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The Aharonov–Bohm effect: the role of tunneling and associated forces

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Abstract

Through tunneling, or barrier penetration, small wavefunction tails can enter a finitely shielded cylinder with a magnetic field inside. When the shielding increases to infinity, the Lorentz force goes to zero together with these tails. However, it is shown, by considering the radial derivative of the wavefunction on the cylinder surface, that a flux-dependent force remains. This force explains in a natural way the Aharonov–Bohm effect in the idealized case of infinite shielding.

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1. Introduction

The counterintuitive Aharonov–Bohm (AB) effect [1] represents one of the most widely discussed issues of quantum physics. It predicts that a charged particle can be influenced by a magnetic field 'even if the particle is nowhere in the region of nonzero field strength' [2]. This intriguing effect has alternatively been attributed to a nonlocal feature of quantum mechanics, to a hitherto unexpected direct physical meaning of an otherwise unphysical vector potential, to a topological cause and so on [3]. It is experimentally well verified [3, 4], and its possible applications have attracted much interest recently; see e.g. [5–10]. A generally accepted intuitive and physical understanding, however, seems to be still lacking.

As a Hamiltonian operator for an electron (without spin) in the presence of a magnetic field, one takes

$$\hat{H} = \left[\hat{\mathbf{P}} + e\mathbf{A}(\hat{\mathbf{x}})\right]^2 / 2m_e, \tag{1}$$

where $\hat{\mathbf{P}}$ is the canonical momentum operator of the electron, m_e is the electron mass and $-e$ is its charge. $\mathbf{A}(\mathbf{x})$ is a vector potential, which is not unique and is related to the magnetic field by $\mathbf{B}(\mathbf{x}) = \text{curl}\ \mathbf{A}(\mathbf{x})$. In classical physics, such a vector potential is an auxiliary quantity without a direct physical meaning. It may happen that a magnetic field vanishes in a region,

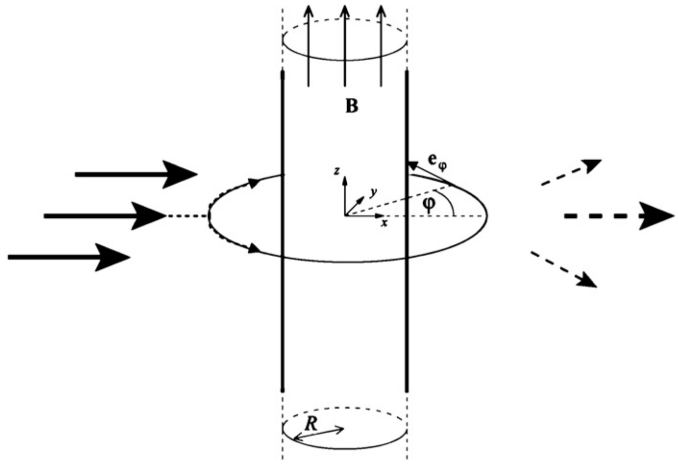

Figure 1. Schematic sketch of the Aharonov–Bohm effect. Electron scattering by an infinite, perfectly shielded cylinder of radius R, with a homogeneous magnetic field $B\mathbf{e}_z$ inside, depends on the magnetic flux.

while the allowed vector potentials do not. An example is given in figure 1 with a constant magnetic field which vanishes outside an infinitely long cylinder of radius R. Since the integral $\oint \mathbf{A}(\mathbf{x}) \cdot \mathrm{d}\mathbf{x}$ over a circle around the cylinder yields the flux, $\mathbf{A}(\mathbf{x})$ cannot identically vanish outside the cylinder.

A quick, heuristic, way to obtain the AB effect is to note that an electron may pass on either side of an impenetrable cylinder (see figure 1), thereby picking up a phase $(e/\hbar) \int \mathbf{A}(\mathbf{x}) \cdot \mathrm{d}\mathbf{x}$, with the integral taken over the electron's path. The resulting phase difference is $(e/\hbar)\Phi$, where Φ is the magnetic flux in the cylinder, and this leads to field-dependent effects for scattering. Related effects in magnetic fields without shielding had been pointed out earlier [11, 12].

A more detailed derivation [1, 19] describes electron scattering by eigenfunctions of the Hamiltonian (1) with $\mathbf{A}(\mathbf{x}) = (\Phi/2\pi r)\,\mathbf{e}_\varphi$, where $r \equiv \sqrt{x^2 + y^2} \geqslant R$. Impenetrability is taken into account by choosing eigenfunctions with zero boundary conditions. Since the vector potential outside does not vanish, the eigenfunctions differ from those for the free Hamiltonian $\hat{H}^{(0)} = \hat{\mathbf{P}}^2/2m_\mathrm{e}$ with the same boundary conditions. This then gives the baffling result that electron scattering depends on the magnetic field inside the cylinder although the electron wavefunction cannot penetrate there. Tonomura *et al* [3] explicitly calculate for a special case the momentum transfer to the electron from the wall of the excluded cylinder, compare it with the momentum transfer implied by the scattering cross section, and conclude that in general the force exerted by the cylinder surface is needed to satisfy Ehrenfest's theorem. It remains, however, physically somewhat puzzling why this force depends on the magnetic field inside the cylinder although the wavefunction vanishes on the surface and inside. Liebowitz [13] invokes a new, previously not considered, classical force to explain the AB effect. This was criticized in [14] and rebutted in [15]. Boyer [16] draws a distinction between the Aharonov–Bohm phase shift and the Aharonov–Bohm effect and suggests that the Aharonov–Bohm phase shift is actually due to classical electromagnetic forces when relativistic effects are taken into account. In a recent experiment [17], the time delay for an electron passing by a 'macroscopic' solenoid has been investigated.

