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Variational methods for complex eigenfrequencies

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Abstract. Variational expressions have been developed for the complex normal-mode frequencies occuring in a variety of physical systems including laboratory and solar plasmas as well as cosmic space.

1. Introduction

The initial growth of instabilities occurring in various plasmas and cosmic situations is often investigated by taking Fourier–Laplace transforms of linearised equations of motion (Vithal and Tandon 1972, 1973, Cap 1976, Vithal 1977a, b). The solution to these equations yields complex eigenfrequencies, the imaginary parts of which determine the growth rates for the unstable modes.

However, if the equations of motion result from a second-order Lagrangian system, the equation for a normal mode reduces to

$$(\omega^2P-2\omega R-Q)\alpha=0$$

where P and Q are real, symmetric matrices and R is imaginary and antisymmetric. When the normal-mode frequency is real, Low (1961) found it using the variational method. Laval *et al* (1964) extended Low's work to a marginally stable situation in the vicinity of the system with real normal-mode frequencies. Later, Barston (1970) studied the systems with imaginary frequencies and found the maximum growth rate of an unstable system to be the least upper bound of a certain functional in the form of a variational expression. Nevertheless, it is still of interest to construct a variational principle for the complex normal-mode frequency which would yield this mode at a stationary point. The method is described in § 2 and illustrated with a simple application to the study of plasma oscillations in a one-dimensional one-component plasma in § 3.

Lin and Lau (1976) have reported that complex eigenfrequencies may also occur when R is real and symmetric. In that case a simplified method leads to a variational expression for the eigenvalue as discussed in § 4 where it is also illustrated with an example based on the Klein paradox (Klein 1929) in the relativistic wave equation for a scalar particle.

Finally, in § 5 a non-holonomic variational principle is presented.

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2. Conservative second-order systems

2.1. Formulation

The equation for a normal mode of a second-order Lagrangian system is

$$(\omega^2 P - 2\omega R - Q)\alpha = A(\omega)\alpha = 0, \tag{1}$$

where P and Q are real, symmetric matrices and R is imaginary and antisymmetric. Hence P, Q and R are all self-adjoint. Thus, for any allowed frequency ω, $-\omega$ and $\pm\omega^*$ will also be allowed, since the determinantal equation $\det A = 0$ can be transposed, turning ω into $-\omega$, and then 'complex conjugated', turning $-\omega$ into ω^*.

It should be noted that if α is a solution of equation (1), and β is any vector, then

$$\omega^2(\beta, P\alpha) - 2\omega(\beta, R\alpha) - (\beta, Q\alpha) = 0 \tag{2}$$

where $(x, z) = \Sigma_i x_i^* z_i$ is Hermitian, (,) being the usual inner product defined over the region of interest, so that

$$\omega = \frac{(\beta, R\alpha)}{(\beta, P\alpha)} \pm \left(\frac{(\beta, R\alpha)^2}{(\beta, P\alpha)^2} + \frac{(\beta, Q\alpha)}{(\beta, P\alpha)}\right)^{1/2}. \tag{3}$$

Similarly, if $\tilde{\alpha}$ is a solution of the equation

$$(\omega^{*2} P - 2\omega^* R - Q)\tilde{\alpha} = 0 \tag{4}$$

and β is any vector, then

$$\omega^2(\tilde{\alpha}, P\beta) - 2\omega(\tilde{\alpha}, R\beta) - (\tilde{\alpha}, Q\beta) = 0. \tag{5}$$

From equation (5), for any β, we have

$$\omega = \frac{(\tilde{\alpha}, R\beta)}{(\tilde{\alpha}, P\beta)} \pm \left(\frac{(\tilde{\alpha}, R\beta)^2}{(\tilde{\alpha}, P\beta)^2} + \frac{(\tilde{\alpha}, Q\beta)}{(\tilde{\alpha}, P\beta)}\right)^{1/2}. \tag{6}$$

2.1.1. If the Lagrangian system possesses a time–reversal invariance, a matrix σ gives the corresponding transformation. Thus, if there exists the matrix σ which commutes with P and Q and anticommutes with R, then it is obvious that

$$\tilde{\alpha} = \sigma^{\dagger}\alpha^*. \tag{7}$$

We can now construct a variational principle for the frequency: evidently, the quantity

$$\Phi(\alpha) = \frac{(\tilde{\alpha}, R\alpha)}{(\tilde{\alpha}, P\alpha)} \pm \left(\frac{(\tilde{\alpha}, R\alpha)^2}{(\tilde{\alpha}, P\alpha)^2} + \frac{(\tilde{\alpha}, Q\alpha)}{(\tilde{\alpha}, P\alpha)}\right)^{1/2} \tag{8}$$

is stationary for α to be a solution of equation (1) and $\tilde{\alpha} = \sigma\alpha^*$, as shown by equations (3) and (6).

