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Electrons in logarithmic potentials I. Solution of the Schrödinger equation

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Abstract. The asymptotic behaviour of the general solution of Schrödinger's equation for an electron in a logarithmic potential is derived from stability theorems, and the energy spectrum is investigated in both the attractive and repulsive cases. The general solution is represented by an uniformly convergent perturbation expansion which may be used to calculate electron interferences.

1. Introduction

The Fresnel biprisma experiment with light may also be performed with electrons, if the optical lens is replaced by some suitable electric field. In this way electron interferences can be observed without using any intermediate crystal (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976). Such an electric field can be generated by means of a cylindrical capacitor consisting of a hollow cylinder and a central straight wire. The electric field inside the cylinder can be derived from the static potential

$$V_{\text{cut}}(r)=\begin{cases}\epsilon \ln(r/b), & a\leqslant r\leqslant b\\ 0, & r>b\end{cases} \tag{1.1}$$

where a and b denote the radii of the wire and hollow cylinder respectively.

To calculate the electron interferences the corresponding (non-) relativistic wave equation must be solved under suitable boundary conditions. To gain an insight into the mathematical structure of these wave equations it is useful to extend the logarithmic behaviour of the potential to the whole space, namely to consider the Schrödinger and Dirac equations with the potential:

$$V(r)=\epsilon \ln(r/b), \qquad 0<r<\infty. \tag{1.2}$$

In this paper we analyse the Schrödinger equation. First we state the self-adjointness of the Schrödinger operator, and then we consider the family of radial operators via the usual expansion with respect to the angular momentum eigenvalues. Subsequently we specify certain fundamental systems of asymptotic solutions as $r\to 0$ and $r\to\infty$, on the basis of stability theorems about linear differential equations. Accordingly we characterise the spectrum of the Schrödinger equation and approximate the electron energy levels by means of connection formulae for our asymptotic solutions.

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Finally we derive a very transparent perturbation expansion of the general solution of each radial Schrödinger equation, and prove its uniform convergence on each compact subset of the half-line $[0, +\infty)$.

In the second paper the Dirac operator with the logarithmic potential V is considered, and the Dirac equation is solved rigorously by methods similar to our treatment of the Schrödinger problem. We show that remarkable differences between these two equations of motion occur, concerning the asymptotic behaviour of their solutions and the spectral properties. These differences are classified with respect to their origin from relativistic kinematics, the electron spin, and the possible existence of positrons.

Our following efforts will be devoted to the restriction of these general solutions by suitable boundary conditions at the radii a and b, in order to verify theoretically the results of electron interference experiments which have been performed by the authors mentioned previously.

2. Self-adjointness and angular momentum expansion

In the Hilbert space $L_2(\mathbb{R}^2)$ we consider the formal differential operator

$$T = -\Delta + V(r) \tag{2.1}$$

with the previously defined logarithmic potential V. This potential is of Stummel type (Stummel 1956), and therefore the following statement holds (Ikebe and Kato 1962).

Theorem 2.1. The restriction $T|C_0^\infty(\mathbb{R}^2)$ is essentially self-adjoint.

We decompose the Hilbert space in the usual manner by means of polar coordinates r and ϕ,

$$L_2(\mathbb{R}^2) = L_2(\mathbb{R}^+, r\,\mathrm{d}r) \otimes L_2([0, 2\pi], \mathrm{d}\phi). \tag{2.2}$$

On functions of the product form $f(r)\eta(\phi)$, the formal differential operator T acts as

$$T(f(r)\eta(\phi)) = -r^{-2}f(r)B\eta(\phi) + \left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) - r^{-1}\frac{\mathrm{d}}{\mathrm{d}r}\right)f(r)\eta(\phi), \tag{2.3}$$

where the Laplace–Beltrami operator $B = \mathrm{d}^2/\mathrm{d}\phi^2$, the restriction $B|C^\infty([0, 2\pi])$ of which is essentially self-adjoint under periodic boundary conditions, possesses the purely discrete spectrum $\{-l^2;\ l = 0, 1, 2, \ldots\}$. Thus we obtain in $L_2(\mathbb{R}^+, r\,\mathrm{d}r)$ the formal differential operators