Some authors have noted that if one starts right away with a perfectly shielded cylinder—corresponding to quantum mechanics in a plane with a hole or in three-dimensional space with an excluded cylinder—the quantum dynamics for a particle outside is not uniquely determined (cf, e.g., [18]). With this point of view, the choice of one particular quantum dynamics then appears somewhat ad hoc since it typically relies on information from the excluded region. This problem does not arise in approaches which consider finite, but increasingly high, barriers and then take a limit [18, 19]. In this case, there are no interpretational problems. But it has also been shown [18, 19] that as the barrier height is increased in the limit, one arrives at exactly the same zero boundary conditions for the wavefunction as before. Thus, the conceptual problem remains by which physical mechanism information about the inside field is transmitted to the outside.

In this paper it is shown that in the case of large, but finite, shielding the small wavefunction tails, which can tunnel into the cylinder and into the magnetic field, determine the force acting on the electron. In the limit of infinite shielding this force remains finite and flux dependent, determines the otherwise under-defined dynamics outside and yields the AB effect.

The paper is organized as follows. In section 2, we review the argument why the quantum dynamics can be viewed as ambiguous if one has a perfectly shielded cylinder right from the beginning. This is due to the fact that classically equivalent Hamiltonians can become physically inequivalent after transition to quantum mechanics. In section 3, expressions for the forces for finite and infinite shielding are given in terms of radial derivatives of the modulus of the wavefunction. These radial derivatives are calculated in section 4 and the resulting forces are determined. In section 5, it is indicated how the forces determine the dynamics and the AB effect. In the appendix expressions for the forces are explicitly derived which are valid for arbitrary geometries, not only cylinders.

2. Indeterminacy of the quantization

We first consider a free *classical* electron outside an impenetrable infinitely long cylinder of radius R. No assumption about a possible magnetic field inside the cylinder is made. By symmetry, one can confine oneself to the $x-y$ plane. A possible classical Hamiltonian function is $H^{(0)} = \mathbf{P}^2/2m_e$, with reflections from the boundary of the excluded region implemented by the configuration space. The Hamiltonian, however, is not unique. Indeed, if $\boldsymbol{\Omega}_{\rm dum}(\mathbf{x})$ is any vector function (a 'dummy field') outside the cylinder, satisfying

$$\text{curl}\,\boldsymbol{\Omega}_{\rm dum}(\mathbf{x}) = 0$$

there, otherwise arbitrary and not connected to any field inside the cylinder, then

$$H_{\rm dum} = [\mathbf{P} + \boldsymbol{\Omega}_{\rm dum}(\mathbf{x})]^2 / 2m_e \tag{2}$$

equals the kinetic energy and also yields[1] $\ddot{\mathbf{x}} = 0$. This is, up to a constant, the most general form of the Hamiltonian yielding $\ddot{\mathbf{x}} = 0$ and equaling the kinetic energy. Classically, all these Hamiltonians are physically equivalent.

This general equivalence, however, is no longer true after transition to the quantum theory (with zero boundary conditions on the cylinder) (cf, e.g., [18, 20]). For a given $\boldsymbol{\Omega}_{\rm dum}(\mathbf{x})$ with $\text{curl}\boldsymbol{\Omega}_{\rm dum}(\mathbf{x}) = 0$ outside the cylinder, we define κ as

$$\kappa \equiv \text{ non-integer part of } \oint \boldsymbol{\Omega}_{\rm dum}(\mathbf{x}) \cdot \mathrm{d}\mathbf{x}/h \tag{3}$$

so that $0 \leqslant \kappa < 1$. Then one can define the continuous and differentiable function of modulus 1:

$$\Lambda(\mathbf{x}) \equiv \exp\left\{\frac{\mathrm{i}}{\hbar}\int_{\mathbf{x}_0}^{\mathbf{x}} \left[\boldsymbol{\Omega}_{\rm dum}(\mathbf{x}') - \frac{\hbar\kappa}{r'}\mathbf{e}_{\varphi'}\right] \cdot \mathrm{d}\mathbf{x}'\right\}, \tag{4}$$

[1] This corresponds to the well-known freedom to add to the Lagrangian a total time derivative. See, e.g., [18].

where $\mathbf{x}_0$ can be chosen as $\mathbf{x}_0 = (R, 0)$; $r, r' \geqslant R$. It is easy to check that $\Lambda(\hat{\mathbf{x}})\hat{H}_{\text{dum}}\Lambda(\hat{\mathbf{x}})^\dagger = \hat{H}^{(\kappa)}_{\text{dum}}$, where

$$\hat{H}^{(\kappa)}_{\text{dum}} = \left[\hat{\mathbf{P}} + \mathbf{\Omega}^{(\kappa)}_{\text{dum}}(\hat{\mathbf{x}})\right]^2 / 2m_{\text{e}}, \qquad \mathbf{\Omega}^{(\kappa)}_{\text{dum}}(\mathbf{x}) \equiv \frac{\hbar\kappa}{r}\mathbf{e}_\varphi \tag{5}$$

with $0 \leqslant \kappa < 1$, and the zero boundary conditions are preserved. The Hamiltonian operators $\hat{H}^{(\kappa)}_{\text{dum}}$ are physically inequivalent for $0 \leqslant \kappa < 1$, and without further input information it is unclear which one to choose. Thus there is an ambiguity when one starts right away with infinite shielding, and this ambiguity can be fixed by imposing an additional boundary condition which arises in a natural way when one takes into account tunneling and associated forces, as seen in the following.

