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EIGENVALUES OF THE KLEIN–GORDON EQUATION

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Consider the Klein–Gordon equation

$$\left[\left(\frac{\partial}{\partial t}-ieq\right)^2-\sum_{j=1}^{n}\left(\frac{\partial}{\partial x_j}-ieA_j\right)^2+m^2\right]u=0 \tag{1}$$

where q, A_j are real valued functions on R^n, m and e positive constants. Equation (1) describes the motion of a relativistic particle of mass m and charge e in an external field described by the electrostatic potential q and the electromagnetic potential $A=(A_j)$; units are chosen so that the speed of light is one.

Assume

$$q\in L^\infty(R^n), \qquad A_j\in L^2_{\text{loc}}(R^n) \tag{2}$$

Denote by K the operator of multiplication by eq in $\mathscr{G}=L^2(R^n)$; K is a bounded selfadjoint operator. $\tilde{H}$ is the natural selfadjoint realisation of

$$-\sum_{j=1}^{n}\left(\frac{\partial}{\partial x_j}-ieA_j\right)^2+m^2 \text{ in } \mathscr{G} \text{ ([3])}, \ H=\tilde{H}-K^2.$$

The equation (1) can be written as

$$\frac{d^2u(t)}{dt^2}-2iK\frac{du(t)}{dt}+Hu(t)=0 \tag{3}$$

or, using the notation

$$U(t)=\begin{bmatrix} u(t) \\ -i\dfrac{du(t)}{dt}\end{bmatrix}, \quad \mathscr{A}=\begin{bmatrix} 0 & \mathrm{I} \\ \mathrm{H} & 2\mathrm{K}\end{bmatrix},$$

we have

$$\frac{dU(t)}{dt}=i\mathscr{A}U(t). \tag{4}$$

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It is easy to see that (3) has an elementary solution of the form $u(t)=e^{i\lambda t}u$, $u\in\mathcal{G}$, if and only if (4) has a solution of the form

$$U(t)=e^{i\lambda t}\begin{bmatrix} u \\ \lambda u \end{bmatrix}.$$

This is the case if and only if λ is an eigenvalue of $\mathscr{A}$; equivalently if and only if

$$(\lambda^2-2\lambda K-H)u=0. \tag{5}$$

We say that λ is an eigenvalue, u an eigenfunction of the Klein–Gordon equation if (5) holds. It is an eigenvalue of geometric (algebraic) multiplicity k if it is an eigenvalue of $\mathscr{A}$ of geometric (algebraic) multiplicity k; here the geometric (algebraic) multiplicity of an eigenvalue of a linear operator is the dimension of the eigenspace (of the space spanned by eigenvectors and the associated vectors). The eigenvalue is simple if it is of algebraic multiplicity one and it is semisimple if its algebraic and geometric multiplicities are equal. If λ is a nonsemisimple eigenvalue, then there is an eigenfunction u and a function v such that $(\lambda^2-2\lambda K-H)v=2(\lambda-K)u$.

If H is positive definite all the eigenvalues are real and semisimple (this follows from the fact that $\mathscr{A}$ is selfadjoint in the Hilbert space to be defined below). In general, there might be nonreal and nonsemisimple eigenvalues; this is the so-called Klein paradox. It cannot happen as long as $\|K\|<m$ (i.e. as long as $\|q\|_{L^\infty}<m/e$; in the usual units m/e should be replaced by mc^2/e). It is known [6] that if $\|q\|_{L^\infty}<m/e\sqrt{2}$ then $\mathscr{A}$ is a spectral operator.

We shall show that, as should be expected, $\|q\|_{L^\infty}$ is not so important; what matters is $\operatorname{diam} q=\operatorname{ess\,sup} q-\operatorname{ess\,inf} q$. If $\operatorname{diam} q<2m/e$ then all the eigenvalues are real and semisimple; there are no eigenvalues in certain intervals; $\mathscr{A}$ is a selfadjoint operator in an appropriate scalar product. A real nonsemisimple eigenvalue can occur if $\operatorname{diam} q=2m/e$; however an eigenfunction must satisfy some additional, very restrictive stipulations, so this case is exceptional. For example if $A=0$ then all the eigenvalues are semisimple even if $\operatorname{diam} q=2m/e$. If $A=0$ then $\mathscr{A}^{-1}$ is a real operator which is positivity preserving if q is of constant sign (more generally if diam q is small enough). In this case some interesting phenomena occur. Assume q is negative and $\tilde{H}$-compact so the essential spectrum of $\mathscr{A}$ is $[-\infty, -m]\cup[m,\infty)$. Then all the discrete eigenvalues originate at m and move to the left as q decreases. The smallest eigenvalue is simple—it is a "ground state". When $\operatorname{diam} q=m/e$, there can be eigenvalues appearing at $-m$ and moving to the right as $\|q\|_{L^\infty}$ increases further. The largest of such eigenvalues is simple: it is another ground state. Thus we have (at most) two ground states.