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2} - r^{-1}\frac{\mathrm{d}}{\mathrm{d}r} + V(r) + l^2r^{-2},$$

which can be transformed unitarily to the family $\{T_l;\ l = 0, 1, 2, \ldots\}$ in $L_2(\mathbb{R}^+, \mathrm{d}r)$,

$$T_l = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + U_l(r), \qquad U_l(r) = V(r) + (l^2 - \tfrac{1}{4})r^{-2}. \tag{2.4}$$

The classical motion generated by the effective potential $V(r) + l^2r^{-2}$ is complete near infinity for $l = 0, 1, 2, \ldots$; in the repulsive case ($\epsilon < 0$) it is complete near zero for

$l=0,1,2,\ldots$, but in the attractive case ($\epsilon>0$) only for $l=1,2,3,\ldots$ (Reed and Simon 1975).

Within the framework of quantum mechanics, the radial potentials U_l are in the limit point case near infinity for $l=0,1,2,\ldots$, and in the limit point case near zero for $l=1,2,3,\ldots$; the potential U_0 is in the limit circle case near zero (Reed and Simon 1975, Dunford and Schwartz 1963). Therefore the restrictions $T_l|C_0^\infty(\mathbb{R}^+)$ are essentially self-adjoint in $L_2(\mathbb{R}^+, \mathrm{d}r)$ for $l=1,2,3,\ldots$; especially we must take the Friedrichs extension of $T_0|C_0^\infty(\mathbb{R}^+)$ to obtain equivalence with the essentially self-adjoint operator $T|C_0^\infty(\mathbb{R}^2)$.

3. Asymptotic solutions and spectral properties

The Schrödinger equation

$$(-\Delta+V(r))\Psi(r,\phi)=E\Psi(r,\phi), \qquad r>0, \quad 0\leqslant\phi\leqslant 2\pi, \tag{3.1}$$

is solved by the product *ansatz*:

$$\Psi(r,\phi)=f_l(r)\,\mathrm{e}^{\pm il\phi}, \qquad l=0,1,2,\ldots, \tag{3.2}$$

if the radial differential equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+U_l(r)\right)g_l(r)=Eg_l(r), \qquad g_l(r)=r^{1/2}f_l(r), \tag{3.3}$$

is satisfied.

In order to solve these radial equations asymptotically near zero and infinity, we perform the transformation

$$g_l(r)=\mathrm{e}^{x/2}y_l(x), \qquad x=\ln(r/b)-\nu, \qquad \nu=E/\epsilon, \tag{3.4}$$

and obtain the linear differential equations

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}-l^2\right)y_l(x)=\lambda x\,\mathrm{e}^{2x}y_l(x), \qquad \lambda=b^2\epsilon\,\mathrm{e}^{2\nu}, \qquad x\in\mathbb{R}, \tag{3.5}$$

the general solutions of which are entire functions. Note that

$$\operatorname{sgn}(\lambda x)=\operatorname{sgn}(V(r)-E), \qquad r>0, \tag{3.6}$$

and that $r\to 0$ means $x\to-\infty$, and $r\to+\infty$ means $x\to+\infty$. Concerning the physical meaning of solutions, bound states are defined by the condition

$$\int_0^\infty \mathrm{d}r|g_l(r)|^2<\infty, \qquad \text{or equivalently} \qquad \int_{-\infty}^{+\infty}\mathrm{e}^{2x}\,\mathrm{d}x\,|y_l(x)|^2<\infty. \tag{3.7}$$

We use the conventional notation of asymptotic approximation, namely, for complex-valued functions f and g on the real line,

$$f(x)\sim g(x) \text{ as } x\to\pm\infty \qquad \text{means} \qquad f(x)=g(x)(1+\mathrm{o}(1)). \tag{3.8}$$

