ON THE SPECTRUM OF V(ρ) = $-\frac{qt}{\rho} + \frac{rt}{\rho^2} + st^{\rho} + t^{\rho^2}$. PHYSICAL IMPLICATIONS FOR A VARIETY OF PROBLEMS

J. A. C. Gallas*

Max-Planck Institut für Quantenoptik D-8046 Garching bei München West Germany

R. F. O'Connell

Department of Physics and Astronomy Louisiana State University Baton Rouge, Louisiana 70803, USA

1. INTRODUCTION

In recent years there has been much interest in obtaining eigenvalues for relatively complicated potentials, particularly for those situations where perturbation theory is not applicable. Motivation for this interest is not hard to discern: On the one hand, there are the various strong-field problems of condensedmatter-, atomic- and astro-physics [1-7]; and, on the other hand, there are the extensive investigations of the charmonium spectrum [8-10]. Many of these studies have been concerned with the onedimensional potential

$$V(\rho) = -\frac{qt}{\rho} + \frac{rt}{\rho^2} + st\rho + t\rho^2$$
(1)

where $r \ge 0$ and $q, t \ge 0$. For simplicity, we may also take $s \ge 0$, since this covers many of the cases of interest.

*Permanent address: Departamento de Fisica Universidade Federal de Santa Catarina 88000 Florianópolis, SC, Brasil 721

S. P. McGlynn et al. (eds.), Photophysics and Photochemistry in the Vacuum Ultraviolet, 721–728. © 1985 by D. Reidel Publishing Company. Table 1 provides a listing of those physical problems encompassed by the potential of Eq. (1). In particular, this potential is precisely that one considered in many investigations of the charmonium energy spectrum [8-10]. When r=s=0, the quasi-Landau spectrum with magnetic quantum number m=0 results [2]; whereas, if only s=0, the more general quasi-Landau spectrum (m≠0) results [3]. If the ρ^2 term is omitted, the potential has the same form as that for the well-known Stark problem [7]. And, finally, this potential is also appropriate for treating the case of electrons at the surface of liquid helium [1,5] in the presence of crossed electric and magnetic fields [6].

In Section 2 we obtain a WKB solution of the eigenvalue problem resulting from Eq. (1); and, in Section 3 we present a brief discussion of some applications.

2. SOLUTION OF THE EIGENVALUE PROBLEM

Our purpose here is to extend a previously employed technique [4] in order to solve the spectral problem for Eq. (1). We start from the well-known WKB result for the energy E:

$$(2M)^{\frac{l_2}{2}} \int_{\rho_1}^{\rho_2} \left[E - V(\rho) \right]^{\frac{l_2}{2}} d\rho = (n + \frac{l_2}{2}) \pi \hbar$$
(2)

where M is a particle mass (usually that of the electron), and where ρ_1 and ρ_2 are the WKB turning points. Thus, from

Table 1. A List of Physical Problems Encompassed by the Potential $V(\rho) = -\frac{qt}{\rho} + \frac{rt}{\rho^2} + st\rho + t\rho^2$.

Physical ProblemsNon-Contributing Terms in $V(\rho)$ Quasi-Landau (m=0)r=s=0Quasi-Landau (m≠0)s=0Stark Effect ρ^2 term is omittedElectrons at the Surface of Li-
quid Helium in an Electric Field ρ^2 term is omittedElectrons at the Surface of Li-
quid Helium in Crossed Electric
and Magnetic Fields---

Eqs. (1,2) we may write

$$I = \int_{\rho_1}^{\rho_2} \frac{d\rho}{\rho} (-\rho^4 - s\rho^3 + p\rho^2 + q\rho - r)^{\frac{1}{2}} = (n + \frac{1}{2}) \frac{\pi\hbar}{(2Mt)^{\frac{1}{2}}}$$
(3)

where $p\equiv E/t,$ and where $\rho_1 < \rho_2$ are the two real and non-negative roots of

$$(4) p^{4} - s\rho^{3} + p\rho^{2} + q\rho - r \equiv (\rho - \rho_{1})(\rho_{2} - \rho)(\rho^{2} - 2X\rho + Y) = 0.$$

It is convenient to define a generic integral

$$I_{i} = \int_{\rho_{1}}^{\rho_{2}} \rho^{i} (-\rho^{4} - s\rho^{3} + p\rho^{2} + q\rho - r)^{-1} d\rho$$
 (5)

which allows us to rewrite Eq. (3) as

$$I = -I_3 - sI_2 + pI_1 + qI_0 - rI_{-1}.$$
 (6)

One may also verify, using integration by parts, that [4]

$$I = I_{3} + \frac{s}{2}I_{2} + \frac{1}{2}qI_{0} - rI_{-1}.$$
 (7)

Combining Eqs. (6,7), we obtain

$$I = -\frac{s}{4}I_2 + \frac{1}{2}pI_1 + \frac{3}{4}qI_0 - rI_{-1}.$$
 (8)

A very useful observation can now be made: Namely, that the *struc*ture of the polynomial occurring in Eq. (4) is the same as that for the s=0 case [4], with the only difference being the numerical values of the four roots ρ_1 , ρ_2 , and X \pm (X²-Y)^{5/2}. Thus, the integrals I₁, I₀ and I₋₁ are exactly the same as described previously [4] and depend only upon K and I (the complete elliptic integrals of the first and third kinds, respectively) [10]. We refer to [4] for explicit results.