3. The forces for finite and infinite shielding

Finite shielding of the cylinder can be modeled by a potential $V(\mathbf{x})$. Just for simplicity we consider $V(\mathbf{x}) = V_0\Theta(R - r)$, with $V_0 \to \infty$ later on, and a homogeneous magnetic field inside the cylinder with vector potential

$$\mathbf{A}_\Phi(\mathbf{x}) = \frac{\Phi}{2\pi}\left[\frac{1}{R^2}\Theta(R - r) + \frac{1}{r^2}\Theta(r - R)\right]\begin{pmatrix}-y\\ x\end{pmatrix}, \tag{6}$$

where Φ is the magnetic flux, but also other magnetic fields can be considered. The Hamiltonian then is

$$\hat{H}_{\Phi,V} = [\hat{\mathbf{P}}^2 + e\mathbf{A}_\Phi(\hat{\mathbf{x}})]^2/2m_{\text{e}} + V(\hat{\mathbf{x}}). \tag{7}$$

We consider a normalized (planar) wavefunction, $\psi_t^{(\Phi,V)}$, corresponding for $t \to -\infty$ to an incoming free particle which is then scattered. Due to tunneling, small tails enter the cylinder. The total force on the electron is

$$\mathbf{F}_t^{(\Phi,V)} = \left\langle\psi_t^{(\Phi,V)}\right| - \nabla V - e\hat{\mathbf{v}} \times \hat{\mathbf{B}}\left|\psi_t^{(\Phi,V)}\right\rangle. \tag{8}$$

Note that only the tails contribute. As the tails, the Lorentz force goes to 0 when $V \to \infty$. For a step potential, the first part becomes $V_0\int_0^{2\pi} R\,\mathrm{d}\varphi|\psi_t^{(\Phi,V)}(R,\varphi)|^2\mathbf{e}_r$. Expanding $\psi_t^{(\Phi,V)}$ in terms of eigenfunctions of $\hat{H}_{\Phi,V}$ and using equations (35)–(40) of [19], one can show explicitly for large V_0 that $V_0^{1/2}\left|\psi_t^{(\Phi,V)}(R,\varphi)\right| = \hbar\partial_r\left|\psi_t^{(\Phi,V)}(R,\varphi)\right|/(2m)^{1/2} + O\left(V_0^{-1}\right)$. Thus,

$$\mathbf{F}_t^{(\Phi,V)} = \frac{\hbar^2}{2m_{\text{e}}}\int_0^{2\pi} R\,\mathrm{d}\varphi\left[\frac{\partial}{\partial r}\left|\psi_t^{(\Phi,V)}(R,\varphi)\right|\right]^2\mathbf{e}_r + O\left(V_0^{-1}\right). \tag{9}$$

This result is also true for more general V and $\mathbf{B}$, e.g. $\mathbf{B}(r) = 0$, $r > R/2$, as well as for the torus and other domains (with a surface integral and normal derivative). This general case is treated in the appendix.

For infinite shielding and a fixed arbitrarily chosen dummy field $\mathbf{\Omega}^{(\kappa)}_{\text{dum}}$, we use $\mathbf{F}_t^{(\kappa)} = \mathrm{d}/\mathrm{d}t\left\langle\psi_t^{(\kappa)}\right|m_{\text{e}}\hat{\mathbf{v}}\left|\psi_t^{(\kappa)}\right\rangle$ for the force and eventually obtain

$$\mathbf{F}_t^{(\kappa)} = \frac{\hbar^2}{2m_{\text{e}}}\int_0^{2\pi} R\,\mathrm{d}\varphi\left[\frac{\partial}{\partial r}\left|\psi_t^{(\kappa)}(R,\varphi)\right|\right]^2\mathbf{e}_r. \tag{10}$$

Again, this carries over to other domains as shown in the appendix. In (9) and (10) one can now let the wavefunction go to a stationary solution.

The as yet underdetermined dummy field $\mathbf{\Omega}^{(\kappa)}_{\text{dum}}$ can be made unique by requiring that the κ-dependent force (10) agrees with (9) in the limit $V \to \infty$ (obtained with the field actually contained in the cylinder). It will now be shown that this requirement uniquely determines κ, and thus also the dynamics of the idealized case.

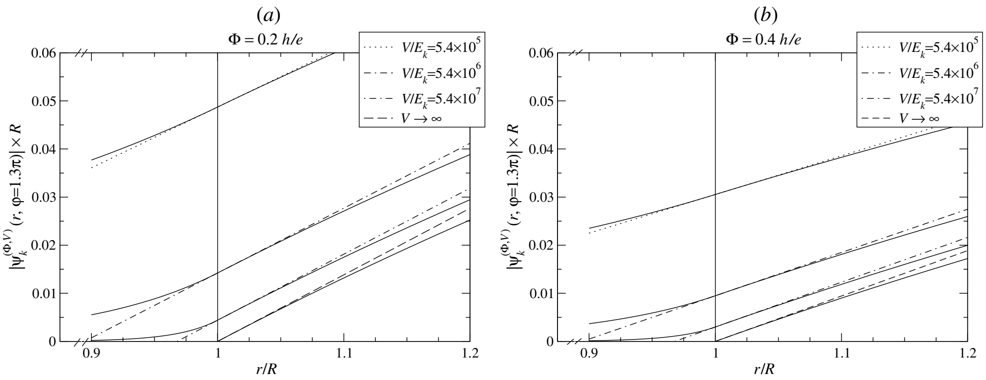

Figure 2. Wavefunction behavior near the boundary: finite shielding. Cylinder of radius R, wavefunction corresponding to incoming electrons of momentum $\hbar k \mathbf{e}_x$ with $kR = 4.3 \times 10^{-3}$. Two different magnetic fluxes: (a) $\Phi = 0.2h/e$ and (b) $\Phi = 0.4h/e$. Solid lines: $|\psi_k^{(\Phi,V)}(r,\varphi)|$ near the cylinder boundary for a fixed polar angle $\varphi = 1.3\pi$ and for increasing barrier heights V as well as for the limit $V \to \infty$. Thick vertical line: cylinder boundary. Broken lines: slope at this point. For the two fluxes the slopes differ significantly, but differ little for a fixed flux and different barrier heights V.