The converse is, however, less obvious. Assuming Φ to be stationary, we obtain

$$0 = \delta\Phi = \frac{1}{\bar{P}}\delta\bar{R} - \frac{\bar{R}}{\bar{P}^2}\delta\bar{P} \pm \frac{1}{2}\frac{1}{[(\bar{R}^2/\bar{P}^2) + (\bar{Q}/\bar{P})]^{1/2}}\left[\frac{2\bar{R}}{\bar{P}}\left(\frac{\delta\bar{R}}{\bar{P}} - \frac{\delta\bar{P}}{\bar{P}^2}\bar{R}\right) + \frac{\delta\bar{Q}}{\bar{P}} - \bar{Q}\frac{\delta\bar{P}}{\bar{P}^2}\right], \tag{9}$$

where $\bar{P} = (\tilde{\alpha}, P\alpha)$, etc. Combining terms, we have

$$0 = \Phi^2\delta\bar{P} - 2\Phi\delta\bar{R} - \delta\bar{Q}. \tag{10}$$

Now

$$\delta\bar{Q} = (\delta\tilde{\alpha}, Q\alpha) + (\tilde{\alpha}, Q\delta\alpha) = (\delta\alpha, \sigma Q\alpha)_{\mathscr{R}} + (\alpha, \sigma Q\delta\alpha)_{\mathscr{R}} \tag{11}$$

where (,) denotes a real inner product. Thus

$$\delta\bar{Q} = (\delta\alpha, [\sigma Q + (\sigma Q)^{\mathrm{T}}]\alpha)_{\mathscr{R}} = (\sigma\alpha, (\sigma + \sigma^{\mathrm{T}})Q\alpha)_{\mathscr{R}} \tag{12}$$

where σ^{T} is the transpose of σ. Similarly

$$\delta\bar{P} = (\delta\alpha, (\sigma + \sigma^{\mathrm{T}})P\alpha)_{\mathscr{R}} \tag{13}$$

and

$$\begin{aligned}\delta\bar{R} &= (\delta\alpha, [\sigma R + (\sigma R)^{\mathrm{T}}]\alpha)_{\mathscr{R}} = (\delta\alpha, [\sigma R - (R\sigma)^{\mathrm{T}}]\alpha)_{\mathscr{R}} \\ &= (\delta\alpha, (\sigma R - \sigma^{\mathrm{T}} R^{\mathrm{T}})\alpha)_{\mathscr{R}} = (\delta\alpha, (\sigma + \sigma^{\mathrm{T}})R\alpha)_{\mathscr{R}}.\end{aligned} \tag{14}$$

Thus from equations (10) and (12)–(14) we have

$$(\delta\alpha, (\sigma + \sigma^{\mathrm{T}})(\Phi^2 P - 2\Phi R - Q)\alpha)_{\mathscr{R}} = 0$$

or (15)

$$(\sigma + \sigma^{\mathrm{T}})(\Phi^2 P - 2\Phi R - Q)\alpha = 0.$$

Provided $\sigma + \sigma^{\mathrm{T}}$ has an inverse, this shows that

$$(\Phi^2 P - 2\Phi R - Q)\alpha = 0 \tag{16}$$

and the expression (8) is fully variational.

2.1.2. Now, suppose that there is no such matrix σ with the desired properties. In this case, evidently, the transformation from α to $\tilde{\alpha}$ requires in some way a separation of odd powers of R from even powers which can be done by enlarging the vector space. To do this a 2×2 matrix $\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ is added, doubling the number of components, and instead of equation (1) a new equation

$$(\omega^2 P - 2\omega R\sigma_1 - Q)\beta = 0 \tag{17}$$

is written. Evidently, equation (17) allows the required transformation with σ of equation (7) given by

