International Journal of Theoretical Physics, Vol. 42, No. 10, October 2003 (© 2003)

Aspects of the Theory and Computation of Resonances, With Applications to Field-Free and Field-Dressed Atomic States[1]

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Received June 30, 2003

A review of certain aspects of the theory and computation of resonance states is presented, from the point of view of the work by the author and his colleagues in atomic physics. Two issues are mainly discussed: one is the understanding and ab initio calculation of resonance states of real systems from a time-dependent point of view. The other is the derivation and application of the *complex eigenvalue Schrödinger equation* from a superposition of the localized wave packet Ψ_0 with the orthogonal to it scattering wave functions $\varphi(\mathrm{E})$, when outgoing-wave boundary conditions are imposed. It is shown how two complex adjoint solutions, the hallmark of resonance state theory, correspond to the Fano solution for a resonance state on the real energy axis, obtained from the application of Hermitian quantum mechanics. The forms of the complex eigenfunctions are used for non-Hermitian calculations of resonance states in polyelectronic atoms. The question of time-asymmetry at the quantum level is tackled by observing that the time-evolution has to be considered with boundary conditions $t \geq 0$ and $\infty > E > 0$ and a complex energy distribution given by the diagonal matrix element of the Green's function with respect to Ψ_0. Using a model whereby the self-energy of the decaying state, $A(z)$, is approximated by $A(z) \approx A(E_0)$, where $E_0 = \langle\Psi_0|H|\Psi_0\rangle$, it is shown that time-asymmetry, if present as defined in this work, should have an effect on the as yet unobserved long-time deviation from exponential decay. Although not described explicitly, it is indicated, via the forms of the trial wave functions and via the references, how polyelectronic calculations have been carried out, for field-free resonance states as well as

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[1] Large portions of this paper are also contained in the Proceedings of the 22nd Solvay conference, Delphi, Greece, November, 24–29 2001.

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for resonance states that are created by the presence of an external electromagnetic field.

KEY WORDS: resonances; localization; complex eigenvalues; time-dependence; nonexponential decay.

1. INTRODUCTION

The excitation of polyelectronic atoms to energies above their first ionization threshold produces structures inside the continuous spectrum which are associated with resonance (or, “autoionizing,” or “Auger” or “compound”) states. The concept of a resonance state and its properties appears in various physical situations, from atoms to elementary particles, and so it has been investigated extensively over many decades. In the case of atoms, the Hamiltonian is known, even when relativistic corrections must be included. So atomic physics is suitable for testing formalisms concerning resonance states. This testing cannot, of course, stop with phenomenology. Rather, the formalism must have a simple and flexible structure so as to provide not only rigorous understanding of the concepts and the related quantities but also to allow their systematic computation in conjunction with suitably developed many-body theory. Fortunately, in atomic physics the accuracy of measurements of the effects of resonance states on observables can be high, thereby placing theory under stringent conditions.

The present paper reviews aspects of the work on atomic, field-free and field-dressed, resonance states by the author and his colleagues since 1972, by examining issues of concepts and fundamental physics as well as of practical calculations. Only a few essentials are gleaned. For complete descriptions, applications and additional references, the reader is referred to (e.g., Bylicki and Nicolaides, 2002; Haritos *et al.*, 2001; Mercouris *et al.*, 2001; Mercouris and Nicolaides, 1990, 1997, 2001, 2002; Nicolaides, 1972; Nicolaides *et al.*, 1981, 1990, 1993; Nicolaides and Beck, 1977a,b, 1978a,b; Nicolaides and Gotsis, 1992; Nicolaides and Mercouris, 1985, 1996; Nicolaides and Piangos, 2001; Nicolaides and Themelis, 1992; Themelis and Nicolaides, 2000, 2001). In this context, one may wonder about the possible advantages of computing resonance states directly in a time-independent framework, rather than obtaining the same information by determining the relevant transition amplitudes. One advantage is the fact that by solving directly for the complex eigenvalues, of the resonance states, very small widths of real states can be established within a nonperturbative framework, thereby allowing identification of new states where other theories fail (e.g., Bylicki and Nicolaides, 2002). Also, solving for the appropriate complex eigenvalue in field-dressed problems allows the all-orders (nonperturbative) calculation of physical properties, such as multiphoton ionization rates of atoms in strong fields (Haritos *et al.*, 2001; Mercouris *et al.*, 2001; Mercouris and Nicolaides, 1990, 2001). We point out that the herein reviewed framework for the solution of problems involving nonstationary states has also been applied to molecular systems, a topic which is outside the scope of this paper (e.g., Petsalakis *et al.* 1990).