Standard theorems about the stability of linear differential equations (Coppel 1965, Olver 1974) can now be applied to analyse the asymptotic behaviour of fundamental systems of solutions of equations (3.5):

$$y_l(x)\sim e^{\pm lx}, \qquad y_l'(x)\sim \pm l\, e^{\pm lx} \qquad \text{as } x\to-\infty \text{ for } l=1,2,3,\ldots;$$
$$y_0(x)\sim 1 \text{ or } x, \qquad y_0'(x)\sim 0 \text{ or } 1 \qquad \text{as } x\to-\infty; \tag{3.9}$$

$$y_l(x)\sim (h_l(x))^{-1/4}\exp\left(\pm\int_0^x d\xi (h_l(\xi))^{1/2}\right)$$

and

$$y_l'(x)\sim \pm(h_l(x))^{+1/4}\exp\left(\pm\int_0^x d\xi (h_l(\xi))^{1/2}\right) \qquad \text{as } x\to+\infty \text{ for } \lambda>0, \tag{3.10}$$

$$y_l(x)\sim (-h_l(x))^{-1/4}\exp\left(\pm i\int_0^x d\xi (-h_l(\xi))^{1/2}\right)$$

and (3.11)

$$y_l'(x)\sim \pm i(-h_l(x))^{+1/4}\exp\left(\pm i\int_0^x d\xi (-h_l(\xi))^{1/2}\right) \qquad \text{as } x\to+\infty \text{ for } \lambda<0,$$

with $h_l(x)=l^2+\lambda x\, e^{2x}$, for $l=0,1,2,\ldots$.

For $l=1,2,3,\ldots$, only one of these two linearly independent solutions (3.9) enables us to satisfy condition (3.7), namely $y_l(x)\sim e^{+lx}$ as $x\to-\infty$; the solution $y_0(x)\sim 1$ as $x\to-\infty$ especially corresponds to the Friedrichs extension of $T_0|C_0^\infty(\mathbb{R}^+)$.

As $x\to+\infty$, this asymptotic behaviour for $l=0,1,2,\ldots$ allows bound states or enforces unphysical solutions in case of attraction ($\lambda>0$), and permits scattering states in case of repulsion ($\lambda<0$).

To evaluate the integrals in the exponents, we use the error function (Abramowitz and Stegun 1972)

$$\Phi(z)=2\pi^{-1/2}\int_0^z dt\, e^{-t^2}, \qquad z\in\mathbb{C}; \tag{3.12}$$

in the attractive case ($\lambda>0$) we obtain by partial integration

$$\int_0^x d\xi (h_0(\xi))^{1/2}=(h_0(x))^{1/2}+\tfrac{1}{2}i(\pi\lambda)^{1/2}\Phi(ix^{1/2}), \qquad x\geqslant 0, \tag{3.13}$$

and further by binomial expansion

$$\int_0^x d\xi (h_l(\xi))^{1/2}=\int_0^x d\xi (h_0(\xi))^{1/2}+O(\text{constant}) \qquad \text{for } l=1,2,3,\ldots, \quad x\geqslant 0. \tag{3.14}$$

In the repulsive case ($\lambda<0$) we may proceed similarly, and by an asymptotic expansion of the error function we obtain finally the fundamental system of solutions:

$$y_l(x)=(\lambda x\, e^{2x})^{-1/4}\exp[\pm(\lambda x)^{1/2}e^x(1-(2x)^{-1}+O(x^{-2}))](1+o(1))$$

and (3.15)

$$y_l'(x)=\pm(\lambda x\, e^{2x})^{+1/4}\exp[\pm(\lambda x)^{1/2}e^x(1-(2x)^{-1}+O(x^{-2}))](1+o(1))$$
$$\text{as } x\to+\infty, \text{ for } l=0,1,2,\ldots.$$

These asymptotic approximations may be rewritten in terms of fundamental systems of asymptotic solutions of the radial equations (3.3):

$$g_l(r) \sim r^{\frac{1}{2}\pm l} \qquad \text{for } l = 1, 2, 3, \ldots,$$
$$g_0(r) \sim r^{1/2} \quad \text{or} \quad r^{1/2} \ln(r/b) \qquad \text{as } r \to 0; \tag{3.16}$$

$$g_l(r) \sim [\ln(r/b) - \nu]^{-1/4} \exp\left\{ \pm \{\epsilon[\ln(r/b) - \nu]\}^{1/2} r \left[1 + O\left(\frac{1}{\ln(r/b)}\right)\right]\right\} \qquad \text{as } r \to \infty. \tag{3.17}$$

This asymptotic behaviour indicates the structure of the energy spectrum. Indeed the dependence of the potential $V(r)$ on large r, and especially the non-oscillating character of the radial equations near zero and infinity imply (Dunford and Schwartz 1963, Weidmann 1967) the following theorem.

