Berry phase in magnetic systems with point perturbations

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Abstract

We study a two-dimensional charged particle interacting with a magnetic field, in general non-homogeneous, perpendicular to the plane, a confining potential, and a point interaction. If the latter moves adiabatically along a loop, the state corresponding to an isolated eigenvalue acquires a Berry phase. We derive an expression for it and evaluate it in several examples such as a homogeneous field, a magnetic whisker, a particle confined at a ring or in quantum dots, a parabolic and a zero-range one. We also discuss the behavior of the lowest Landau level in this setting obtaining an explicit example of the Wilczek–Zee phase for an infinitely degenerated eigenvalue. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

A non-trivial Berry phase [4] can be demonstrated in different situations. There is a growing interest recently to this effect in mesoscopic systems (see, e.g., [22,24] and references therein). These papers investigate theoretically and experimentally how the phase is manifested in quantum dynamics of a particle with spin interacting with a time-dependent magnetic field. In the present paper, we are going to discuss a simple model in which the Berry phase emerges even if the spin–orbital coupling is neglected.

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The model describes a charged particle confined to a potential well and placed into a magnetic field of constant direction, which is independent of time and may be homogeneous. The phase will appear when the well is moving adiabatically. A similar situation appears in the Born–Oppenheimer approach for the study of molecules (see, e.g., [17] and references therein) and impurities in semiconductors [30]. For the sake of simplicity, we suppose that the well represents a zero-range interaction, i.e., it is given by a point interaction in the plane. This makes it possible to derive explicit formulae for the Berry potential. The idea of employing point interactions to this purpose is not new: some solvable models exhibiting a non-trivial Berry phase have been constructed earlier. For instance, the geometric phase resulting from a cyclical motion of the boundary condition for the Dirac and Schrödinger equations on an interval $[0, \ell]$ was computed in [7,16]. On the other hand, Cheon and Shigehara [9] investigated the Berry phase which arises when a pointlike scatterer is adiabatically moved in a rectangular billiard in such a way that the energy levels encircle a "diabolic point".

In our cases, the results are simpler and rather illustrative. In particular, we shall show that moving the zero-radius potential well–defined in accordance with [1,31]–along a closed curve in the plane, the eigenfunctions of a particle trapped by the well and exposed to a homogeneous field perpendicular to the plane acquire a phase which coincides with the number of magnetic field quanta through the area restricted by the curve. This picture changes if an additional confining potential is added, say, in the form of an annular potential "ditch". In the limiting case of an infinitely thin ring, the motion of the point interaction induces a geometric phase which differs from the above one on a quantity proportional to the persistent current in the annulus. Recall that persistent currents in a ring with a point perturbation were investigated (see, e.g., [8]), but the relation to the Berry phase was not noticed.

Let us describe briefly the contents of the paper. In the next section, we shall recall briefly how the zero-range interaction in a magnetic system is constructed and how its spectrum is determined by means of the Krein's formula. For simplicity, we suppose always that the magnetic field as well as the possible confining scalar potential are rotationally symmetric. The central part of the paper is Section 3, where we derive a general expression for the Berry potential corresponding to a point interaction moving along a smooth curve (cf. Eq. (3.18)).

This result is illustrated on a number of examples in the next section. We show that the Berry phase for the perturbation moving along a closed loop C in a homogeneous field without a scalar potential is proportional to the number of flux quanta through C. In distinction to that, the phase corresponding to a magnetic whisker contains an extra term proportional to the persistent current in the loop C. For comparison, we analyze an electron confined to a circular ring and find the same Berry phase expression containing the persistent-current term, in this case independently of the field profile. Finally, we discuss a harmonic quantum dot in a homogeneous field. We show that if the point interaction is strong, the effect of the confining potential is small and the Berry phase is again given by the number of the flux quanta through C, up to an error term. We compare this with the situation, where the quantum dot itself is zero-range.

The behavior of degenerate eigenvalues under adiabatic change of parameters is more complicated and less understood. In the final section, we address this question in the present

setting and discuss what happens in this situation with the lowest Landau level. We compute the generalized Berry potential which determines the corresponding Wilczek–Zee phase, and find the latter for adiabatic evolution around a small loop. It appears to be non-trivial for the angular momentum $m = 1$, while the states with higher momenta are not affected. Moreover, the phase which arises here differs in sign from the one corresponding to the isolated energy level; we explain this effect as a sort of topological charge conservation.

2. Magnetic systems with a point perturbation

As indicated above, we shall consider a charged particle of charge e and mass m_* (which may be thought of as the effective mass of an electron in a crystal) living in the plane with Cartesian coordinates x, y and exposed to a magnetic field perpendicular to the plane, $\mathbf{B} = B(x, y)\mathbf{e}_z$. We also assume that the particle may be confined to a part of the plane by a non-negative potential W. The main simplifying assumption we shall make concerns the *rotational symmetry*: we suppose that there is a system of polar coordinates r, φ such that the magnetic field and the confining potential depend on the radial coordinate only, $B = B(r)$ and $W = W(r)$. In this case one can choose a gauge in such a way that the radial component of the vector potential vanishes, $A_r(r, \varphi) = 0$, and $A_\varphi(r, \varphi) = A_\varphi(r)$ depends on r only. In particular, $\nabla \mathbf{A} = 0$.

It is convenient to single out the uniform component of the magnetic field, $\mathbf{B} = \mathbf{B}_0 + \mathbf{B}_1$ with $\mathbf{B}_0$ being a fixed vector. Of course, such a decomposition is arbitrary, but, mostly we will have in mind situations when $\mathbf{B}$ has a finite limit as $r \to \infty$; then the non-uniqueness is removed by the requirement $\mathbf{B}_1 \to 0$. We shall also employ the corresponding decomposition of the vector potential, $\mathbf{A} = \mathbf{A}_0 + \mathbf{A}_1$. In view of the assumed symmetry, it is natural to use the circular gauge, $\mathbf{A}_0(r) = \frac{1}{2}B_0 r \mathbf{e}_\varphi$. As for the non-constant part, we are particularly interested in the example of an infinitely thin Aharonov–Bohm solenoid, or a magnetic flux line with $A_{1\varphi}(r) = \Phi/2\pi r$, where Φ is the magnetic flux through the solenoid. It is convenient to use a dimensionless parameter η, $\eta = \Phi/\Phi_0$, where

$$\Phi_0 = \frac{2\pi \hbar c}{|e|}$$

is the magnetic flux quantum; so η is the number of quanta carried by the solenoid. The corresponding magnetic field is concentrated at the origin of the coordinates, $\mathbf{B}_1 = \Phi\delta(r)\mathbf{e}_z$.

In the following considerations, however, we assume only that $A_{1\varphi}$ is a smooth function of the variable r on the half-line $(0, \infty)$. Under the stated assumption, the particle Hamiltonian has the following form:

$$
\begin{aligned}
H &= \frac{1}{2m_*}\left(-\mathrm{i}\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2 + W \\
&= -\frac{\hbar^2}{2m_*}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right] + \frac{e\hbar}{2m_*c}\left(B_0 + \frac{2}{r}A_{1\varphi}(r)\right)\left(\mathrm{i}\frac{\partial}{\partial\varphi}\right) \\
&\quad + \frac{e^2}{2m_*c^2}\left(\frac{1}{4}B_0^2 r^2 + B_0 r A_{1\varphi}(r) + A_{1\varphi}(r)^2\right) + W(r).
\end{aligned}
\tag{2.1}
$$

The potential W is non-negative by assumption, and therefore H is a well-defined self-adjoint operator, which can be understood, e.g., as the Friedrichs extension of the operator defined on $C_0^\infty(\mathbb{R}^2 \setminus \{0\})$ by the RHS of Eq. (2.1).