The Klein paradox occurs when two ground states meet or when the right ground state hits $-m$ or the left ground state hits m. A precise statement concerning the multiplicity of such eigenvalues can be made.†

†There is some overlapping of our results with those of K. Veselić in [11].

Define $\mathscr{H}=\mathscr{D}(\tilde{H}^{1/2})\times\mathscr{G}$; $\mathscr{H}$ is a Hilbert space in the norm $\|u\|=(\|\tilde{H}^{1/2}u_1\|^2+\|u_2\|^2)^{1/2}$ where $u=[u_1\ u_2]$; we denote the norms in $\mathscr{H}$ and $\mathscr{G}$ by the same symbol, since it will always be clear to what space a vector belongs.

Define $\mathscr{A}$ on $\mathscr{D}(\mathscr{A})=\mathscr{D}(H)\times\mathscr{D}(\tilde{H}^{1/2})$ by

$$\mathscr{A}\begin{bmatrix}u\\v\end{bmatrix}=\begin{bmatrix}v\\Hu+2Kv\end{bmatrix}.$$

If H is positive definite, the norm in $\mathscr{H}$ can be defined using H instead of $\tilde{H}$; $\mathscr{A}$ is selfadjoint in the corresponding scalar product.

If $\lambda\neq 0$ define

$$H_\lambda=H+2\lambda K-\lambda^2,\ K_\lambda=K-\lambda,\ \mathscr{S}_\lambda=\begin{bmatrix}I&0\\-\lambda&I\end{bmatrix},\ \mathscr{A}_\lambda=\begin{bmatrix}0&I\\H_\lambda&2K_\lambda\end{bmatrix}\ \text{on}\ \mathscr{D}(\mathscr{A}_\lambda)=\mathscr{D}(\mathscr{A}).$$

Then $\mathscr{A}_\lambda=\mathscr{S}_\lambda\mathscr{A}\mathscr{S}_\lambda^{-1}-\lambda I$. Thus μ is an eigenvalue of $\mathscr{A}$ if and only if $\mu-\lambda$ is an eigenvalue of $\mathscr{A}_\lambda$. This can be seen equivalently by setting $u(t)=e^{i\lambda t}v(t)$ in (3). Then $v(t)$ satisfies (3) with K,H replaced by K_λ,H_λ. This translation of spectral parameter represents the arbitrariness of choosing the zero potential.

Our results are contained in the next two theorems.

Theorem A. *Let* $\min\sigma(K)=1/e\operatorname{ess\,inf}q=k_2$, $\max\sigma(K)=1/e\operatorname{ess\,sup}q=k_1$.

(a) *The set of all* $\lambda\in R$ *such that* H_λ *is positive semidefinite is either empty or a closed interval* $[\lambda_-,\lambda_+]$. *If the latter is the case, then* H_{λ_-} *and* H_{λ_+} *are semidefinite,* H_λ *is positive definite if* $\lambda_-<\lambda<\lambda_+$ *and indefinite if* $\lambda<\lambda_-$ *or* $\lambda>\lambda_+$.

(b) *There are no eigenvalues in* (λ_-,λ_+) *if* $\lambda_-<\lambda_+$.

(c) *If* $k_1-k_2\leqq 2m$ *then* $\lambda_-<k_1-m\leqq k_2+m<\lambda_+$ *and all the eigenvalues are real and semisimple.*

(d) *If* $\lambda_-<\lambda_+$ *then* $k_2>\lambda_-$ *implies* $\lambda_+\geqq m$, $k_1<\lambda_+$ *implies* $\lambda_-\leqq -m$.

(e) *All the nonreal and nonsemisimple eigenvalues are contained in* $\{z\in C: k_2\leqq \operatorname{Re} z\leqq k_1, |z|\leqq m\}$.

Theorem B. *Assume additionally* $A=0$.

