CERN-TH. 5914/90
UW ThPh-1990-50

November 1990

ORDER OF ENERGY LEVELS FOR THE KLEIN-GORDON EQUATION

H. GROSSE

*Institut für Theor. Physik
Universität Wien*

A. MARTIN

*Theoretical Physics Division, CERN
1211 Geneva 23, Switzerland*

J. STUBBE

*Département de Physique Théorique
Université de Genève*

ABSTRACT

We generalize to the case of the Klein-Gordon equation results on the order of energy levels of the Schrödinger equation for a given sign of the Laplacian of the potential. In particular we obtain modified versions of the theorems on the order of energy levels for a negative, vector-like, central potential with a Laplacian of a given sign. For the case of a positive Laplacian, a positive scalar potential, with a positive Laplacian, can be included too.

Some years ago, Baumgartner, Grosse and Martin [1] proved that the Coulomb degeneracy of the Schrödinger equation is lifted in a way which depends on the sign of the *Laplacian* of the spherically symmetric potential. Specifically if n is the number of nodes of the radial wave function and ℓ the orbital angular momentum

$$\begin{aligned} E(n, \ell) &\gtrless E(n-1, \ell+1) \\ \text{if } \Delta V(r) &\gtrless 0 \quad \forall \quad r > 0. \end{aligned} \tag{1}$$

For the pure Coulomb case $\Delta V(r) = \delta^3(\vec{r})$ and hence we get degeneracy and the energy levels depend only on the principal quantum number

$$N = n + \ell + 1 \tag{2}$$

More recently, Martin und Stubbe [2] have obtained the following inequality for purely angular excitations of the Schrödinger equation

$$\frac{E(0, \ell_3) - E(0, \ell_2)}{E(0, \ell_2) - E(0, \ell_1)} > \frac{-\frac{1}{(\ell_3+1)^2} + \frac{1}{(\ell_2+1)^2}}{-\frac{1}{(\ell_2+1)^2} + \frac{1}{(\ell_1+1)^2}} \tag{3}$$

with $\ell_3 > \ell_2 > \ell_1$, not necessarily integers, if $\Delta V(r) \gtrless 0 \quad \forall \quad r > 0$.

In the special case $V(r) < 0$, $V(r) \rightarrow 0$ for $r \rightarrow \infty$ $E(0, \ell_3) \rightarrow 0$ for $\ell_3 \rightarrow \infty$ when $\Delta V(r)$ has a given sign, and we get

$$E(0, \ell_2) (\ell_2 + 1)^2 \gtrless E(0, \ell_1) (\ell_1 + 1)^2 \tag{4}$$

$$\text{if } V(r) < 0, \quad V(r) \rightarrow 0 \quad \text{and} \quad \Delta V(r) \gtrless 0 \quad \forall \quad r > 0 \quad \text{with} \quad \ell_2 > \ell_1$$

A question we are often asked is what happens if relativistic effects are taken into account. The next simple cases to treat are those of the Klein-Gordon equation and of the Dirac equation, but, while (1) (3) and (4) become equalities in the case of a pure Coulomb potential in the Schrödinger equation, this is not anymore the case if one uses the Klein-Gordon or the Dirac equation.

For the Dirac equation with a vector-like potential, the energy levels depend on N , J , the total angular momentum and k , or equivalently N , J and ℓ the orbital angular momentum. It has been shown by Grosse [3] that when the Coulomb potential is perturbed by a potential with a given sign of the Laplacian the degeneracy in k is lifted :

$$\begin{aligned} E(N, J, -k) &\geq E(N, J, k) \\ \text{if } \Delta V(r) &\geq 0 \quad \forall r > 0 \quad k > 0 \end{aligned} \quad (5)$$

This means that, in spectroscopic notation, the $Ns_{1/2}$ level is above the $Np_{1/2}$ level if $\Delta V(r) > 0 \quad \forall r > 0$. However this result is only established in first order of perturbation theory and there is no inequality connecting energy levels with the same N but different J 's. For the pure Coulomb case we know that for fixed N , the energies increase as J increases.

There is a result obtained by Palladino and Leal Ferreira for the special case of a 50 % 50 % mixture of scalar and vector potential [4], but this does not tell us what happens in the neighbourhood of a pure Coulomb potential, which is vector like.