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Hence $\tilde{\beta} = \sigma_3 \beta^*$ satisfies the equation

$$(\omega^{*2} P - 2\omega^* \sigma_1 R - Q)\tilde{\beta} = 0 \tag{18}$$

provided β satisfies equation (17). Thus our variational principle holds for β with

$$\Phi = \frac{(\tilde{\beta}, R\beta)}{(\tilde{\beta}, P\beta)} \pm \left(\frac{(\tilde{\beta}, R\beta)^2}{(\tilde{\beta}, P\beta)^2} + \frac{(\tilde{\beta}, Q\beta)}{(\tilde{\beta}, P\beta)}\right)^{1/2}. \tag{19}$$

Now we need merely prove that if β satisfies equation (17) we can write solutions of equation (1) with the same frequency, and vice versa. Let

$$(\omega^2 P - 2\omega R\sigma_1 - Q)\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = 0, \tag{20}$$

or

$$(\omega^2 P - Q)\beta_1 = 2\omega R\beta_2$$

and

$$(\omega^2 P - Q)\beta_2 = 2\omega R\beta_1.$$

Then $\alpha = \beta_1 + \beta_2$ satisfies equation (1) so that ω is an allowed frequency of equation (1).

Conversely, let

$$(\omega^2 P - 2\omega R - Q)\alpha = 0.$$

We know that an α' must exist, since if ω is an allowed frequency of (1) so is $-\omega$. Thus

$$(\omega^2 P + 2\omega R - Q)\alpha' = 0. \tag{21}$$

Then

$$\beta_1 = \mu\alpha + \nu\alpha' \tag{22}$$

and

$$\beta_2 = \mu\alpha - \nu\alpha' \tag{23}$$

clearly satisfy equation (20) with arbitrary μ, ν. The arbitrariness of μ and ν corresponds to the invariance of equation (17) under transformations of the form $E + F\sigma_1$. Any $\beta = (\beta_1, \beta_2)$ is satisfactory for use in the variational principle (20) except

$$\beta_1 = \beta_2 = \alpha(\nu = 0), \qquad \text{or} \qquad \beta_1 = -\beta_2 = \alpha'(\mu = 0),$$

since for those two choices our equation (19) for Φ becomes indeterminate. As for say $(\nu = 0)$,

$$\bar{P} = \left((\alpha, \alpha)\sigma_3 P\begin{pmatrix}\alpha\\ \alpha\end{pmatrix}\right)_{\mathfrak{R}} = (\alpha, P\alpha)_{\mathfrak{R}} - (\alpha, P\alpha)_{\mathfrak{R}} = 0. \tag{24}$$

Similarly, $\bar{Q} = 0$, and

$$\bar{R} = \left((\alpha, -\alpha)\sigma_1 R\begin{pmatrix}\alpha\\ \alpha\end{pmatrix}\right)_{\mathfrak{R}} = \left((\alpha, -\alpha)\begin{pmatrix}R\alpha\\ R\alpha\end{pmatrix}\right)_{\mathfrak{R}} = 0 \tag{25}$$

so that this choice of β as a trial expression must be avoided.

2.2. *Discussion*

2.2.1. There are obviously no positivity properties to be expected from this variational expression. Nevertheless, we give an interesting relation for the second variation of Φ.

Supposing β_0 to be a solution of equation (17), we obtain

$$\bar{P} = (\tilde{\beta}_0, P\beta_0) + (\tilde{\beta}_0, P\delta\beta) + (\delta\tilde{\beta}, P\beta_0) + (\delta\tilde{\beta}, P\delta\beta) \tag{26}$$

with similar expressions for $\bar{Q}$ and $\bar{R}$.

From equations (2) and (5) we know that $\Phi(\beta)$ calculated with the first three terms of (26) is independent of $\delta\beta$. Hence the only contribution to the second variation of Φ will be from the second variations of $\bar{P}$, $\bar{Q}$ and $\bar{R}$. Analogous to equation (9), it will be given by

$$\delta^2\Phi = \frac{\mp 1}{2\bar{P}[(\bar{R}/\bar{P})^2 + (\bar{R}/\bar{P})]^{1/2}}((\Phi^2\delta^2\bar{P} - 2\Phi\delta^2\bar{R} - \delta^2\bar{Q}) \tag{27}$$

with

$$\delta^2\bar{P} = (\delta\tilde{\beta}, P\delta\beta) \text{ etc.}$$

2.2.2. We know that in problems with translational invariance the wavenumber basis diagonalises the dependence upon spatial coordinates. In this basis the variational expression is slightly modified by the procedure illustrated below for one coordinate.