If $\lambda_-<\lambda_+$ *then* λ_-,λ_+ *can be only simple eigenvalues. If* $\lambda_-=\lambda_+=\tilde{\lambda}$ *then* $k_2\leqq\tilde{\lambda}\leqq k_1$, $|\tilde{\lambda}|\leqq m$. *If* $\tilde{\lambda}$ *is an eigenvalue, then* $k_2<\tilde{\lambda}<k_1$ *and it is an eigenvalue of geometric multiplicity one and algebraic multiplicity one or two. If*

$$q^2 \text{ is } \Delta^2\text{-compact} \tag{5}$$

and $\lambda_->-m$ $(\lambda_+<m)$ *then* λ_- *(respectively* λ_+*) is an eigenvalue. If* $\lambda_-=\lambda_+=\tilde{\lambda}$ *then* $\tilde{\lambda}$ *is an eigenvalue (even if* $|\tilde{\lambda}|=m$*). If* $|\tilde{\lambda}|<m$ *the algebraic multiplicity of* $\tilde{\lambda}$ *is two.*

Proof of Theorem A. For $u \in \mathscr{G}$ with $\|u\|=1$ denote $p_u(\lambda) = -(H_\lambda u \mid u) = \lambda^2 - 2\lambda(Ku \mid u) - (Hu \mid u)$. If $p_u(\lambda)$ has real zeros denote the smaller by $\lambda_-(u)$, the larger by $\lambda_+(u)$. If λ_0 is an eigenvalue and u_0 an eigenfunction then $p_{u_0}(\lambda_0)=0$.

Now define

$$\lambda_+ = \inf_{\|u\|=1} \lambda_+(u), \quad \lambda_- = \sup_{\|u\|=1} \lambda_-(u).$$

Since H is unbounded, p_u must have real zeros for some u, so λ_+ and λ_- are well defined. Assume $\lambda_- \leqq \lambda_+$ and let $\lambda_- \leqq \lambda \leqq \lambda_+$. For any $u \in \mathscr{G}$ with $\|u\|=1$ we find

$$(H_\lambda u \mid u) = -p_u(\lambda) = (\lambda_+(u) - \lambda)(\lambda - \lambda_-(u)) \geqq (\lambda_+ - \lambda)(\lambda - \lambda_-) \geqq 0.$$

This means $(H_\lambda u \mid u) \geqq (\lambda_+ - \lambda)(\lambda - \lambda_-)\|u\|^2$ for every $u \in \mathscr{G}$. We conclude that H_λ is positive definite if $\lambda \in (\lambda_-, \lambda_+)$. If $\lambda > \lambda_+$ or $\lambda < \lambda_-$ then there exists u such that $p_u(\lambda) > 0$ (this is the case as soon as $\lambda > \lambda_+(u)$ or $\lambda < \lambda_-(u)$), hence $(H_\lambda u \mid u) < 0$ so H_λ is indefinite. Now H_λ is analytic in λ and therefore $H_{\lambda-}$ and $H_{\lambda+}$ are semidefinite. This proves (a); part (b) follows from (a).

Now let λ be a nonsemisimple eigenvalue. Then we can find $u, v \in \mathscr{G}$ with $\|u\| = 1$, $H_\lambda u = 0$, $H_\lambda v = 2(K-\lambda)u$, hence $p_u(\lambda) = 0$ and $((K-\lambda)u \mid u) = \frac{1}{2}(H_\lambda v \mid u) = 0$. Since $p_u'(\lambda) = 2((\lambda - K)u \mid u)$, it follows that $p_u'(\lambda) = 0$. This implies $\lambda_-(u) = \lambda_+(u)$ so the discriminant of p_u is zero. If u is an eigenfunction of a nonreal eigenvalue then evidently p_u has no real zeros, hence its discriminant is negative.

From this it follows that an eigenvalue λ is real and semisimple if and only if the discriminant of p_u is positive for every eigenfunction u with $\|u\|=1$. The discriminant is

$$(Hu \mid u) + (Ku \mid u)^2 = (\tilde{H}u \mid u)^2 - q_K(u) \quad \text{where} \quad q_K(u) = \|Ku\|^2 - (Ku \mid u)^2.$$

Evidently $q_K(u) \leqq \|K\|^2$; if $k_1 = -k_2$ the equality holds if and only if $\|Ku\| = \|K\|$, $(Ku \mid u) = 0$. This is possible if and only if

$$u = u_1 + u_2, \quad \|u_1\| = \|u_2\| = \frac{1}{\sqrt{2}}, \quad Ku_1 = \|K\|u_1, \quad Ku_2 = -\|K\|u_2.$$

