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An asymptotic formula for energy eigenvalues in the bound-state Aharonov–Bohm effect

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Abstract. An asymptotic formula for the energy eigenvalues of a charged particle contained in a cylindrical shell is derived. The formula is used to estimate the eigenvalues when there is a cylindrically symmetric static magnetic-induction field present and the system exhibits the bound-state Aharonov–Bohm effect. It is shown that the errors involved form an ℓ^2 sequence with terms labelled by the radial quantum number. Numerical approximations obtained from the asymptotic formula are compared to those obtained from analytical solutions of Schrödinger's equation in the following two cases. (i) There is no magnetic-induction field in the shell itself but there is a field inside the inner cylinder. (ii) There is a constant magnetic-induction field in the shell as well as a (possibly different) field inside the inner cylinder. In these cases, the radial eigenfunctions are expressible in terms of Bessel functions and confluent hypergeometric functions, respectively. The numerical results are consistent with the asymptotic character of the formula for the energy eigenvalues.

1. Introduction

The bound-state Aharonov–Bohm effect is manifest in the shifts that occur in the discrete energy spectrum of a charged particle when a static magnetic-induction field threads a multiply connected space region to which the particle is restricted. The energy eigenfunctions and associated position probability densities are also changed by the field. This effect is the bound-state counterpart of the well known scattering Aharonov–Bohm effect [1]. Both effects are periodic in the flux of the threading field with period equal to London's natural unit of magnetic flux. Several aspects of the bound-state effect have been considered by Peshkin [2, 3], Peshkin and Tonomura [4] and O'Raifeartaigh *et al* [5, 6].

In this paper, we derive an asymptotic formula for the energy eigenvalues when the particle is contained in a cylindrical shell and the magnetic-induction field is cylindrically symmetric and parallel to the axis of the shell. The formula gives an arbitrarily close approximation to the energy for sufficiently large values of the radial quantum number and fixed values of both the angular-momentum quantum number and the quantum number for motion parallel to the axis. It is shown that the bound-state Aharonov–Bohm effect exists and that the asymptotic formula can be applied when there is a magnetic-induction field in the shell as well as one inside the inner cylinder. Numerical comparisons are made in two cases for which analytical solutions of Schrödinger's equation can be found. In the first case, there is no field in the shell and in the second, there is a constant field in the shell that may differ in magnitude and sense from the field inside the inner cylinder. In both cases, the results indicate that the approximations obtained from the asymptotic formula improve as the radial quantum number increases while the other quantum numbers and parameters of the system are fixed.

2. Bound-state Aharonov–Bohm effect

We consider a particle of mass m and charge e† constrained by perfectly reflecting walls to remain in the cylindrical shell S defined in terms of cylindrical polar coordinates (ρ, θ, z) by $a \leqslant \rho \leqslant b$, $0 \leqslant \theta < 2\pi$ and $0 \leqslant z \leqslant d$, where a, b and d are positive constants and $a < b$. It will be assumed that there is a cylindrically symmetric static magnetic-induction field $\boldsymbol{B}$ of the form $B\hat{\boldsymbol{z}}$ present. B must be a function of ρ only in order for $\boldsymbol{B}$ to satisfy the Maxwell equation $\nabla \cdot \boldsymbol{B} = 0$. It is possible [3] to express $\boldsymbol{B}$ in terms of a vector potential $\boldsymbol{A}$ of the form $A\hat{\boldsymbol{\theta}}$ where A also is a function of ρ only. A is continuous, if B is piecewise continuous. The vector potential satisfies not only $\nabla \times \boldsymbol{A} = \boldsymbol{B}$ but also the Coulomb-gauge condition $\nabla \cdot \boldsymbol{A} = 0$. In the shell S,

$$A(\rho) = \frac{\Phi}{2\pi}\frac{1}{\rho} + A_0(\rho) \tag{1}$$

where Φ is the magnetic flux (in the sense of $\hat{\boldsymbol{z}}$) through a cross section of the inner cylinder $\rho = a$ and

$$A_0(\rho) = \frac{1}{\rho}\int_a^\rho B(\rho')\rho' \, \mathrm{d}\rho'. \tag{2}$$

It should be noted that $A_0\hat{\boldsymbol{\theta}}$ is the vector potential in S when the confined flux Φ is zero. It will be convenient to scale the confined flux with respect to London's unit hc/e (in which h is Planck's constant and c is the speed of light *in vacuo*) and to define the dimensionless flux constant f by $f = e\Phi/(hc)$.

