Aharonov-Bohm effects on nearly-localized quantum states

1991 J. Phys. A: Math. Gen. 24 4093

(http://iopscience.iop.org/0305-4470/24/17/026)

J. Phys. A: Math. Gen. 24 (1991) 4093-4108. Printed in the UK

Aharonov–Bohm effects on nearly-localized quantum states

Yasuhiro Nagoshi† and Shin Takagi
Department of Physics, Tohoku University, Sendai 980, Japan

Received 17 April 1991

Abstract. We consider a charged particle confined to a ring encircling a magnetic flux. Supposing that the particle is trapped by a delta-function potential located on the ring, we examine the flux dependence of the energy and the wavefunction of the bound state. This offers a simple explicit model for the Aharonov-Bohm effect on a system localized, but not completely confined, to a simply connected region off a magnetic flux. The result is used to show that Berry's phase for the bound state, when the delta-function potential is slowly transported around the ring, consists not only of the Aharonov-Bohm phase proportional to the flux, but also of an extra term which reflects the incomplete localization of the state; in the limit of strong binding the extra term depends sinusoidally on the flux.

1. Introduction

We consider two closely related questions concerning the Aharonov-Bohm effect (Aharonov and Bohm 1959, 1961, Peshkin and Tonomura 1989 and references therein). Suppose that a localized system such as an atom is placed in the field-free region outside a magnetic flux (e.g. a solenoid). We ask two questions: (i) is the energy spectrum of the system affected by the flux? (ii) if the system has a non-vanishing total charge, will it acquire the Aharonov-Bohm phase (hereafter called the AB phase) when it is slowly transported around the flux back to its original position? Here, by the AB phase, we mean 2π times the flux in units of fluxons (see section 2). The answer to (i) is no, because the vector potential can be eliminated by a suitable gauge transformation. The answer to (ii) has been shown to be yes by Berry (1984), who argued that this particular version (to be called Berry's version in this paper) of Aharonov-Bohm effect can be interpreted as an example of Berry's phase (see Berry 1990 and references therein). Both conclusions, however, depend on the assumption that the wavefunction of the system is *completely confined to a simply connected region* outside the solenoid. This assumption does not hold for a realistic localized system, whose wavefunction always has a tail. Therefore we drop this assumption, although we continue to suppose that the solenoid is impenetrable. It is then expected that the answer to (i) is yes; the energy spectrum will exhibit a typically exponentially small dependence on the flux. The answer to (ii) might not be obvious, but there seems to be no reason why Berry's phase should be exactly equal to the AB phase; after all Berry's gedanken experiment deals with a different physical situation from the more traditional case of the scattering in the flux line's vector potential originally treated by Aharonov and Bohm (1959).

† Present address: Ube-Kohsan Co Ltd, Ube, Japan.

0305-4470/91/174093+16$03.50

The purpose of this paper is to demonstrate the validity of these expectations with a simple model, that is, a charged particle confined to a ring around a localized magnetic flux; the particle does not move freely along the ring, but can be trapped by a potential well. We calculate the energy level for some simple potentials and answer (i) affirmatively. A particularly interesting case consists of two delta-function potentials of the same depth; if they are sufficiently deep, there are two bound states and the energy splitting between them depends sinusoidally on the flux. We also compute Berry's phase for the bound state of a delta-function potential supposing that the position of the potential is slowly transported along the ring. It is shown that Berry's phase does not coincide with the AB phase but acquires an exponentially small correction, which depends sinusoidally on the flux. The computation is done in two ways. The first method uses Berry's connection, and the second method solves the time-dependent Schrödinger equation directly with the help of a rotating frame of reference. The second method sheds light on the origin of the correction term; it is caused by the Coriolis effect which, being of the first order in the angular velocity of the transportation, cannot be neglected however small the speed of transportation may be. We conclude that Berry's phase in Berry's version of the AB effect is in general different from the AB phase.

2. Model

We consider a particle of mass m and charge q described by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r}, t) = H(t)\psi(\boldsymbol{r}, t) \tag{2.1a}$$

$$H(t) \equiv -\frac{\hbar^2}{2m}[\nabla - i\boldsymbol{A}(\boldsymbol{r})]^2 + V(\boldsymbol{r}, t). \tag{2.1b}$$

The factor $q/\hbar c$ has been absorbed into the vector potential $\boldsymbol{A}$. Let $\boldsymbol{r}$ be represented by the cylindrical coordinates (ρ, φ, z), and introduce a toroidal domain D defined by

$$D \equiv \{\boldsymbol{r} \mid (\rho - a)^2 + z^2 < d^2\}$$

where a and d are constants satisfying $a > d > 0$. We suppose that

$$V(\boldsymbol{r}, t) = V_0(\boldsymbol{r}, t) + V_D(\boldsymbol{r}) \tag{2.1c}$$

where V_0 is arbitrary at this stage, and V_D confines the particle to D, that is, V_D vanishes in D and is infinite outside D. A time-independent magnetic field with flux $\tilde{\Phi}$ is supposed to thread through the hole of the torus D. The field is supposed to vanish in D, but it is otherwise arbitrary. Under this condition it is possible to choose the gauge so that the vector potential in D takes the form (see appendix)

$$\boldsymbol{A}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = A(\varphi)\,\mathrm{d}\varphi \tag{2.2}$$

where $A(\varphi)$ is an arbitrary 2π-periodic function such that

$$\int_0^{2\pi} A(\varphi)\,\mathrm{d}\varphi = 2\pi\Phi \equiv 2\pi q\tilde{\Phi}/hc. \tag{2.3}$$

The dimensionless parameter Φ represents the flux in units of fluxons hc/q. Being an arbitrary function, $A(\varphi)$ can be chosen to be a constant, namely Φ. Unless otherwise

mentioned, however, we shall work with a generic $A(\varphi)$ in order to make the gauge-invariant nature of our treatment manifest. (It is easy to work with a completely general gauge; the use of gauge (2.2) is just to simplify the notation.)

Equation (2.1) must of course be solved for a solution which is single-valued in D. For the most part of this paper we restrict φ to the interval $[0, 2\pi]$ and impose the boundary condition $\psi(\rho, 0, z, t) = \psi(\rho, 2\pi, z, t)$.