Because of $q_{K+\lambda} = q_K$ we conclude that for arbitrary K $\|Ku\|^2 - (Ku \mid u)^2 \leqq \frac{1}{4}(k_1 - k_2)^2$ for all u with $\|u\|=1$; the equality holds if and only if $\tilde{u} = u_1 + u_2$, $\|u_1\| = \|u_2\|$, $Ku_i = k_i u_i$, $i = 1, 2$. Therefore the discriminant is strictly positive if $k_1 - k_2 < 2m$; it is nonnegative if $k_1 - k_2 = 2m$; if there is an eigenfunction $\tilde{u}$ such that $p_{\tilde{u}}$ has double zero then this zero is necessarily equal to $(K\tilde{u} \mid \tilde{u}) = (k_1 + k_2)/2$. In this case $(K - (k_1 + k_2)/2)^2 \tilde{u} = \frac{1}{4}(k_1 - k_2)^2 \tilde{u}$, so

$$\tilde{H}u = (K - k_0)^2 u = m^2 u, \; u = u_1 + u_2, \; \|u_1\| = \|u_2\|, \; Ku_i = k_i u_i, \; i = 1, 2 \tag{6a}$$

holds for some $u \neq 0$ and $k_0 = (k_1 + k_2)/2$.

If $\|K - \lambda\| < m$ then $\tilde{H}_\lambda = \tilde{H} - (K - \lambda)^2$ is positive definite; this is the case if $k_1 - m < \lambda < k_2 + m$. This is possible only if $k_1 - k_2 < 2m$; if this is the case and $k_1 - m$ is an eigenvalue, then obviously $\lambda_- = k_1 - m$ and $\tilde{H}u = m^2 u = (K - k_1 + m)^2 u$ for any eigenfunction u. Since $2m-k_1+K\geqq 2m-k_1+k_2>0$ we conclude that in this case there is $u\neq 0$ such that

$$\tilde{H}u=m^2u,\ Ku=k_1u. \tag{6b}$$

In the same way, if k_2+m is an eigenvalue, then there is $u\neq 0$ such that

$$\tilde{H}u=m^2u,\ Ku=k_2u. \tag{6c}$$

Now by Kato's inequality ([7, II]) $(\tilde{H}-m^2)u=0$ implies

$$0=((\tilde{H}-m^2)u\,|\,u)=\sum_j\left\|\left(\frac{\partial}{\partial x_j}-ieA_j\right)u\right\|^2\geqq\sum_j\left\|\frac{\partial}{\partial x_j}|u|\right\|^2,$$

hence $|u|$ is a constant, so $u=0$. Thus (6a), (6b) and (6c) are impossible and the sharp inequalities in (c) are proved.

Part (e) is proved in [**6**], and one part of (d) follows from the next lemma; the other part is proved in the same way.

Lemma. *Let* $\lambda\in(\lambda_-,\lambda_+)$ *and* $K\geqq\lambda$. *Then* $\lambda_+\geqq m$. *Moreover all the eigenvalues in* $(-m,m)$ *are nondecreasing functions of* K *as long as* $K\geqq\lambda>\lambda_-$ (λ_- *depends on* K).

Proof. Without loss of generality (translating the spectral parameter) we can assume $\lambda=0$. Define

$$H(\mu)=\tilde{H}-\mu^2K^2,\ (u\,|\,v)_\mu=(H(\mu)^{1/2}u_1\,|\,H(\mu)^{1/2}v_1)+(u_2\,|\,v_2),$$

$$\mathscr{H}(\mu)=(\mathscr{H},(\,|\,)_\mu),\ \mathscr{A}(\mu)=\begin{bmatrix}0 & I\\ H(\mu) & 2\mu K\end{bmatrix}\text{ on }\mathscr{D}(\mathscr{A}).$$

Then

$$\mathscr{A}(\mu)^{-1}=\begin{bmatrix}-2\mu H(\mu)^{-1}K & H(\mu)^{-1}\\ I & 0\end{bmatrix}$$

and

$$f_u(\mu)=\frac{(\mathscr{A}(\mu)^{-1}u\,|\,u)_\mu}{2(u\,|\,u)_\mu}=\frac{\operatorname{Re}(u_1\,|\,u_2)-\mu(Ku_1\,|\,u_1)}{(\tilde{H}u_1\,|\,u_1)+\|u_2\|^2-\mu^2\|Ku_1\|^2}.$$

We shall prove that f_u is monotone decreasing for all $u\in\mathscr{H}$ in $[0,m/\|K\|]$. By the min–max theorem this means that $\lambda_+(\mu)\geqq m$ for all μ in this interval (where $\lambda_+(\mu)$ is λ_+ associated with $\mathscr{A}(\mu)$). Assume $K'\geqq K>0$, $\tilde{H}-K'^2>0$ (implying $\lambda'_-<0$). Define $\mathscr{A}'$, $(\,|\,)'$ using K' and let $f_u(K)=(\mathscr{A}^{-1}u\,|\,u)/2(u\,|\,u)$, $f_u(K')=(\mathscr{A}'^{-1}u\,|\,u)'/2(u\,|\,u)'$. Since $\sigma_p(A')\cap(-m,m)\subset(-m,0)$ it suffices to show $f_u(K)<0$ implies $f_u(K')<0$ (by the min–max theorem, it follows that the spectrum of $\mathscr{A}'^{-1}$ is to the left of the spectrum of