The θ- and z-dependent parts of the energy eigenfunction for a given stationary state are independent of f but the radial part $R_{n\lambda}(\rho)$ is flux dependent. It satisfies the radial Schrödinger equation

$$\rho^2 R''_{n\lambda} + \rho R'_{n\lambda} + \left[\alpha^2_{n\lambda}\rho^2 - \left(\lambda - \frac{2\pi e}{hc}\rho A_0\right)^2\right] R_{n\lambda} = 0. \tag{3}$$

Here the positive integer n is the radial quantum number and $\lambda = l - f$, where the integer l is the quantum number for the z component of the canonical angular momentum. The eigenvalues $\alpha^2_{n\lambda}$ are determined by the boundary conditions

$$R_{n\lambda}(a) = 0 = R_{n\lambda}(b). \tag{4}$$

That these eigenvalues must be non-negative can be seen from the fact that they are independent of the quantum number s for motion parallel to the z axis ($s = 1, 2, \ldots$) and from the fact that the energy eigenvalues, which are given by

$$E_{n\lambda s} = \frac{h^2}{8\pi^2 m}\left[\alpha^2_{n\lambda} + \left(\frac{s\pi}{d}\right)^2\right] \tag{5}$$

are non-negative‡ for arbitrarily large values of the height d of the cylindrical shell. We will take $\alpha_{n\lambda}$ also to be non-negative. Sturm–Liouville theory [7] guarantees that for given

† We use e to denote the signed charge of the particle. Thus, for an electron $e = -e_0$ where $e_0 \simeq 4.803 \times 10^{-10}$ esu.

‡ This follows from the form $\frac{1}{2}m\dot{\boldsymbol{r}}^2$ of the Hamiltonian and the fact that with the given boundary conditions the velocity operator $\dot{\boldsymbol{r}}$ is Hermitian. The energy must in fact be positive. For if it were zero, the ground state of the system would be an eigenstate of $\dot{\boldsymbol{r}}$ with eigenvalue zero. This, however, would contradict the uncertainty relations that follow from the commutation relations between the components of $\boldsymbol{r}$ and $\dot{\boldsymbol{r}}$.

A_0 and λ, the constants $\alpha_{n\lambda}$ form an unbounded denumerable set and hence that they may be labelled by the positive integer n. Furthermore, the eigenfunctions $R_{n\lambda}$ (again for fixed A_0 and λ) form an orthogonal set on $[a, b]$ with respect to the weight function ρ and may be chosen to be normalized with respect to this weight function.

The effect of the confined field is determined solely by the scaled flux f and is manifest by the appearance of λ, or $l - f$, in equations (3) and (5) where only l would otherwise occur. For a given field in the cylindrical shell, the wave functions and energy levels of the system depend on the confined field and the charge of the particle through f, even though the particle cannot penetrate the confined field†. This is the bound-state Aharonov–Bohm effect‡. Only values of f in the interval $[0, 1)$ need be considered, as the eigenvalue spectrum and the set of eigenstates are invariant under the addition of an arbitrary integer to f [4].

3. Asymptotic formula

In this section we derive an asymptotic formula for the energy eigenvalues by transforming the radial Schrödinger equation (3) and the boundary conditions (4) into the boundary-value problem

$$\begin{aligned} -y_n'' + q y_n &= \nu_n y_n \\ y_n(0) = 0 &= y_n(1) \end{aligned} \tag{6}$$

where n is a positive integer, dashes denote derivatives with respect to the independent variable x and the coefficient q is a function of x. Approximations to the eigenvalues of this problem can be obtained by using the following result [7].