2. THE COMPLEX EIGENVALUE SCHRÖDINGER EQUATION FOR RESONANCE STATES

2.1. Superposition of Wave Functions in the Continuous Spectrum Fano's Standing Wave Solution

Fundamental to the existence and description of an isolated resonance state is the formation of a localized wave packet, Ψ_0, at $t = 0$. This formation breaks the continuity from $t = -\infty$ to $t = +\infty$ of the overall reaction or scattering process and introduces the concept of a decaying state, provided the lifetime of this state (for its definition see below), is much longer than the excitation–interaction mechanism. Heuristic arguments as to the existence and significance of Ψ_0 and methods for its consistent calculation to a high degree of accuracy in excited atomic systems, are discussed in the references already cited. The formation of Ψ_0 implies the beginning of a nonstationary process of decay with the initial condition $\Psi(t = 0) \equiv \Psi_0$. The time-evolution is caused by the interaction of Ψ_0 with the (formally) orthogonal to it scattering wave functions, $\varphi(E)$, via the Hamiltonian, H, of the system. Neither Ψ_0 nor $\varphi(E)$ are stationary eigenstates of H. Such a stationary state, $\Psi(E)$, is a superposition of Ψ_0 and $\varphi(E)$ with energy dependent probability amplitudes:

$$\Psi(\mathbf{r}; E) = a(E)\Psi_0(\mathbf{r}) + \int b_E(E')\varphi(\mathbf{r}; E')dE' \tag{1}$$

Fano (1961) obtained the coefficients $a(E)$ and b_E for boundary conditions of a standing wave, i.e., for real functions. To do so, he followed the method of Dirac (Section 50 of Dirac, 1958), whereby the division by $(E - E')$ in the continuous spectrum introduces an unknown function, $\lambda(E)$, which is determined by the boundary conditions. In this way, Fano (1961) obtained

$$\lambda(E) = \frac{E - E_0 - \Delta(E)}{|V(E)|^2} \tag{2}$$

and

$$|a(E)|^2 dE = \frac{1}{2\pi} \frac{\Gamma(E)}{(E - E_0 - \Delta(E))^2 + \frac{\Gamma^2(E)}{4}} dE \tag{3}$$

where,

$$\langle\Psi_0|H|\varphi(E)\rangle \equiv V(E),\ E_0 = \langle\Psi_0|H|\Psi_0\rangle \tag{4}$$

$$\Gamma(E) = 2\pi|V(E)|^2 \quad \text{(the energy width)} \tag{5a}$$

and

$$\Delta(E) = \text{P.V.} \int dE' \frac{|V(E)|}{E - E'} \quad \text{(the energy shift).} \tag{5b}$$

P.V. stands for principal value. The probability distribution in the energy spectrum, $|a(E)|^2$, is equal to $|\langle\Psi(E)|\Psi_0\rangle|^2$. Its form is the result of energy normalization of $\Psi(E)$, satisfying

$$H\Psi(\mathbf{r}; E) = E\Psi(\mathbf{r}; E), \quad \langle\Psi(E)|\Psi(E')\rangle = \delta(E - E'), \tag{6}$$

and has the property that it is normalized to one

$$\int dE|a(E)|^2 = \int dE|\langle\Psi_0|\Psi(E)\rangle|^2 \equiv \int dE g(E) = 1 \tag{7}$$

The structure of Fano's treatment is Hermitian and time symmetric. It uses real functions and real energies. The standing wave boundary conditions imply the use of the Hermitian K-matrix rather than the S-matrix[5] (Goldberger and Watson, 1964; Newton, 1982). The position of the resonance is given by $E_r = E_0 + \Delta(E_r)$ and is found by solving self-consistently the transcendental equation (numerator of Eq. (2))

$$E - E_0 - \Delta(E) = 0. \tag{8}$$

Indeed, such calculations have been carried out for a variety of polyelectronic resonance states, even for those with multiply excited electronic structures, where, in addition, total as well as partial widths were obtained (Nicolaides *et al.*, 1993; Nicolaides and Piangos, 2001). Crucial to such many-body calculations is the computation of accurate Ψ_0 and E_0. (More on Ψ_0 in Section 5).

The energy distribution, $g(E)$, is real and drives the survival amplitude $G(t)$:

$$G(t) = \langle\Psi_0|e^{-iHt}|\Psi_0\rangle = \int dE|\langle\Psi(E)|\Psi_0\rangle|^2 e^{-iEt} \equiv \int dE g(E) e^{-iEt} \tag{9}$$

where the integral over energy is obtained by inserting the Hermitian unit operator of the stationary states, $I = \int dE|\Psi(E)\rangle\langle\Psi(E)|$. The significant relevant property of $g(E)$ is that it has complex poles at z_0 and z_0^* (Eqs. (10), (16), and (21)) and that it *does not differentiate between positive and negative times* (Nicolaides and Beck, 1977, 1978, p. 492).

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[5] Even though in the discussions on resonance states the emphasis has been on S-matrix-type theories, the use of K-matrix type formalism, with its Hermitian structure, can have advantages. For example, for real multiparticle systems, such as the polyelectronic atoms, where scattering theory must be combined with the particularities of the many-body problem, it is possible to unite, formally and computationally, within the K-matrix formalism, properties of the discrete and of the continuous spectrum, using basis sets of bound and scattering functions. (Komninos *et al.*, 1995; Komninos and Nicolaides, 1987; Sinanis *et al.*, 1998).