3. Energy spectrum

In this section we suppose that V_0 is time independent and has the form

$$V_0(\boldsymbol{r}, t) = \hbar^2 v(\varphi)/2m\rho^2. \tag{3.1}$$

The stationary state of energy E can then be separated in the form $\psi = u_D(\rho, z)u(\varphi)\exp(-iEt/\hbar)$, where

$$\{-[\mathrm{d}/\mathrm{d}\varphi - iA(\varphi)]^2 + v(\varphi)\}u(\varphi) = \pi^{-2}\varepsilon u(\varphi) \tag{3.2}$$

$$\left(H_D + \frac{\hbar^2\varepsilon}{2m\pi^2\rho^2}\right)u_D(\rho, z) = Eu_D(\rho, z) \tag{3.3}$$

and

$$H_D \equiv -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2}\right) + V_D(\rho, z) \tag{3.4}$$

with ε being a separation constant. Let E_D be an eigenvalue of H_D, then E can be expressed as

$$E = E_D + (\hbar^2/2m\pi^2a^2)[\varepsilon + O(d/a)]. \tag{3.5}$$

Note that E_D is of the order of $\hbar^2/md^2$. If $a \gg d$, that is, if D is a ring of radius a and thickness d, then the low lying energy levels are determined by ε. With such a situation in mind, we shall calculate ε for some simple potentials v. In the rest of this section we choose the range of φ to be $[-0, 2\pi - 0]$, where -0 is an infinitesimal negative number, without loss of generality.

3.1. Single delta-function potential

First we treat the case of

$$v(\varphi) = -\pi^{-1}g\delta(\varphi) \tag{3.6}$$

where g is a dimensionless parameter, the potential being attractive if $g > 0$. We perform a singular gauge transformation

$$u(\varphi) = \exp\left[i\int_0^{\varphi} A(\varphi')\,\mathrm{d}\varphi'\right]\tilde{u}(\varphi) \tag{3.7}$$

to find that $\tilde{u}$ obeys

$$\tilde{u}''(\varphi) = -\pi^{-2}\varepsilon\tilde{u}(\varphi) \tag{3.8}$$

in the interval $[+0, 2\pi-0]$, where the prime denotes differentiation with respect to φ. It is necessary that $\tilde{u}$ satisfies the boundary condition

$$\tilde{u}(+0)-\exp(2\pi i\Phi)\tilde{u}(2\pi-0)=0 \tag{3.9a}$$

$$\tilde{u}'(+0)-\exp(2\pi i\Phi)\tilde{u}'(2\pi-0)=-\pi^{-1}g\tilde{u}(+0). \tag{3.9b}$$

It follows that

$$\tilde{u}(\varphi)=\sin(k-\pi\Phi)\exp[ik(\varphi/\pi-1)]+\sin(k+\pi\Phi)\exp[-ik(\varphi/\pi-1)] \tag{3.10}$$

modulo a normalization factor, where $k=\varepsilon^{1/2}$, and that allowed values of k are determined by

$$\cos 2k-\cos 2\pi\Phi-(g/2k)\sin 2k=0. \tag{3.11}$$

Evidently the spectrum is an even periodic function of Φ with period 1; it is sufficient to restrict Φ to the interval $[0, \frac{1}{2}]$.

The overall behaviour of the spectrum may be understood by a graphical method. In particular a bound state, with the convention that a state with negative ε is to be so called, may be found from the equation

$$\frac{2\kappa}{g}=\frac{\sinh 2\kappa}{\cosh 2\kappa-\cos 2\pi\Phi} \tag{3.12}$$

where we have put $k=i\kappa$. From now on we use κ and $(-\varepsilon)^{1/2}$ interchangeably. It follows that there is one bound state if and only if

$$g>g_c\equiv 1-\cos 2\pi\Phi.$$

The energy of the bound state are analytically found, when $g\simeq g_c$, as

$$\varepsilon\simeq-\tfrac{3}{2}(g-g_c)/(2+\cos 2\pi\Phi)$$

and, when $g\gg 1$, as

$$\varepsilon\simeq-\tfrac{1}{4}g^2\{1+4\,e^{-g}\cos 2\pi\Phi-4\,e^{-2g}[1+(2g-3)(\cos 2\pi\Phi)^2]\}. \tag{3.13}$$

Let us also write down the normalized bound state wavefunction

$$\tilde{u}(\varphi)=(2\pi Z)^{-1/2}\{\sinh[\kappa(2-\varphi/\pi)]+\exp(-2\pi i\Phi)\sinh(\kappa\varphi/\pi)\} \tag{3.14a}$$

$$Z\equiv\frac{1}{4\kappa}\sinh 4\kappa+\left(\cosh 2\kappa-\frac{1}{2\kappa}\sinh 2\kappa\right)\cos 2\pi\Phi-1. \tag{3.14b}$$

When $g\gg 1$ this is approximately given by

$$\tilde{u}(\varphi)\simeq(\kappa/\pi)^{1/2}\{\exp(-\kappa\varphi/\pi)+\exp[-2\pi i\Phi-\kappa(2-\varphi/\pi)]\}. \tag{3.15}$$

It is interesting to compare (3.13) and (3.15) with the bound-state solution ε^∞, u^∞ of the purely one-dimensional problem, that is, the solution of (3.2) with (3.6) when φ ranges over the entire real axis and u^∞ satisfies the boundary condition $u^\infty(\pm\infty)=0$;

$$\varepsilon^\infty=-\tfrac{1}{4}g^2 \qquad \tilde{u}^\infty(\varphi)=(\kappa/\pi)^{1/2}\exp(-\kappa|\varphi|/\pi).$$

Thus, the periodic boundary condition gives rise to an exponentially small correction to the binding energy, and the flux causes a correction of the same order of magnitude. (When $\Phi=\frac{1}{4}$ the two effects happen to cancel each other to the leading order of $\exp(-g)$.) Both are due to the overlap of the tail of the wavefunction as is seen from the relationship

$$e^{-g}\sim|u^\infty(\pm\pi)|^2.$$

In figure 1 we depict the square of the absolute value of the normalized bound-state wavefunction

$$|u(\varphi)|^2 = (2\pi Z)^{-1}\{(\cosh 2\kappa - \cos 2\pi\Phi)\cosh[2\kappa(\varphi/\pi - 1)] + \cosh 2\kappa \cos 2\pi\Phi - 1\} \tag{3.16}$$

for $g = 3$ and for three typical values of Φ. When $\Phi \neq 0$, the wavefunction is not symmetric with respect to the reflection at $\varphi = \pi$ as seen from (3.10); *parity* is not a good quantum number in the presence of a flux. But the absolute value is symmetric. Note that

$$|u(\pi)/u(0)| = |\cos \pi\Phi|/\cosh \kappa. \tag{3.17}$$

For completeness we show in figure 2 the result of the numerical solution of equation (3.12) as a function of Φ for three typical values of g. In figure 3 the same solution is plotted as a function of g for three typical values of Φ.