Lemma. If $q \in L^2[0, 1]$, the eigenvalues ν_n of the regular Sturm–Liouville problem (6) satisfy the asymptotic relationship

$$\nu_n = n^2\pi^2 + \int_0^1 q(x)\,\mathrm{d}x + \ell^2(n) \qquad n = 1, 2, \ldots\,. \tag{7}$$

In other words

$$\sum_{n=1}^{\infty} \left| \nu_n - n^2\pi^2 - \int_0^1 q(x)\,\mathrm{d}x \right|^2 < \infty. \tag{8}$$

We remark that both the eigenvalues ν_n and the ℓ^2 sequence appearing above are functionals of the coefficient function q. The self-adjoint form of the radial Schrödinger equation (3), together with the boundary conditions (4) constitute the regular Sturm–Liouville problem

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}R_{n\lambda}}{\mathrm{d}\rho}\right) + \rho Q_\lambda R_{n\lambda} &= \alpha_{n\lambda}^2 \rho R_{n\lambda} \\ R_{n\lambda}(a) = 0 &= R_{n\lambda}(b) \end{aligned} \tag{9}$$

in which

$$Q_\lambda(\rho) = \left[\frac{\lambda}{\rho} - \frac{2\pi e}{hc} A_0(\rho)\right]^2. \tag{10}$$

† See also the discussion in [4]. Here we do not assume that the field in the shell has to be zero.

‡ Since it is energy differences rather than energy levels that are observable, the effect is manifest in the spectrum only if the change in energy due to the confined field is not the same for every state. That this is indeed the case can be seen from the asymptotic formula developed in section 3 and from the numerical results of sections 4 and 5.

Under the change of variables

$$x = \frac{\rho - a}{b - a} \qquad \text{and} \qquad y_n(x) = \sqrt{\rho} R_{n\lambda}(\rho) \tag{11}$$

where a, b, A_0 and λ are all fixed, the Sturm–Liouville problem (9) is transformed into (6) with

$$q(x) = (b-a)^2 \left[Q_\lambda(\rho) - \frac{1}{4\rho^2} \right] \tag{12}$$

and

$$\nu_n = (b-a)^2 \alpha_{n\lambda}^2. \tag{13}$$

In our applications, B is piecewise continuous and A_0 is continuous and so the function q defined by equation (12) is certainly in the class $L^2[0, 1]$. It follows from the lemma and equations (10), (12) and (13) that

$$\alpha_{n\lambda}^2 = \frac{n^2\pi^2}{(b-a)^2} - \frac{1}{4ab} + \frac{1}{b-a} \int_a^b \left[\frac{\lambda}{\rho} - \frac{2\pi e}{hc} A_0(\rho) \right]^2 \mathrm{d}\rho + \frac{1}{(b-a)^2} \ell^2(n) \tag{14}$$

where the ℓ^2 sequence depends on A_0, λ, a, b and e. Omission of the nth term of the ℓ^2 sequence in equation (14) gives an approximation to $\alpha_{n\lambda}^2$ that is arbitrarily close to the exact value when n is sufficiently large and other quantum numbers and parameters are fixed. The expression (5) will then give a corresponding approximation to the energy eigenvalues $E_{n\lambda s}$. For given a, b, e and A_0, the first term on the right-hand side of equation (14) depends on n only, the second term is constant and the third term depends on l and f through their difference λ but is independent of n.