The only new integral we must evaluate is I_2 ; and, we find that this integral depends not only upon K and \mathbb{H}^2 but also upon E(the complete elliptic integral of the second kind). As in all problems of this nature [2-4], there are two cases to consider, namely $E>V_C$ and $E\leq V_C$, where V_C is the relative minimum of $V(\rho)$ along the negative ρ -axis. As before [4], we use the results of Byrd and Friedman [11] to obtain:

(i) if
$$E > V_{c}$$

$$I_{2} = g \left\{ d^{2} K(k) + 2d(\rho_{2}-d) \Pi(\alpha^{2},k) + \frac{(\rho_{2}-d)^{2}}{2(\alpha^{2}-1)(k^{2}-\alpha^{2})} \right\}$$

$$\times \left[\alpha^{2} E(k) + (k^{2}-\alpha^{2}) K(k) + (2\alpha^{2}k^{2}+2\alpha^{2}-\alpha^{4}-3k^{2}) \Pi(\alpha^{2},k) \right] \right\} (9)$$

(ii) if
$$E \leq V_{c}$$

$$I_{2} = g \frac{(\rho_{1}A - \rho_{2}B)^{2}}{(A - B)^{2}} \left\{ 2K(k) + \frac{2(\rho_{2} - \rho_{1})(A + B)}{(\rho_{1}A + \rho_{2}B)} \Pi(\alpha_{1}^{2}, k) - \frac{2AB(A + B)^{2}}{(\rho_{1}A + \rho_{2}B)^{2}} X \left[\frac{(A - B)^{2} - 2(\rho_{1} - \rho_{2})^{2}}{4AB} \Pi(\alpha_{1}^{2}, k) + \left(\frac{\rho_{1} - \rho_{2}}{A + B} \right)^{2} K(k) - \left(\frac{A - B}{A + B} \right)^{2} E(k) \right] \right\}$$
(10)

The various symbols introduced in Eqs. (9,10) are defined in [4], with the exception of α :

$$\alpha^{2} = (\rho_{1} - \rho_{2}) / (\rho_{1} - d) .$$
 (11)

To summarize, we have analyzed a relatively complicated four term potential, using WKB techniques, and have succeeded in obtaining an analytic solution for the eigenvalues in terms of elliptic functions, of which there are only three kinds. We restricted ourselves to s>0 (which is the actual case for many applications and, in particular, for those discussed below) in order to avoid a double-well potential and the associated tunneling and energy shifts [12,13]. In the future, we will return to the s<0situation in order to consider potentials similar to those depicted in Fig. 2 of [12]. This will require an extension of the work of [12], which was restricted to a harmonic double-well potential, by inclusion of the more general potential. For now, we turn to a brief discussion of a variety of physical problems to which our results are applicable.

3. APPLICATIONS

3.1 Quasi-Landau Resonances

A problem which has attracted enormous interest in recent years is that of the motion of a spinless electron in combined Coulomb and magnetic fields. It is relevant to investigations in such diverse areas as condensed-matter-, atomic- and astrophysics; and, it is fascinating per se, from a theoretical point of view, because it is an outstanding example of a nonseparable problem. If the Schrödinger equation for this combined-field problem is written in cylindrical coordinates, it can be shown that the problem is reducible to two-dimensional motion in ρ -z space, where $\rho^2 = x^2 + y^2$. However, if we set z=0, motion in a one-dimensional potential results [2]:

$$V(\rho) = \frac{\pi^2}{2M\rho^2} \frac{T}{\rho^2} - \frac{e^2}{\rho} + \frac{1}{8} M\omega^2 \rho^2$$
(12)

where $\omega = eB/Mc$ is the cyclotron frequency; B is the magnetic field strength; and T is a known function of the magnetic quantum

number m.

The z=0 approximation has been shown to give good agreement with the experimental results of Garton and Tomkins [14]. These authors [14] studied the absorption spectrum of barium in a magnetic field of 24 kG, for n values as high as 75, and found broad resonances spaced by approximately 1.5 fix near E=0. These socalled quasi-Landau resonances were observed only in the σ spectrum (Δ m=±1); and, since the σ lines result from states which are essentially localized in the x-y plane, we obtain a better appreciation of why the z=0 approximation works so well.