3.2. Double delta-function potentials

Next we consider the case of

$$v(\varphi) = -\pi^{-1}[g_1\delta(\varphi) + g_2\delta(\varphi - \theta\pi)] \tag{3.18}$$

where $0 < \theta \leqslant 1$. In this case condition (3.9) need be supplemented by a similar condition appropriate at $\varphi = \theta\pi$. The spectrum is determined by

$$\cos 2k - \cos 2\pi\Phi - [(g_1 + g_2)/2k]\sin 2k = (g_1 g_2/4k^2)\{\cos 2k - \cos[2(1-\theta)k]\}. \tag{3.19}$$

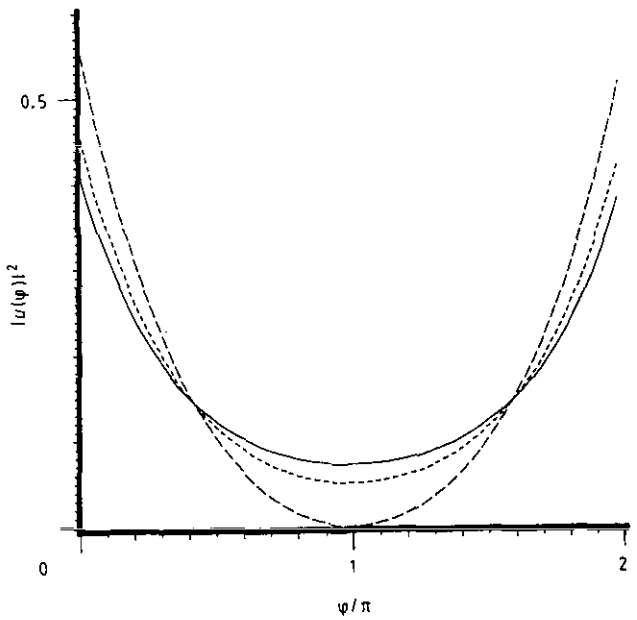

Figure 1. The absolute value squared of the normalized bound-state wavefunction for the single delta-function potential with $g = 3$ for $\Phi = 0$ (full curve), $\Phi = \frac{1}{4}$ (dotted curve) and $\Phi = \frac{1}{2}$ (dashed curve).

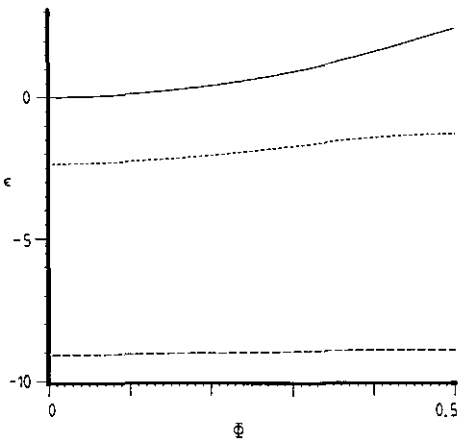

Figure 2. The ground-state energy for the single delta-function potential with $g=0$ (full curve), $g=3$ (dotted curve) and $g=6$ (dashed curve).

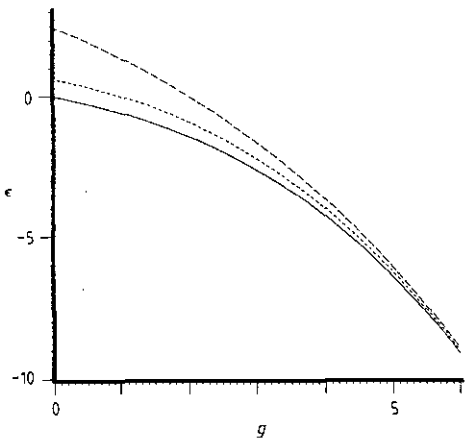

Figure 3. The same energy as in figure 2 plotted as a function of g for $\Phi=0$ (full curve), $\Phi=\frac{1}{4}$ (dotted curve) and $\Phi=\frac{1}{2}$ (dashed curve).

As in the previous section we restrict Φ to the interval $[0, \frac{1}{2}]$ without loss of generality. In what follows we treat the symmetric case only:

$$g_1=g_2=g.$$

Let us first examine the case of the two potentials located diametrically, namely $\theta=1$. We put $k=\mathrm{i}\kappa$ to cast (3.19) into the form

$$\frac{2\kappa}{g}=\frac{\sinh\kappa}{\cosh\kappa\pm\cos\pi\Phi}. \tag{3.20}$$

It follows that there is one bound state if

$$2(1-\cos\pi\Phi)<g<2(1+\cos\pi\Phi)$$

and there are two bound states if

$$g>2(1+\cos\pi\Phi).$$

Suppose that the last inequality holds. Let ε_- be the energy of the ground state and ε_+ be that of the first excited state. Let $\varepsilon(\Phi; g)$ be the bound-state energy for the case of the single delta-function potential treated in the previous section. Comparison of equations (3.12) and (3.20) shows that

$$\varepsilon_+ = 4\varepsilon\left(\frac{1-\Phi}{2}; \frac{g}{2}\right) \qquad \varepsilon_- = 4\varepsilon\left(\frac{\Phi}{2}; \frac{g}{2}\right).$$

In particular, for $g \gg 1$, we find

$$\varepsilon_\pm \simeq -\tfrac{1}{4}g^2(1 \mp 4\,\mathrm{e}^{-g/2}\cos\pi\Phi). \tag{3.21}$$

The energy splitting $\varepsilon_+ - \varepsilon_-$ is thus seen to depend sensitively on the flux. A part of the numerically calculated spectrum is shown as a function of Φ in figure 4.