4. Zero field in shell

If there is no magnetic-induction field in the shell S, the function A_0 in equation (2) is identically zero and the asymptotic formula (14) gives

$$\alpha_{n\lambda}^2 \simeq \frac{n^2\pi^2}{(b-a)^2} + \frac{\lambda^2 - \frac{1}{4}}{ab} \tag{15}$$

for large n. Numerical approximations obtained from this expression will now be compared to those obtained from the analytical solution of Schrödinger's equation. For in this case the radial equation (3) reduces to Bessel's equation of order λ with parameter $\alpha_{n\lambda}$, which is positive†. An unnormalized eigenfunction is given by

$$J_\lambda(\alpha_{n\lambda} a) Y_\lambda(\alpha_{n\lambda}\rho) - Y_\lambda(\alpha_{n\lambda} a) J_\lambda(\alpha_{n\lambda}\rho). \tag{16}$$

This obviously satisfies the boundary condition at $\rho = a$ and will satisfy the boundary condition at $\rho = b$ also if $\alpha_{n\lambda}$ $(n = 1, 2, \ldots)$ is a positive root of the equation

$$J_\lambda(\alpha a) Y_\lambda(\alpha b) - Y_\lambda(\alpha a) J_\lambda(\alpha b) = 0 \tag{17}$$

in which a, b and λ are fixed. Approximations to $\alpha_{n\lambda}^2$ for several values of n and λ were obtained by using the computer algebra system *Maple*‡ to solve equation (17) numerically. For comparison purposes, the approximations are tabulated in table 1, together with the

† We have seen in section 2 that $\alpha_{n\lambda}$ may always be taken to be non-negative. If $\alpha_{n\lambda}$ is zero, then the radial Schrödinger equation is a Cauchy–Euler differential equation (rather than the parametric form of Bessel's equation) of which only the zero solution satisfies the boundary conditions at a and b.

‡ *Maple V*, Release 4 was used. The relevant *Maple* commands are **BesselJ**, **BesselY** and **fsolve**.

Table 1. Approximations to $\alpha^2_{n\lambda}$ obtained from the asymptotic formula are shown in columns labelled A and those obtained from the solution of the parametric form of Bessel's equation are shown in columns labelled B. n is the radial quantum number and $\lambda = l - f$, where l is the angular-momentum quantum number and f is the scaled flux of the confined field. The field in the cylindrical shell is zero and the inner and outer radii a and b of the shell are taken to be 1 and 2, respectively, in arbitrary length units.

	$\lambda = 0$		$\lambda = -0.35$		$\lambda = 4.65$	
n	A	B	A	B	A	B
1	9.744 60	9.753 32	9.805 85	9.810 31	20.555 85	19.609 67
2	39.353 42	39.356 00	39.414 67	39.415 98	50.164 67	49.982 56
3	88.701 44	88.702 63	88.762 69	88.763 30	99.512 69	99.446 42
4	157.788 67	157.789 35	157.849 92	157.850 27	168.599 92	168.566 09
5	246.615 11	246.615 55	246.676 36	246.676 58	257.426 36	257.405 78
6	355.180 76	355.181 07	355.242 01	355.242 16	365.992 01	365.978 13
7	483.485 62	483.485 84	483.546 87	483.546 98	494.296 87	494.286 85
8	631.529 68	631.529 85	631.590 93	631.590 12	642.340 93	642.333 36
9	799.312 96	799.313 09	799.374 21	799.374 28	810.124 21	810.118 27
10	986.835 44	986.835 55	986.896 69	986.896 75	997.646 69	997.641 91

corresponding approximations obtained from the expression (15). In calculating the table entries, the inner and outer radii a and b of the cylindrical shell were set to 1 and 2, respectively. The unit of length to be used for a and b (and for the cylinder height d) is arbitrary†. The table contains approximations to $\alpha^2_{n\lambda}$ in units of the square of the reciprocal of the chosen unit of length; approximations to $E_{n\lambda s}$ in the corresponding energy units can then be obtained from equation (5). It is clear from table 1 that for the parameter values considered, the asymptotic formula gives better approximations to $\alpha^2_{n\lambda}$ as n increases, with λ being fixed.

It is interesting to note that when $\lambda = \frac{1}{2}$, the asymptotic expression (15) is exact for all positive integers n. This may be shown by using the identities [9]

$$J_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}}\sin x \qquad \text{and} \qquad Y_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}}\cos x \tag{18}$$

to obtain the exact solutions

$$\alpha_{n,\frac{1}{2}} = \frac{n\pi}{b-a} \tag{19}$$

of equation (17) for this case. The corresponding normalized radial eigenfunctions are given by

$$R_{n,\frac{1}{2}}(\rho) = \sqrt{\frac{2}{(b-a)\rho}}\sin\left(n\pi\frac{\rho-a}{b-a}\right) \tag{20}$$

and obviously satisfy the boundary conditions (4).