Theorem 3.1. For $l = 0, 1, 2, \ldots$, in the case of attraction ($\epsilon > 0$) the radial operators in equations (3.3) are bounded from below and their essential spectra are empty, whereas in the case of repulsion ($\epsilon < 0$) the spectra of these operators are continuous and cover the whole real line.

This theorem tells us that in the case of attraction only isolated eigenvalues of finite multiplicities occur, but it contains no information about their distribution over the real axis. To get some feeling about their location we apply the semi-classical approximation method, which yields exact results for both the harmonic oscillator and the hydrogen atom. For this purpose we introduce the action integral

$$I_l = \int_{r_1}^{r_2} \mathrm{d}r (W_l(r))^{1/2}, \qquad W_l(r) = E - V(r) - l^2 r^{-2}, \tag{3.18}$$

where l denotes the classical angular momentum, and r_1, r_2 are the classical turning points defined by the zeros of the function $r^2 W_l(r)$, $r \geqslant 0$. The desired approach then follows from the Bohr–Sommerfeld quantisation rule:

$$I_l = (n + \tfrac{1}{2})\pi, \qquad l, n = 0, 1, 2, \ldots. \tag{3.19}$$

Inserting our logarithmic potential we calculate especially

$$I_0 = \int_0^{b\,\mathrm{e}^{\nu}} \mathrm{d}r [E - \epsilon \ln(r/b)]^{1/2} = \tfrac{1}{2} b (\pi\epsilon)^{1/2} \mathrm{e}^{\nu}, \qquad \epsilon > 0, \tag{3.20}$$

and approximate the s-state energy levels by

$$E_{n,l=0} \approx \epsilon \ln\left[\left(\frac{2}{b}\right)\left(\frac{\pi}{\epsilon}\right)^{1/2}\left(n + \frac{1}{2}\right)\right], \qquad n = 0, 1, 2, \ldots. \tag{3.21}$$

This heuristic consideration can be confirmed by means of connection formulae for solutions of linear differential equations (Olver 1974). The discrete eigenvalues of equations (3.5) with $\lambda > 0$ are determined rigorously by the asymptotic relation

$$\int_{x_1}^{x_2} \mathrm{d}x (-l^2 - \lambda x\, \mathrm{e}^{2x})^{1/2} + O(\lambda^{-1/2}) = (n + \tfrac{1}{2})\pi, \qquad n = 0, 1, 2, \ldots, l = 1, 2, 3, \ldots, \tag{3.22}$$

with x_1, x_2 denoting the two zeros of $l^2+\lambda x\,e^{2x}$, $x\in\mathbb{R}$. Via the transformation (3.4) this relation turns out to be just the quantisation rule (3.19).

4. Uniformly convergent perturbation expansion

In this section we represent the general solution of equation (3.5) by some suitable series of exponential polynomials. The most convenient *ansatz* for such an expansion is suggested partly by the asymptotic behaviour (3.9) of these solutions.

Theorem 4.1. The regular differential equation

$$\left(\frac{d^2}{dx^2}-l^2\right)y_l(x)=\lambda x\,e^{2x}y_l(x), \qquad x\in\mathbb{C}, \quad l=0,1,2,\ldots, \tag{4.1}$$

is solved by the convergent series

$$y_l(x)=e^{lx}\sum_{n=0}^{\infty}\lambda^n\,e^{2nx}p_{n,l}(x), \qquad x\in\mathbb{C}, \tag{4.2}$$

with the polynomials $p_{n,l}$ of degree n defined recursively by

$$\begin{aligned}&\left(4n(n+l)+2(2n+l)\frac{d}{dx}+\frac{d^2}{dx^2}\right)p_{n,l}(x)=xp_{n-1,l}(x), \qquad n=1,2,3,\ldots,\\ &p_{0,l}(x)=1, \qquad x\in\mathbb{C}, \quad l=0,1,2,\ldots.\end{aligned} \tag{4.3}$$