Now we shall introduce a point perturbation of the above Hamiltonian located at a point $\mathbf{s} \in \mathbb{R}^2$ with the polar coordinates (ρ, θ). (Further we will assume that $\mathbf{s} \neq 0$ if $\mathbf{A}_1$ has a singularity at the point $r = 0$.) The perturbed operator $H_{\alpha,\mathbf{s}}$ is conventionally obtained as a self-adjoint extension of the symmetric operator S which is a restriction of H to the domain

$$\mathcal{D} := \{\psi \in \mathcal{D}(H) : \psi(\mathbf{s}) = 0\}, \tag{2.2}$$

since the deficiency indices of S are $(1, 1)$, the extensions are characterized by a single parameter α. Under rather general assumptions about the Hamiltonian [15], the Green's function $G_{\alpha,\mathbf{s}}(\mathbf{r}, \mathbf{r}'; E)$ of $H_{\alpha,\mathbf{s}}$ is given by the Krein formula

$$G_{\alpha,\mathbf{s}}(\mathbf{r}, \mathbf{r}'; E) = G(\mathbf{r}, \mathbf{r}'; E) - [Q(E; \mathbf{s}) + \alpha]^{-1} G(\mathbf{r}, \mathbf{s}; E) G(\mathbf{s}, \mathbf{r}'; E), \tag{2.3}$$

where $Q(E; \mathbf{s})$ is the so-called Krein Q-function or renormalized Green's function at the diagonal point $(\mathbf{s}, \mathbf{s})$,

$$Q(E; \mathbf{s}) := \lim_{\mathbf{r} \to \mathbf{s}} \left[G(\mathbf{r}, \mathbf{s}; E) - \frac{m_*}{\pi \hbar^2} \ln |\mathbf{r} - \mathbf{s}|^{-1} \right], \tag{2.4}$$

and α is the mentioned parameter. The latter is related to the scattering length λ of the point interaction by the formula

$$\alpha = \frac{m_*}{\pi \hbar^2} \ln \lambda^{-1}. \tag{2.5}$$

Less formally, the point perturbation at a point $\mathbf{s}$ may be defined via the Fermi pseudopotential of the form

$$\mu \delta(\mathbf{r} - \mathbf{s})(1 - \ln |\mathbf{r} - \mathbf{s}|(\mathbf{r} - \mathbf{s})\nabla_{\mathbf{r}}), \tag{2.6}$$

where the coupling constant μ is related to the parameter α by $\mu = \alpha^{-1}$.

Under rather weak regularity requirements on the potentials $\mathbf{A}(r)$ and $W(r)$, the Green's function is of the form

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{m_*}{\pi \hbar^2} \ln |\mathbf{r} - \mathbf{r}'|^{-1} + G_0(\mathbf{r}, \mathbf{r}'; E), \tag{2.7}$$

where G_0 is continuous in the variables $\mathbf{r}, \mathbf{r}'$ and analytic with respect to E in the resolvent set, $\mathbb{C} \setminus \sigma(H)$, of the free operator. It is the case, e.g., if $\mathbf{A}_1$ and W are smooth functions (see, e.g., [3], Chapter III, Theorem 5.1). If $\mathbf{A}_1$ has a singularity at the origin, then every point $\mathbf{r}, \mathbf{r} \neq 0$, has a neighborhood such that Eq. (2.7) is true for $\mathbf{r}'$ in this neighborhood.

Since the singular term in Eq. (2.7) is energy independent, $\partial G / \partial E$ needs no renormalization and we have

$$\frac{\partial Q(E; \mathbf{s})}{\partial E} = \frac{\partial G}{\partial E}(\mathbf{s}, \mathbf{s}; E). \tag{2.8}$$

Due to the well-known Weyl theorem, the essential spectra of H and $H_{\alpha,\mathbf{s}}$ coincide. As for the discrete spectrum, it may happen that H and $H_{\alpha,\mathbf{s}}$ have a common eigenvalue. Let E be an

isolated eigenvalue of H such that there exists a corresponding eigenfunction ψ satisfying $\psi(\mathbf{s}) = 0$ (in particular, this can be always achieved if E is a degenerate eigenvalue). Then E belongs to the spectrum of $H_{\alpha,\mathbf{s}}$ as an isolated eigenvalue; moreover, the multiplicity m' of E in the spectrum of $H_{\alpha,\mathbf{s}}$ obeys the inequality $m' \geq m - 1$, where m is the multiplicity of E in the spectrum of H. This assertion may be proven following the arguments from [10], where a special case of our claim has been considered. In addition, the spectrum of $H_{\alpha,\mathbf{s}}$ contains all solutions of the equation

$$Q(E; \mathbf{s}) + \alpha = 0 \tag{2.9}$$

(the true levels of the zero-range well). Every solution of this equation lies in a gap of the unperturbed spectrum and is a simple isolated eigenvalue of $H_{\alpha,\mathbf{s}}$. The corresponding eigenfunction ψ has the form

$$\psi(\mathbf{r}) = \left[\frac{\partial Q}{\partial E}(E, \mathbf{s}) \right]^{-1/2} G(\mathbf{r}, \mathbf{s}; E). \tag{2.10}$$

Recall that in the real part of the resolvent set, the derivative is positive, $(\partial Q/\partial E)(E) > 0$ for $E \in \mathbb{R} \setminus \sigma(H)$ (cf. [20]). Therefore, Eq. (2.10) has at most one solution in every gap of the spectrum $\sigma(H)$. Generally speaking, Eq. (2.9) may have no solutions (see, e.g., [2]). It is straightforward to see that if E_0 is an isolated eigenvalue of H and $\psi(\mathbf{s}) \neq 0$ holds for at least one eigenfunction corresponding to E_0, then E_0 is a pole of the function $Q(\cdot; \mathbf{s})$. Hence if $\sigma(H)$ is purely discrete, solutions of Eq. (2.10) exist in infinitely many spectral gaps.

A simple but important particular case of the considered problem, $\mathbf{A}_1 = 0$ and $W = 0$, concerns a free motion in a uniform magnetic field. In this situation, the Green function acquires the following explicit form:

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{m_*}{2\pi \hbar^2} \Gamma\left(\frac{1}{2} - \frac{E}{\hbar \omega_c} \right) \exp\left[-\pi i \xi_0 \mathbf{r} \wedge \mathbf{r}' - \frac{(\mathbf{r} - \mathbf{r}')^2}{4 a_0^2} \right]$$
$$\times \Psi\left(\frac{1}{2} - \frac{E}{\hbar \omega_c}, 1; \frac{(\mathbf{r} - \mathbf{r}')^2}{4 a_0^2} \right), \tag{2.11}$$

where

$$\omega_c := \frac{|e B_0|}{m_* c}$$

is the cyclotronic frequency,

$$\xi_0 := \frac{e B_0}{2\pi \hbar c}$$

is the flux density of the uniform component of the magnetic field,

$$a_0 := \left(\frac{\hbar}{m_* \omega_c} \right)^{1/2} = (2\pi |\xi_0|)^{-1/2} \tag{2.12}$$

is the magnetic length, and Ψ is the Tricomi confluent hypergeometric function (cf. [11]). The Q-function now obviously does not depend on $\mathbf{s}$ and equals [12,14]:

$$Q(E) = -\frac{m_*}{2\pi\hbar^2}\left[\psi\left(\frac{1}{2} - \frac{E}{\hbar\omega_c}\right) + 2\gamma - \ln 2 - 2\ln a_0\right], \tag{2.13}$$

where $\psi(x) = (\ln\Gamma(x))'$ and $\gamma = -\psi(1)$ is the Euler constant. Up to a scaling and a shift in the argument, the behavior of $Q(E)$ is given by that of the digamma function ψ; this shows that in a uniform magnetic field, the zero-range potential with any fixed $\alpha \in \mathbb{R}$ induces existence of an energy level on the half-line $(-\infty, \varepsilon_0)$ as well as in each interval $(\varepsilon_\ell, \varepsilon_{\ell+1})$, where $\varepsilon_\ell := (\ell + \frac{1}{2})\hbar\omega_c$ are the Landau levels.