2.2. Superposition of Wave Functions in the Continuous Spectrum: Traveling Wave Solutions

As is well known from the theory of scattering (Dirac, 1958; Goldberger, and Watson, 1964; Newton, 1982), the alternative to standing wave boundary conditions is the use of traveling waves. Then, one obtains two Green's functions, one for the "in" and one for the "out" state. These are time-reversed and both are needed to secure unitarity of the S-matrix. I will show how the solution of the problem of Eqs. (1) and (6) produces naturally and rigorously two complex eigenvalue Schrödinger equations (CESE) with adjoint solutions, $\Psi(\mathbf{r}; z_0)$ and $\Psi^t(\mathbf{r}; z_0^*)$, one corresponding to a decaying state and one to a growing state for $t \geq 0$, when outgoing and incoming wave boundary conditions are imposed. In doing so, no definitions or assumptions anticipating the result are made. In this way, the real energy, Hermitian problem on the real energy axis, incorporating information for $t > 0$ as well as for $t < 0$, is split into two complex eigenvalue non-Hermitian problems, each being the time-reversed of the other. The two complex eigenvalues are obtained below as

$$z_0 = E_0 + \Delta - \frac{i}{2}\Gamma, \quad z_0^* = E_0 + \Delta + \frac{i}{2}\Gamma \tag{10}$$

where Δ and Γ are defined in terms of the matrix elements of eqs. (5) at the solution of eq. (8), $E_r = E_0 + \Delta(E_r) = \Re(z_0) = \Re(z_0^*)$. It is then clear that E_r, z_0 and z_0^* have as their reference point the real energy E_0.

By solving formally for the coefficient b_E, the $\Psi(\mathbf{r}; E)$ of Eq. (1) can be written as

$$\Psi(\mathbf{r}; E) = a(E)\left[\Psi_0(\mathbf{r}) + \text{P.V.} \int dE' \frac{V(E')}{E - E'}\varphi(\mathbf{r}; E') + \lambda(E)V(E)\varphi(\mathbf{r}; E')\right] \tag{11}$$

where the unknown function $\lambda(E)$ is to be defined by the boundary conditions of the physical problem of interest. In the case of the decaying state, for $t \geq 0$ the boundary conditions are those of regularity at the origin and of an asymptotically outgoing wave with no incoming part. The opposite is true for the adjoint state, namely we have an incoming wave with no outgoing part. Since it is the $r \to \infty$ region that matters, it is the asymptotic form of $\varphi(E)$ that enters Eq. (11), depending on the scattering potentials of interest. For example, for the linear potential, (effect of an electric field), one has the Airy function, for the Coulomb potential the Coulomb function and for the short-range potential, used in nuclear physics and in atomic negative ions, the Bessel function. By substituting these asymptotic forms into Eq. (11) and by carrying out the required algebraic manipulations, $\Psi(\mathbf{r}; E)$ in the asymptotic region acquires the following form (the term $a(E)\Psi_0(\mathbf{r})$ goes to zero for $r \to \infty$):

$$\Psi(r) \underset{r\to\infty}{\approx} -\sqrt{\frac{\pi}{2k}} Va \left[\left(1 - \frac{\lambda(E)}{i\pi}\right) e^{iN} + \left(1 + \frac{\lambda(E)}{i\pi}\right) e^{-iN} \right] \tag{12}$$

where the r-dependent N stands for the slightly different result for each potential. The conclusion is immediate: Eq. (12) contains both an outgoing wave, e^{iN}, (decaying state for $t \geq 0$), and an incoming wave, e^{-iN}, (unphysical, growing state). In order for only one or the other to survive, $\lambda(E)$ must be

$$\lambda(E) = -i\pi \quad \text{outgoing wave boundary condition} \tag{13a}$$

$$\lambda(E) = +i\pi \quad \text{incoming wave boundary condition} \tag{13b}$$

Therefore, by combining the expression for E, Eq. (2),

$$E = E_0 + \Delta(E) + \lambda(E)|V(E)|^2, \tag{14}$$

with Eqs. (13), one obtains directly the corresponding complex eigenvalues of Eq. (10). Furthermore, one also obtains the exact form for the asymptotic part of the resonance eigenfunction, which, using Eqs. (12) and (13a), is

$$\Psi(\mathbf{r}; z_0) \sim -Va\sqrt{\frac{2\pi}{k_r}} e^{iN} \tag{15}$$

where a is the complex coefficient of Ψ_0 and k_r is the complex momentum, $(2z_0)^{1/2}$. The combination of Eqs. (11) and (15) yields the form of the resonance eigenfunction over the full coordinate space. It follows that, under the boundary conditions extracted from Eq. (12) when either (13a) or (13b) are applied, the standing wave real eigenvalue Schrödinger equation (6) is converted into two complex eigenvalue Schrödinger equations (CESE) for the two adjoint states:

$$(H - z_0)\Psi(\mathbf{r}; z_0) = 0, \quad \text{outgoing wave condition} \tag{16a}$$

$$(H - z_0^*)\Psi^\dagger(\mathbf{r}; z_0^*) = 0, \quad \text{incoming wave condition} \tag{16b}$$

The non Hermitian CESEs (16) involve complex eigenfunctions that are not square-integrable and do not belong to, or constitute elements of, Hilbert space. Considered separately, each solution is a manifestation of nonunitarity, brought about by the fact that due to the formation of Ψ_0, there is a singularity at $t = 0$ when the TDSE is used to determine the physics. This breakdown of continuity creates the two solutions of Eqs. (16). When the parameter of time is introduced, then for $t \geq 0$ one of these states is physical, representing the decay, and one, its adjoint state, is unphysical. The use of these states in defining the norm of time-dependent wave functions is demonstrated below. I add here that the above treatment and derivation has led to the following relations which have been used as constraints for the optimization of trial resonance wave functions. The first has used the expectation values of H and of H^2 (Nicolaides and Beck, 1978a,b): From Eq. (16) it follows that

$$I(z_0) = \frac{\langle\Psi(z_0|H^2|\Psi(z_0\rangle}{\langle\Psi(z_0|\Psi(z_0\rangle} = z_0^2 \tag{17}$$

Then,

$$\Re(I(z_0) = E^2 - \frac{1}{4}\Gamma^2 \tag{18a}$$

$$\Im(I(z_0) = -E\Gamma \tag{18b}$$

Application of these equations to the calculation of the Stark effect in Hydrogen was presented in (Nicolaides and Gotsis, 1992).