It is clear that Eq. (12) is a special case of the general potential given in Eq. (1) and corresponds to taking s=0. Since we have already discussed the solution to this problem at length, we refer to our previous work [2-4] for details.

3.2 Stark Effect

This is a classic problem which has recently returned to the forefront of interest because of the plethora of experimental investigations of highly-excited states (Rydberg states) brought about by the availability of laser techniques. For many of these investigations, perturbation theory is no longer adequate because of the relative weakness of the Coulomb field, vis-à-vis the electric field, for high-Rydberg states. It is well-known that the Hamiltonian for this problem can be separated in parabolic coordinates, resulting in two Schrödinger radial-like equations in the now familiar $\xi = r+z$ and $\eta = r-z$ coordinates. The corresponding potentials are special cases of Eq. (1) [the ρ^2 term is missing] and a detailed WKB solution, in terms of the elliptic integrals discussed above, has recently been presented [7].

3.3 Electrons at the Surface of Liquid Helium

Electrons outside a free surface of liquid helium are trapped in an image potential, which is essentially one-dimensional Coulombic [1,5,6]. In addition, there is a 1 eV potential barrier at the surface which prevents electron penetration. As a result, the electrons are trapped in a one-dimensional well, giving rise to quantized states in a direction (z say) perpendicular to the surface. The potential is given by

$$V(z) = -Ze^2/z \tag{13}$$

where $Z = \frac{1}{4}(\varepsilon-1)/(\varepsilon+1) = 6.951 \times 10^{-3}$. If we now assume that the barrier is infinite at the origin, we are led to a "hydrogenic" spectrum for electrons trapped at the surface. Some interesting characteristics of this spectrum have been discussed by Grimes, *et al.* [15]. It was found to be convenient experimentally to

apply an electric field F to the system [15] since this configuration permitted investigations to be carried out at a fixed frequency, while the energy separations were varied by means of the electric field. However, the presence of an electric field gives rise to an extra term in the potential, namely eFz. We have already presented a WKB solution to this problem [5], the potential being the same as that of Eq. (1) with the ρ^2 term omitted; the corresponding z^{-2} term which arises in this problem comes from the Langer-type correction to the potential [4,16], a correction which is necessary if one wishes to use the WKB method, derived for the one-dimensional range $(-\infty, +\infty)$, in problems where the range is restricted to $(0, +\infty)$.

Zipfel, Brown and Grimes [6] next applied a magnetic field along the surface ($B=B_y$ say). Following these authors [6], if one chooses a gauge A = (zB,0,0), the Hamiltonian can be written as

$$H = \frac{1}{2M} (p_x - \frac{e}{c}Bz)^2 + \frac{1}{2M} (p_y^2 + p_z^2) - \frac{Ze^2}{z} + eFz . (14)$$

Since p_x and p_y commute with H, it is clear that they are both constants of the motion. Moreover, the motion in the z-direction is governed by the potential

$$V(z) = (-\omega p_{x} + eF)z + \frac{1}{2} M\omega^{2} z^{2} - \frac{Ze^{2}}{z}$$
(15)

where, again, $\omega = eB/Mc$, and where p_x now refers to the eigenvalue rather than to the operator.

Finally, since $0 \le x \le \infty$, the Langer correction contributes a z^{-2} term to Eq. (15); hence, the potential which results is similar to that of Eq. (1), provided F is large enough (or else p_x and/or B are small enough) that the coefficient of z in Eq. (15) is positive. In essence, then, the problem is solved and a detailed exposition of the numerical predictions will be presented in another venue.

3.4 Charmonium

The suggestion, by Gell-Mann and Zweig in 1964, that quarks are the fundamental building blocks of elementary particles has had a profound influence on high-energy physics research. The original proposal was a three-quark model (up, down and strange quarks) but, shortly thereafter, Bjorken and Glashow suggested the existence of a fourth quark (called "charm"). Then, in 1974, a revolution occured in high-energy physics following the discovery of the famous ψ/J particle. It is now well-established that this particle is a particular bound state of the charmed quark and its anti-particle. Such a bound state, the net charm quantum number of which is zero, is called "charmonium". The ψ/J particle is simply the 1^3S_1 state of the charmonium spectrum, a spectrum which, at least as far as nomenclature is concerned, can be compared to the positronium spectrum. Our knowledge of the interquark forces is still somewhat phenomenological but it is generally accepted that the potential is of the form

$$V(\mathbf{r}) = -\frac{\beta}{\mathbf{r}} + \mu \mathbf{r} + \lambda \mathbf{r}^2 + \cdots \qquad (16)$$