3. The Berry phase

Let us return to the condition (2.9). In what follows, we will keep α fixed (and drop it mostly from the notation) and move the point $\mathbf{s}$ along a smooth path $C : \mathbf{s} = \mathbf{s}(t), t \in [0, 1]$, in the plane $\mathbb{R}^2$ (or in the punctured plane $\mathbb{R}^2 \setminus \{\mathbf{0}\}$ if $\mathbf{A}_1$ has a singularity at the point $\mathbf{0}$) in such a way that Eq. (2.9) has a solution $E_0(\mathbf{s}, \alpha)$ lying in a gap of the unperturbed Hamiltonian H. Denote

$$\psi_{\mathbf{s}}(\mathbf{r}) = \left[\frac{\partial Q}{\partial E}(E_0(\mathbf{s}, \alpha), \mathbf{s})\right]^{-1/2} G(\mathbf{r}, \mathbf{s}; E_0(\mathbf{s}, \alpha)), \tag{3.1}$$

the corresponding normalized eigenfunction of the perturbed operator $H_{\alpha,\mathbf{s}}$ (see (2.10)). If the path C is a closed loop, $\mathbf{s}(0) = \mathbf{s}(1)$, the initial and final state, $\psi_{\mathbf{s}(0)}$ and $\psi_{\mathbf{s}(1)}$, respectively, differ by a phase factor,

$$\psi_{\mathbf{s}(1)} = \psi_{\mathbf{s}(0)}\exp\left(-\frac{i}{\hbar}\int_0^1 E_0(\mathbf{s}(t))\,\mathrm{d}t + i\gamma(C)\right), \tag{3.2}$$

where the Berry phase $\gamma(C)$ depends only on the path C; in accordance with Ref. [4], it equals

$$\gamma(C) = \int_C \mathbf{V}(\mathbf{s})\,\mathrm{d}\mathbf{s}, \tag{3.3}$$

where

$$\mathbf{V}(\mathbf{s}) := i\langle\psi_{\mathbf{s}}|\boldsymbol{\nabla}_{\mathbf{s}}|\psi_{\mathbf{s}}\rangle \tag{3.4}$$

is the so-called Berry vector potential. Recall that from the differential-geometric point of view $\mathrm{Im}\,\langle\psi_{\mathbf{s}}|\boldsymbol{\nabla}_{\mathbf{s}}|\psi_{\mathbf{s}}\rangle$ is a connection 1-form in a principal fiber bundle over $\mathbb{R}^2$ (or $\mathbb{R}^2 \setminus \{\mathbf{0}\}$) associated with the eigenfunction fibration $\psi_{\mathbf{s}} \mapsto \mathbf{s}$ [26]; in other words, this quantity is a gauge potential with the gauge group $\mathbf{U}(1)$. We shall express $\mathbf{V}(\mathbf{s})$ in the polar coordinates:

$$\mathbf{V}(\mathbf{s}) = V_\rho(\rho, \theta)\mathbf{e}_\rho + V_\theta(\rho, \theta)\mathbf{e}_\theta \tag{3.5}$$

with

$$V_\rho = \mathrm{i}\langle \psi_\mathbf{s} | \nabla_\rho | \psi_\mathbf{s} \rangle, \qquad V_\theta = \frac{\mathrm{i}}{\rho} \langle \psi_\mathbf{s} | \nabla_\theta | \psi_\mathbf{s} \rangle. \tag{3.6}$$

To proceed further, we need more information about the structure of the Green's function $G(\mathbf{r}, \mathbf{r}'; E)$. First of all, we decompose the state space $L^2(\mathbb{R}^2)$ into partial waves, i.e., we represent it as $L^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes L^2(\mathbb{S}^1, \mathrm{d}\varphi)$ and perform the Fourier transform on the second component, $L^2(\mathbb{S}^1, \mathrm{d}\varphi) \to \ell^2(\mathbb{Z})$ with

$$g \mapsto \{g_m\}_{m\in\mathbb{Z}}, \qquad g_m = \frac{1}{(2\pi)^{1/2}} \int_0^{2\pi} g(\varphi)\,\mathrm{e}^{-\mathrm{i}m\varphi}\,\mathrm{d}\varphi. \tag{3.7}$$

Then $L^2(\mathbb{R}^2)$ decomposes into an orthogonal sum of subspaces each of which is isomorphic to the radial component:

$$L^2(\mathbb{R}^2) \simeq \bigoplus_{m=-\infty}^{\infty} L^2(\mathbb{R}_+, r\,\mathrm{d}r). \tag{3.8}$$

The unperturbed operator H commutes with rotations around the origin, and therefore it decomposes correspondingly into the orthogonal sum

$$H = \bigoplus_{m=-\infty}^{\infty} H_m, \tag{3.9}$$

where the partial-wave parts H_m are self-adjoint operators in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ obtained as the Friedrichs extensions of the operators (2.1) with the domain $C_0^\infty(\mathbb{R}_+, r\,\mathrm{d}r)$ and $-\mathrm{i}\partial/\partial\varphi$ replaced by m. It is obvious that each H_m is a real operator, i.e., that it commutes with the operator of complex conjugation in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$. It follows that its Green's function $G_m(r, r'; E)$ is real-valued for a real E.

The full Green's function can be expressed through its partial-wave components as

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}m(\varphi-\varphi')} G_m(r, r'; E). \tag{3.10}$$

It follows that $\langle \psi_\mathbf{s} | \nabla_\rho | \psi_\mathbf{s} \rangle$ is a real number. On the other hand, differentiating the identity $\langle \psi_\mathbf{s}|\psi_\mathbf{s}\rangle = 1$, we see that the real part of $\langle \psi_\mathbf{s} | \nabla_\rho | \psi_\mathbf{s} \rangle$ (as well as $\langle \psi_\mathbf{s} | \nabla_\theta | \psi_\mathbf{s} \rangle$) vanishes. Consequently, the radial component of the Berry potential $V_\rho(\mathbf{s}) = 0$. To find the angular one, let us differentiate the identity

$$(H - E)G(\mathbf{r}, \mathbf{s}; E) = \delta(\mathbf{r} - \mathbf{s}) \tag{3.11}$$

with respect to the constant component B_0 of the magnetic field, keeping E and $\mathbf{s}$ fixed; this yields

$$\frac{\partial H}{\partial B_0} G + (H - E)\frac{\partial G}{\partial B_0} = 0. \tag{3.12}$$

Notice that $\partial G/\partial B_0$ is a smooth function in view of (2.7). Hence

$$\left\langle G\,|(H-E)|\,\frac{\partial G}{\partial B_0} \right\rangle = \left\langle \delta(\mathbf{r}-\mathbf{s})\,\left|\,\frac{\partial G(\mathbf{r},\mathbf{s};E)}{\partial B_0} \right.\right\rangle = \frac{\partial G}{\partial B_0}(\mathbf{s},\mathbf{s};E) = \frac{\partial Q}{\partial B_0}(E,\mathbf{s}),$$

and therefore

$$\left\langle G \left| \frac{\partial H}{\partial B_0} \right| G \right\rangle + \frac{\partial Q}{\partial B_0} = 0. \tag{3.13}$$

Dividing both terms of this expression by $\partial Q / \partial E$ and putting $E = E_0(\mathbf{s})$, we arrive at the relation

$$\left\langle \psi_{\mathbf{s}} \left| \frac{\partial H}{\partial B_0} \right| \psi_{\mathbf{s}} \right\rangle + \frac{\partial Q}{\partial B_0} \left(\frac{\partial Q}{\partial E} \right)^{-1} = 0. \tag{3.14}$$

Since $E_0(\mathbf{s})$ solves Eq. (2.9), the last term at the LHS can be expressed as

$$\frac{\partial Q}{\partial B_0} \left(\frac{\partial Q}{\partial E} \right)^{-1} \bigg|_{E=E_0} = -\frac{\partial E_0}{\partial B_0},$$

so

$$\left\langle \psi_{\mathbf{s}} \left| \frac{\partial H}{\partial B_0} \right| \psi_{\mathbf{s}} \right\rangle = \frac{\partial E_0}{\partial B_0}. \tag{3.15}$$

Now we shall employ the formula (2.1) which yields

$$\frac{\partial H}{\partial B_0} = \mathrm{i} \frac{e\hbar}{2m_*c} \frac{\partial}{\partial \varphi} + \frac{e^2 B_0}{4m_*c^2} r^2 + \frac{e^2}{2m_*c^2} r A_{1\varphi}(r). \tag{3.16}$$

It follows from (3.10) that $(\partial/\partial\theta)G(\mathbf{r}, \mathbf{s}; E) = -(\partial/\partial\varphi)G(\mathbf{r}, \mathbf{s}; E)$, and furthermore, that $Q(E, \mathbf{s})$ is independent of the angular variable, $Q(E, \mathbf{s}) = Q(E, \rho)$. The last claim means that $E_0(\mathbf{s})$ also does not depend on θ. As a result we have that $\nabla_\theta \psi_{\mathbf{s}} = -\nabla_\varphi \psi_{\mathbf{s}}$. Finally, we express the angular momentum operator from (3.16) as

$$-\mathrm{i} \frac{\partial}{\partial \varphi} = -\frac{2m_*c}{e\hbar} \frac{\partial H}{\partial B_0} + \pi \xi_0 r^2 + (\mathrm{sgn}\, e) \frac{2\pi}{\Phi_0} r A_{1\varphi}(r), \tag{3.17}$$

which allows us to cast the sought angular component into the form

$$V_\theta(\rho) = \frac{1}{\rho} \left[-\frac{2m_*c}{e\hbar} \frac{\partial E_0(\mathbf{s})}{\partial B_0} + \pi\xi_0 \langle \psi_{\mathbf{s}} | r^2 | \psi_{\mathbf{s}} \rangle + (\mathrm{sgn}\, e) \frac{2\pi}{\Phi_0} \langle \psi_{\mathbf{s}} | r A_{1\varphi}(r) | \psi_{\mathbf{s}} \rangle \right]$$

$$= \frac{1}{\rho} \left[-\frac{m_*}{\pi\hbar^2} \frac{\partial E_0(\mathbf{s})}{\partial \xi_0} + \pi\xi_0 \langle \psi_{\mathbf{s}} | r^2 | \psi_{\mathbf{s}} \rangle + (\mathrm{sgn}\, e) \frac{2\pi}{\Phi_0} \langle \psi_{\mathbf{s}} | r A_{1\varphi}(r) | \psi_{\mathbf{s}} \rangle \right]. \tag{3.18}$$

We stress that in view of (3.10), V_θ is independent of θ.

