamma 2}\right)V^{\gamma}\delta a \delta b\ . \qquad (12)$$

In a similar vein, the last leg, $dV^{\alpha}{}_{\mathrm{DA}}$, is obtained by reversing the direction of integration, yielding $dV^{\alpha}{}_{\mathrm{DA}} = \Gamma^{\alpha}{}_{\gamma 2}V^{\gamma}\delta b$. Combining this with $dV^{\alpha}{}_{\mathrm{BC}}$ from eqn (7) yields

$$dV^{\alpha}{}_{\mathrm{BC}} + dV^{\alpha}{}_{\mathrm{DA}} = -\left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 2}}{\partial q^1} - \Gamma^{\alpha}{}_{\delta 2}\Gamma^{\delta}{}_{\gamma 1}\right)V^{\gamma}\delta a \delta b\ . \qquad (13)$$

The net change for the closed circuit is obtained by adding eqns (12) and (13):

$$dV^{\alpha} = -\left(\frac{\partial \Gamma^{\alpha}{}_{\gamma 2}}{\partial q^{1}} - \frac{\partial \Gamma^{\alpha}{}_{\gamma 1}}{\partial q^{2}} + \Gamma^{\alpha}{}_{\delta 1} \Gamma^{\delta}{}_{\gamma 2} - \Gamma^{\alpha}{}_{\delta 2} \Gamma^{\delta}{}_{\gamma 1} \right) V^{\gamma} \delta a \delta b \tag{14}$$

This was obtained by using the two spatial coordinates q^1 and q^2. For the general 4D case it follows that dV^{α} is

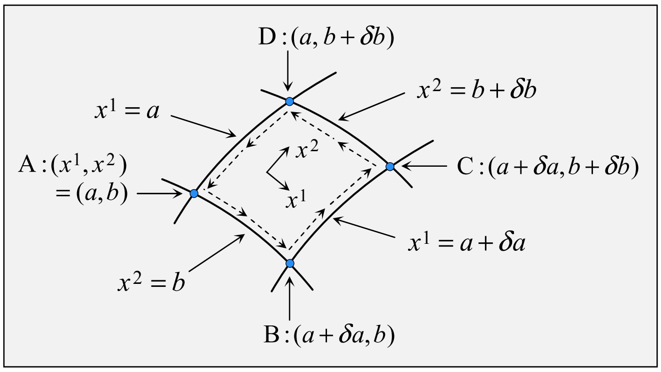
$$dV^{\alpha} = -\left(\frac{\partial \Gamma^{\alpha}{}_{\gamma \beta}}{\partial q^{\sigma}} - \frac{\partial \Gamma^{\alpha}{}_{\gamma \sigma}}{\partial q^{\beta}} + \Gamma^{\alpha}{}_{\delta \sigma} \Gamma^{\delta}{}_{\gamma \beta} - \Gamma^{\alpha}{}_{\delta \beta} \Gamma^{\delta}{}_{\gamma \sigma} \right) V^{\gamma} dS^{\sigma\beta} . \tag{15}$$

The incremental surface area is $dS^{\sigma\beta}$.

The contents of the large parentheses comprise the Riemann curvature tensor: $R^{\alpha}{}_{\gamma\beta\sigma}$. This is discussed in: *Gravitation*, by Misner, Thorne, and Wheeler. As mentioned above, a discussion focused on the present case is in Aitchison and Hey. When every element $R^{\alpha}{}_{\gamma\beta\sigma}$ is zero the space is flat. When at least one of these elements is nonzero the space is curved. Working this out for polar coordinates illustrates the fact that the space is flat, despite the fact that the basis vectors vary with location.