The force between quarks is propagated by gluons, in analogy to the photon propagation of electromagnetic forces, but here the situation is more complicated in that one must deal with a non-Abelian gauge theory (known as quantum chromodynamics, QCD). However, in the non-relativistic limit it is known that a Coulombtype force arises at small distances, which rationalizes the first term of Eq. (16), where β is a measure of the gluon force (observations imply that $\beta \approx 0.25$). The other terms in Eq. (16) represent the "confining potential" which prevents break-up of the system; these terms are introduced, without any basic theoretical underpinning, to understand the observed level spacings. Perhaps it should be emphasized that the potential given in Eq. (16) is inserted into the three-dimensional Schrödinger equation; then, the usual transformation $R(r) \rightarrow \xi(r) = r R(r)$ provides a one-dimensional equation for the modified radial wavefunction $\xi(\mathbf{r})$, with the potential also being modified by the addition of a centrifugal term $\hbar^2 \ell(\ell+1)/2Mr^2$. This latter term is further modified by the Langer correction to give $\hbar^2 (\ell + 1/2)^2 / 2Mr^2$. Such a term, when added to the V(r) appearing in Eq. (16), results in, once more, a potential which is a particular example of Eq. (1).

4. SUMMARY

We have used WKB techniques to obtain analytic solutions, in terms of elliptic functions, for the eigenvalues of the potential given in Eq. (1). In addition, we have shown that this solution provides a general framework which can be used for the consideration of a large class of problems, the so-called strong-field problems: That is, problems in which more than one field makes comparable contributions to the basic forces and energies. Also, for some of these strong-field problems we have already demonstrated in detail the accuracy of our results, by comparison with experiment and other theoretical investigations [2-5].

ACKNOWLEDGMENT

JACG acknowledges support from the UFSC-Florianopolis/Brasil

J. A. C. GALLAS AND R. F. O'CONNELL

and DAAD/Germany. RFO'C acknowledges support from the Department of Energy, Division of Material Sciences, contract DE-AS05-79ER10459; he would also like to thank the Max-Planck Institute of Quantum Optics for hospitality during the summer of 1982, when this work was completed.

REFERENCES

- R. F. O'Connell, Phys. Lett. <u>60A</u>, 481 (1977); J. A. C. Gallas, E. Gerck and R. F. O'Connell, Phys. Rev. Lett. <u>50</u>, 324 (1983).
- J. A. C. Gallas and R. F. O'Connell, J. Phys. B: At. Mol. Phys. 15, L75 (1982).
- 3. J. A. C. Gallas and R. F. O'Connell, J. Phys. B: At. Mol. Phys. <u>15</u>, L309 (1982).
- J. A. C. Gallas and R. F. O'Connell, J. Phys. B: At. Mol. Phys., <u>15</u>, L593 (1982).
- 5. R. F. O'Connell, in: Proceedings of the Colloque International C.N.R.S. (Aussois, France, 1982), J. de Physique (France), Colloque C2, Supplement 11, C2-81 (1982).
- 6. C. L. Zipfel, T. R. Brown and C. C. Grimes, Phys. Rev. Lett. 37, 1760 (1976).
- J. A. C. Gallas, H. Walther and E. Werner, Phys. Rev. A26, 1775 (1982); Phys. Rev. Lett. 49, 867 (1982).
- C. Quigg and J. L. Rosner, Phys. Reports <u>56C</u>, 167 (1979);
 J. Killingbeck, J. Phys. A: Math. Gen. <u>13</u>, L393 (1980).
- D. P. Datta and S. Mukherjee, J. Phys. A: Math. Gen. <u>13</u>, L221 (1980).
- 10. J. Killingbeck and S. Galicia, J. Phys. A: Math. Gen. <u>13</u>, 3419 (1980); G. P. Flessas, J. Phys. A: Math. Gen. <u>15</u>, <u>L1</u> (1982).
- 11. B. P. Byrd and M. D. Friedman, Handbook of Elliptic Integrals for Engineers and Scientists, 2nd rev. ed. (Springer-Verlag, Berlin, 1975); in particular, see p. 124 and also Eq. (336.02), p. 201.
- 12. J. H. Weiner, J. Chem. Phys. 69, 4743 (1978).
- 13. J. H. Weiner and S. T. Tse, J. Chem. Phys. 74, 2419 (1981).
- 14. W. R. S. Garton and F. S. Tomkins, Astrophys. J. <u>158</u>, 839 (1969).
- C. C. Grimes and T. R. Brown, Phys. Rev. Lett. <u>32</u>, 280 (1974); C. C. Grimes, T. R. Brown, M. L. Burns and C. L. Zipfel, Phys. Rev. B <u>13</u>, 140 (1976).
- 16. R. E. Langer, Phys. Rev. 51, 669 (1937).