For the Klein-Gordon equation

$$(p^2 + (m + S)^2 - (E - V)^2) \psi = 0 \quad (6)$$

we know the solutions for the pure Coulomb case

$$S = 0, \quad V = -\frac{Z\alpha}{r}, \quad Z\alpha < 1/2, \quad (7)$$

which are obtained by noticing that the term V^2 can be incorporated in the centrifugal term in the reduced radial equation :

$$\left(-\frac{d^2}{dr^2} + \frac{\ell'(\ell' + 1)}{r^2} + m^2 - E^2 - 2E\frac{Z\alpha}{r} \right) u = 0 \quad (8)$$

with

$$(\ell' + 1/2)^2 = (\ell + 1/2)^2 - (Z\alpha)^2 \quad (9)$$

Hence (8) looks like a Schrödinger equation with Coulomb potential, and one gets

$$E(n, \ell) = \frac{m}{\sqrt{1 + \frac{(Z\alpha)^2}{(n+1/2 + \sqrt{(\ell+1/2)^2 - (Z\alpha)^2})^2}}} \quad (10)$$

Here, naturally, E is the total energy. It is easy to see that for fixed $N = n + \ell + 1$, E increases as ℓ increases.

In this paper we shall present some results on the level ordering and also find an analogue of (4) for the Klein-Gordon case. Proofs will only be sketched and details given elsewhere.

A prerequisite is to notice that the energy levels can still be labelled by n and ℓ and to make sure that the "trivial" ordering properties:

$$E(n+1, \ell) > E(n, \ell) \quad (11)$$

and

$$E(n, L) > E(n, \ell) \quad \text{for } L > \ell \quad (12)$$

are satisfied. They are indeed provided $V \leq 0$ and $E(n, \ell) > 0$. Then the coefficient of u , the reduced wave function, in the Klein-Gordon equation is an *increasing* function of E and this suffices to establish (11). (12) follows from the Feynman Hellmann theorem applied to dE/dl and the positivity of $E - V$ [see equ. (24) below].

In what follows, we shall take $S = 0$. However, as we shall see at the end, some results are valid for $S > 0$.

THEOREM I

If $\Delta V(r) \leq 0$, $V(r) < 0$ and $V(r) \rightarrow 0$ for $r \rightarrow \infty$ and if $\lim_{r \rightarrow 0} rV(r) > 1/2$, $E(n, \ell) < E(n-1, \ell+1)$ (notice the strict inequality!).

To prove this, we look at the Klein-Gordon equation as a Schrödinger equation depending on the parameter E :

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + m^2 - E^2 + (2VE - V^2) \right) u = 0. \quad (13)$$

Under the assumptions made, the Laplacian of the effective potential $2VE - V^2$ (we restrict ourselves to *positive* energy states !) is *negative* because :

$$\Delta V^2 = 2 \left(V \Delta V + \left(\frac{dV}{dr} \right)^2 \right) \quad (14)$$

Now, since $\Delta V < 0$ and $V < 0$, rV has a negative limit for $r \rightarrow 0$ and this means that the effective potential has a $-1/r^2$ singularity. However, the results of reference (1) can be easily extended to a potential $U(r)$ such that $\lim_{r \rightarrow 0} r^2 U(r) > -1/4$. On the other hand, the non-linear dependence of (10) in the energy can be overcome by using a fixed point argument.

The weakness of Theorem I is that it has no counterpart for $\Delta V \geq 0$. To circumvent this difficulty we follow the analogue of what was done in (8), i.e. transfer a part of the "potential" into the angular momentum term. We shall define, by analogy to the Coulomb case :

$$-Z\alpha = \lim_{r \rightarrow \infty} rV(r) \quad (15)$$

and keep the definition (9) of ℓ' . Then the Klein-Gordon equation becomes :

$$\left(-\frac{d^2}{dr^2} + \frac{\ell'(\ell'+1)}{r^2} + m^2 - E^2 + \hat{V} \right) u = 0 \quad (16)$$

$$\text{with } \hat{V} = 2EV - V^2 + \frac{(Z\alpha)^2}{r^2}. \quad (17)$$

It is easy to prove the

LEMMA :

$$\text{if } \Delta V \gtrless 0 \forall r > 0, \quad V(r) < 0, \lim_{r \rightarrow \infty} rV(r) = -Z\alpha, \text{ then } \Delta \hat{V} \gtrless 0, \text{ and } V^2 \leq \frac{(Z\alpha)^2}{r^2} \quad (18)$$

Let us now make the change of variables :

$$\hat{E}(n, \ell') = E(n, \ell) \quad (19)$$

Then the two-sided theorem can be formulated.