The other relation is obtained from the form of the resonance wave function, and relates the mixing coefficients a and b to the width and the complex momentum (Nicolaides *et al.*, 1981; Nicolaides and Mercouris, 1985). Thus, the coefficient $b(z_0)$, representing the flux of emitted particles, is equal to

$$|b|^2 = |a|^2\frac{\Gamma}{|k_r|} \tag{19}$$

In Eq. (19), I used the total width, Γ, and the complex momentum, k_r. However, the same relation holds for each partial width separately. Application to the calculation of single- and multichannel decaying states is described in Nicolaides *et al.* (1981) and Nicolaides and Mercouris (1985).

3. NORMS AND ENERGY DISTRIBUTIONS

For a purely scattering state, the energy distribution on the real energy axis is just the Dirac δ function. In the case of the Fano resonance state, the requirement that $\Psi(E)$ of Eq. (1) is normalized as in Eq. (6), produces the exact form of the real energy distribution as Eq. (3). In this treatment, the usual rules of Hermitian quantum mechanics apply, unitarity is satisfied and the formalism and results contain information for both $t \geq 0$ and $t \leq 0$. However, if we consider the sectionally analytic resolvent operator $R(z) \equiv (z - H)^{-1}$ with z complex, and obtain from it the two diagonal Green's functions defined above and below the cut of the real axis (Goldberger and Watson, 1964; Newton, 1982):

$$\langle\Psi_0|R(z)|\Psi_0\rangle = \begin{cases} {}^dG^{+}(E - H + i0)^{-1} = {}^dG^{+}(E) \\ {}^dG^{-}(E - H + i0)^{-1} = {}^dG^{-}(E) \end{cases} \tag{20}$$

then, it is their combination which equals $g(E)$:

$$g(E) = \frac{1}{2\pi i}[{}^dG^{-}(E) - {}^dG^{+}(E)] = \mp\frac{1}{\pi}\Im({}^dG^{\pm}(E)) \tag{21}$$

If only one of the two complex Green's functions is considered, whose analytic continuation through the cut of the real axis yields the pole z_0 on the second sheet, (or z_0^* for the other function), the hallmark of resonance state theory, then no unit normalization is obtained. Unit normalization of the real energy distribution holds only for Hermitian systems.

If we use the standing wave solution, $\Psi(\mathbf{r}; E)$, in order to construct the time-dependent wave function, $\Psi(\mathbf{r}; E, t) = \Psi(\mathbf{r}; E)e^{-iEt}$, the norm is one for all t:

$$\langle\Psi(t)|\Psi(t)\rangle = \int dE \int \Psi^*(\mathbf{r}; E)e^{iEt}\Psi(\mathbf{r}; E)e^{-iEt}d\mathbf{r} = 1 \tag{22}$$

On the other hand, the following values for the norms are obtained when considering the use of the resonance eigenfunction:

1. If only the decaying state solution is used, then flux is not conserved since decay occurs. This is seen by assuming the form of the time-dependent resonance eigenfunction to be

   $$\Psi(\mathbf{r}; z_0, t) = \Psi(\mathbf{r}; z_0)\exp(-iz_0 t). \tag{23}$$

   Then,

   $$\begin{aligned}&\int \Psi^*(\mathbf{r}; z_0, t)\Psi(\mathbf{r}; z_0, t)d\mathbf{r}\\ &= \{\exp[(z_0^* - z_0)it]\} \int \Psi^*(\mathbf{r}; z_0)\Psi(\mathbf{r}; z_0)d\mathbf{r}\\ &= e^{-\Gamma t} \int \Psi^*(\mathbf{r}; z_0)\Psi(\mathbf{r}; z_0)d\mathbf{r}\end{aligned} \tag{24}$$

   Eq. (24) demonstrates the exponential decay, under the assumption of Eq. (23). The resolution of the problem that the integral over space is infinite, is discussed below.
2. The second type of norm is the one that has to show conservation of flux for the whole system, just like the norm of Eq. (22) shows. Following the line of argument about the equivalence between the one solution on the real axis with both solutions in the complex plane, it is evident that the *flux-conserving* norm must involve both the decaying state and its adjoint, $\Psi^\dagger(\mathbf{r}; z_0^*)$. In this case,

$$\begin{aligned}\int \Psi^\dagger(\mathbf{r}; z_0^*, t)\Psi(\mathbf{r}; z_0, t)d\mathbf{r} &= \{\exp[(z_0 - z_0)it]\} \int \Psi(\mathbf{r}; z_0)\Psi(\mathbf{r}; z_0)d\mathbf{r}\\ &= \int \Psi(\mathbf{r}; z_0)\Psi(\mathbf{r}; z_0)d\mathbf{r}\end{aligned} \tag{25}$$

Hence, the use of both eigenfunctions of Eq. (16) produces a norm which is independent of time. Furthermore, Eq. (25) shows a characteristic feature of the properties of resonance states represented by complex eigenfunctions, namely that the integral over position space involves the square of the function itself and not of its absolute value. Again, this integral is infinite.