4. Examples

Let us now illustrate the Berry phase behavior on several examples.

4.1. An homogeneous field

Suppose that the magnetic field is uniform, i.e., $\mathbf{A}_1 = 0$. Since the Green and Krein functions are explicitly known in this case, it is convenient to evaluate the Berry potential directly from the relation (3.4). It follows from (2.11) that $\psi_\mathbf{s}$ is of the form

$$\psi_\mathbf{s}(\mathbf{r}) = \exp[-\pi\,\mathrm{i}\xi_0(\mathbf{r} \wedge \mathbf{s})] f(|\mathbf{r} - \mathbf{s}|), \tag{4.1}$$

and therefore

$$\nabla_\theta \psi_\mathbf{s}(\mathbf{r}) = -\pi\,\mathrm{i}\xi_0\, r\rho\,(\cos\varphi\cos\theta + \sin\varphi\sin\theta) \exp[-\pi\,\mathrm{i}\xi_0(\mathbf{r} \wedge \mathbf{s})] f(|\mathbf{r} - \mathbf{s}|)$$
$$+ \exp[-\pi\,\mathrm{i}\xi_0(\mathbf{r} \wedge \mathbf{s})] \nabla_\theta f(|\mathbf{r} - \mathbf{s}|). \tag{4.2}$$

Inspecting the explicit form of the function f, we see that it is real-valued and normalized, $\|f\|^2 = 1$. It follows that

$$\langle\psi_\mathbf{s}|\exp[-\pi\,\mathrm{i}\xi_0(\mathbf{r} \wedge \mathbf{s})]\nabla_\theta|f\rangle = \langle f|\nabla_\theta|f\rangle = \tfrac{1}{2}\nabla_\theta\|f\|^2 = 0,$$

so the sought quantity is given by the first term only:

$$\langle\psi_\mathbf{s}|\nabla_\theta|\psi_\mathbf{s}\rangle = -\pi\,\mathrm{i}\xi_0 \int_{\mathbb{R}^2} \mathbf{r}\cdot\mathbf{s}\,|f(|\mathbf{r}-\mathbf{s}|)|^2\,\mathrm{d}\mathbf{r} = -\pi\,\mathrm{i}\xi_0 \int_{\mathbb{R}^2} (\mathbf{s}^2 + \mathbf{r}\cdot\mathbf{s})|f(|\mathbf{r}|)|^2\,\mathrm{d}\mathbf{r}$$

$$= -\pi\,\mathrm{i}\xi_0\left(\rho^2\int_{\mathbb{R}^2}|f(|\mathbf{r}|)|^2\,\mathrm{d}\mathbf{r} + \rho\int_{\mathbb{R}^2} r(\cos\varphi\cos\theta\right.$$

$$\left. + \sin\varphi\sin\theta)|f(|\mathbf{r}|)|^2\,\mathrm{d}\mathbf{r}\right). \tag{4.3}$$

The first integral obviously equals 1 and the second 0, hence

$$V_\theta(\rho) = \frac{\mathrm{i}}{\rho}\langle\psi_\mathbf{s}|\nabla_\theta|\psi_\mathbf{s}\rangle = \pi\xi_0\rho \tag{4.4}$$

and the Berry phase is given by

$$\gamma(C) = 2\pi\xi_0 S, \tag{4.5}$$

where S is the area encircled by the loop C. We can write it also as

$$\gamma(C) = 2\pi\,\mathrm{sgn}\,e\,\frac{\Phi_C}{\Phi_0}, \tag{4.6}$$

where Φ_C is the full magnetic flux through the loop. Comparing (4.4) which corresponds to $\mathbf{A}_1 = 0$ with the general expression (3.18) derived in the previous section, we get in the limit $\rho \to 0$, the relation

$$\frac{\partial E_0}{\partial B_0} = \frac{m_*}{4B_0}\,\omega_\mathrm{c}^2\langle\psi_\mathbf{0}\,|r^2|\,\psi_\mathbf{0}\rangle. \tag{4.7}$$

Let us finish the example with a remark concerning an extension of the above result to three-dimensional systems. Suppose that the field is parallel to the z-axis and $\mathbf{B}(\rho, \varphi, z) = \mathbf{B}(\rho)$ holds in the cylindrical coordinates. Then we have $V_\rho = 0$, $V_\theta = \pi\xi_0\rho$, and $V_\zeta = 0$,

where (ρ, θ, ζ) are the cylindrical coordinates of the point $\mathbf{s}$. Consequently, the Berry phase along a closed loop C is again $\gamma(C) = 2\pi\Phi_C/\Phi_0$, up to a sign, where Φ_C is now the magnetic flux through the projection of C to a plane perpendicular to the field.

4.2. A magnetic whisker

The opposite extreme corresponds to the situation, where the homogeneous component is absent and the field is concentrated into a flux line (sometimes called Aharonov–Bohm solenoid), i.e., $\mathbf{B}_0 = 0$ and $\mathbf{A}_1 = (\eta\Phi_0/2\pi r)\mathbf{e}_\varphi$. Then (3.18) yields

$$V_\theta(\rho) = -\frac{m_*}{\pi\hbar^2\rho}\frac{\partial E_0}{\partial\xi_0} + \frac{\eta}{\rho}\operatorname{sgn} e. \tag{4.8}$$

Suppose, in particular that the point perturbation moves along a circle C of radius R centered at the origin of coordinates. In that case, the Berry phase equals

$$\gamma(C) = -\frac{2m_*}{\hbar^2}\frac{\partial E_0}{\partial\xi_0}\bigg|_{B_0=0} + 2\pi(\operatorname{sgn} e)\eta. \tag{4.9}$$

The total flux Φ_C of the field $\mathbf{B}$ through the circle C is $(\pi R^2\xi_0 + \eta)\Phi_0$. Keeping the flux Φ fixed, we have $\partial/\partial\xi_0 = \pi R^2\Phi_0(\partial/\partial\Phi_C)$. Hence

$$\gamma(C) = \left[-\frac{2\pi m_* R^2\Phi_0}{\hbar^2}\frac{\partial E_0}{\partial\Phi_C} + 2\pi(\operatorname{sgn} e)\frac{\Phi_C}{\Phi_0}\right]_{B_0=0}. \tag{4.10}$$

Recall that for a particle confined to the loop C, the derivative $\partial E_0/\partial\Phi_C$ equals $-(1/c)I_0$, where I_0 is the corresponding persistent current. To understand better the meaning of Eq. (4.10), we consider the following example.