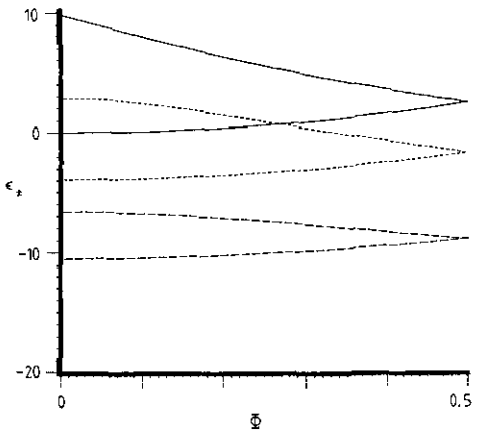

Figure 4. The energies of the ground state and the first excited state for the diametrically located double delta-function potentials with $g = 0$ (full curve), $g = 3$ (dotted curve) and $g = 6$ (dashed curve).

When $\Phi = \frac{1}{2}$, equation (3.20) becomes identical to (3.12), that is, the spectrum is identical to that of the single-potential case and each energy level is doubly degenerate. The reason of this degeneracy may be understood from equation (3.17), which shows that the bound-state wavefunction for the single potential located at $\varphi = 0$ vanishes at $\varphi = \pi$; the presence of another potential at $\varphi = \pi$ does not affect the problem in this special case.

For a generic value of θ results are more complicated. Let us write down only the energies of the two bound states in the case of $g \gg 1$ and $\frac{1}{2} < \theta < \frac{3}{4}$:

$$\varepsilon_\pm \simeq -\tfrac{1}{4}g^2\{1-(\theta g-1)\,\mathrm{e}^{-\theta g} \mp 2\,\mathrm{e}^{-\theta g/2}[1+\mathrm{e}^{-(1-\theta)g}\cos 2\pi\Phi]\} \tag{3.22}$$

where quantities of order $\exp(-\frac{3}{4}g)$ or less have been neglected.

3.3. A square well potential

Since delta-function potentials are rather special, we supplement our study by briefly describing the case of a square well potential

$$v(\varphi) = \begin{cases} -g/\theta\pi^2 & \text{for } 0 < \varphi < \theta\pi \\ 0 & \text{for } \theta\pi < \varphi < 2\pi \end{cases} \tag{3.23}$$

where $0<\theta<2$. Putting $k=\varepsilon^{1/2}$ and $K=(\varepsilon+g/\theta)^{1/2}$, we find that the spectrum is determined by

$$\cos[(2-\theta)k]\cos(\theta K)-\cos 2\pi\Phi-\frac{k^2+K^2}{2kK}\sin[(2-\theta)k]\sin(\theta K)=0. \tag{3.24}$$

We have chosen the parameter g so that

$$\int_0^{2\pi} \mathrm{d}\varphi\, v(\varphi)=-g/\pi$$

in order to facilitate comparison with the delta function potential considered in section 3.1; equation (3.24) reduces to (3.11) as θ tends to zero. In figure 5 we show the ground-state energy as a function of Φ for the case of $\theta=\frac{1}{2}$ with $g=3$ and 6.

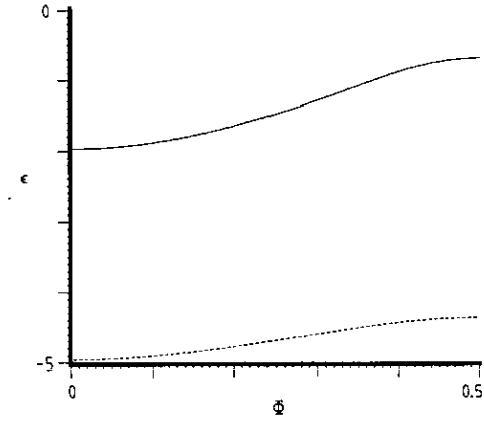

Figure 5. The ground-state energy for the square-well potential with $\theta=\frac{1}{2}$ for $g=3$ (full curve) and $g=6$ (dotted curve).

4. Berry's phase

In this section we discuss Berry's version of the AB effect. Let us begin with reviewing Berry's argument in a slightly simplified situation. We consider the model described by equations (2.1*a–c*) with the potential V_0 now having the form

$$V_0(\boldsymbol{r}, t)=V_B(\rho, \varphi-\varphi_0(t), z) \tag{4.1}$$

where $V_B(\rho, \varphi, z)$ is infinite for $\theta\pi<\varphi<2\pi$, with θ being a constant less than 2, and is otherwise arbitrary. The function $\varphi_0(t)$ is arbitrary except that it is supposed to satisfy $\varphi_0(0)=0$ and $\varphi_0(T)=2\pi$, where T is a positive constant. The potential V_0 thus represents a box which completely confines the particle to it and is transported once around the flux in time T. (By a box we always mean a *hard box* as defined above.) Let $\Psi_n^{(0)}(\boldsymbol{r})$ be the normalized nth eigenstate of $H^{(0)}(0)$, namely $H(0)$ defined by (2.1) and (4.1) but in the absence of the vector potential, and the associated energy eigenvalue be E_n. It is possible to choose $\Psi_n^{(0)}(\boldsymbol{r})$ to be real. For convenience we extend $\Psi_n^{(0)}(\rho, \varphi, z)$

periodically with period 2π to the entire real value of φ and denote the extended function by the same symbol. Now define

$$\Psi_n(\boldsymbol{r};\varphi_0)\equiv\exp\left[\mathrm{i}\int_{\varphi_0}^{\varphi}A(\varphi')\,\mathrm{d}\varphi'\right]\Psi_n^{(0)}(\rho,\varphi-\varphi_0,z). \tag{4.2}$$