4. The radial derivative and resulting forces

It suffices to consider electron beams of definite incoming kinetic momentum, $\hbar k \mathbf{e}_x$ say. The corresponding scattering solution is a stationary state, denoted by $\psi_k^{(\Phi,V)}$ and $\psi_k^{(\kappa)}$, respectively. To calculate these we note that around the backward direction, $\varphi = \pi$, the incident wave should behave as an eigenfunction of $\hat{\mathbf{P}}_{\text{kin}}$. This implies that the incident wave should behave as

$$\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x} - \mathrm{i}e\Phi(\varphi-\pi)/h} \qquad \text{for} \quad kr \gg 1, \quad |\varphi - \pi| < \varepsilon, \tag{11}$$

and similarly for $\psi_k^{(\kappa)}$. The asymptotics in [1], based on the probability current, is the same[2].

The wavefunction $\psi_k^{(\Phi,V)}(r,\varphi)$ can be calculated analytically as a series and evaluated numerically. Note that the wavefunction is gauge dependent while its absolute value is not. Although the tails go to zero inside and on the cylinder when V tends to infinity, the behavior of the wavefunction in the vicinity of the cylinder depends sensitively on the value of Φ, as seen in figures 2(a) and (b). There we consider two different magnetic fields inside the cylinder, with fluxes Φ_1 and Φ_2, and increasing barrier heights V. For each flux and barrier height $\psi_k^{(\Phi,V)}(r,\varphi)$ is calculated and its absolute value is plotted as a function of r for $\varphi = 1.3\pi$. With increasing barrier height V the wavefunctions are indeed seen to converge to zero inside the cylinder ($r \leqslant R$). The form of the tails depends on the specific $\mathbf{B}$ and V, while the limiting slope depends only on Φ, or rather on

$$\alpha \equiv \text{ non-integer part of } e\Phi/h. \tag{12}$$

With infinite shielding and a dummy field $\mathbf{\Omega}_{\text{dum}}^{(\kappa)}$, the scattering solutions $\psi_k^{(\kappa)}(r,\varphi)$ vanish on the cylinder ($r = R$), but the rate with which 0 is approached when $r \to R$ depends on κ. To see this we calculate $\psi_k^{(\kappa)}(r,\varphi)$ by expressing it as a linear combination of eigenfunctions of

[2] One can also start with an incident plane wave $|\mathbf{k}\rangle \hat{=} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$ and use the Lippmann–Schwinger equation to obtain the corresponding scattering solution. We have determined the necessary Green's functions and have shown that one obtains the same expression as with (11). This generalizes a result for a magnetic string [21] and will be published elsewhere.

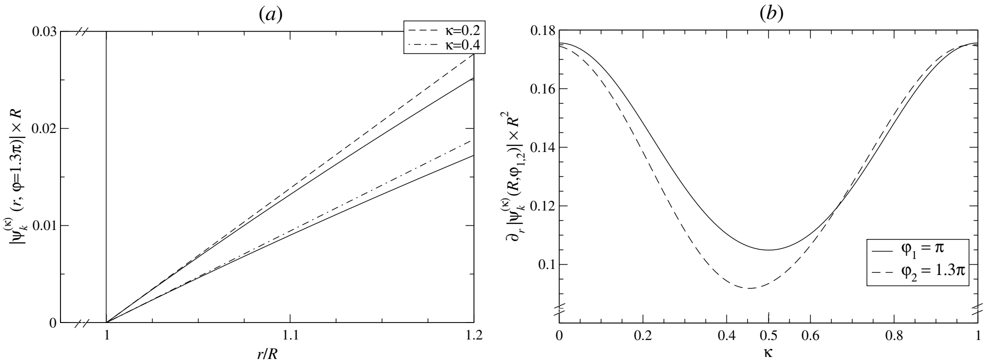

Figure 3. Infinite shielding with dummy field. kR as in figure 2. (*a*) Solid lines: $|\psi_k^{(\kappa)}(r,\varphi)|$ near the boundary as a function of r for a fixed polar angle $\varphi = 1.3\pi$ and for two different values of κ which labels inequivalent dummy fields $\mathbf{\Omega}_{\text{dum}}^{(\kappa)}$ from (5). The slope at $r = R$ (dashed, dot-dashed lines) depends on κ. (*b*) The slope at $r = R$ plotted as a function of κ for two polar angles $\varphi_1 = \pi$ and $\varphi_2 = 1.3\pi$. The value of κ is uniquely determined if the slope is known for two different angles φ.

$\hat{H}_{\text{dum}}^{(\kappa)}$ of fixed canonical angular momentum, with unknown coefficients. Using the asymptotics of Bessel and Hankel functions and (11), one can determine the coefficients and obtain

$$\psi_k^{(\kappa)}(r,\varphi) = \sum_{n=-\infty}^{\infty} (-\mathrm{i})^{|n+\kappa|}\, \mathrm{e}^{\mathrm{i}n(\varphi+\pi)} \left[J_{|n+\kappa|}(kr) - \frac{J_{|n+\kappa|}(kR)}{H_{|n+\kappa|}(kR)} H_{|n+\kappa|}(kr) \right]. \tag{13}$$

The rate is given by the tangent slope of $\left|\psi_k^{(\kappa)}(r,\varphi)\right|$ at the cylinder, i.e. by the radial derivative $\partial_r \left|\psi_k^{(\kappa)}(r=R,\varphi)\right|$ which can be calculated from (13). Since $\psi_k^{(\kappa)} = 0$ on the boundary of the cylinder, one easily sees that

$$\partial_r \left|\psi_k^{(\kappa)}(r,\varphi)\right| = \left|\partial_r \psi_k^{(\kappa)}(r,\varphi)\right| \qquad \text{if} \quad r = R. \tag{14}$$

With this identity and using the Wronskian for Bessel and Hankel functions, one obtains from (13)

$$\partial_r \left|\psi_k^{(\kappa)}(R,\varphi)\right| = \frac{2}{\pi R} \left| \sum_n \frac{(-\mathrm{i})^{|n+\kappa|}}{H_{|n+\kappa|}(kR)} \mathrm{e}^{\mathrm{i}n(\varphi+\pi)} \right|. \tag{15}$$

We note that this derivative is invariant under the unitary transformation $\Lambda(\hat{\mathbf{x}})$ in (4).