4.3. Electron in a ring

Up to now the confining potential of (2.1) was trivial. The previous example inspires us to analyze another extreme situation in which W is a very deep and narrow well. To get a solvable model, we employ the usual idealization and suppose that the particle is confined to an infinitely thin circular ring C pierced by the magnetic field. In that case, the Hamiltonian H becomes one-dimensional. Having in mind an electron, $e < 0$, we can write H as

$$H = \frac{\hbar^2}{2m_* R^2}\left(-\mathrm{i}\frac{\partial}{\partial\varphi} + \eta\right)^2, \tag{4.11}$$

where R is the ring radius and $\Phi = \eta\Phi_0$ is the total flux of the field $\mathbf{B}$ through the circle; the field profile is irrelevant here. The Green and Krein functions are of the form

$$G(\varphi, \varphi'; E) = \frac{m_* R}{\pi\hbar^2}\sum_{m=-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}m(\varphi-\varphi')}}{(m+\eta)^2 - (2m_* R^2/\hbar^2)E}, \tag{4.12}$$

$$Q(E; \eta) = \frac{m_* R}{\pi \hbar^2} \sum_{m=-\infty}^{\infty} \left[(m + \eta)^2 - \frac{2m_* R^2}{\hbar^2} E \right]^{-1}$$

$$= \frac{m_*}{\hbar (m_* E)^{1/2}} \frac{\sin(2\pi R/\hbar)(2m_* E)^{1/2}}{\cos(2\pi R/\hbar)(2m_* E)^{1/2} - \cos 2\pi \eta}. \tag{4.13}$$

Consider now a point perturbation of the operator H,

$$H_\theta = H + \alpha^{-1} \delta(\varphi - \theta). \tag{4.14}$$

As above the Green's function for H_θ is given by the Krein formula

$$G_\theta(\varphi, \varphi'; E) = G(\varphi, \varphi'; E) - [Q(E) + \alpha]^{-1} G(\varphi, \theta; E) G(\theta, \varphi'; E). \tag{4.15}$$

A solution to the spectral condition

$$Q(E) + \alpha = 0 \tag{4.16}$$

exists in each interval $(\tilde{E}_\ell, \tilde{E}_{\ell+1})$, where $\{\tilde{E}_\ell\}_{\ell \geq 0}$ is the sequence of "free" eigenvalues

$$\tilde{E}^{(m)} = \frac{\hbar^2}{2m_* R^2} (m + \eta)^2 \tag{4.17}$$

arranged in the ascending order. In addition, for $\alpha < 0$, Eq. (4.16) has a solution also on the half-line $(-\infty, \tilde{E}_0)$.

Consider a fixed solution $E_0(\theta)$ of (4.16). It is clearly independent of θ and represents a non-degenerate eigenvalue of H_θ with the eigenfunction

$$\psi_\theta(\varphi) = \left[\frac{\partial Q}{\partial E} (E_0) \right]^{-1/2} G(\varphi, \theta; E_0). \tag{4.18}$$

Let us evaluate the Berry phase when the perturbation site θ travels once around the ring. The Berry potential is given by

$$V(\theta) = i \langle \psi_\theta | \nabla_\theta | \psi_\theta \rangle. \tag{4.19}$$

We express ψ_θ in the form

$$\psi_\theta(\varphi) = \frac{m_* R c_0}{\pi \hbar^2} \sum_{m=-\infty}^{\infty} \frac{\exp[im(\varphi - \theta)]}{(m + \eta)^2 - (2m_* R^2 / \hbar^2) E} \tag{4.20}$$

with $c_0 := [(\partial Q / \partial E)(E_0)]^{-1/2}$. Then

$$V(\theta) = \frac{2m_*^2 R^3 c_0^2}{\pi \hbar^4} \sum_{m=-\infty}^{\infty} \frac{m}{((m + \eta)^2 - (2m_* R^2 / \hbar^2) E)^2}. \tag{4.21}$$

On the other hand,

$$\frac{\partial Q}{\partial E} (E_0) = \frac{2m_*^2 R^3}{\pi \hbar^4} \sum_{m=-\infty}^{\infty} \left[(m + \eta)^2 - \frac{2m_* R^2}{\hbar^2} E \right]^{-2}, \tag{4.22}$$

so

$$V(\theta) = \sum_{m=-\infty}^{\infty} \frac{m}{((m+\eta)^2 - (2m_*R^2/\hbar^2)E)^2}$$

$$\times \left\{ \sum_{m=-\infty}^{\infty} \left[(m+\eta)^2 - \frac{2m_*R^2}{\hbar^2}E \right]^{-2} \right\}^{-1}. \tag{4.23}$$

Differentiating now Q with respect to η we get

$$\frac{\partial Q}{\partial \eta} = -\frac{2m_*R}{\pi\hbar^2} \sum_{m=-\infty}^{\infty} \frac{m+\eta}{((m+\eta)^2 - (2m_*R^2/\hbar^2)E)^2} \tag{4.24}$$

which yields the identity

$$\sum_{m=-\infty}^{\infty} \frac{m}{((m+\eta)^2 - (2m_*R^2/\hbar^2)E)^2}$$

$$= -\frac{\pi\hbar^2}{2m_*R}\frac{\partial Q}{\partial \eta} - \sum_{m=-\infty}^{\infty} \frac{\eta}{((m+\eta)^2 - (2m_*R^2/\hbar^2)E)^2}. \tag{4.25}$$

In combination with (4.22) and (4.23) this formula gives

$$V(\theta) = -\frac{m_*R^2}{\hbar^2}\frac{\partial E_0}{\partial \eta} - \eta \tag{4.26}$$

and the corresponding Berry phase accumulated while θ moves once anticlockwise around C is

$$\gamma(C) = -\frac{2\pi m_*R^2}{\hbar^2}\frac{\partial E_0}{\partial \eta} - 2\pi\eta. \tag{4.27}$$

Taking into account that the total flux through the ring is $\Phi_C = \eta\Phi_0$, we see that the obtained expression is fully analogous to the formula (4.10) valid in the whisker case.

4.4. A parabolic quantum dot

As the next example of this section, we shall discuss a quantum dot in a uniform magnetic field $\mathbf{B}_0$. To get a solvable model, we suppose that the confining potential which determines the dot is parabolic, $W(r) = \frac{1}{2}m_*\omega_0^2 r^2$. The frequency ω_0 is related to the effective radius R of the dot by

$$\zeta = \frac{1}{2}m_*\omega_0^2 R^2, \tag{4.28}$$

where ζ is the chemical potential of the system [5]. The spectrum of H is discrete with the eigenvalues (usually called the Fock–Darwin levels)

$$E_{mn} = \hbar\omega(\tfrac{1}{2}(|m|+1)+n) + \hbar\omega_c n, \quad m \in \mathbb{Z}, \ n \in \mathbb{N}, \tag{4.29}$$

where $\omega := (\omega_c^2 + \omega_0^2)^{1/2}$. We can employ the known propagator kernel [19] of the operator H:

$$K(\mathbf{r}, \mathbf{r}'; t) = \frac{m_* \omega}{4\pi i \hbar \sin \frac{1}{2}\omega t} \exp \left\{ \frac{i m_* \omega}{4\hbar \sin \frac{1}{2}\omega t} \left[(r^2 + r'^2) \cos \frac{1}{2}\omega t \right. \right.$$

$$\left. \left. - 2\mathbf{r} \cdot \mathbf{r}' \cos \frac{1}{2}\omega_c t - 2i\mathbf{r} \wedge \mathbf{r}' \sin \frac{1}{2}\omega_c t \right] \right\}. \tag{4.30}$$

To find an integral representation of the Green's functions of H, one has to perform the Wick rotation in (4.30), i.e., to pass to the imaginary time $t \to -it$. This yields the heat kernel of e^{-tH}; applying the Laplace transformation to it we get

$$G(\mathbf{r}, \mathbf{r}'; t) = \frac{m_* \omega}{2\pi \hbar^2} \int_0^\infty \exp \left\{ \frac{2tE}{\hbar} \right\} \exp \left\{ -\frac{m_* \omega}{4\hbar \sinh \omega t} \left[(r^2 + r'^2) \cosh \omega t \right. \right.$$

$$\left. \left. - 2\mathbf{r} \cdot \mathbf{r}' \cosh \omega_c t + 2i\mathbf{r} \wedge \mathbf{r}' \sinh \omega_c t \right] \right\} \frac{\mathrm{d}t}{\sinh \omega t}. \tag{4.31}$$

We shall also need the Krein function. It is obtained by the following trick: we observe that replacing ω_c at the RHS of (4.31) by ω, we get the Green's function of the Landau–Hamiltonian with the cyclotronic frequency ω. We add and subtract this function at the RHS, then we subtract the singularity, $(m_*/\pi\hbar^2) \ln |\mathbf{r} - \mathbf{r}'|^{-1}$, and pass to the limit $\mathbf{r}, \mathbf{r}' \to \mathbf{s}$. In accordance with (2.13), we obtain

$$Q(E; \mathbf{s}) = \frac{m_* \omega}{2\pi \hbar^2} \int_0^\infty \exp \left\{ \frac{2tE}{\hbar} \right\} \exp \left\{ -\frac{m_* \omega}{2\hbar \sinh \omega t} \rho^2 (\cosh \omega t - \cosh \omega_c t) - 1 \right\}$$

$$\times \frac{\mathrm{d}t}{\sinh \omega t} - \frac{m_*}{2\pi \hbar^2} \left[\psi \left(\frac{1}{2} - \frac{E}{\hbar \omega} \right) + 2\gamma - \ln 2 - 2 \ln a \right], \tag{4.32}$$

where $a := (\hbar/m_* \omega)^{1/2}$.