Since $\Psi_n^{(0)}$ vanishes outside the box, the phase factor is single-valued with respect to $\boldsymbol{r}$, and $\Psi_n(\boldsymbol{r},\varphi_0(t))$ is the nth eigenstate of $H(t)$ with the same energy eigenvalue E_n as $\Psi_n^{(0)}(\boldsymbol{r})$. It also follows from the above definition that $\Psi_n(\boldsymbol{r};\varphi_0)$ is also single-valued in the parameter space. By use of this construction Berry computed Berry's connection (or 1-form)

$$\beta\equiv-\mathrm{Im}\int\mathrm{d}\boldsymbol{r}\,\Psi_n^*(\boldsymbol{r};\varphi_0)\,\mathrm{d}\Psi_n(\boldsymbol{r};\varphi_0) \tag{4.3}$$

where $\mathrm{d}\Psi_n\equiv(\partial\Psi_n/\partial\varphi_0)\,\mathrm{d}\varphi_0$, as

$$\begin{aligned}\beta&=-\left[\mathrm{Im}\int\mathrm{d}\boldsymbol{r}\,\Psi_n^{(0)}(\rho,\varphi-\varphi_0,z)\{-iA(\varphi_0)+\partial/\partial\varphi_0\}\Psi_n^{(0)}(\rho,\varphi-\varphi_0,z)\right]\mathrm{d}\varphi_0\\&=\left[A(\varphi_0)+\mathrm{Im}\int\mathrm{d}\boldsymbol{r}\,\Psi_n^{(0)}(\boldsymbol{r})\frac{\partial}{\partial\varphi}\Psi_n^{(0)}(\boldsymbol{r})\right]\mathrm{d}\varphi_0.\end{aligned} \tag{4.4}$$

Since $\Psi_n^{(0)}$ is real, the integral in the second term is real (and is in fact zero). Hence only the first term survives. Consequently Berry's phase γ is found to be

$$\gamma=\oint\beta=\int_0^{2\pi}A(\varphi_0)\,\mathrm{d}\varphi_0=2\pi\boldsymbol{\Phi}. \tag{4.5}$$

Berry's phase in this gedanken experiment thus coincides with the AB phase $2\pi\boldsymbol{\Phi}$.

In this argument of Berry, it is essential that the potential V_B confines the particle completely to the box. Let us now drop this condition and replace the box by a well, that is,

$$V_0(\boldsymbol{r},t)=V_W(\rho,\varphi-\varphi_0(t),z) \tag{4.6}$$

supposing that $V_W(\rho,\varphi,z)$ vanishes except for $0<\varphi<\theta\pi$, where it takes finite negative values. (By a well we always mean a well of finite depth.) Everything else is supposed to remain the same as before. Note in particular that the particle is always in the field-free region. We shall treat this problem with two alternative methods.

Before doing so, however, a preparation is in order. Let $H(t)$ be the Hamiltonian defined by (2.1) and (4.6), and $\psi_n(\boldsymbol{r})$ be the normalized nth eigenstate of $H(0)$ with energy eigenvalue $E_n(0)$. We extend $\psi_n(\boldsymbol{r})$ periodically with period 2π to the entire real value of φ and denote the extended function by the same symbol. Then, $\psi_n(\rho,\varphi-\varphi_0(t),z)$ is the nth eigenstate of $H'(t)$ with the same energy $E_n(0)$, where $H'(t)$ is obtained from $H(t)$ by replacing $A(\varphi)$ with $A(\varphi-\varphi_0(t))$:

$$H'(t)=\exp[-\mathrm{i}G(\varphi_0(t))]H(t)\exp[\mathrm{i}G(\varphi_0(t))] \tag{4.7a}$$

$$G(\varphi_0)\equiv\int_0^{\varphi}\mathrm{d}\varphi'\{A(\varphi')-A(\varphi'-\varphi_0)\}. \tag{4.7b}$$

If we define

$$\psi_n(\boldsymbol{r};\varphi_0)\equiv\exp[\mathrm{i}G(\varphi_0)]\psi_n(\rho,\varphi-\varphi_0,z) \tag{4.8}$$

then $\psi_n(\boldsymbol{r}; \varphi_0(t))$ is the nth eigenstate of $H(t)$ with energy $E_n(0)$. Consequently the spectrum $\{E_n(t)\}$ of $H(t)$ is independent of t. From the above definition it follows that $\psi_n(\boldsymbol{r}; \varphi_0)$ is single-valued with respect to $\boldsymbol{r}$ and also in the parameter space of φ_0. It is to be noted that equation (4.8) is different from (4.2); the phase factor is different, and moreover $\psi_n(\boldsymbol{r})$ cannot be taken real in general because the vector potential is still present in $H(0)$.

4.1. Method of Berry's connection

Let us specialize to the model of section 3.1 and identify V_W with the delta-function potential via equations (3.1) and (3.6). We want to compute Berry's connection for the bound state. We denote by $u(\varphi; \varphi_0)$ the bound state wavefunction when the potential is located at $\varphi = \varphi_0$. We fix its phase by use of construction (4.8) so that $u(\varphi; \varphi_0)$ becomes single-valued in the parameter space thus:

$$u(\varphi; \varphi_0) = u_{\pm}(\varphi; \varphi_0) \exp\left[\mathrm{i} \int_0^{\varphi} \mathrm{d}\varphi' \, A(\varphi') - \mathrm{i} \int_{2\pi-\varphi_0}^{2\pi} \mathrm{d}\varphi' \, A(\varphi') \right] \tag{4.9}$$

where u_+ is appropriate for $\varphi_0 < \varphi < 2\pi$ and u_- is appropriate for $0 < \varphi < \varphi_0$. They are given in terms of $\tilde{u}$ defined by (3.14) as

$$u_+(\varphi; \varphi_0) = \tilde{u}(\varphi - \varphi_0)$$

$$u_-(\varphi; \varphi_0) = \exp(2\pi \mathrm{i}\Phi)\tilde{u}(2\pi - \varphi_0 + \varphi)$$

or explicitly as

$$u_{\pm}(\varphi; \varphi_0) = (2\pi Z)^{-1/2}\{\sinh[2\kappa \mp \kappa(\varphi - \varphi_0)/\pi] \pm \exp(\mp 2\pi \mathrm{i}\Phi) \sinh[\kappa(\varphi - \varphi_0)/\pi]\}.$$