3.1. Normalization of Ψ(r; z_0) and Calculation of Ψ(r; *zo*) and of z_0

As it was recognized already in 1928, as soon as the Gamow outgoing wave was introduced (Gamow, 1928), matrix elements involving functions with such asymptotic behavior cannot be defined in position space. Since the reliable solution of Eq. (16a) presupposes the possibility of dealing effectively with all difficulties of the many-body problem and open channel mixing, the lack of norm in the usual sense reduced for many decades the possibility and/or the interest in tackling problems of resonance states as a complex eigenvalue problem. For example, Kemble (1937), in his book on quantum mechanics, briefly discussed this issue and conjectured the possibility of defining a new norm by introducing the attenuating factor $\exp(-ar^n)$. This idea, and further analysis using short range potentials, was much later examined by Zel'dovich (1961) and Berggren (Berggren, 1968). In fact, a simple and practical solution to the norm problem was provided in 1961 by Dykhne and Chaplik (1961) by extending integration into the upper half of complex coordinate plane, i.e., by changing r into $re^{i\theta}$. They showed that for the simple model used by Zel'dovich, the same norm is obtained. They concluded that *in spite of the fact that the wave functions vanish at infinity, the energy values are complex because of the non-Hermitian character of the Hamiltonian in V* (the volume of integration). About a decade later, the same result was obtained in a mathematical language which analyzed the spectral properties of the rotated Coulomb Hamiltonian $H(\theta) = e^{-2i\theta}T + e^{-i\theta}V$ in the Hilbert space of L^2 functions (Aguilar and Combes, 1972; Balslev and Combes, 1972). It was shown that the complex eigenvalues of $H(\theta)$ correspond to the second sheet poles of the resolvent, i.e., to resonance states. Even though the mathematical proofs of (Aguilar and Combes, 1972; Balslev and Combes, 1972) concerned the Coulomb Hamiltonian, it has since become clear that *complex scaling* of the Hamiltonian coordinates works for other situations as well, including models, (Moiseyev, 1998 and references therein).

However, for the many-body problem in real systems, and for the calculation of partial widths to all orders, the use of complex-scaled Hamiltonians in conjunction with single sets of square-integrable functions runs into trouble. As a solution, we have proposed and implemented a many-electron (for field-free) or a many-electron, many-photon (for field-dressed states) theory, where the coordinates of the Hamiltonian are real. It is the function spaces that are chosen appropriately so as to follow the two-part form of the resonance wave function discussed in this section. This means that there is one L^2 space which consists of real functions with real coordinates (the undecayed part) and another L^2 space consisting of both real and complex functions (the decayed part)—see Eq. (27) below. The theory emphasizes the use of optimized spaces for these two parts, whether for isoated or for strongly coupled states. Lack of space does not allow the presentation of the related methodologies and results. So the reader is referred to (Bylicki and Nicolaides, 2002; Haritos *et al.*, 2001; Mercouris *et al.*, 2001; Mercouris and Nicolaides, 1990, 2001; Nicolaides *et al.*, 1981; Nicolaides and Beck, 1977a,b, 1978a,b; Nicolaides and Gotsis, 1992; Nicolaides and Mercouris, 1985; Nicolaids and Themelis, 1992; Themelis and Nicolaides, 2000, 2001) for essential information and applications. Here I give only two formulae, which contain the basic idea of introducing the non-Hermiticity via the proper choice of the function space rather than via the scaling of the Hamiltonian coordinates. The first is Eq. (3) of Nicolaides and Beck, 1978a, which emphasizes the fact that it is only the asymptotic part of the resonance wave function that has to be dealt with special methods. Thus the norm was defined as

$$\int_{\text{all space}} \Psi^2 dr = \int_0^R \Psi^2 dr = \int_{\mathrm{C}} \Psi^2 dr \tag{26}$$

where R is a point on the real axis at the edge of the inner region and R $R < \Re(s) < \infty$. This type of regularization, which has since been named *exterior scaling*, has been applied analytically and numercally to a number of different potentials e.g., Nicolaides *et al.*, (1990). The second formula concerns the form of the multiparticle resonance wave function. For an isolated resonance state it is given by (Bylicki and Nicolaides, 2002; Haritos *et al.*, 2001; Mercouris *et al.*, 2001; Mercouris and Nicolaides, 1990, 2001; Nicolaides *et al.*, 1981, 1990; Nicolaides and Beck, 1977a,b, 1978a,b; Nicolaides and Gotsis, 1992; Nicolaides and Mercouris, 1985; Nicolaids and Themelis, 1992; Themelis and Nicolaides, 2000, 2001).

$$\Psi(r, \rho^*) = \alpha(\theta)\Psi_0(r) + \sum_n \beta(\theta) u_n(r, \rho^*), \tag{27}$$

where $\rho^* = re^{i\theta}$, and $\Psi(r, \rho^*)$ is square-integrable. The complex functions $u_n(r, \rho^*)$ are products of basis functions with real coordinates for the bound part of the channel and with complex coordinates for the outgoing particle in that channel. It is important to emphasize here that it is the use of forms (26) and (27) that has made the solution of difficult many-body problems with resonance states possible. For coupled states, Ψ_0 is replaced by a sum over the corresponding wave functions.