We shall not analyze the last expression generally and restrict ourselves to showing that if the point-interaction is strong enough in the sense that $E_0 \ll -\hbar\omega$, the confinement potential has an insignificant effect on the Berry potential only. To this aim, we denote $2E/\hbar = -\varepsilon$ and split the integral I in RHS of (4.31) into a sum $I = I_1(\varepsilon) + I_2(\varepsilon)$ of integrals corresponding to the intervals $(0, \varepsilon^{-1/2})$ and $(\varepsilon^{-1/2}, \infty)$. It is easy to see that the first integral obeys the inequality $I_1(\varepsilon) \geq c_1(\mathbf{r}, \mathbf{r}') \exp[-(\varepsilon)^{1/2}]$ with a constant c_1 depending on $\mathbf{r}$ and $\mathbf{r}'$ only. On the other hand, using an integration by parts, we find that $I_2(\varepsilon) \leq c_2(\mathbf{r}, \mathbf{r}') \varepsilon^{-1} \exp[-(\varepsilon)^{1/2}]$. Neglecting for large $|E|$ the second integral, we have

$$G(\mathbf{r}, \mathbf{r}'; t) \simeq \frac{m_* \omega}{2\pi \hbar^2} \exp \left\{ -i\frac{m_* \omega_c}{2\hbar} \mathbf{r} \wedge \mathbf{r}' \right\}$$

$$\times \int_0^{\varepsilon^{-1/2}} \exp \left\{ \frac{2tE}{\hbar} \right\} \exp \left\{ -\frac{m_* \omega}{4\hbar t} (\mathbf{r} - \mathbf{r}')^2 \right\} \frac{\mathrm{d}t}{t}. \tag{4.33}$$

Since the integral depends on $|\mathbf{r} - \mathbf{r}'|^2$ only, we can repeat the considerations of Section 4.1 obtaining thus

$$V_\theta = \pi \xi_0 \rho + \mathcal{O}(|E|_0^{-1}). \tag{4.34}$$

4.5. A zero-range quantum dot

The results of the previous section may be better understood by considering the zero-range limit of the confinement potential $W(r)$ of the dot. Specifically, let

$$W(r) = \mu_0 \delta(\mathbf{r})(1 - (\ln r)\mathbf{r}\nabla_\mathbf{r}), \tag{4.35}$$

in accordance with Eq. (2.6). Then the Green's function of H has the form (see (2.3))

$$G(\mathbf{r}, \mathbf{r}'; E) = G_0(\mathbf{r}, \mathbf{r}'; E) - [Q_0(E) + \alpha_0]^{-1} G_0(\mathbf{r}, 0; E) G_0(0, \mathbf{r}'; E), \tag{4.36}$$

where $\alpha_0 = \mu_0^{-1}$, $G_0(\mathbf{r}, \mathbf{r}'; E)$ is given by the RHS of (2.11) and $Q_0(E)$ is equal to the expression at RHS of Eq. (2.13). Hence

$$Q(\mathbf{s}; E) = Q_0(E) - [Q_0(E) + \alpha_0]^{-1} G_0^2(\mathbf{s}, 0; E), \tag{4.37}$$

$$\psi_\mathbf{s}(\mathbf{r}) = \left(\frac{\partial Q(\mathbf{s}; E)}{\partial E} \right)^{-1/2} \left[G_0(\mathbf{r}, \mathbf{s}; E) - (Q_0(E) + \alpha_0)^{-1} G_0(\mathbf{r}, 0; E) G_0(0, \mathbf{s}; E) \right]. \tag{4.38}$$

Since $G_0(\mathbf{s}, 0; E)$ is independent of θ, we have

$$\nabla_\theta \psi_\mathbf{s} = \left(\frac{\partial Q(\mathbf{s}; E)}{\partial E} \right)^{-1/2} \nabla_\theta G_0(\mathbf{r}, \mathbf{s}; E).$$

Using now the results of Section 4.1, we obtain

$$\langle \psi_\mathbf{s} | \nabla_\theta | \psi_\mathbf{s} \rangle = \left(\frac{\partial Q(\mathbf{s}; E)}{\partial E} \right)^{-1} \left[\left(\frac{\partial Q_0(E)}{\partial E} \right) (-\pi i \xi_0 \rho^2) \right.$$
$$\left. - (Q_0(E) + \alpha_0)^{-1} G_0(0, \mathbf{s}; E) \langle G_0(\mathbf{r}, 0; E) | \nabla_\theta | G_0(\mathbf{r}, \mathbf{s}; E) \rangle \right]. \tag{4.39}$$

It is clear that

$$\langle G_0(\mathbf{r}, 0; E) | \nabla_\theta | G_0(\mathbf{r}, \mathbf{s}; E) \rangle = \nabla_\theta \langle G_0(\mathbf{r}, 0; E) | G_0(\mathbf{r}, \mathbf{s}; E) \rangle. \tag{4.40}$$

On the other hand, the scalar product $\langle G_0(\mathbf{r}, 0; E) | G_0(\mathbf{r}, \mathbf{s}; E) \rangle$ has the form

$$\langle G_0(\mathbf{r}, 0; E) | G_0(\mathbf{r}, \mathbf{s}; E) \rangle = \int_{\mathbb{R}^2} \exp(-\pi i \xi_0 \mathbf{r} \wedge \mathbf{s}) f(|\mathbf{r}|) g(|\mathbf{r} - \mathbf{s}|) \, d\mathbf{r}, \tag{4.41}$$

and therefore it is invariant with respect to rotations of the vector $\mathbf{s}$ around the origin. Indeed, let T be such a rotation, then

$$\int_{\mathbb{R}^2} \exp(-\pi i \xi_0 \mathbf{r} \wedge T\mathbf{s}) \, f(|\mathbf{r}|) \, g(|\mathbf{r} - T\mathbf{s}|) \, d\mathbf{r}$$
$$= \int_{\mathbb{R}^2} \exp(-\pi i \xi_0 T\mathbf{r} \wedge T\mathbf{s}) f(|T\mathbf{r}|) g(|T\mathbf{r} - T\mathbf{s}|) \, d\mathbf{r}$$
$$= \int_{\mathbb{R}^2} \exp(-\pi i \xi_0 \mathbf{r} \wedge \mathbf{s}) f(|\mathbf{r}|) g(|\mathbf{r} - \mathbf{s}|) \, d\mathbf{r}.$$

As a result, Eqs. (4.39) and (4.40) lead to the following expression for the non-zero component of the Berry potential:

$$V_\theta(\rho) = \left(\frac{\partial Q(\mathbf{s}; E)}{\partial E}\right)^{-1} \left(\frac{\partial Q_0(E)}{\partial E}\right)(\pi\xi_0\rho). \tag{4.42}$$

Using the asymptotics

$$Q_0(E) = \mathcal{O}(\ln|E|), \qquad G_0(\mathbf{s}, 0; E) = \mathcal{O}(|E|^{-1}) \quad \text{as} \quad E \to -\infty,$$

we see from Eqs. (4.37) and (4.42) that in a deep zero-range well, in the sense that $E_0 \ll -\hbar\omega_c$, we get

$$V_\theta = \pi\xi_0\rho + \mathcal{O}(|E|_0^{-2}) \tag{4.43}$$

in accordance with the result (4.34) of the previous example.

5. Wilczek–Zee phase

It was essential in the above considerations that the energy level in question was non-degenerate. In the opposite case, the behavior of the system with respect to a moving perturbation is more complex, the degenerate levels may form different linear combinations and the change includes more than a simple phase factor. Nevertheless, the effect is usually labeled as the Wilczek–Zee phase [28].

In magnetic systems with a homogeneous field, a prime example of a degenerate eigenvalue are the Landau levels which constitute the spectrum of the unperturbed operator (2.1) with $\mathbf{B}_1 = 0$ and $W = 0$; they are

$$\varepsilon_\ell = (\ell + \tfrac{1}{2})\hbar\omega_c, \quad \ell = 0, 1, 2, \ldots. \tag{5.1}$$

In this section, we will briefly discuss how the corresponding eigenfunctions behave under the influence of a moving point interaction.