Let

$$\alpha(k)=\frac{1}{(2\pi)^{1/2}}\int \exp(-iky)\alpha(y)\,dy \tag{28}$$

and

$$\Gamma(k)=\int \exp(ik\Delta y)\Gamma(\Delta y)\,d(\Delta y), \tag{29}$$

where the labels for other degrees of freedom have been suppressed and $\Gamma(y, y')=\Gamma(y-y')$ refer to P, R or Q. The hermiticity and symmetry/antisymmetry properties of P, Q and R in the original coordinate basis can now be expressed as

$$\begin{aligned} &P(k)=P^{\mathrm{T}}(-k)=P^*(-k),\\ &Q(k)=Q^{\mathrm{T}}(-k)=Q^*(-k),\\ \text{and}\quad &R(k)=-R^{\mathrm{T}}(-k)=-R^*(-k). \end{aligned} \tag{30}$$

The expression defining $\tilde{\alpha}$ can be written, as in equation (7), as

$$\tilde{\alpha}(k)=\sigma^{\dagger}\alpha^*(k) \tag{31}$$

where

$$\begin{aligned} &\sigma P(k)=P(-k)\sigma,\\ &\sigma Q(k)=Q(-k)\sigma,\\ \text{and}\quad &\sigma R(k)=-R(-k)\sigma. \end{aligned} \tag{32}$$

If the matrix σ cannot be found in the original space it can be constructed in a manner similar to that described earlier in this section. To do this one begins by dividing the operators P, Q and R into parts that are even and odd under $k\to -k$ here as

$$\begin{aligned} &P(k)=P_e(k)+P_0(k),\\ &Q(k)=Q_e(k)+Q_0(k),\\ \text{and}\quad &R(k)=R_e(k)+R_0(k). \end{aligned} \tag{33}$$

The problem is next reformulated by doubling the basis with the substitutions

$$\begin{aligned} &P(k)=P_e(k)+\sigma_1 P_0(k),\\ &Q(k)=Q_e(k)+\sigma_1 Q_0(k),\\ &R(k)=\sigma_1 R_e(k)+R_0(k),\\ &\alpha(k)\to\begin{pmatrix}\beta_1(k)\\ \beta_2(k)\end{pmatrix}, \end{aligned}$$

and

$$\tilde{\alpha}(k) \to \sigma_3 \begin{pmatrix} \beta_1^*(k) \\ \beta_2^*(k) \end{pmatrix} = \begin{pmatrix} \beta_1^*(k) \\ -\beta_2^*(k) \end{pmatrix}.$$

The related eigensolutions of the original problem are now reconstructed from β_1 and β_2 in accordance with

$$\alpha(k) = \beta_1(k) + \beta_2(k) \tag{34}$$

corresponding to a frequency ω and wavenumber k,

$$\alpha'(k) = \beta_1(k) - \beta_2(k) \tag{35}$$

corresponding to a frequency $-\omega$ and wavenumber $-k$,

$$\alpha^*(k) = \beta_1^*(k) + \beta_2^*(k) \tag{36}$$

corresponding to a frequency $-\omega^*$ and wavenumber $-k$, and

$$\alpha'^*(k) = \beta_1^*(k) - \beta_2^*(k) \tag{37}$$

corresponding to a frequency ω^* and wavenumber k.

3. Plasma oscillations

As an illustration consider a homogeneous one-dimensional one-component plasma undergoing small oscillations in the presence of a self-induced field. The equation for small displacements $y(k, v)$ of the plasma having a frequency ω and wavenumber k is

$$(\omega - kv)^2 y = \omega_p^2 \int_{-\infty}^{\infty} dv' y(k, v') f(v') \tag{38}$$

where $\omega_p^2 = 4\pi n z^2 e^2/m$ is the square of the plasma frequency and f is the unperturbed velocity distribution function. The exact solution is

$$y = (\omega - kv)^{-2} \tag{39}$$

when

$$1 = \omega_p^2 \int_{-\infty}^{\infty} \frac{dv f(v)}{(\omega - kv)^2}.$$

On a Hermitian basis $\hat{y} = y f^{1/2}$ the equation for $\hat{y}$ becomes

$$\omega^2 \hat{y} - 2\omega k v \hat{y} + \left[(kv)^2 \hat{y} - \omega_p^2 f^{1/2}(v) \int_{-\infty}^{\infty} dv' [f(v')]^{1/2} \hat{y}(v') \right] = 0. \tag{40}$$