Finally, as regards the theoretical foundations, a conclusion from the contents of the above subsection can perhaps be summarized by quoting from the 1978 paper (Nicolaides and Beck, 1978a): *In general, the mathematical properties of resonance states are maniifestations of non self-adjoint systems due to the radiation boundary conditions with complex energies. Such systems can be treated in terms of biorthogonal expansions, i.e., with the use of adjoint functions. In such cases, the norm can be defined over both direct and adjoint spaces. As the resonant state* *tends to a bound state, the two spaces merge into one, the Hilbert space, where the norm is defined as in the textbooks.*

4. A COMMENT ON RESONANCE STATE-LIKE FORMS AND COMPUTATION

According to the previous discussion, the crucial element in the conceptual and computational framework for a theory of resonance states is the possibility of establishing the existence of a localized square-integrable Ψ_0 containing the information from all the interactions creating stability and leaving out the contribution of the part of function space causing fragmentation (Nicolaides, 1972; Nicolaides and Beck, 1977a,b, 1978a,b; Bylicki and Nicolaides, 2002; Nicolaides and Mercouris, 1996; Mercouris and Nicolaides, 1977, 2000). Consequences of using (Ψ_0, E_0) as the origin are the computationally practical resonance wave function forms of Eqs. (26) and (27). A similar to (27) form, including photon states, is used when treating as a resonance problem the *many-electron, many-photon* problem, for which the reader is referred to Mercouris and Nicolaides, 1990, 2001. Except for cases of calculation of partial widths to all orders, a nearly equivalent formulation of the quest for the computation of resonance states as complex eigenvalue problems is achieved and facilitated by using non Hermitian Hamiltonians consisting of two parts, one real and one complex. This physically meaningful and economic approach was emphasized in Nicolaides and Beck, 1978b. The real part, H_0, produces via diagonalization in Hilbert space the real energy E_0. When the complex part is added, the function space corresponding to H_0 need not be recalculated. Optimization for the complex eigenvalue calculation can be done in terms of the additional space of L^2 functions on which the complex part of the Hamiltonians is projected. Two Hamiltonians of the aforementioned form were suggested in Nicolaides and Beck, 1978b. The first emerges naturally from the formal treatment of decaying states. Its form was written as (Eq. 3.51 of Nicolaides and Beck, 1978b)

$$M(z) = H_0 + A(z) \tag{28}$$

where $A(z)$ is the self-energy operator (Goldberger and Watson, 1964; Nicolaides and Beck, 1977a,b, 1978a,b). The position and the width of the resonance are given by the complex eigenvalue of $M(z)$ for which the imaginary part is negative and the vector is closest to Ψ_0. The second Hamiltonian form refers to the scaled Hamiltonian $H(\theta)$ (Aguilar and Combes, 1972; Balslev and Combes, 1972; Dykhne and Chaplik, 1961; Moiseyev, 1998) and is written as (Eq. 5.26 of Nicolaides and Beck, 1978b)

$$H(\theta) = (T + V) + [(e^{-2i\theta} - 1)T + (e^{-i\theta} - 1)V] \equiv H(0) + V(\theta) \tag{29}$$

where T is the kinetic energy operator V is the local potential for the nucleus–electron and electron–electron interactions and θ is the angle of coordinate rotation. By comparing the forms of Eqs. (28) and (29) we see that the complex part $V(\theta)$ corresponds to the non Hermitian self-erergy matrix $A(z)$.

5. ON THE EXISTENCE AND CALCUATION OF THE LOCALIZED WAVE FUNCTION Ψ_0, REPRESENTING THE NON STATIONARY STATE AT $t = 0$

The essential element in the theory of resonance states is the presence of Ψ_0 whose energy E_0 is embedded in the continuous spectrum of scattering states with which Ψ_0 interacts. However, although the phenomenology resulting from resonance scattering theory or from decaying state theory is satisfied by the mere adoption of any bound wave function Ψ_0, two important questions remain

(i) Is there a physically realized Ψ_0? This would imply the momentary formation of a localized (square-integrable) wave packet which is practically decoupled from the excitation mechanism and where all the interactions of the Hamiltonian act, but which is non stationary due to its coupling with, and dissipation into, the continuum. Obviously, the longer the lifetime compared to the collision (production) time the better Ψ_0 can be understood conceptually. Furthermore, the deeper the binding potential, the easier it is to compute Ψ_0 for multielectron states (Nicolaides *et al.*, 1993; Nicolaides and Piangos, 2001). For an artificial one-particle system, say the barrier penetration model of alpha particle decay, it is indeed possible to choose a potential for which a Ψ_0 can be computed exactly, analytically or numerically. However, for real polyelectronic systems it is impossible to write out explicitly the potential responsible for the formation of Ψ_0. Therefore, for most physically relevant systems the above question is challenging. Among other things, it was raised and discussed in the work on atomic systems cited here. Physical as well as formal arguments have been given in favor of the existence of Ψ_0 as a maximum but finite localized projection out of the exact (complex) resonance eigenfunction, for which the variance $\langle\Psi_0|(H - \langle H\rangle)^2|\Psi_0\rangle$ is minimum. This variance, named *stationarity coefficient* in Mercouris and Nicolaides, 2002, is the coefficient of the t^2 term in the small-t series expansion of the time-dependent survival probability, $P(t) = |G(t)|^2$. When $P(t)$ was computed from first principles via the numerical solution of the time-dependent Schrödinger equation (TDSE) for polyelectronic non stationary atomic states, it was found that the short-time, preexponential decay regime is dominated by the t^2 term (Mercouris and Nicolaides, 2002).