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$\mathscr{A}^{-1}$). This is evident since $f_u(K)<0$ implies

$$|f_u(K)|=\frac{(Ku_1\,|\,u_1)-\mathrm{Re}(u_1\,|\,u_2)}{(\tilde{H}u_1\,|\,u_1)+\|u_2\|^2-\|Ku_1\|^2}$$

and the denumerator is increasing while the denominator is decreasing with K.

To prove that $f_u(\mu)$ is monotone denote $\mathrm{Re}(u_1\,|\,u_2)=a$, $(Ku_1\,|\,u_1)=b$, $(\tilde{H}u_1\,|\,u_1)+\|u_2\|^2=c$, $\|Ku_1\|^2=d$. Then $f_u(\mu)=(a-b\mu)/(c-d\mu^2)$, $f_u'(\mu)=-h(\mu)/(c-d\mu^2)^2$ with $h(\mu)=bd\mu^2-2ad\mu+bc$. If u is such that $a<0$ then $h(\mu)>0$ for all μ and f_u *is* decreasing on $[0,\infty)$. If $a>0$ then f_u is decreasing on $[0,\mu_1(u)]$ where $\mu_1(u)=ad-\sqrt{(a^2d^2-b^2dc)}/bd$ is the smaller root of $h(\mu)=0$. Now

$$\mu_1(u)=\frac{bc}{ad+\sqrt{(a^2d^2-b^2dc)}}\geqq\frac{bc}{2ad},$$

$$c\geqq m^2\|u_1\|^2+\|u_2\|^2\geqq 2m\|u_1\|\,\|u_2\|\geqq 2ma,$$

$$d=\|K^{1/2}K^{1/2}u_1\|^2\leqq\|K^{1/2}\|^2\|K^{1/2}u_1\|^2=b\|K\|,$$

hence $bc/2ad\geqq m/\|K\|$, so f_u is decreasing in $[0,m/\|K\|]$ for all u.

Remarks

1. If

$$q^2 \text{ is } \tilde{H}^2 \text{ compact} \tag{7}$$

then K and K^2 are $\tilde{H}^2$-compact, so $\sigma_e(H_\lambda)=\sigma_e(H-\lambda^2)$ ([**10**]), therefore $\sigma_e(H_\lambda)=[m^2-\lambda^2,\infty)$. It follows that $(-m,m)\cap\sigma(\mathscr{A})$ consists only of eigenvalues which are increasing (respectively decreasing) functions of q as long as q is positive (respectively negative) and small enough; if $\lambda_+<m$ (or $\lambda_->-m$) then λ_+ (respectively λ_-) is an eigenvalue.

2. If $A=0$, the conclusion that (6) has no solutions follows also from the unique continuation theorem except in the trivial case when q is a constant or a step function attaining only two values.

3. The estimates in (c) can easily be strenghtened. Note that $H_\lambda=\tilde{H}^{1/2}(I-X_\lambda^*X_\lambda)\tilde{H}^{1/2}$ where $X_\lambda=K_\lambda\tilde{H}^{-1/2}$. Hence if $\|X_\lambda\|<1$ then $\lambda\in(\lambda_-,\lambda_+)$. Now Kato's inequality implies that a sufficient condition for $\|X_\lambda\|<1$ is $\|K_\lambda f\|^2<\|\nabla|f|\|^2+m^2\|f\|^2$ for every $f\in H^1(R^n)$. Now $\|\nabla|f|\|\geqq\|f/2r\|$, so a sufficient condition is $(K-\lambda)^2<m^2+1/4r^2$, i.e.

$$\lambda-\sqrt{\left(m^2+\frac{1}{4|x|^2}\right)}<q(x)<\lambda+\sqrt{\left(m^2+\frac{1}{4|x|^2}\right)}.$$

In other words, if $q_1(x)=q(x)-\sqrt{(m^2+1/4|x|^2)}$, $q_2(x)=q(x)+\sqrt{(m^2+1/4|x|^2)}$ then $\operatorname{ess\,sup} q_1 \geqq \lambda_-$, $\operatorname{ess\,inf} q_2 \leqq \lambda_+$.