In figure 3(*a*) $\left|\psi_k^{(\kappa)}(r,\varphi)\right|$ is plotted as a function of r for two values of κ and for fixed $\varphi = 1.3\pi$, and it is seen that the slope at $r = R$ depends on κ. In figure 3(*b*) the slope at $r = R$ is plotted as a function of κ for two values of φ (solid curve: $\varphi_1 = \pi$, dashed curve: $\varphi_2 = 1.3\pi$), and it is seen that the values of the slope at the two different angles determine κ uniquely. Moreover, this slope agrees with the limiting slope for a magnetic flux Φ if κ equals the non-integer part of $e\Phi/h$ (i.e. if $\kappa = \alpha$), and then the corresponding forces on the electron beam are equal, by equations (9) and (10); conversely the condition $\kappa = \alpha$ is also necessary for this. Thus, requiring the equality of the forces determines the previously underdetermined dummy field $\mathbf{\Omega}_{\text{dum}}^{(\kappa)}$.

The force on the electron beam can easily be calculated for $V \to \infty$ by means of (15) (with $\kappa = \alpha$) as a rapidly converging sum involving Hankel functions. There is both a component in the backward direction as well as a perpendicular component. The former is repulsive and invariant under the replacement $\alpha \to 1-\alpha$. The latter reverses sign under $\alpha \to 1-\alpha$ and under charge reversal, vanishes for $\alpha = 0, 1/2, 1$, and for small Φ points in the same direction a Lorentz force would do for an electron inside the cylinder. For $kR \ll 1$ one obtains for the force per unit cylinder length on an electron beam of incoming momentum $\hbar k\mathbf{e}_x$ and density ρ

$$\mathbf{F}^{(\Phi,V\to\infty)} = \rho\frac{\hbar^2 k}{m_e}\begin{pmatrix} -2\sin^2(\pi e\Phi/h) \\ \sin(2\pi e\Phi/h) \end{pmatrix} + O(R^{\alpha'}), \tag{16}$$

where $\alpha' = \min(2\alpha, 4-4\alpha)$. The higher order terms in R contain the reflecting force by the cylinder and they vanish for $R \to 0$ (magnetic string). For $kR \sim 1$, F_2 is several orders of magnitude smaller than F_1 since reflection by the cylinder dominates. Subtracting this gives about the same order of magnitude, but the remainder is overall much smaller than in (16).

5. Forces and the AB effect

These results yield a physical explanation of the AB effect as follows. For the idealized case of an impenetrable cylinder, the quantum (but not the classical) dynamics in the outside region is underdetermined since it contains a largely arbitrary 'dummy' field. Although tempting, there is no *a priori* reason to relate this field to an (in principle unknown) magnetic field inside the cylinder. This leads to physically inequivalent Hamiltonians $\hat{H}^{(\kappa)}_{\text{dum}}$, $0 \leqslant \kappa < 1$, and a κ-dependent force. To derive an additional boundary condition which removes the indeterminacy we consider high, but finite, barriers. Then, by tunneling, minute tails of the scattering wavefunction can enter the cylinder. The shielding and a magnetic field inside the cylinder exert a force on these tails and on the electron. By the combined influence of magnetic field and increasing shielding on the form of the wavefunction, this force remains finite and flux dependent even when the shielding goes to infinity and it can be expressed by the radial wavefunction derivative at the cylinder. Requiring that the force for the directly tackled idealized case (with infinite shielding from the outset) be equal to this limiting force fixes the former's as yet underdetermined dynamics (i.e. κ). Alternatively, the limit slope of the scattering solution at the boundary can be considered as an additional boundary condition for the ideal case which also removes the indeterminacy. The dummy field determined in this way is, up to a factor e, just the vector potential customarily used right away in the discussion of the AB effect.

6. Summary

It has been shown that the AB effect for cylinders arises quite naturally when one considers tunneling and the force exerted on the small wavefunction tails of the electron inside the cylinder. Although the Lorentz force vanishes when the tails go to zero in the limit of infinite shielding, the flux dependence of the remaining force persists and precisely yields the AB effect. It has also been shown that the limit slope of the scattering solution at the boundary can be considered as an additional boundary condition for the ideal case which also removes the indeterminacy of the quantization procedure. The same results are expected to carry over to the torus and other domains.

Appendix. General case: forces in a magnetic and scalar field

A.1. Magnetic and large, but finite, scalar potential

We first consider a general time-independent magnetic field $\mathbf{B}(\mathbf{x})$ in a region G, with a vector potential $\mathbf{A}(\mathbf{x})$ vanishing at infinity and a scalar potential $V(\mathbf{x})$ which is nonzero in the same region G and vanishes outside. Later, we will remark on the more general case that the scalar potential may also vanish on parts of the interior of G.