We therefore find that

$$\begin{aligned} \beta &= -\mathrm{Im} \int_0^{2\pi} \mathrm{d}\varphi \, u^*(\varphi; \varphi_0) \, \mathrm{d}u(\varphi; \varphi_0) \\ &= A(-\varphi_0) \, \mathrm{d}\varphi_0 - \mathrm{Im}\left\{ \int_{\varphi_0}^{2\pi} \mathrm{d}\varphi \, u_+^*(\varphi; \varphi_0) \, \mathrm{d}u_+(\varphi; \varphi_0) \right. \\ &\quad \left. + \int_0^{\varphi_0} \mathrm{d}\varphi \, u_-^*(\varphi; \varphi_0) \, \mathrm{d}u_-(\varphi; \varphi_0) \right\}. \end{aligned}$$

By use of the property

$$\mathrm{Im}\, u_{\pm}^* \, \mathrm{d}u_{\pm} = \{(2\pi^2 Z)^{-1} \kappa \sinh 2\kappa \sin 2\pi\Phi\} \, \mathrm{d}\varphi_0$$

Berry's phase is obtained as

$$\gamma = \oint \beta = 2\pi\Phi + \delta\gamma \tag{4.10a}$$

where

$$\delta\gamma \equiv -2Z^{-1} \kappa \sinh 2\kappa \sin 2\pi\Phi \tag{4.10b}$$

gives the deviation of Berry's phase from the AB phase. Note that κ is a function of g and Φ as defined by equation (3.12), and that $\delta\gamma$ is an odd periodic function of Φ

with period 1. In figure 6 we show $\delta\gamma$ as a function of Φ for typical values of g. When $g \gg 1$, $\delta\gamma$ is exponentially small and depends sinusoidally on Φ:

$$\delta\gamma \simeq -2g^2 \mathrm{e}^{-g} \sin 2\pi\Phi \tag{4.11a}$$

in other words

$$\delta\gamma \simeq -\pi^{-1}\partial\varepsilon/\partial\Phi \tag{4.11b}$$

where ε is the bound-state energy (3.13).

4.2. Method of rotating frame

In order to obtain a deeper insight into the origin of the correction term $\delta\gamma$, we reconsider the same problem from a different point of view. We attempt to solve the time-dependent Schrödinger equation (2.1) with the potential (4.6) under the initial condition

$$\psi(\boldsymbol{r}, 0) = \psi_n(\boldsymbol{r})$$

where $\psi_n(\boldsymbol{r})$ is the eigenstate of $H(0)$ introduced just before equation (4.7).

It is convenient to introduce a rotating frame of reference with cylindrical coordinates (ρ, φ', z) such that

$$\varphi' = \varphi - \varphi_0(t).$$

With the definition

$$\psi'(\rho, \varphi', z, t) \equiv \psi(\rho, \varphi' + \varphi_0(t), z, t) \tag{4.12}$$

Schrödinger equation (2.1) takes the form

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi'(\boldsymbol{r}, t) = \left[H_D + V_W(\boldsymbol{r}) + \frac{\mathscr{L}_t^2}{2m\rho^2} - \omega(t)\mathscr{L}_t + \hbar\phi_s(\varphi, t)\right]\psi'(\boldsymbol{r}, t) \tag{4.13}$$

where H_D is defined by (3.4), $\boldsymbol{r}$ stands for (ρ, φ, z) as before, and

$$\begin{aligned} &\omega(t) = \mathrm{d}\varphi_0(t)/\mathrm{d}t \\ &\mathscr{L}_t = \frac{\hbar}{\mathrm{i}}\left\{\frac{\partial}{\partial\varphi} - \mathrm{i}A(\varphi + \varphi_0(t))\right\} \\ &\phi_s(\varphi, t) = -\omega(t)A(\varphi + \varphi_0(t)). \end{aligned} \tag{4.14}$$

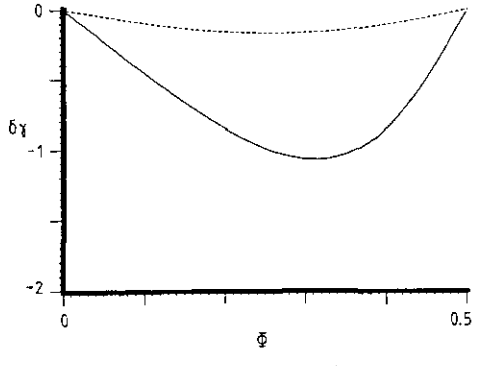

Figure 6. The deviation of Berry's phase from the AB phase for $g = 3$ (full curve) and $g = 6$ (dotted curve).

The last term $\hbar\phi_s(\varphi, t)$ is the electric scalar potential induced by the motion of the reference frame. This is most easily seen from

$$A(\varphi)\,\mathrm{d}\varphi = A(\varphi' + \varphi_0(t))[\mathrm{d}\varphi' + \omega(t)\,\mathrm{d}t].$$

This scalar potential may be eliminated by the transformation

$$\tilde{\psi}(\boldsymbol{r}, t) \equiv \exp\left[\mathrm{i}\int_0^t \mathrm{d}t'\,\phi_s(\varphi, t')\right]\psi'(\boldsymbol{r}, t). \tag{4.15}$$

Recall that A is a 2π-periodic function of φ, hence the phase factor is a single-valued function of $\boldsymbol{r}$. By use of the property

$$\int_0^t \mathrm{d}t'\,\phi_s(\varphi, t') = -\int_0^{\varphi_0(t)} \mathrm{d}\varphi_0\,A(\varphi + \varphi_0) \tag{4.16}$$

equation (4.13) may be converted into

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial t}\tilde{\psi}(\boldsymbol{r}, t) &= \left[H_D + V_W(\boldsymbol{r}) + \frac{\mathscr{L}^2}{2m\rho^2} - \omega(t)\mathscr{L}\right]\tilde{\psi}(\boldsymbol{r}, t) \\ &= [H(0) - \omega(t)\mathscr{L}]\tilde{\psi}(\boldsymbol{r}, t)\end{aligned}$$

where

$$\mathscr{L} \equiv \mathscr{L}_0 = \frac{\hbar}{\mathrm{i}}\left\{\frac{\partial}{\partial\varphi} - \mathrm{i}A(\varphi)\right\} \tag{4.17}$$

is the gauge-invariant mechanical angular momentum around the z-axis.