4. If $\lambda_-=\lambda_+=\tilde{\lambda}$ and if $\tilde{\lambda}$ is an eigenvalue, it cannot have a Jordan chain of length more than two. To prove this, we can again assume $\tilde{\lambda}=0$. Suppose $\mathscr{A}e_1=0$, $\mathscr{A}e_i=e_{i-1}$, $i=2,3$ where $e_i=[x_i\ y_i]^T$, $i=1,2,3$. We immediately find $y_1=0$, $y_i=x_{i-1}$, $i=2,3$ and $Hx_1=0$, $Hx_2+2Kx_1=0$, $Hx_3+2Kx_2=x_1$. Multiply the second equation by x_2, the third by x_1. We find

$$2(Kx_1\,|\,x_2)=-(Hx_2\,|\,x_2),\ 2(Kx_2\,|\,x_1)=\|x_1\|^2,$$

i.e. $\|x_1\|^2=-(Hx_2\,|\,x_2)$. Since H is semidefinite we have $x_1=0$, so $e_1=0$ and this is a contradiction.

Proof of Theorem B. If λ_- is an eigenvalue, the corresponding eigenfunction of H_{λ_-} is a ground state of a Schrödinger operator (note that $(H+2\lambda K+\alpha)^{-1}$ is positivity improving for appropriate α; cf. [7, IV]); therefore it is positive and the eigenvalue is simple.

Note that (5) coincides with (7) if $A=0$ so we can use Remark 1 above to prove that if $\lambda_->-m$ then it is a simple eigenvalue. All that is left to prove are the two last statements (the rest follows from Theorem A(e) and Remark 4 above). Assume $\tilde{\lambda}=-m$ ($\tilde{\lambda}=m$ is treated in the same way). Pick $\lambda_0>-m$ such that H_{λ_0} is an indefinite operator with $0\in\rho(H_{\lambda_0})$ and with one dimensional negative part; define $\hat{H}(\mu)=\tilde{H}-\mu^2(K-\lambda_0)^2$ so that $\hat{H}(1)=H_{\lambda_0}$. Since $\hat{H}(\mu)$ is analytic in μ, there is $\mu_0<1$ such that $0\in\rho(\hat{H}(\mu))$ and $\hat{H}(\mu)$ has one dimensional negative part for all $\mu\in[\mu_0,1]$. Define

$$[u\,|\,v]_\mu=(\operatorname{sgn}\hat{H}(\mu)|\hat{H}(\mu)|^{1/2}u_1\,|\,|\hat{H}(\mu)|^{1/2}v_1)+(u_2\,|\,v_2),$$

$$\mathscr{H}(\mu)=(\mathscr{H},[\ \,|\ \,]_\mu),\ K(\mu)=\mu(K-\lambda_0),$$

$$\mathscr{A}(\mu)=\begin{bmatrix}0 & I\\ \hat{H}(\mu) & 2K(\mu)\end{bmatrix}\text{ on }\mathscr{D}(\mathscr{A}(\mu))=\mathscr{D}(\mathscr{A}).$$

Then $\mathscr{H}(\mu)$ is a Pontrjagin space of index 1 ([1]), $\mathscr{A}(\mu)$ is selfadjoint in $\mathscr{H}(\mu)$. Therefore $\mathscr{A}(\mu)$ has a one dimensional invariant subspace $\mathscr{L}(\mu)$ such that $[\ \,|\ \,]_\mu$ is nonpositive on $\mathscr{L}(\mu)$. It is easy to see that this subspace is just the eigenspace associated with the simple eigenvalue $\lambda_+(\mu)$. Since $K(\mu)\leqq K(1)$ we have $\lambda_+(\mu)>\lambda_-(\mu)=-m-\lambda_0$. Now $K(\mu)$ and $\hat{H}(\mu)^{-1}$ converge in norm to $K(1)$ and $\hat{H}(1)^{-1}$, $[u|v]_\mu$ converges to $[u|v]_1$ (for all u, $v\in\mathscr{H}$) as $\mu\to 1$. The results of [2] imply that $\lim_{\mu\to 1}\lambda_+(\mu)=\hat{\lambda}$ is an eigenvalue of $\mathscr{A}(1)=\mathscr{A}_{\lambda_0}$. This eigenvalue cannot have a Jordan chain of length larger than three. Now $\lambda_+(\mu)$ is less than zero so $\hat{\lambda}\leqq 0$; in fact $\hat{\lambda}<0$ since $0\in\rho(H_{\lambda_0})$. If $[u\ \hat{\lambda}\hat{u}]^T$ is the eigenvector associated to $\hat{\lambda}$ then it is nonpositive in $\mathscr{H}(1)$, i.e. $((H_{\lambda_0}+\hat{\lambda}^2)\hat{u}\,|\,\hat{u})<0$. This immediately implies $\hat{\lambda}=\lambda_+(1)=-m-\lambda_0$. It follows that $-m$ is an eigenvalue of $\mathscr{A}$.