The force, $\mathbf{F}_t^{(V)}$, on an electron of charge $-e$ at time t is then the sum of the scalar and Lorentz force:

$$\mathbf{F}_t^{(V)} = \langle \psi_t^{(V)}, (-\nabla V - e\mathbf{v} \times \mathbf{B})\psi_t^{(V)} \rangle, \tag{A.1}$$

where $\psi_t^{(V)}$ denotes the wavefunction under the time development with the Hamiltonian H_V, of an electron coming in from infinity. The Hamiltonian is

$$H_V = (\mathbf{P} + e\mathbf{A})^2/2m + V. \tag{A.2}$$

We will investigate the behavior of the force in (A.1) for large scalar potential V and will show that it can be expressed as an integral over the surface, ∂G, of the region G:

$$\mathbf{F}_t^{(V)} = \frac{\hbar^2}{2m} \int_{\partial G} \mathrm{d}\mathbf{o} \left| \frac{\partial \psi_t^{(V)}}{\partial n} \right|^2 + \text{terms} \to 0 \qquad \text{for} \quad V \to \infty. \tag{A.3}$$

Note that the dependence of this expression on the magnetic field comes through the time development via the Hamiltonian. In two dimensions and if the region G is a circle, one arrives at (9) and one can let $\psi_t^{(V)}$ go to a stationary solution of H_V.

To prove (A.3), we first consider the scalar part in (A.1) and show that

$$\langle \psi_t^{(V)}, -\nabla V \psi_t^{(V)} \rangle = -\frac{1}{2m} \int_G \mathrm{d}^d x \nabla \overline{\psi_t^{(V)}} \mathbf{P}^2 \psi_t^{(V)} + \text{c.c.} + \text{terms} \to 0 \quad \text{for} \quad V \to \infty. \tag{A.4}$$

To show this, we use partial integration to write

$$\begin{aligned} \langle \psi_t^{(V)}, -\nabla V \psi_t^{(V)} \rangle &= \int \mathrm{d}^d x \, V(\mathbf{x}) \nabla \left| \psi_t^{(V)}(\mathbf{x}) \right|^2 \\ &= \int_G \mathrm{d}^d x \nabla \overline{\psi_t^{(V)}} V \psi_t^{(V)} + \text{c.c.} \end{aligned} \tag{A.5}$$

V can now be expressed by the Hamiltonian in (A.2). For the latter, we have

$$\begin{aligned} \langle \psi_t^{(V)}, H_V \psi_t^{(V)} \rangle &= \frac{1}{2m} \langle (\mathbf{P} + e\mathbf{A})\psi_t^{(V)}, (\mathbf{P} + e\mathbf{A})\psi_t^{(V)} \rangle + \langle \psi_t^{(V)}, V \psi_t^{(V)} \rangle \\ &= \frac{1}{2m} \langle (\mathbf{P} + e\mathbf{A})\psi_t^{(V)}, (\mathbf{P} + e\mathbf{A})\psi_t^{(V)} \rangle_{\mathbb{R}^d \setminus G} \\ &\quad + \frac{1}{2m} \langle (\mathbf{P} + e\mathbf{A})\psi_t^{(V)}, (\mathbf{P} + e\mathbf{A})\psi_t^{(V)} \rangle_G + \langle \psi_t^{(V)}, V \psi_t^{(V)} \rangle_G, \end{aligned} \tag{A.6}$$

where the indices denote integration over the respective regions. The term $\langle \psi_t^{(V)}, H_V \psi_t^{(V)} \rangle$ is independent of t and therefore equals the incoming kinetic energy. The first term after the last equality sign converges for $V \to \infty$ to the corresponding expression with Dirichlet boundary conditions on G, by standard results [18, 22], e.g. if $\mathbf{A}$ is bounded and if the initial incoming wavefunction is in the domain of the Hamiltonian. This limit also equals the incoming kinetic energy. Since all terms are non-negative, the remaining terms in (A.6) have to go to zero when $V \to \infty$. Hence for $V \to \infty$,

$$\langle \psi_t^{(V)}, H_V \psi_t^{(V)} \rangle_G \to 0 \tag{A.7}$$

$$\langle \psi_t^{(V)}, V \psi_t^{(V)} \rangle \to 0, \qquad \langle \psi_t^{(V)}, \psi_t^{(V)} \rangle_G \to 0 \tag{A.8}$$

$$\langle (\mathbf{P} + e\mathbf{A})\psi_t^{(V)}, (\mathbf{P} + e\mathbf{A})\psi_t^{(V)} \rangle_G \to 0. \tag{A.9}$$

With this one obtains for bounded **A** and with the inequality

$$\|(\mathbf{P}+e\mathbf{A})\psi_t^{(V)}\|_G^2 \geqslant \big|\|\mathbf{P}\psi_t^{(V)}\|_G - \|e\mathbf{A}\psi_t^{(V)}\|_G\big|^2$$

that also

$$\|\mathbf{P}\psi_t^{(V)}\|_G \to 0 \qquad \text{for} \quad V \to \infty. \tag{A.10}$$

This and Schwartz's inequality then imply that

$$\langle \nabla\psi_t^{(V)}, H_V\psi_t^{(V)}\rangle_G \to 0 \qquad \text{for} \quad V \to \infty \tag{A.11}$$

if the initial wavefunction is in the domain of H_V. Inserting

$$V = H_V - (\mathbf{P}^2 + e\mathbf{A})^2/2m$$

into (A.5), one obtains from (A.11)

$$\begin{aligned}\langle \psi_t^{(V)}, -\nabla V\psi_t^{(V)}\rangle &= -\frac{1}{2m}\int_G \mathrm{d}^d x \nabla\overline{\psi_t^{(V)}}(\mathbf{P}+e\mathbf{A})^2\psi_t^{(V)} + \text{c.c.}\\ &\quad + \text{terms} \to 0 \qquad \text{for} \quad V \to \infty.\end{aligned} \tag{A.12}$$

Using (A.10) and Schwartz's inequality, this yields the claim in (A.4).