Let us first observe that the perturbation preserves the Landau levels as infinitely degenerate eigenvalues. Let L_ℓ be the eigenspace of H referring to an eigenvalue ε_ℓ. It is straightforward to see that the eigenspace of $H_\mathbf{s}$ corresponding to the same eigenvalue has the following form

$$L_\ell(\mathbf{s}) = \{\psi \in L_\ell : \psi(\mathbf{s}) = 0\}. \tag{5.2}$$

Since L_ℓ is invariant with respect to translations of the eigenfunctions, it is possible to select an orthonormal basis $\psi_1^{(\ell)}(\mathbf{s}), \psi_2^{(\ell)}(\mathbf{s}), \ldots, \psi_n^{(\ell)}(\mathbf{s}), \ldots$ in $L_\ell(\mathbf{s})$ which depends smoothly on the point $\mathbf{s} \in \mathbb{R}^2$. We suppose that $\mathbf{s}$ is adiabatically moving along a smooth closed contour, $\mathbf{s} = \mathbf{s}(t), t \in [0, 1]$, and that at the initial moment $t = 0$, the system is in a state $\psi_m^{(\ell)}(\mathbf{s}(0))$. Then the state $\psi(t)$ at an instant t is given by the formula

$$\psi(t) = \exp\left\{\frac{\varepsilon_\ell t}{\mathrm{i}\hbar}\right\} \sum_n U_{nm}^{(\ell)}(t)\psi_n^{(\ell)}(\mathbf{s}(t)), \tag{5.3}$$

where $(U_{nm}^{(\ell)}(t))$ is a unitary matrix generalizing the Berry phase factor $\mathrm{e}^{\mathrm{i}\gamma(t)}$ (see [28]). The role of Berry potential is played by the infinite self-adjoint matrix

$$V_{mn}^{(\ell)}(\mathbf{s}) = \mathrm{i}\langle\psi_m^{(\ell)}(\mathbf{s})|\nabla_{\mathbf{s}}|\psi_n^{(\ell)}(\mathbf{s})\rangle, \tag{5.4}$$

which is related to $U^{(\ell)}(t) \equiv U(t)$ by

$$(U^{-1}(t)\dot{U}(t))_{mn} = \mathrm{i}V_{nm}^{(\ell)}(\mathbf{s}(t)). \tag{5.5}$$

The solution to Eq. (5.5) along the curve $C : \mathbf{s} = \mathbf{s}(t)$ is given by the path integral (the Wilson loop)

$$U(C) = \mathcal{P}\exp\left(\mathrm{i}\oint_C V(\mathbf{s})\,\mathrm{d}\mathbf{s}\right), \tag{5.6}$$

where $\mathcal{P}$ indicates a time-ordered exponential.

The Wilczek–Zee theory has the following differential-geometric interpretation [27]. Consider the trivial vector bundle $\mathcal{E}_\ell = \mathbb{R}^2 \times L_\ell$, then $\mathcal{F}_\ell = \cup\{\{\mathbf{s}\} \times L_\ell(\mathbf{s}) : \mathbf{s} \in \mathbb{R}^2\}$ is a subbundle of $\mathcal{E}_\ell$ with the infinite-dimensional typical fiber ℓ^2. Denote by $\mathfrak{u}(\infty)$ the Lie algebra of the unitary group of ℓ^2 (the Lie algebra of skew-Hermitian infinite-dimensional matrices). Then it is convenient to regard $-\mathrm{i}V_{mn}(\mathbf{s})$ as coefficients of the differential form $\omega = \omega_k\,\mathrm{d}x^k$ assuming values in $\mathfrak{u}(\infty)$:

$$\omega_k = \langle\psi_m^{(\ell)}(\mathbf{s})|\nabla_{x^k}|\psi_n^{(\ell)}(\mathbf{s})\rangle, \quad \mathbf{s} = (x^1, x^2). \tag{5.7}$$

This form is a connection form in the bundle $\mathcal{F}_\ell$, and the operators $U(C)$ are the holonomy operators in the principal $\mathcal{U}(\infty)$-bundle associated with $\mathcal{F}_\ell$. According to the Ambrose–Singer theorem [18], the curvature form Ω, $\Omega = \mathrm{d}\omega + \omega \wedge \omega$ determines completely the operators $U(C)$ (the tensor $F_{jk} = \mathrm{i}\Omega_{jk}$ is the strength of the gauge potential V_k). Notice that there is an explicit formula (analogous to the Stokes formula) which expresses the RHS of Eq. (5.6) in terms of the coefficients of Ω [23]; nevertheless, it is difficult to use this formula when the components of ω are not commuting (which is the case for the matrices (5.7)). However, we can gain some insight into the behavior of the Wilczek–Zee phase considering infinitely small loops. In particular, for such a loop C encircling a point $\mathbf{s}_0$, the holonomy operator is given by an ordinary exponential

$$U(C) = \exp(\Omega_{12}(\mathbf{s}_0)S), \tag{5.8}$$

where S is the area encircled by the loop S.

In the following, we shall consider for simplicity the lowest Landau level ε_0 and drop the subscript 0 for the notations. Normalized eigenfunctions of the ground state L_0 may be chosen in the form [21]

$$\Psi_m(r, \varphi) = \left(\frac{|\xi_0|}{2^m m!}\right)^{1/2}\mathrm{e}^{\sigma\mathrm{i}m\varphi}\exp\left\{\frac{-r^2}{4a_0^2}\right\}\left(\frac{r}{a_0}\right)^m, \quad m \geq 0, \tag{5.9}$$

where $\sigma = \mathrm{sgn}\,\xi_0$. The integral kernel $P_0(\mathbf{r}, \mathbf{r}')$ of the projection operator onto the subspace

L_0 equals [13]

$$P_0(\mathbf{r}, \mathbf{r}') = |\xi_0| e^{-\pi i \xi_0 \mathbf{r} \wedge \mathbf{r}'} \exp\left\{\frac{-(\mathbf{r} - \mathbf{r}')^2}{4a_0^2}\right\}. \tag{5.10}$$

The condition $\psi(\mathbf{s}) = 0$ can be then written as

$$\int_{\mathbb{R}^2} P_0(\mathbf{s}, \mathbf{r})\psi(\mathbf{r})\, d\mathbf{r} = 0, \tag{5.11}$$

and a comparison with (5.9) shows that this is equivalent to

$$\langle [\mathbf{s}, \zeta]\Psi_0 | \psi \rangle = 0, \tag{5.12}$$

where $[\mathbf{s}, \zeta]$ with $\mathbf{s} \in \mathbb{R}^2$ and $\zeta \in \mathbb{S}^1$ denotes the operator of magnetic translation [29] which acts on $f \in L^2(\mathbb{R}^2)$ as

$$[\mathbf{s}, \zeta]f(\mathbf{r}) = \zeta \exp(-\pi i \xi_0 \mathbf{r} \wedge \mathbf{s})f(\mathbf{r} - \mathbf{s}). \tag{5.13}$$

This shows that one can choose a family of functions

$$\psi_m(\mathbf{s}) = [\mathbf{s}, 1]\Psi_m, \quad k = 1, 2, \ldots \tag{5.14}$$

for orthonormal basis in $L_0(\mathbf{s})$. Let us calculate the corresponding matrix elements $V_{mn}(\mathbf{s})$. It is convenient to perform the calculation in the Cartesian coordinates. Let $\mathbf{r} = (x, y)$, $\mathbf{s} = (x', y')$; then

$$\psi_m(\mathbf{s})(\mathbf{r}) = \exp(-\pi i \xi_0(xy' - x'y))\Psi_m(x - x', y - y'). \tag{5.15}$$

Writing Ψ_m as

$$\Psi_m(x, y) = \left(\frac{|\xi_0|}{2^m m!}\right)^{1/2} \exp\left\{\frac{-(x^2 + y^2)}{4a_0^2}\right\}\left(\frac{x + \sigma i y}{a_0}\right)^m, \tag{5.16}$$

we find

$$\frac{\partial \Psi_m}{\partial x} = -\frac{x}{2a_0^2}\Psi_m + \frac{1}{a_0}\left(\frac{m}{2}\right)^{1/2}\Psi_{m-1},$$

$$\frac{\partial \Psi_m}{\partial y} = -\frac{y}{2a_0^2}\Psi_m + \frac{\sigma i}{a_0}\left(\frac{m}{2}\right)^{1/2}\Psi_{m-1}. \tag{5.17}$$