The infinite series (4.2) converges uniformly on each compact subset of $\mathbb{C}$, and it converges uniformly on the negative real line. Therefore

$$\lim_{x\to-\infty} y_l(x)\,e^{-lx}=1, \qquad l=0,1,2,\ldots. \tag{4.4}$$

The first step of this recursion yields

$$p_{1,l}(x)=\left(x-\frac{2+l}{2(1+l)}\right)[4(1+l)]^{-1}, \qquad x\in\mathbb{C}, \quad l=0,1,2,\ldots. \tag{4.5}$$

Proof. Write the polynomials $p_{n,l}$ as

$$p_{n,l}(x)=\sum_{\nu=0}^{n}c_\nu^{(n,l)}x^\nu, \qquad n,l=0,1,2,\ldots. \tag{4.6}$$

Inserting these polynomials into equations (4.3) for $l=0,1,2,\ldots$, we get the coefficient recursion scheme

$$\begin{aligned}&4n(n+l)c_n^{(n,l)}=c_{n-1}^{(n-1,l)}, \qquad n\geqslant1, \qquad c_0^{(0,l)}=1;\\ &4n(n+l)c_{n-1}^{(n,l)}+2(2n+l)nc_n^{(n,l)}=c_{n-2}^{(n-1,l)}, \qquad n\geqslant2;\\ &4n(n+l)c_{n-k}^{(n,l)}+2(2n+l)(n-k+1)c_{n-k+1}^{(n,l)}+(n-k+2)(n-k+1)c_{n-k+2}^{(n,l)}\\ &\quad=c_{n-k-1}^{(n-1,l)}, \qquad k=2,3,\ldots,n-1;\\ &4n(n+l)c_0^{(n,l)}+2(2n+l)c_1^{(n,l)}+2c_2^{(n,l)}=0.\end{aligned} \tag{4.7}$$

This linear system of equations can be converted to

$$c_n^{(n,l)}=\frac{l!}{4^n n!(n+l)!}, \qquad n\geqslant 0;$$

$$c_{n-1}^{(n,l)}=-\frac{2n+l}{2(n+l)}c_n^{(n,l)}+\frac{1}{4n(n+l)}\bigg(-\frac{2(n-1)+l}{2(n-1+l)}c_{n-1}^{(n-1,l)}+\frac{1}{4(n-1)(n-1+l)}$$

$$\times\bigg(-\frac{2(n-2)+l}{2(n-2+l)}c_{n-2}^{(n-2,l)}+\ldots+\frac{1}{4\,.\,2(2+l)}\bigg(-\frac{2+l}{2(1+l)}c_1^{(1,l)}\bigg)\ldots\bigg)$$

$$=-c_n^{(n,l)}\sum_{\nu=1}^{n}\frac{2\nu+l}{2(\nu+l)},$$

$$c_{n-1}^{(n,0)}=-nc_n^{(n,0)}, \qquad n\geqslant 1;$$

$$c_0^{(1,l)}=-\frac{2+l}{2(1+l)}c_1^{(1,l)}, \qquad c_1^{(1,l)}=\frac{1}{4(1+l)}; \tag{4.8}$$

$$c_{n-k}^{(n,l)}=-\frac{(2n+l)(n-k+1)}{2n(n+l)}c_{n-k+1}^{(n,l)}-\frac{(n-k+2)(n-k+1)}{4n(n+l)}c_{n-k+2}^{(n,l)}$$

$$+\frac{1}{4n(n+l)}\bigg(-\frac{(2n-2+l)(n-k)}{2(n-1+l)(n-1)}c_{n-k}^{(n-1,l)}-\frac{(n-k+1)(n-k)}{4(n-1)(n-1+l)}c_{n-k+1}^{(n-1,l)}+\ldots$$