THEOREM II

If $\Delta V \gtrless 0$, $V < 0$, $\lim_{r \rightarrow \infty} rV(r) = -Z\alpha > -\frac{1}{2} - \ell$, $\hat{E}(n, \ell') \gtrless \hat{E}(n-1, \ell'+1)$, and more generally $\hat{E}(n, \ell') \gtrless \hat{E}(n-k, \ell'+k)$

Remark

In the case $\Delta V \leq 0$ a prerequisite for Theorem II is that the Klein-Gordon equation makes sense, i.e. that $\lim_{r \rightarrow 0} rV(r) > -\frac{1}{2} - \ell$.

Naturally Theorem II can be translated into the variable ℓ

$$E(n, \ell) \gtrless E(n-k, \ell + \Delta(\ell, k)) \quad (20)$$

with

$$\sqrt{(\ell + \frac{1}{2})^2 - (Z\alpha)^2} + k = \sqrt{(\ell + \Delta + 1/2)^2 - (Z\alpha)^2} \quad (21)$$

Naturally, in general, Δ is not an integer when k is an integer. One has

$$0 < \Delta(\ell, k) < k \quad (22)$$

and in that sense this means that Theorem I is a consequence of Theorem II. Indeed, for $\Delta V < 0$, etc., one has :

$$E(n, \ell) < E(n - k, \ell + \Delta(\ell, k)) < E(n - k, \ell + k) \quad (23)$$

because of the monotonicity of the energies with respect to angular momentum, which still holds for the Klein-Gordon case for negative potentials because of the equation :

$$\frac{dE(n, \ell)}{d\ell} < E - V > = (\ell + 1/2) < \frac{1}{r^2} > . \quad (24)$$

It should be noted that in "normal" situations $\Delta(\ell, k)$ is always very close to k .

- if $Z\alpha < 1/2$ (which is required for $\ell = 0$), one has :

$$k - 1/2 < \Delta(\ell, k) < k \quad (25)$$

- if $Z\alpha < 1$, $\ell \geq 1$

$$k - 0.4 < \Delta(\ell, k) < k \quad (26)$$

Using these remarks, one can transform theorem II into a theorem connecting *physical* angular momenta :

COROLLARY

$$\text{if } \Delta V > 0, \quad V < 0, \quad \lim_{r \rightarrow \infty} Vr > -1/2, \quad E(n, \ell) > E(n - k, \ell + k - 1)$$

This is somewhat crude and does not reduce to the correct limit when V approaches a pure Coulomb potential.

However, we can do better by first proving a relativistic analogue of inequality (4):

THEOREM IIIa

if $\Delta V \leq 0$ $V(r) < 0$, $\lim_{r \rightarrow \infty} rV(r) = -Z\alpha > -1/2 - \ell_1$

$$\left(\frac{m^2}{\widehat{E}(0, \ell'_1)^2} - 1 \right) (\ell'_1 + 1)^2 > \left(\frac{m^2}{\widehat{E}(0, \ell'_2)^2} - 1 \right) (\ell'_2 + 1)^2 \text{ with } \ell'_2 > \ell'_1 \quad (27)$$

THEOREM IIIb

if $\Delta V \geq 0$ $V(r) < 0$, $\lim_{r \rightarrow \infty} rV(r) > -\ell_1 - 1/2$

$$\left(\frac{m^2}{\widehat{E}(n, \ell'_1)^2} - 1 \right) (\ell'_1 + 1)^2 < \left(\frac{m^2}{\widehat{E}(n, \ell'_2)^2} - 1 \right) (\ell'_2 + 1)^2 \text{ with } \ell'_2 > \ell'_1 \quad (28)$$

The proofs of (27) and (28) involve a chain of inequalities :

- 2 forms of the virial theorem, for the initial Klein-Gordon equation and for the modified Klein-Gordon equation, combined with the fact that $V < 0$ and that ΔV has a given sign :

$$E(E - \langle V \rangle) \gtrless m^2 \quad \text{for } \Delta V \gtrless 0 \quad (29)$$

$$\langle \widehat{T} \rangle_{n, \ell'} \gtrless -E \langle V \rangle \quad \text{for } \Delta V \gtrless 0 \quad (30)$$

where $\langle \widehat{T} \rangle_{n, \ell'}$ is the expectation value of $-\frac{d^2}{dr^2} + \frac{\ell'(\ell' + 1)}{r^2}$.