(ii) How can one define systematically and compute Ψ_0 for a real polyelectronic atom? Since the exact Hamiltonian, H, of an N-electron atom is

> given by the sum of one- and two-electron operators, and since, for a given symmetry, H has only a continuous spectrum above the first ionization threshold, it is impossible to write an explicit form of a local operator of which Ψ_0 is an eigenfunction. In other words, the standard formal separation of the Hamiltonian operator, $H = H_0 + V$, which is necessary for the mathematical treatment of discrete states embedded in the continuum, is not accompanied by explicit forms for the operators corresponding to H_0 or V. (In fact, H_0 and V are effective matrix operators, constructed by projecting onto appropriate function spaces). For example, a mathematical device that has often been used in the literature is to assume that the *interaction is turned off* and that Ψ_0 is the eigenfunction of a fictitious interactionless Hamiltonian, H_0. The coupling operator for the interactions is then allowed to enter and to produce the off-diagonal coupling matrix elements. However, this artificial device cannot be physically or computationally justified, since the presence of the interelectronic interactions is continuous. (This concept is acceptable when the interaction is induced by the sudden introduction of an external perturbation, such as the application of an electromagnetic field).

The question stated above has been addressed consistently in a series of our publications reporting practical calculations on a variety of resonance states, starting with Nicolaides 1972. For atoms, the shell structure, state-specific multiconfigurational Hartree–Fock theory as well as the virial theorem have been used as practical criteria. The energy E_0 is found as a local minimum inside the continuous spectrum. The minimization of the variance, $\langle\Psi_0|(H - \langle H\rangle)^2|\Psi_0$, has also been used. An additional criterion is given below: the interpretation of Ψ_0 as a wave packet localized at $t = 0$ is discussed in Section 5C of Nicolaides and Beck, 1978b. Starting with a superposition of outgoing waves with complex coefficients, a(ϵ), and writing

$$\Psi(\mathbf{r}, t) = \int a(\epsilon)\exp(-i\epsilon t)\phi(\mathbf{r};\epsilon)d\epsilon \tag{30}$$

where

$$\phi(\mathbf{r};\epsilon) = \text{constant} \times \exp(ikr), \quad k = (2E)^{1/2} \tag{31}$$

and

$$a(\epsilon) = \int \exp(i\epsilon t)\exp(-iz_0 t)dt = i(\epsilon - z_0)^{-1}, \quad z_0 = E_r - \frac{i}{2}\Gamma \tag{32}$$

it is shown that $\Psi(\mathbf{r}, t)$ has no outgoing component if the position, $\mathbf{r}$, of the emitted particle satisfies $r < t(2E_r)^{1/2}$. Given the recent analysis on the stationarity coefficients ΔE, Mercouris and Nicolaides (2002), I take as a reasonable estimate for the duration t to be $1/(\Delta E)^{1/2}$. Therefore, a useful heuristic criterion of localization is that

$$\text{extent of } \Psi_0 < (2E_0/(\Delta E)^{1/2} \tag{33}$$

In the next section I focus on the time-evolution of $\Psi_0(t)$, with initial condition $\Psi(0) = \Psi_0$.

6. NONEXPONENTIAL DECAY AND TIME-ASYMMETRY

The celebrated law of exponential decay results from Eqs. (3) and (9) if two approximations are made:

1. The functions $\Gamma(E)$ and $\Delta(E)$ are assumed to have a very weak energy dependence, so that $\Gamma(E) \approx \Gamma(E_0)$ and $\Delta(E) \approx \Delta(E_0)$, since the resonance occurs around E_0. Then the distribution of Eq. (3) is Lorentzian. Ab initio calculations of interaction matrix elements and of $g(E)$ for polyelectronic atomic resonance states were carried out for the first time in Mercouris and Nicolaides, 1997, 2002; Nicolaides, and Mercouris, 1996.
2. The lower limit of the integral in Eq. (9) is taken to be $-\infty$ instead of 0. A mathematical proof that $G(t)$ of Eq. (9) cannot decay exponentially if there is a lower bound, regardless of the form of $g(E)$, was given in Khalfin 1958, Nicolaides and Beck, 1978b.