We will now investigate the first term on the right-hand side of (A.4) and will show that it can be expressed as a surface integral, i.e. for the ith component

$$\begin{aligned}&-\frac{1}{2m}\int_G \mathrm{d}^d x\, \partial_i\overline{\psi_t^{(V)}}\mathbf{P}^2\psi_t^{(V)} + \text{c.c.}\\ &\qquad = \frac{\hbar^2}{2m}\left\{\int_{\partial G}\partial_i\overline{\psi_t^{(V)}}\nabla\psi_t^{(V)}\cdot \mathbf{do} + \text{c.c.} - \mathbf{e}_i\cdot\int_{\partial G}\mathbf{do}\,\nabla\overline{\psi_t^{(V)}}\cdot\nabla\psi_t^{(V)}\right\}.\end{aligned} \tag{A.13}$$

To prove this we use partial integration, i.e. Gauss's theorem in the form

$$\int_G f\partial_j g = -\int_G(\partial_j f)g + \int_{\partial G}\mathbf{e}_j\cdot \mathbf{do}\, fg. \tag{A.14}$$

Then

$$\int_G \mathrm{d}^d x\,\partial_i\overline{\psi_t^{(V)}}\partial_j\partial_j\psi_t^{(V)} = -\int_G \mathrm{d}^d x\,\partial_j\partial_i\overline{\psi_t^{(V)}}\partial_j\psi_t^{(V)} + \int_{\partial G}\mathbf{e}_j\cdot\mathbf{do}\,\partial_i\overline{\psi_t^{(V)}}\partial_j\psi_t^{(V)} \tag{A.15}$$

and

$$\int_G \mathrm{d}^d x\,\partial_i\psi_t^{(V)}\partial_j\partial_j\overline{\psi_t^{(V)}} = -\int_G \mathrm{d}^d x\,\partial_j\partial_i\psi_t^{(V)}\partial_j\overline{\psi_t^{(V)}} + \int_{\partial G}\mathbf{e}_j\cdot\mathbf{do}\,\partial_i\psi_t^{(V)}\partial_j\overline{\psi_t^{(V)}}. \tag{A.16}$$

Applying (A.14) to the first term on the rhs of (A.16) yields

$$\begin{aligned}\int_G \mathrm{d}^d x\,\partial_i\psi_t^{(V)}\partial_j\partial_j\overline{\psi_t^{(V)}} &= \int_G \mathrm{d}^d x\,\partial_j\psi_t^{(V)}\partial_i\partial_j\overline{\psi_t^{(V)}}\\ &\quad - \int_{\partial G}\mathbf{e}_i\cdot\mathbf{do}\,\partial_j\psi_t^{(V)}\partial_j\overline{\psi_t^{(V)}} + \int_{\partial G}\mathbf{e}_j\cdot\mathbf{do}\partial_i\psi_t^{(V)}\partial_j\overline{\psi_t^{(V)}}.\end{aligned} \tag{A.17}$$

Adding equations (A.15) and (A.17), the first terms cancel and one obtains

$$\begin{aligned}\int_G \mathrm{d}^d x\,\partial_i\overline{\psi_t^{(V)}}\partial_j\partial_j\psi_t^{(V)} + \text{c.c.} &= \int_{\partial G}\mathbf{e}_j\cdot\mathbf{do}\,\partial_i\overline{\psi_t^{(V)}}\partial_j\psi_t^{(V)}\\ &\quad + \int_{\partial G}\mathbf{e}_j\cdot\mathbf{do}\,\partial_j\overline{\psi_t^{(V)}}\partial_i\psi_t^{(V)} - \int_{\partial G}\mathbf{e}_i\cdot\mathbf{do}\,\partial_j\overline{\psi_t^{(V)}}\partial_j\psi_t^{(V)},\end{aligned} \tag{A.18}$$

which gives (A.13).

For large V, (A.13) can be further simplified. Indeed, one has $\psi_t^{(V)} \to 0$ on ∂G for $V \to \infty$ and hence

$$\begin{aligned} \nabla\psi_t^{(V)} &\to \frac{\partial\psi_t^{(V)}}{\partial n}\mathbf{n} \qquad (\mathbf{n} = \text{normal}) \\ \partial_i\psi_t^{(V)} &= \mathbf{e}_i \cdot \nabla\psi_t^{(V)} \to \mathbf{e}_i \cdot \mathbf{n}\frac{\partial\psi_t^{(V)}}{\partial n} \end{aligned} \tag{A.19}$$

for $V \to \infty$. Insertion into (A.13) gives

$$-\frac{1}{2m}\int_G \mathrm{d}^d x\, \partial_i \overline{\psi_t^{(V)}} \mathbf{P}^2 \psi_t^{(V)} + \text{c.c.} = \frac{\hbar^2}{2m}\int_{\partial G} \mathbf{e}_i \cdot \mathbf{n}\, \mathrm{d}o \frac{\partial\overline{\psi_t^{(V)}}}{\partial n}\frac{\partial\psi_t^{(V)}}{\partial n} \tag{A.20}$$

plus terms going to 0 for $V \to \infty$.

For the Lorentz force, one has

$$\left\langle\psi_t^{(V)}, e\mathbf{B} \times \mathbf{v}\psi_t^{(V)}\right\rangle = \left\langle\psi_t^{(V)}, e\mathbf{B} \times m^{-1}(\mathbf{P} + e\mathbf{A})\psi_t^{(V)}\right\rangle_G$$

and one finds from (A.10) and Schwartz‘s inequality together with the boundedness of $\mathbf{B}$ that it decreases to 0 when $V \to \infty$. This, together with equations (A.20) and (A.4), yields (A.3).