The term linear in ω has been made real by the unitary transformation. The general treatment of the problem in the wavenumber basis is not required in such an elementary example as this, since it is evident that the solutions for ω and ω^* are merely complex conjugate pairs at the same real value of k. Thus the operator σ in (32) may be replaced by the identity, since P and Q are even in k and $R = kv$ is odd in this example. Although the system under consideration is not necessarily invariant under time-reversal, it is invariant under time and space inversion and so the condition for the existence of σ is realised. The expectation values appearing in the variational expression are then given by

$$\bar{P} = \int y^2 f \, \mathrm{d}v, \tag{41}$$

$$\bar{Q} = \omega_{\mathrm{p}}^2 \left(\int fy \, \mathrm{d}v \right)^2 - \int (kv)^2 f y^2 \, \mathrm{d}v \tag{42}$$

and

$$\bar{R} = \int kvy^2 f \, \mathrm{d}v \tag{43}$$

where no complex conjugation appears, even though y may in general be complex.

We may try

$$y = (\xi - kv)^{-2} \tag{44}$$

as the trial expression for y where ξ is a complex variational parameter.

The stationary point of the variational expression

$$\Phi(\alpha) = \frac{\bar{R}}{\bar{P}} \pm \left[\left(\frac{\bar{R}}{\bar{P}} \right)^2 + \frac{\bar{Q}}{\bar{P}} \right]^{1/2} \tag{45}$$

is determined by direct differentiation from

$$0 = \Phi \bar{P}'(\xi) - 2\Phi \bar{R}'(\xi) - \bar{Q}'(\xi) \tag{46}$$

where the primes refer to differentiation with respect to ξ. The above condition on the integrals in equations (41)–(43) is actually satisfied by the integrand in v itself, namely

$$\frac{4\Phi^2 f}{(\xi - kv)^5} - \frac{8\Phi kvf}{(\xi - kv)^5} + \frac{4(kv)^2 f}{(\xi - kv)^5} - \omega_{\mathrm{p}}^2 \int \frac{4f}{(\xi - kv)^3} \cdot \frac{f(v') \, \mathrm{d}v'}{(\xi - kv')^2} = 0, \tag{47}$$

provided that $\Phi = \xi = \omega$, where ω satisfies equation (38). Thus the exact solution is recovered at the stationary point, and the variational principle gives the correct dispersion relation. It is rather interesting that the above example also succeeds when the oscillations are stable and damped. In the general case variations in ξ are restricted to the Riemann sheet cut along $\mathrm{Im}\, \xi = 0$ as the integrals in equations (41)–(43) are undefined on the real axis in ξ. If the contour integrals in v are distorted analytically as ξ crosses the real axis, complex solutions on the second sheet in ω can be reached and correspond to stationary points of the variational expression, even though the operators P, Q and R are not all Hermitian along such distorted contours. Since the variational expression (8) depends on α and not α^*, it may be analytic in the variational parameters defining α, if α itself is analytic in these parameters. Thus the possibility of analytic continuation should exist in a general application.

4. Non-conservative second-order systems

If in equation (1) R is real and symmetric along with P and Q, the eigenfrequencies may still be complex. It is then trivial to formulate a variational principle for the eigenvalues. To each eigenfrequency ω and eigenvector α, there corresponds an eigenfrequency ω^* and eigenvector α^*. Hence equation (7) reduces simply to

$$\tilde{\alpha} = \alpha^*$$

so that the matrix elements in expression (8) become simply real inner products in the notation (11). For instance

$$(\tilde{\alpha}, R\alpha) = (\alpha, R\alpha)_{\mathscr{R}}. \tag{48}$$

As an illustration of the use of this variational principle in a non-conservative system, we consider the Klein–Gordon equation for a massive particle of charge e moving in a strongly attractive Coulomb potential which reads as

$$[(\omega - V)^2 - p^2 - m^2]\psi = 0 \tag{49}$$

where

$$V = -ze^2/r,$$
$$p^2 = p_0^2 + l(l+1)/r^2,$$
$$p_0^2 = -\frac{1}{r}\frac{\partial^2}{\partial r^2}r.$$