Now we obtain from Eq. (5.17):

$$\frac{\partial \psi_m}{\partial x'}(\mathbf{s})(x, y) = \pi i \xi_0 y \psi_m(\mathbf{s})(x, y) + \exp(-\pi i \xi_0(xy' - x'y))$$

$$\times \left[\frac{x - x'}{2a_0^2}\Psi_m(x-x', y-y') - \frac{1}{a_0}\left(\frac{m}{2}\right)^{1/2}\Psi_{m-1}(x - x', y - y')\right], \tag{5.18}$$

$$\frac{\partial \psi_m}{\partial y'}(\mathbf{s})(x, y) = -\pi i \xi_0 x \psi_m(\mathbf{s})(x, y) + \exp(-\pi i \xi_0 (xy' - x'y))$$

$$\times \left[\frac{y - y'}{2a_0^2} \Psi_m(x - x', y - y') - \frac{\sigma i}{a_0} \left(\frac{m}{2}\right)^{1/2} \Psi_{m-1}(x - x', y - y') \right].$$

(5.19)

Hence

$$\langle \psi_n | \nabla_{x'} | \psi_m \rangle = \pi i \xi_0 y' \delta_{mn} + \pi i \xi_0 \langle \Psi_n | y | \Psi_m \rangle$$
$$+ \frac{1}{2a_0^2} \langle \Psi_n | x | \Psi_m \rangle - \frac{1}{a_0} \left(\frac{m}{2}\right)^{1/2} \delta_{n, m-1},$$

(5.20)

$$\langle \psi_n | \nabla_{y'} | \psi_m \rangle = -\pi i \xi_0 x' \delta_{mn} - \pi i \xi_0 \langle \Psi_n | x | \Psi_m \rangle + \frac{1}{2a_0^2} \langle \Psi_n | y | \Psi_m \rangle$$
$$- \frac{\sigma i}{a_0} \left(\frac{m}{2}\right)^{1/2} \delta_{n, m-1}.$$

(5.21)

To find the matrix elements $\langle \Psi_n | x | \Psi_m \rangle$ and $\langle \Psi_n | y | \Psi_m \rangle$, we make use of the following observations: the matrices $(i \langle \psi_n | \nabla_{x'} | \psi_m \rangle)$ and $(i \langle \psi_n | \nabla_{y'} | \psi_m \rangle)$ are Hermitian, and at the same time, the numbers $\langle \Psi_n | x | \Psi_m \rangle$ and $\langle \Psi_n | y | \Psi_m \rangle$ are real. Taking these facts into account, we get from Eqs. (5.20) and (5.21)

$$\frac{i}{2a_0^2} \langle \Psi_n | x | \Psi_m \rangle - \frac{i}{a_0} \left(\frac{m}{2}\right)^{1/2} \delta_{n, m-1} = -\frac{i}{2a_0^2} \langle \Psi_n | x | \Psi_m \rangle + \frac{i}{a_0} \left(\frac{n}{2}\right)^{1/2} \delta_{m, n-1}, \quad (5.22)$$

$$\frac{i}{2a_0^2} \langle \Psi_n | y | \Psi_m \rangle + \frac{\sigma}{a_0} \left(\frac{m}{2}\right)^{1/2} \delta_{n, m-1} = -\frac{i}{2a_0^2} \langle \Psi_n | y | \Psi_m \rangle + \frac{\sigma}{a_0} \left(\frac{n}{2}\right)^{1/2} \delta_{m, n-1}. \quad (5.23)$$

Thus

$$\langle \Psi_n | x | \Psi_m \rangle = \frac{1}{\sqrt{2}} a_0 (\sqrt{n} \, \delta_{m, n-1} + \sqrt{m} \, \delta_{n, m-1}),$$

(5.24)

$$\langle \Psi_n | y | \Psi_m \rangle = \frac{1}{\sqrt{2}} \sigma i a_0 (\sqrt{m} \delta_{n, m-1} - \sqrt{n} \delta_{m, n-1}).$$

(5.25)

Since $|\xi_0|^{-1} = 2\pi a_0^2$, we have finally

$$\langle \psi_n | \nabla_{x'} | \psi_m \rangle = \pi i \xi_0 y' \delta_{mn} + \frac{1}{\sqrt{2} a_0} (\sqrt{n} \delta_{m, n-1} - \sqrt{m} \delta_{n, m-1}),$$

(5.26)

$$\langle \psi_n | \nabla_{y'} | \psi_m \rangle = -\pi i \xi_0 x' \delta_{mn} - \frac{\sigma i}{\sqrt{2} a_0} (\sqrt{n} \delta_{m, n-1} + \sqrt{m} \delta_{n, m-1}).$$

(5.27)

Because the matrices $(\langle \psi_n | \nabla_{x'} | \psi_m \rangle)$ and $(\langle \psi_n | \nabla_{y'} | \psi_m \rangle)$ do not commute, it is not easy to calculate the path integral (5.6), and we turn to Eq. (5.8) to gain some insight into the behavior of the Wilczek–Zee phase. For this purpose, let us calculate the curvature form Ω. Since Ω_{jk} is skew-symmetric (w.r.t. the indices jk) it is enough to find the component

Ω_{12}. It is clear from Eqs. (5.26) and (5.27) that $d\omega = -\pi i \xi_0 \delta_{mn} dx^1 \wedge dx^2$. Since the first terms in Eqs. (5.26) and (5.27) are scalar matrices, in order to find $\omega \wedge \omega$, we must have to calculate the commutator of the matrices $(\sqrt{2}a_0)^{-1}(\sqrt{n}\delta_{m,n-1} - \sqrt{m}\delta_{n,m-1})$ and $-\sigma i (\sqrt{2}a_0)^{-1}(\sqrt{n}\delta_{m,n-1} + \sqrt{m}\delta_{n,m-1})$ only. As a result we obtain that

$$\Omega_{12} = 2\pi i \xi_0 \delta_{1m} \delta_{1n} dx^1 \wedge dx^2. \tag{5.28}$$

Therefore, for an infinitely small loop C in the plane $\mathbb{R}^2$, the operator $U(C)$ has the diagonal matrix

$$U_{mn}(C) = \text{diag}(\exp(-2\pi i \xi_0 S), 1, 1, \ldots, 1, \ldots), \tag{5.29}$$

where S is the area encircled by the loop C. Hence during an adiabatic evolution along the loop C, the state $\psi_1^{(0)}$ with the angular momentum $m = 1$ is modified by the Berry-like factor $\exp(-2\pi i \xi_0 S)$; the states with the other angular momenta $m = 2, 3, \ldots$ remain unchanged. This behavior of the Wilczek–Zee phase is similar to the spectral behavior of the Aharonov–Bohm Hamiltonian with an infinitely thin solenoid with anomalous magnetic flux, which is described in analogy with a delta-perturbed Hamiltonian by a self-adjoint extension of a symmetric operator. Namely, the infinitely thin Aharonov–Bohm solenoid perturbs only two states with neighbor angular momenta (see, e.g., [6]). Similarly, in the case of the Wilczek–Zee phase, the point potential changes two states with neighbor angular momenta: $m = 0$ and $m = 1$. The opposite signs in (4.5) and (5.29) can be interpreted as a "topological charge conservation". More specifically, the mappings $\mathbb{R}^2 \ni \mathbf{s} \mapsto [\mathbf{s}, 1]\Psi_m$, $m = 0, 1, \ldots$ form a basis section of the vector bundle $\mathcal{E}_0$. Formula (5.4) with $m, n \geq 0$ defines a connection in this bundle, and it is easy to show that this connection is flat (i.e., its curvature vanishes). Thus in accordance with the Ambrose–Singer theorem, all the Wilson loops (5.6) are identity operators, i.e., the "Berry phase" for this connection is equal to zero. Adding the point potentials of the same strength α to each point $\mathbf{s} \in \mathbb{R}^2$, we split the bundle $\mathcal{E}_0$ into a sum of the line bundle $\mathcal{L}_0$ of the eigenfunctions in the zero-range well and the bundle $\mathcal{F}_0$ of the eigenfunctions remaining on the zeroth Landau level: $\mathcal{E}_0 = \mathcal{L}_0 \oplus \mathcal{F}_0$. Eqs. (4.5) and (5.29) show that the sum of Berry phases related to the summands is still zero. This effect is similar to the Berry phase conservation in the Born–Openheimer problem [30]. On the other hand, we have here an analogy with the Novikov formula for the Chern numbers of a sum of vector bundles of magneto-Bloch functions [25]. In physical terms, the Novikov formula states that the quantized Hall conductivity of a Bloch–Landau band is the sum of conductivities of the all magnetic subbands of this band. It remains to note that the mentioned Chern numbers are integrals of the curvature form.

Acknowledgements

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