Now we assume that φ_0 changes so slowly that $|\omega(t)|$ remains small all the time. We may then use the perturbation theory to obtain

$$\tilde{\psi}(\boldsymbol{r}, t) = \exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\{E_n(0) - \omega(t')\langle\mathscr{L}\rangle_n\}\right]\psi_n(\boldsymbol{r}) \tag{4.18}$$

where $\langle\mathscr{L}\rangle_n$ is the expectation value of $\mathscr{L}$ with respect to the initial state $\psi_n(\boldsymbol{r})$. By use of $E_n(t) = E_n(0)$ and equations (4.12) and (4.15) we find

$$\psi(\boldsymbol{r}, t) = \exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\{E_n(t') + \hbar\phi_s(\varphi - \varphi_0(t), t') - \omega(t')\langle\mathscr{L}\rangle_n\}\right]\psi_n(\rho, \varphi - \varphi_0(t), z). \tag{4.19}$$

Note that the argument of φ_0 occurring in ϕ_s is not t' but t. The first term on the exponential gives the adiabatic dynamical phase associated with the Hamiltonian in the inertial frame. Since $\psi_n(\boldsymbol{r})$ is 2π-periodic with respect to φ, we have

$$\psi_n(\rho, \varphi - \varphi_0(T), z) = \psi_n(\rho, \varphi - 2\pi, z) = \psi_n(\rho, \varphi, z).$$

Similar relationship holds for ϕ_s. Consequently Berry's phase γ is identified as

$$\gamma = -\int_0^T \mathrm{d}t\,\phi_s(\varphi, t) + \delta\gamma \tag{4.20a}$$

where

$$\delta\gamma = \hbar^{-1}\int_0^T \mathrm{d}t\,\omega(t)\langle\mathscr{L}\rangle_n = 2\pi\hbar^{-1}\langle\mathscr{L}\rangle_n. \tag{4.20b}$$

Equation (4.16) shows that the first term of γ coincides with the AB phase; in the present method it appears as the dynamical phase due to the electric scalar potential as viewed from the rotating frame: compare a related consideration by Mondragon and Berry (1989). It may thus be concluded that the deviation of Berry's phase from the AB phase can be interpreted to arise from the Coriolis coupling $-\omega\mathscr{L}$ of the circular motion of the potential to the mechanical angular momentum; since the coupling is linear in the angular velocity, its effect does not vanish even in the adiabatic limit. If the potential V_0 represents a box, then it is intuitively obvious that the mechanical angular momentum under consideration vanishes. When V_0 represents a well, on the other hand, the wavefunction may encircle the z-axis and may support a finite angular momentum, giving rise to a non-vanishing $\delta\gamma$.

Let us confirm that formula (4.20) gives the same Berry's phase as computed by use of Berry's connection. From formula (4.20) and definition (4.17) of $\mathscr{L}$, we have

$$\gamma=\int_0^{2\pi} \mathrm{d}\varphi\, A(\varphi)+2\pi\int \mathrm{d}\boldsymbol{r}\,\psi_n^*(\rho,\varphi,z)\left\{\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi}-A(\varphi)\right\}\psi_n(\rho,\varphi,z).$$

Since the functions $A(\varphi)$ and $\psi_n(\boldsymbol{r})$ are 2π-periodic with respect to φ, we can rewrite this as

$$\gamma=\int_0^{2\pi} \mathrm{d}\varphi_0\, A(-\varphi_0)-2\pi\int \mathrm{d}\boldsymbol{r}\,\psi_n^*(\rho,\varphi-\varphi_0,z)\left\{\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi_0}+A(\varphi-\varphi_0)\right\}\psi_n(\rho,\varphi-\varphi_0,z).$$

Since the first term is independent of $\boldsymbol{r}$ and the second term is independent of φ_0, we may further rewrite the above equation as

$$\gamma=\mathrm{i}\int_0^{2\pi} \mathrm{d}\varphi_0\int \mathrm{d}\boldsymbol{r}\,\psi_n^*(\rho,\varphi-\varphi_0,z)\{\partial/\partial\varphi_0+\mathrm{i}[A(\varphi-\varphi_0)-A(-\varphi_0)]\}\psi_n(\rho,\varphi-\varphi_0,z).$$

Finally we use definition (4.8) to find

$$\gamma=\mathrm{i}\int_0^{2\pi} \mathrm{d}\varphi_0\int \mathrm{d}\boldsymbol{r}\,\psi_n^*(\boldsymbol{r};\varphi_0)\frac{\partial}{\partial\varphi_0}\psi_n(\boldsymbol{r};\varphi_0)=\oint\beta \tag{4.21a}$$

where

$$\beta=\mathrm{i}\int \mathrm{d}\boldsymbol{r}\,\psi_n^*(\boldsymbol{r};\varphi_0)\,\mathrm{d}\psi_n(\boldsymbol{r};\varphi_0). \tag{4.21b}$$

We recall that $\psi_n(\boldsymbol{r};\varphi_0)$ is single-valued in the parameter space. It follows that the above β is nothing but Berry's connection for the nth eigenstate of H. Therefore, when applied to the model of section 3.1, formula (4.21) is guaranteed to reproduce previous result (4.10).

8. Concluding remarks

(i) The models considered in section 3 might be experimentally realizable in future by use of an electron confined to a mesoscopic (or even microscopic) ring. Actual observation of the energy splitting (see figure 6), for instance, would be a fairly direct way to see the behaviour of the tails of bound state wavefunctions and to prove that the overlapping of the tails is essential for the AB effect. Although similar phenomena are well known in other systems such as a superconducting ring with a normal function,

and so on, it would still be interesting to see the phenomenon in the context of a single-particle quantum mechanics. To get a rough idea on a possible experimental value of the strength g of the potential, suppose that the potential $v(\varphi)$ is prepared by locally varying the thickness of the otherwise uniform ring. If the thickness is augmented by δd for $0<\varphi<\theta\pi$, then $v(\varphi)$ is of form (3.23) with

$$g \sim \theta a^2 \delta \mathrm{d}/\mathrm{d}^3.$$

(Note that this g is independent of the effective mass m of the electron in the ring if m is isotropic.) In view of this result it seems reasonable to expect that g can be varied over a wide range.