- the Feynman-Hellmann relation for $\widehat{E}$ as a function of ℓ' :

$$2 \langle \hat{E} - V \rangle \frac{d\hat{E}(n, \ell')}{d\ell'} = (2\ell' + 1) \langle \frac{1}{r^2} \rangle \quad (31)$$

- and finally an inequality connecting the total kinetic energy and the angular kinetic energy established in the Schrödinger case by Common [5].

$$\langle \hat{T} \rangle_{n, \ell'} > (\ell' + 1/2) (\ell' + 1) \langle \frac{1}{r^2} \rangle_{n, \ell'} \text{ for } \Delta V > 0, \text{ etc.} \quad (32)$$

$$\langle \hat{T} \rangle_{0, \ell'} < (\ell' + 1/2) (\ell' + 1) \langle \frac{1}{r^2} \rangle_{0, \ell'} \text{ for } \Delta V < 0, \text{ etc.} \quad (33)$$

By combining these results one obtains a differential inequality which gives Theorems (IIIa) or (IIIb) according to the case. The dissymmetry between these theorems is the dissymmetry between (32) and (33). (33) holds only for $n = 0$ with $\Delta V < 0$, (32) holds for any n , but is optimal in the Coulomb case *only* for $n = 0$.

Now, combining Theorem II and Theorem IIIb with $\ell_1 = \ell + \Delta(\ell, k)$, $\ell_2 = \ell + k$, one gets inequalities involving only physical angular momenta which reduce to the normal one in the non-relativistic limit, which gives for the case $k = 1$, for a potential with positive Laplacian :

$$\left(\frac{m^2}{(E(n, \ell))^2} - 1 \right) < \left(\frac{m^2}{(E(n-1, \ell+1))^2} - 1 \right) \left(\frac{1/2 + \sqrt{(\ell + 3/2)^2 - (Z\alpha)^2}}{3/2 + \sqrt{(\ell + 1/2)^2 - (Z\alpha)^2}} \right)^2 \quad (34)$$

For the case of a negative Laplacian we have the opposite inequality, but it holds only for $n = 1$. But then, we have anyway Theorem I. Naturally one can write an analogue of (34) for an increase of k units in ℓ .

One may wonder what is the field of application of these inequalities. It would be tempting to apply these to pionic atoms, but, unfortunately, in that case, contrary to the case of muonic atoms, the major distorsion is not due to the size of the nucleus, but to strong interactions including absorption by the nucleus. Another application would be quarkonium if it makes sense to describe it by the Klein-Gordon equation. This has been done by Schnitzer [6], but the price he had to pay, using a pure vector confining interaction, was that the energy levels were only metastable. A possibility, somewhat along the lines of

Ref. 4 would be to use a negative vector potential V going to zero at infinity and a scalar part S , added to m . Then if $\Delta V > 0, V < 0$ and $\Delta S > 0, S > 0, dS/dr > 0$, Theorem II applies to this situation.

Probably the most interesting conclusion is that we have found a case where the obstacles in going from a non-relativistic situation to a relativistic situation are not insurmountable. We hope that in the future it will be possible to do the same for the Dirac case, though the technical difficulties seems, for the time being, considerable.

ACKNOWLEDGEMENTS

H. Grosse thanks the CERN Theory Division for the kind hospitality extended to him. J. Stubbe acknowledges the support of the Swiss National Science Foundation.

REFERENCES

1. B.Baumgartner, H. Grosse and A. Martin, *Phys. Letters*, **146B** (1984) 363.
2. A. Martin and J. Stubbe, CERN preprint TH. 5843/90 (1990) submitted to Europhysics Letters
3. H. Grosse, *Phys. Letters*, **197B** (1987) 413
4. B.E. Palladino and P. Leal-Ferreira, *Phys. Letters*, **185B** (1987) 118
5. A.K. Common, *J. Phys A, Math. Gen.*, **18** (1985) 2219
6. J.S. Kang and H.J. Schnitzer, *Phys. Rev.*, **D 12** (1975) 841