The exact solution to this problem is easily found by considering a similar non-relativistic situation represented by

$$\left(\frac{p_0^2}{2m_0} + \frac{l_0(l_0+1)}{2m_0 r^2} + V(r)\right) = \epsilon\psi \tag{50}$$

which can be obtained from equation (49) with the substitution

$$\omega = m_0, \tag{51}$$

$$l(l+1) - z^2e^4 = l_0(l_0+1) \tag{52}$$

and

$$(\omega^2 - m^2)/2\omega = \epsilon. \tag{53}$$

Hence we are led to consider solutions for non-relativistic motion in a Coulomb potential with stationary mass m_0 and angular momentum l_0. Since equation (52) gives complex values for l_0 when z is sufficiently large, complex eigenvalues ω are expected. In the Hilbert space of normalisable states the usual discrete spectrum for ϵ occurs, as

$$\epsilon = -\frac{1}{2}\frac{z^2e^4m_0}{(l_0+n_r)^2}, \tag{54}$$

$$\psi_{r\to\infty} \sim \exp(-\mathscr{K}r); \qquad \psi_{r\to 0} \sim r^{l_0}, \qquad \mathscr{K}^2 = -2m_0\epsilon \tag{55}$$

where $n_r = 1, 2, \ldots$ is the radial quantum number. The sign of $\mathscr{K}$ is chosen so that Re $\mathscr{K} > 0$, since for the boundary condition at the origin Re $l_0 \geqslant -1$ permits a normalisable wavefunction. It is conventional to define current and charge densities as

$$\boldsymbol{J} = \mathrm{Re}(\psi^* \mathrm{i}^{-1}\nabla\psi)$$

and

$$\rho = \mathrm{Re}[\psi^*(\omega - V)\psi]. \tag{56}$$

The condition for a finite flux through a surface around the origin is Re $l_0 \geqslant -\frac{1}{2}$. Under these conditions the eigenfrequencies are found from equations (51), (53) and (54) as

$$\omega^2 = \frac{m^2}{1+z^2e^4/(l_0+n_r)^2}, \qquad (57)$$

when

$$l_0 = -\tfrac{1}{2}+\tfrac{1}{2}[1+4l(l+1)-4z^2e^4]^{1/2}.$$

The eigenfrequencies are complex when

$$z^2e^4 \geqslant l(l+1)+\tfrac{1}{4} \qquad (58)$$

and now occur in complex conjugate pairs corresponding to

$$l_0 = -\tfrac{1}{2}\pm\tfrac{1}{2}\mathrm{i}[4z^2e^4-4l(l+1)-1]^{1/2}. \qquad (59)$$

Normally the current and charge densities defined by equations (56) satisfy the conservation law

$$\nabla \cdot \boldsymbol{J} + 2(\mathrm{Im}\,\omega)\rho = 0 \qquad (60)$$

for all r as a result of ψ's satisfying equation (50). However, when Re $l_0 = -\frac{1}{2}$, i.e. when the eigenfrequency becomes complex, the conservation law fails at the origin $r = 0$. The usual derivation of current conservation breaks down as

$$\nabla \cdot (\psi^*\nabla\phi - \psi\nabla\psi^*) \neq \psi^*\nabla^2\psi - \psi\nabla^2\psi^*. \qquad (61)$$

The behaviour of $\boldsymbol{J}$ at the origin is given by

$$\boldsymbol{J}_{r\to 0} \sim \hat{r}/r^2. \qquad (62)$$

Thus the left-hand side of inequality (61) contains a δ function singularity at the origin but the right-hand side does not. Ordinarily in quantum mechanics, these states would be excluded from the physical Hilbert space for this reason. In the relativistic wave equation they correspond to an instability of the vacuum caused by the strong potential at the origin, in complete analogy with that of the Klein paradox in the Dirac equation (Klein 1929). We are of course interested in keeping these complex eigenmodes in the present example. Depending on the sign of Im ω, the solutions with complex eigenfrequency may be interpreted as representing an incoming charge with a decreasing amplitude and a sink at the origin or an escaping charge with a growing amplitude and a source at the origin.