Transporting ψ

Next, a wave function is transported around the circuit indicated in the figure. Equation (3.13) gives the change: $d\psi = -iqA_{\mu}\psi dx^{\mu}$ for each leg of the journey. One could also use $d\psi = -iqA^{\mu}\psi dx_{\mu}$. In either case, the result is expressed in terms of the electromagnetic field strength tensor $F_{\mu\nu}$ or $F^{\mu\nu}$. The change for A $\rightarrow$ B is



$$(d\psi)_{\mathrm{AB}} = -\int_{x^1=a,\, x^2=b}^{x^1=a+\delta a,\, x^2=b} dx^1 iqA_1 \psi = -iqA_1(a,b)\psi(a,b)\delta a \tag{16}$$

Again, all legs are expressed relative to (a, b), and contributions are summed to obtain the closed circuit result. To start, expressions analogous to eqns (2) – (4) are written:

$$(d\psi)_{\mathrm{BC}} = -iqA_2(a+\delta a, b)\,\psi(a+\delta a, b)\,\delta b \tag{17}$$

$$(d\psi)_{\mathrm{CD}} = -iqA_1(a+\delta a,\, b+\delta b)\,\psi(a+\delta a,\, b+\delta b)(-\delta a) \tag{18}$$

$$(d\psi)_{\mathrm{DA}} = -iq\,A_2(a,\, b+\delta b)\,\psi(a,\, b+\delta b)(-\delta b) \tag{19}$$

Referring to eqn (17), write $A_2(a+\delta a,b)$ in terms of $A_2(a,b)$ and its derivative with respect to x^1, and $\psi(a+\delta a,b)$ in terms of $\psi(a,b)$ and its connection along x^1:

$$(d\psi)_{\mathrm{BC}} = -iq\left(A_2 + \frac{\partial A_2}{\partial x^1}\delta a\right)(\psi - iqA_1\psi\delta a)\delta b\,. \tag{20}$$

Retaining the lowest order terms gives

$$(d\psi)_{\mathrm{BC}} = -iqA_2\psi\delta b - qqA_1A_2\psi\delta a\delta b - iq\frac{\partial A_2}{\partial x^1}\psi\delta a\delta b\,. \tag{21}$$

Likewise for $(d\psi)_{\mathrm{CD}}$:

$$(d\psi)_{\mathrm{CD}} = iqA_1(a,\, b+\delta b)\,\psi(a, b+\delta b)\,\delta a \tag{22}$$

$$= iq\left(A_1 + \frac{\partial A_1}{\partial x^2}\delta b\right)(\psi - iqA_2\psi\delta b)\delta a \tag{23}$$

$$= iqA_1\psi\delta a + qqA_1A_2\psi\delta a\delta b + iq\frac{\partial A_1}{\partial x^2}\psi\delta a\delta b \tag{24}$$

Finally, $(d\psi)_{\mathrm{DA}}$ is equal to $iq\,A_2\psi\,\delta b$. Combining the four legs of the journey yields

$$d\psi = (d\psi)_{\mathrm{AB}} + (d\psi)_{\mathrm{BC}} + (d\psi)_{\mathrm{CD}} + (d\psi)_{\mathrm{DA}} \tag{25}$$

$$= -iq\cancel{A_1\psi}\,\delta a - iq\cancel{A_2\psi}\,\delta b - qqA_1\cancel{A_2\psi}\,\delta a\delta b - iq\frac{\partial A_2}{\partial x^1}\psi\delta a\delta b$$

$$+\; iq\cancel{A_1\psi}\,\delta a + qq\cancel{A_1A_2}\psi\delta a\delta b + iq\frac{\partial A_1}{\partial x^2}\psi\delta a\delta b + iq\cancel{A_2\psi}\,\delta b\,. \tag{26}$$

Thus, parallel transport of the wave function around the infinitesimal closed circuit has resulted in a compact form for the change $d\psi$:

$$d\psi = -iq\left(\frac{\partial A_2}{\partial x^1} - \frac{\partial A_1}{\partial x^2}\right)\psi\delta a\delta b\,. \tag{27}$$

For a general infinitesimal closed loop, this is $-iq(\partial_\mu A_\nu - \partial_\nu A_\mu)\psi dS$, or

$$d\psi = -iqF_{\mu\nu}\psi dS\,. \tag{28}$$