These results can be generalized to the situation when the potential V vanishes on a part of the interior of the region G, e.g. one could have a magnetic field in a cylinder of radius R while the shielding would be only in a cylindrical ring $R_1 \leqslant r \leqslant R$. Then for particles coming in from infinity, one obtains the same results as above since the incoming wavefunction will less and less penetrate through the ring. This can be made mathematically precise by a similar reasoning as above.

A.2. Forces in the case of infinite shielding

If one starts right away with infinite shielding, the particle motion takes place completely outside the region G and there is no regular expression for the force acting at the boundary. We therefore use $\mathrm{d}/\mathrm{d}t\langle m\mathbf{v}\rangle$ as definition for the force. Moreover, the Hamiltonian is not uniquely determined, as pointed out before, and we arbitrarily pick for it a particular H_{dum} with a dummy field $\boldsymbol{\Omega}_{\text{dum}}$, analogous to (2). Then

$$m\mathbf{v} = \mathbf{P} + \boldsymbol{\Omega}_{\text{dum}}. \tag{A.21}$$

Now let ψ_t be a normalizable wavefunction coming in from infinity (and being in the domain of H_{dum}). We will show that then

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, m\mathbf{v}\psi_t\rangle = \frac{\hbar^2}{2m}\int_{\partial G} \mathrm{d}\mathbf{o}\left|\frac{\partial\psi_t}{\partial n}\right|^2. \tag{A.22}$$

Note again that the dependence of this expression on the dummy field $\boldsymbol{\Omega}_{\text{dum}}$ comes through the time development via the Hamiltonian. In two dimensions and if the region G is a circle, one arrives at (10) if one lets ψ_t go to a stationary solution of H_{dum}.

To show (A.22), we write the left-hand side as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, m\mathbf{v}\psi_t\rangle = \frac{\mathrm{i}m}{\hbar}\{\langle H_{\text{dum}}\psi_t, \mathbf{v}\psi_t\rangle - \langle\psi_t, \mathbf{v}H_{\text{dum}}\psi_t\rangle\}. \tag{A.23}$$

At this point it is *crucial* that in the first term H_{dum} cannot be moved over to the other side by hermiticity since then one would be led to $[H_{\text{dum}}, \mathbf{v}] = \ddot{\mathbf{x}} = 0$, and thus there would be no force. The underlying mathematical reason why this is not allowed is that $\mathbf{v}\psi_t$ need not lie in the domain of $H_{\rm dum}$. However, one can move $\mathbf{\Omega}_{\rm dum}\cdot\mathbf{P}$ over by partial integration since the boundary terms vanish. Thus,

$$\frac{\rm d}{{\rm d}t}\langle\psi_t, m\mathbf{v}\psi_t\rangle = \frac{{\rm i}m}{2m\hbar}\int_{\mathbb{R}^d\setminus G}{\rm d}^d x\left\{\overline{\mathbf{P}^2\psi_t}\mathbf{v}\psi_t + \overline{\psi_t}\left(2\mathbf{\Omega}_{\rm dum}\cdot\mathbf{P}+\mathbf{\Omega}^2_{\rm dum}\right)\mathbf{v}\psi_t - \overline{\psi_t}\mathbf{v}H_{\rm dum}\psi_t\right\}. \tag{A.24}$$

Inserting $0=\overline{\psi_t}\hbar^2\nabla^2(\mathbf{v}\psi_t)-\overline{\psi_t}\hbar^2\nabla^2(\mathbf{v}\psi_t)$ gives

$$\frac{\rm d}{{\rm d}t}\langle\psi_t, m\mathbf{v}\psi_t\rangle = \frac{{\rm i}m}{2m\hbar}\int_{\mathbb{R}^d\setminus G}{\rm d}^d x\{-\hbar^2(\nabla^2\overline{\psi_t})\mathbf{v}\psi_t+\overline{\psi_t}\hbar^2\nabla^2(\mathbf{v}\psi_t)+\overline{\psi_t}[H_{\rm dum},\mathbf{v}]\psi_t\}.$$

Note that the last commutator vanishes. Inserting (A.21) the $\mathbf{\Omega}_{\rm dum}$ terms cancel, by partial integration as in (A.14), since the boundary terms vanish. Thus, one obtains for the ith component of the force in (A.23)

$$\begin{aligned}\frac{\rm d}{{\rm d}t}\langle\psi_t, m v_i\psi_t\rangle &= \frac{-\hbar^2}{2m}\int_{\mathbb{R}^d\setminus G}{\rm d}^d x\{\nabla^2\overline{\psi_t}\partial_i\psi_t-\overline{\psi_t}\nabla^2\partial_i\psi_t\}\\ &= \frac{-\hbar^2}{2m}\left\{-\int_{\mathbb{R}^d\setminus G}{\rm d}^d x\nabla\overline{\psi_t}\cdot\nabla\partial_i\psi_t - \int_{\partial G}{\rm d}\mathbf{o}\cdot\nabla\overline{\psi_t}\partial_i\psi_t\right.\\ &\quad\left.+\int_{\mathbb{R}^d\setminus G}{\rm d}^d x\nabla\overline{\psi_t}\cdot\nabla\partial_i\psi_t+\int_{\partial G}{\rm d}\mathbf{o}\cdot\overline{\psi_t}\nabla\partial_i\psi_t\right\},\end{aligned}$$

where the last equality results from partial integration. The first and third terms cancel, while the last one is zero since ψ vanishes on the boundary. This yields

$$\frac{\rm d}{{\rm d}t}\langle\psi_t, m\mathbf{v}\psi_t\rangle = \frac{\hbar^2}{2m}\int_{\partial G}{\rm d}\mathbf{o}\cdot\nabla\overline{\psi_t}\nabla\psi_t. \tag{A.25}$$

Since $\nabla\psi_t$ is perpendicular to the boundary ∂G, this gives (A.22).

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