† The cylindrical-shell geometry used to model the bound-state Aharonov–Bohm effect is topologically equivalent to the toroidal geometry used in experimental verifications of the scattering Aharonov–Bohm effect by Tonomura *et al* (see [4] and references therein). In these experiments, the dimensions of the toroidal ferromagnet covered with superconducting material and used to scatter the electrons were of the order of a few microns. Similarly, recent experimental studies of Aharonov–Bohm rings containing quantum dots (see [8] and references therein) involve approximations to the cylindrical-shell geometry with inner and outer radii of less than 1 micron.

5. Constant non-zero field in shell

If there is a constant non-zero longitudinal magnetic-induction field in S, then equation (2) implies that

$$\frac{2\pi e}{hc}\rho A_0 = f'\left[\left(\frac{\rho}{a}\right)^2 - 1\right] \tag{21}$$

where f' is the scaled flux (in units of hc/e) that the field in the shell would have if this field were inside the inner cylinder. The asymptotic formula (14) now gives

$$\alpha_{n\lambda}^2 \simeq \frac{n^2\pi^2}{(b-a)^2} + \frac{(\lambda+f')^2 - \frac{1}{4}}{ab} - \frac{2f'(\lambda+f')}{a^2} + \frac{f'^2(a^2+ab+b^2)}{3a^4}. \tag{22}$$

As expected, this reduces to the asymptotic formula (15) of section 4 in the limit as $f' \to 0$. It will be assumed in what follows that the sense of the z axis is chosen so that $f' > 0$. For numerical comparison purposes, it will also be assumed that the difference between the scaled fluxes f and f' is not an integer†. For the general solution of equation (3) can then be expressed‡ in terms of the confluent hypergeometric function F, which has two parameters and one argument. The eigenfunction $R_{n\lambda}$ is proportional to

$$\exp\left(-\frac{f'}{2a^2}\rho^2\right)\left[\left(\frac{\rho}{a}\right)^{\mu} F_2(\beta_{n\lambda}, a)F_1(\beta_{n\lambda}, \rho) - \left(\frac{a}{\rho}\right)^{\mu} F_1(\beta_{n\lambda}, a)F_2(\beta_{n\lambda}, \rho)\right] \tag{23}$$

where the functions F_1 and F_2 are defined by

$$F_1(\beta, \rho) = F\left(-\beta + \frac{1}{2}\mu + \frac{1}{2}, 1+\mu, \frac{f'}{a^2}\rho^2\right) \tag{24}$$

and

$$F_2(\beta, \rho) = F\left(-\beta - \frac{1}{2}\mu + \frac{1}{2}, 1-\mu, \frac{f'}{a^2}\rho^2\right). \tag{25}$$

Also $\beta_{n\lambda}$ is given in terms of $\alpha_{n\lambda}$ by

$$\beta_{n\lambda} = \frac{a^2}{4f'}\alpha_{n\lambda}^2 + \frac{1}{2}\mu \tag{26}$$

and $\mu = \lambda + f'$. Expression (23) obviously satisfies the boundary condition at $\rho = a$ and will satisfy the boundary condition at $\rho = b$ also if $\beta_{n\lambda}$ is a root of the equation

$$\left(\frac{b}{a}\right)^{\mu} F_2(\beta, a)F_1(\beta, b) - \left(\frac{a}{b}\right)^{\mu} F_1(\beta, a)F_2(\beta, b) = 0. \tag{27}$$

It should be noted from equation (26) that $\beta_{n\lambda}$ cannot be less than $\mu/2$.

† The asymptotic formula (22) is of course valid whether $f - f'$ is an integer or not.