Similarly, if $|\tilde{\lambda}|<m$ set $H(\mu)=\tilde{H}-\mu^2(K-\tilde{\lambda})^2$

$$\mathscr{A}(\mu)=\begin{bmatrix} 0 & I \\ H(\mu) & 2\mu(K-\tilde{\lambda}) \end{bmatrix} \text{ on } \mathscr{D}(\mathscr{A}).$$

Then $\lim_{\mu\to 1}\lambda_{\pm}(\mu)=0$. Since $\lambda_{\pm}(\mu)$ are simple eigenvalues of $\mathscr{A}(\mu)$ by the above argument, it follows from the analytic perturbation theory ([4]) that zero is an eigenvalue of $\mathscr{A}(1)$ of algebraic multiplicity at least two. Now $\mathscr{A}(1)$ is similar to $\mathscr{A}-\tilde{\lambda}$, so the algebraic multiplicity of $\tilde{\lambda}$ is exactly two.

Remarks

1. The simplicity of eigenvalues $\lambda_{\pm}$ follows also by another argument. Let $\lambda\in(\lambda_-,\lambda_+)$. Then H_λ^{-1} is positivity improving (Theorem XIII.45 in [7, IV]). Define $\mathscr{B}_\lambda$ as the extension of $\mathscr{A}_\lambda$ to $\mathscr{G}^2$: $\mathscr{D}(\mathscr{B}_\lambda)=\mathscr{D}(\mathscr{A}_\lambda)$, $\mathscr{B}_\lambda u=\mathscr{A}_\lambda u$, $\mathscr{B}_\lambda u$ is regarded as a vector in $\mathscr{G}^2$. Then $\mathscr{B}_\lambda$ is closable and its closure is boundedly invertible. The inverse is

$$\bar{\mathscr{B}}_\lambda^{-1}=\begin{bmatrix} -2H_\lambda^{-1}K_\lambda & H_\lambda^{-1} \\ I & 0 \end{bmatrix}.$$

Now

$$\begin{bmatrix} 0 & H_\lambda^{-1} \\ I & 0 \end{bmatrix}$$

is positivity improving, so there is a real number v such that $v+\bar{\mathscr{B}}_\lambda^{-1}$ is positivity improving. This implies that if $\operatorname{spr}\bar{\mathscr{B}}_\lambda^{-1}$ is equal to the largest eigenvalue, then this eigenvalue is simple. It is easy to see that the eigenvalues of $\mathscr{A}_\lambda$ and $\bar{\mathscr{B}}_\lambda$ coincide. Therefore we conclude: if λ_+ is an eigenvalue of $\mathscr{A}$, then $1/(\lambda_+-\lambda)$ is the largest eigenvalue of $\bar{\mathscr{B}}_\lambda^{-1}$, hence it is simple. Since

$$-\begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix}\bar{\mathscr{B}}_\lambda^{-1}\begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix}=\begin{bmatrix} 2H_\lambda^{-1}K_\lambda & H_\lambda^{-1} \\ I & 0 \end{bmatrix},$$

the same is true for the smallest eigenvalue of $\bar{\mathscr{B}}_\lambda^{-1}$.

2. If $\|q\|_{L^\infty}$ is small enough and q tends to zero at infinity, then there are no eigenvalues ([5]).

3. Sufficient conditions for (5) can be found in [7, II] and [8].

4. If $A\neq 0$ and λ_+ is a discrete eigenvalue, then $\lambda_+>\lambda_+^0$ where λ_+^0 is λ_+ for the case $A=0$. In fact, assume $H_{\lambda_+}u=0$, i.e.

$$D^2u=(K-\lambda_+)^2u-m^2u \quad \text{where} \quad D^2=\sum_j\left(\frac{\partial}{\partial x_j}-ieA_j\right)^2.$$

By Kato's inequality (generalised to forms: [9]),

$$\operatorname{Re}[\arg u D^2 u] = \operatorname{Re}\{[(K-\lambda_+)^2 - m^2] u \arg u\} = [(K-\lambda_+)^2 - m^2]|u| \geqq -\Delta |u|$$

in the distribution sense. It follows that $\|\operatorname{grad}|u|\|^2 - \|K|u|\|^2 + 2\lambda_+(K|u|\,|\,|u|) + (m^2-\lambda_+^2)\|\,|u|\,\|^2 \leqq 0$, so $H^0_{\lambda_0}$ is not positive definite; hence $\lambda^0_+ < \lambda_+$. Analogously $\lambda_- < \lambda^0_-$. In other words, the magnetic potentials postpone the occurrence of the Klein paradox.