(ii) Even in the case of a box, there is a subtle difference between Berry's version of AB effect as originally discussed by Berry and that discussed at the beginning of section 4 in the present paper. In Berry's original consideration the box was not allowed to rotate around its own centre (*translational transportation*), while in our treatment the box rotates once around its centre (*rotational transportation*), during the transportation of the centre round the flux. Our result (4.5) shows that the rotation of the box does not matter. Indeed, in the case of a box, it is not difficult to show that Berry's phase is independent of the mode of transportation. In the case of a well, on the other hand, we have been able to deal only with the rotational transportation. The treatment of the translational transportation is not trivial; as the well is translated around the flux, the tail of the wavefunction becomes heavily distorted due to its exclusion from the flux region. Also, we have dealt only with a delta-function well. It would be interesting to study whether equation (4.11*b*) is valid or not for a generic deep well.

(iii) So far the box (or the well) has been supposed to be *non-magnetic*, that is, to carry no magnetic field of its own. If it is magnetic, a rotation around its centre without translation may give rise to Berry's phase intrinsic to it. One may then ask whether or not the total Berry phase for the rotational transportation is the sum of Berry's phase for the translational transportation and the intrinsic Berry phase.

Acknowledgments

We thank K Ohnishi, S Ohtsuka, T Tanzawa, T Tsuzuki and N Yamada for useful comments. We are also grateful to Professor M V Berry for sending us a copy of his lecture note (Berry 1990) before publication. Many thanks are due to N Yamagata for typing the manuscript.

Appendix

In order to show the validity of gauge choice (2.2), we give a constructive proof of the following theorem, which is applicable to a more general geometry than that considered in the text. As a preparation of the statement of the theorem we introduce a toroidal region D. Let (ρ, φ, z) be cylindrical coordinates representing point $\boldsymbol{r}$. Let $a(\varphi)$ and $b(\varphi)$ be arbitrary 2π-periodic functions satisfying $a_0 < a(\varphi) < b(\varphi)$ with a_0 being a positive constant. Let $c_\pm(\rho, \varphi)$ be arbitrary functions 2π-periodic in φ such that $c_-(\rho, \varphi) < 0 < c_+(\rho, \varphi)$ for $a(\varphi) < \rho < b(\varphi)$ and that $c_\pm(\rho, \varphi) = 0$ for $\rho \leqslant a(\varphi)$ and $\rho \geqslant b(\varphi)$. Region D is then defined by

$$D = \{\boldsymbol{r} \mid c_-(\rho, \varphi) < z < c_+(\rho, \varphi)\}.$$

Theorem. Suppose that divergence-free vector field $B(r)$ is given everywhere in space, that it vanishes identically in D, and that its flux through the hole surrounded by D is $\tilde{\Phi}$, that is,

$$\int_0^{2\pi} d\varphi\, F(\varphi) = \tilde{\Phi} \tag{A.1}$$

where

$$F(\varphi) = \int_0^{a(\varphi)} d\rho\, \rho B_z(\rho, \varphi, 0). \tag{A.2}$$

Let $A(\varphi)$ be an arbitrary 2π-periodic function satisfying

$$\int_0^{2\pi} d\varphi\, A(\varphi) = \tilde{\Phi} \tag{A.3}$$

then there exists a vector field $A(r)$ such that

$$A(r)\, dr = A(\varphi)\, d\varphi \qquad \text{in } D \tag{A.4}$$

and that

$$\nabla \times A(r) = B(r) \qquad \text{everywhere.} \tag{A.5}$$

Proof. We begin by defining a vector field $A'(r)$ as

$$A'_\rho(r) = \int_0^z dz'\, B_\varphi(\rho, \varphi, z') \tag{A.6a}$$

$$A'_\varphi(r) = -\int_0^z dz'\, B_\rho(\rho, \varphi, z') + \frac{1}{\rho}\int_0^\rho d\rho'\, \rho' B_z(\rho', \varphi, 0) \tag{A.6b}$$

$$A'_z(r) = 0. \tag{A.6c}$$

A direct substitution shows that $A'(r)$ is a solution of (A.5). Next, let $A(\varphi)$ be an arbitrary 2π-periodic function satisfying (A.3), and let $f(\rho)$ be an arbitrary smooth function such that $f(\rho) = 1$ for $\rho > a_0$ and $f(0) = 0$. We define

$$\Lambda(r) = f(\rho) \int_0^\varphi d\varphi' \{A(\varphi') - F(\varphi')\}. \tag{A.7}$$

By construction this function is well-defined everywhere; it is single-valued. Hence we may perform the gauge transformation

$$A(r)\, dr \equiv A'(r)\, dr + d\Lambda(r). \tag{A.8}$$

When r is in D, the integrand of (A.6*a*) and that of the first term of (A.6*b*) vanish identically, and the upper limit of the second integral of (A.6*b*) can be replaced by $a(\varphi)$. Consequently

$$A'(r)\, dr = F(\varphi)\, d\varphi \qquad \text{in } D. \tag{A.9}$$

Since $f(\rho) = 1$ for $\rho > a_0$ and *a fortiori* in D, we also have

$$d\Lambda(r) = \{A(\varphi) - F(\varphi)\}\, d\varphi \qquad \text{in } D. \tag{A.10}$$

Equations (A.8)–(A.10) prove (A.4). □

References

Aharonov Y and Bohm D 1959 *Phys. Rev.* **115** 485
—— 1961 *Phys. Rev.* **123** 1511
Berry M V 1984 *Proc. R. Soc.* A **392** 45
—— 1990 *Anomalies, Phases, Defects* ed M Bregola, G Marmo and G Morandi (Naples: Bibliopolis) p 125
Mondragon R J and Berry M V 1989 *Proc. R. Soc.* A **424** 263
Peshkin M and Tonomura A 1989 *The Aharonov–Bohm Effect* (Berlin: Springer)