‡ If $f - f'$ is an integer, one of the two solutions appearing in equation (23) is either undefined or a multiple of the other solution and any second linearly independent solution contains a logarithmic term as well as another power series. This case occurs in the derivation of the Landau levels of a charged particle in an everywhere-constant magnetic-induction field (see [10]), since then $f' = f$. However, a second independent solution is not required in this problem, as only the first solution gives a wavefunction that is bounded as $\rho \to \infty$. Moreover, the confluent hypergeometric function in the first solution reduces to an associated Laguerre polynomial. In the cylindrical-shell problem considered here, two independent solutions are required in order to satisfy the boundary conditions at a and b.

Table 2. Approximations to $\alpha^2_{n\lambda}$ obtained from the asymptotic formula are shown in columns labelled A and those obtained from the solution of the confluent hypergeometric equation are shown in columns labelled C. n is the radial quantum number and $\lambda = l - f$, where l is the angular-momentum quantum number and f is the scaled flux of the confined field. The scaled flux f' corresponding to the field in the cylindrical shell is taken to be 0.3 and the inner and outer radii a and b of the shell are taken to be 1 and 2, respectively, in arbitrary length units.

	$\lambda = 0$		$\lambda = -0.35$		$\lambda = 4.65$	
n	A	C	A	C	A	C
1	9.819 60	9.820 49	9.985 85	9.989 75	19.235 85	18.137 26
2	39.428 42	39.428 97	39.594 67	39.596 13	48.844 67	48.639 27
3	88.776 44	88.776 72	88.942 69	88.943 40	98.192 69	98.120 68
4	157.863 67	157.863 84	158.029 92	158.030 33	167.279 92	167.243 94
5	246.690 11	246.690 22	246.856 36	246.856 63	256.106 36	256.084 73
6	355.255 76	355.255 83	355.422 01	355.422 19	364.672 01	364.657 52
7	483.560 62	483.560 67	483.726 87	483.727 00	492.976 87	492.966 46
8	631.604 68	631.604 73	631.770 93	631.771 04	461.020 93	461.013 09
9	799.387 96	799.387 99	799.554 20	799.554 29	808.804 21	808.798 07
10	986.910 44	986.910 47	987.076 69	987.076 76	996.326 69	996.321 76

Numerical solutions of equation (27) with $a = 1$, $b = 2$ and $f' = 0.3$ were obtained by using *Maple*†. Approximations to $\alpha^2_{n\lambda}$ were then calculated from the relation

$$\alpha^2_{n\lambda} = \frac{2f'}{a^2}\left(2\beta_{n\lambda} - \lambda - f'\right) \tag{28}$$

which follows from inversion of equation (26). These approximations may be compared in table 2 with the approximations obtained from the asymptotic formula (22). The increasing accuracy of the asymptotic formula for fixed f' and λ and increasing n is evident from the table.

6. Conclusions

Analytical solutions of the radial Schrödinger equation for the bound-state Aharonov–Bohm effect in a cylindrical shell are known only in certain simple cases and even in these cases there is no formula for calculating the energy eigenvalues exactly. We have derived an asymptotic formula that enables numerical approximations to the energy eigenvalues to be obtained when the radial quantum number is large and the other quantum numbers and parameters of the system are fixed. The errors involved in making these approximations form an ℓ^2 sequence with terms labelled by the radial quantum number.

The general solution of the radial equation is expressible in terms of Bessel functions for the case in which there is no field in the cylindrical shell. Numerical approximations obtained by using this solution confirm the validity of the asymptotic formula for this case; in particular, for the parameter values used, the formula becomes more accurate as the radial quantum number increases. Similar numerical confirmation was obtained for the case in which there is a constant non-zero field in the shell as well as a confined field inside the inner cylinder. Here the general solution of the radial equation is expressible in terms of confluent hypergeometric functions. The computer algebra system *Maple* was used to

† The hypergeometric functions may be evaluated in *Maple* by first entering the command **readlib(hypergeom)** and then using the **hypergeom** command.

obtain numerical solutions of the transcendental equations resulting from imposition of the boundary conditions in these two cases.

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