5. If $|\tilde{\lambda}| = m$, then $\mathscr{A}$ is a spectral operator (the same conclusion trivially holds if $|\tilde{\lambda}| < m$): $\mathscr{A} = \mathscr{S} + \mathscr{N}$ where $\mathscr{S}$ is a spectral operator of scalar type and $\mathscr{N} = 0$ (if the algebraic multiplicity of $\tilde{\lambda}$ is one) or $\mathscr{N}$ is an operator of rank one (if the algebraic multiplicity is two).

To prove this pick λ_0 such that $0 \in \rho(H_{\lambda_0})$ and H_{λ_0} has one dimensional negative part. Define

$$[u\,|\,v] = (u\,|\,v)_{\mathscr{H}} + 2\lambda_0(Ku_1\,|\,v_1) - \lambda_0[(u_1\,|\,v_2) + (u_2\,|\,v_1)].$$

Then $\mathscr{K} = (\mathscr{H}, [\;|\;])$ is a Pontrjagin space of index 1. It is sufficient to prove that the principal subspace (i.e. the generalised eigenspace) X associated to $\tilde{\lambda}$ is nondegenerate in $\mathscr{K}$; the construction and the facts we use can be found in [6] and its references). If $\dim X = 1$ this is evident; then $\mathscr{A}x = \tilde{\lambda}x$ implies $[x\,|\,x] < 0$. If $\dim X = 2$ let $\mathscr{A}e = \tilde{\lambda}e$, $\mathscr{A}f = \tilde{\lambda}f + e$. We find

$$e = \begin{bmatrix} x \\ \tilde{\lambda}x \end{bmatrix}, \quad f = \begin{bmatrix} y \\ \tilde{\lambda}y + x \end{bmatrix} \quad \text{where} \quad H_{\tilde{\lambda}}x = 0,\; H_{\tilde{\lambda}}y + 2K_{\tilde{\lambda}}x = 0.$$

Now $[e\,|\,e] = 0$ (this is a general fact);

$$[e\,|\,f] = (\tilde{\lambda} - \lambda_0)[\|x\|^2 - 2(K_{\tilde{\lambda}}x\,|\,y)] = (\tilde{\lambda} - \lambda_0)[\|x\|^2 + (H_{\tilde{\lambda}}y\,|\,y)] \neq 0,$$

so X is nondegenerate.

6. From Theorems A and B we have the following picture: assume $A = 0$, q is positive and zero at infinity. Consider μq and increase μ from zero to infinity. As long as μ is sufficiently small, there are no eigenvalues. For some μ_0 a negative eigenvalue appears at $-m$ and moves to the right as μ increases. After some time it is (possibly) followed by another eigenvalue appearing in the same manner, etc. The largest eigenvalue $\lambda_-(\mu)$ remains simple. All the eigenvalues move to the right until $\lambda_-(\mu)$ becomes zero (this cannot happen as long as $\mu < \|q\|_{L^\infty}/e$). As μ increases further the eigenvalues are not monotone in μ any more; it is possible that eigenvalues emerge at m. If this is the case, the smallest of them, $\lambda_+(\mu)$, is simple. As μ increases, two cases are possible. In the first case $\lambda_+(\mu)$ and $\lambda_-(\mu)$ meet at $\tilde{\lambda}$, $\tilde{\lambda}$ is between $-m$ and m, to produce an eigenvalue of geometric multiplicity one and algebraic multiplicity two. If μ is increased further this eigenvalue splits into a nonreal pair, symmetric with respect to the real axis (this follows from the analytic perturbation theory ([4]); the author is indebted to Prof. K. Veselić for this remark).

In the second case $\lambda_-(\mu)$ hits m ($\lambda_+(\mu)$ cannot hit $-m$ by (d) of Theorem A). In that case an eigenvalue of geometric multiplicity one and algebraic multiplicity one or two is produced.

The last statement is particularly interesting since it concerns an eigenvalue embedded in a continuous spectrum; such eigenvalues are usually difficult to handle. Thus the Klein paradox occurs for the first time either by a collision of simple eigenvalues $\lambda_+(\mu)$ and $\lambda_-(\mu)$ between $-m$ and m or by the "negative" eigenvalue $\lambda_-(\mu)$ entering the positive essential spectrum at m.

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