$$+\frac{1}{4(k+1)(k+1+l)}\bigg(-\frac{2k+l}{2(k+l)k}c_1^{(k,l)}-\frac{2}{4k(k+l)}c_2^{(k,l)}\bigg)\ldots\bigg),$$

$$k=2,3,\ldots,n.$$

By induction with respect to k these coefficients can be estimated rather roughly as

$$\tfrac{1}{2}nc_n^{(n,l)}<|c_{n-1}^{(n,l)}|\leqslant nc_n^{(n,l)}, \qquad c_{n-1}^{(n,l)}<0, \qquad n\geqslant 1;$$

$$\tfrac{1}{8}(n-1)|c_{n-1}^{(n,l)}|\leqslant c_{n-2}^{(n,l)}, \qquad n\geqslant 2; \tag{4.9}$$

$$|c_{n-k}^{(n,l)}|\leqslant 2^{k-1}\frac{n!}{(n-k)!}c_n^{(n,l)}, \qquad k=1,2,\ldots,n,$$

by means of the inequality

$$\sum_{\nu=k}^{n}\frac{(\nu-1)!}{(\nu-k)!}\leqslant\frac{n!}{(n-k)!}, \qquad k=1,2,\ldots,n. \tag{4.10}$$

Thus we obtain the result

$$|p_{n,l}(x)|\leqslant\frac{(2+|x|)^n}{4^n n!}, \qquad x\in\mathbb{C}, \quad n,l=0,1,2,\ldots. \tag{4.11}$$

The corresponding majorant with respect to the series (4.2),

$$m(x)=\sum_{n=0}^{\infty}[(\tfrac{1}{4}|\lambda|)\,\mathrm{e}^{2x}(2+|x|)]^n/n!, \qquad x\in\mathbb{C}, \tag{4.12}$$

converges uniformly on each compact subset of $\mathbb{C}$, and also on the negative real axis. This completes the proof.

The infinite series

$$\bar{y}_l(x)=\mathrm{e}^{-lx}\sum_{n=0}^{\infty}\lambda^n\,\mathrm{e}^{2nx}\bar{p}_{n,l}(x),\qquad x\in\mathbb{C},\quad l=1,2,3,\ldots,\tag{4.13}$$

with polynomials $\bar{p}_{n,l}$ defined by the recursion

$$\begin{aligned}&\left(4n(n-l)+2(2n-l)\frac{\mathrm{d}}{\mathrm{d}x}+\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\bar{p}_{n,l}(x)=x\bar{p}_{n-1,l}(x),\qquad n=1,2,3,\ldots,\\&\bar{p}_{0,l}(x)=1,\end{aligned}\tag{4.14}$$

is also uniformly convergent on each compact subset of $\mathbb{C}$ and on the negative real line, as can be proved in quite the same manner as theorem 4.1. Therefore the series (4.13) represents the solution on $\mathbb{C}$ of equation (4.1) with the limit

$$\lim_{x\to-\infty}\bar{y}_l(x)\,\mathrm{e}^{+lx}=1,\qquad l=1,2,3,\ldots.\tag{4.15}$$

Obviously the two solutions y_l and $\bar{y}_l$ are linearly independent.

Again in terms of the polar coordinate r, the perturbation expansion

$$\begin{aligned}g_l(r)&=\mathrm{e}^{x/2}y_l(x)\\&=\left(\frac{r}{b\,\mathrm{e}^{E/\epsilon}}\right)^{l+\frac{1}{2}}\sum_{n=0}^{\infty}\epsilon^n r^{2n}p_{n,l}\left[\ln\left(\frac{r}{b}\right)-\frac{E}{\epsilon}\right],\qquad l=0,1,2,\ldots,\end{aligned}\tag{4.16}$$

with the above defined polynomials $p_{n,l}$ of degree n,

$$p_{n,l}(x)=\frac{l!}{4^n n!(n+l)!}x^n+\mathrm{O}(x^{n-1}),\tag{4.17}$$

converges uniformly on each compact subset of the non-negative real line ($r\geqslant 0$); the solution $\bar{y}_l$ may be rewritten similarly in terms of the radius r. These expansions will enable us to compute the electron interferences quoted in the introduction, of course only in the non-relativistic limit.

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