As a test of the variational principle we consider the solution for $l = 0$, $n_r = 1$. The exact solution is given by

$$\psi = Dr^{l_0}\exp(-\xi r) \qquad (63)$$

where

$$\xi = \frac{ze^2\epsilon}{l_0+1}, \qquad (64)$$

$$\epsilon^2 = \frac{m^2}{1+z^2e^4/(l_0+1)^2}, \qquad (65)$$

and D is an irrelevant normalisation constant. We take ψ from equation (63) to be the trial function with ξ as a complex variational parameter. The matrix elements in equation (8) are given by the real inner products

$$\bar{P}(\xi)=\int_0^\infty \psi^2 r^2\,\mathrm{d}r,$$

$$\bar{Q}(\xi)=\int_0^\infty r^2\psi\left[p_0^2+\frac{l_0(l_0+1)}{r^2}+m^2\right]\psi\,\mathrm{d}r,$$

$$\bar{R}(\xi)=\int_0^\infty \left(\frac{-ze^2}{r}\right)\psi^2 r^2\,\mathrm{d}r,$$

so that

$$\Phi(\xi)=\phi\xi\pm(\gamma\xi^2+m^2)^{1/2}, \tag{66}$$

where

$$\phi=-ze^2/(l_0+1),$$

and

$$\gamma=\phi^2+1.$$

The stationary point in Φ occurs at

$$\xi_0=\mp m\phi/\gamma^{1/2} \tag{67}$$

when

$$\Phi(\xi_0)=\pm m/[1+z^2e^4/(l_0+1)^2]^{1/2}. \tag{68}$$

The choices of sign in equations (66)–(68) are correlated. The results (67) and (68) agree exactly with (64) and (65).

5. Non-holonomic variational expression for Im ω

Consider again the equation

$$(\omega^2P-2\omega R-Q)\alpha=0 \tag{69}$$

with R imaginary and ω complex.

We note as in Low (1961) that if α satisfies equation (1), then

$$\omega=\frac{(\alpha,R\alpha)}{(\alpha,P\alpha)}\pm\left(\frac{(\alpha,R\alpha)^2}{(\alpha,P\alpha)^2}+\frac{(\alpha,Q\alpha)}{(\alpha,P\alpha)}\right)^{1/2}$$

is stationary for real values of ω, but not for complex ones. Also, if the square root is imaginary, it gives the imaginary part of ω as

$$\operatorname{Im}\omega=\pm\frac{1}{\mathrm{i}}\left(\frac{(\alpha,R\alpha)^2}{(\alpha,P\alpha)^2}+\frac{(\alpha,Q\alpha)}{(\alpha,P\alpha)}\right)^{1/2}, \tag{70}$$

provided the argument of the square root is negative, and the inner product is Hermitian.

The stationary quantity for complex ω is in fact

$$\Lambda=\frac{(\alpha,R\alpha)^2}{(\alpha,P\alpha)^2}+\frac{(\alpha,Q\alpha)}{(\alpha,P\alpha)} \tag{71}$$

with the non-integrable constraint

$$\mathrm{Im}[(\delta\alpha, R\alpha)\bar{P} - (\delta\alpha, P\alpha)\bar{R}] = 0.$$

To see this, let us consider

$$\delta\Lambda = \delta\bar{P}\left[-\frac{2\bar{R}^2}{\bar{P}^3} - \frac{\bar{Q}}{\bar{P}^2}\right] + \delta\bar{R}\frac{2\bar{R}}{\bar{P}^2} + \frac{\delta\bar{Q}}{\bar{P}}. \tag{72}$$

On the other hand, for α to be a solution of equation (1),

$$(\delta\alpha, \omega^2 P\alpha - 2\omega R\alpha - Q\alpha) = 0 \tag{73}$$

and

$$\omega^{*2}(\alpha, P\delta\alpha) - 2\omega^*(\alpha, R\delta\alpha) - (\alpha, Q\delta\alpha) = 0 \tag{74}$$

so that on adding (73) and (74), we obtain

$$(\omega - \omega^*)\{\tfrac{1}{2}(\omega + \omega^*)[(\delta\alpha, P\alpha) - (\alpha, P\delta\alpha)] - [(\delta\alpha, R\alpha) - (\alpha, R\delta\alpha)]\}$$
$$+ \tfrac{1}{2}(\omega^2 + \omega^{*2})\delta\bar{P} - (\omega + \omega^*)\delta\bar{R} - \delta\bar{Q} = 0. \tag{75}$$

Using equation (69), and remembering that the square root is imaginary, we see that the coefficient of $\omega - \omega^*$ vanishes by virtue of equation (71). The remainder is just $-\bar{P}\delta\Lambda$.

This expression is evidently of considerably less significance than the one described in § 2, as

(i) the converse does not hold, i.e. Λ can be stationary for all variations subject to the constraints without α being a solution of equation (1), and
(ii) the constraint itself is non-holonomic, and hence, awkward to meet.

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