The concept, which is also a measurable quantity, that is related to exponential decay (ED) is the lifetime, defined by $\tau = 1/\Gamma(\hbar = 1)$. However, as it was demonstrated from the numerical solution of the TDSE (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Mercouris, 1996), for certain states which were chosen because of their proximity to threshold, there is long-time deviation from ED after only a few exponential lifetimes. Therefore, a better definition of the lifetime is

$$\langle t \rangle = \bar{\tau} = \frac{\int_0 tP(t)dt}{\int_0 P(t)dt} \tag{34}$$

where $P(t)$ is the survival probability obtained by solving exactly the TDSE. Eq. (34) implies that $P(t)$ can also be interpreted as expressing the probability for a measurement to reveal that a length of time t has elapsed after the preparation of Ψ_0 at $t = 0$. Mercouris and Nicolaides (1997) demonstrated from ab initio calculations that in exceptional cases of atomic decaying states, $\langle t \rangle$ of Eq. (34) differs from τ.

Although $g(E)$ is a physically meaningful quantity, its presence in Eq. (9) does not reveal the subtleties of *time-asymmetry* that the quantum system follows. When the system is treated in terms of Eq. (6) and of the corresponding $g(E)$ and $G(t)$, (Eq. 9), unitarity is satisfied and the physics is time-symmetric. However, departure from the real axis and from Eq. (6), effected by imposing physically meaningful constraints, such as causality and appropriate boundary conditions, turns the physics into non Hermitian and non unitary. This happens when the concept of a decaying state is adopted implying the discontinuity at $t = 0$ on the solution of the TDSE. If we write for the time evolution operator $T(t) = e^{-iHt}$, then Hermitian quantum mechanics implies that its use is valid for $t > 0$ as well as for $t < 0$. This is equivalent to closing the contour over the cut of the continuous spectrum in both directions, counter clockwise (Goldberger and Watson, 1964; Nicolaides and Beck, 1978b). However, as the breakdown of the density g(E) into the two Green's functions (Eq. (21)) shows, when only the $t > 0$ (or only the $t < 0$) direction is required, only half of the contour over the sepctrum of stationary states must be considered, in conjunction with the fact that the continuous spectrum starts from $E = 0$. In this case, the energy distribution is given by only one of the Green's functions and is, therefore, complex. Correspondingly, using the property of the step function, $\theta(t) + \theta(-t) = 1$, $T(t)$ is split into two parts, T^+ and T^-, and the case of decay, where $t \geq 0$, is described rigorously by the TDSE for T^+, as

$$(i\partial_t - H)T^+(t) = i\delta(t) \tag{35}$$

Thus, the physics involving each of the dual spaces and each of the Green's functions representing mutually time-reversed states, leads to time-asymmetric evolution from the point $t = 0$. It is perhaps needless to add that these observations are in harmony with the previously analyzed solution of the resonance state problem under Fano boundary conditions (standing wave) and under traveling boundary conditions, as well as with the wave packet description connected to Eqs. (30)–(32).

In calculating the propagator $G(t)$, whether the real $g(E)$ is used or the complex Green's function $G^+(E)$, the decay is driven by the same pole, z_0. For both cases, the main result is exponential decay. However, the effect of time-asymmetry, as defined here, is revealed in the, as yet, undetectable long-time nonexponential decay (NED) part. This argument was made in Nicolaides and Beck, 1977, 1978b. Since then, a few related results have been published, and so I return to the issue.

For the sake of the argument it suffices to consider the approximation of the Lorentzian, namely that the energy dependence of $g(E)$ and of $G^+(E)$ is simple and so these functions are determined by choosing $\Gamma(E) \approx \Gamma(E_0)$ and $\Delta(E) \approx \Delta(E_0)$. Let us consider $g(E)$ first. When the limits of integration are put explicitly, Eq. (9) is written as

$$G(t) = \int_0^\infty dEg(E)e^{-iEt} \tag{36}$$

Assuming a Lorentzian distribution, this integral was first done by Khalfin (1958), in his discussion of NED. The same integral with a different distribution was discussed at the same time by Höhler (1958). Since then, a large number of publications have been devoted to this problem, having as common characteristic the assumption of a particular form for $g(E)$ and the production of analytical results concerning deviations from the law of exponential decay. In fact, the essential recognition of the breakdown of this law for long times was formally discussed for the first time in 1953 in the context of radiation damping by Hellund (1953) and by Namiki and Mugibayashi (1953).

The integral (36) using the approximation $\Gamma(E) \approx \Gamma(E_0)$ and $\Delta(E) \approx \Delta(E_0)$ was also done by Nicolaides and Beck by a different method (Eq. 8.54 of Nicolaides and Beck, 1978b- the misprint is corrected here). The object of that work was not just mathematical manipulations concerning the calculation of $G(t)$. Instead, it aimed at showing two things: First, that for NED to acquire significant magnitude, one has to look for special cases very close to threshold. Second, that not only the lower bound in the energy must be accounted for, but also the discontinuity at $t = 0$. The latter constraint implies the use of a complex energy distribution connected to only one pole. When the integral (36) is calculated, the lowest order long-time NED correction to $P(t)$, after the oscillating terms are eliminated, is (Nicolaides and Beck, 1978b)

$$P_{\mathrm{NED}}(\rightarrow \infty) \approx \frac{h^2\Gamma^2}{4\pi^2\left(E^2 + \frac{\Gamma^2}{4}\right)^2 t^2} \tag{37}$$

This result represents two cases, expressing an intrinsic symmetry in the physics of resonance states: Since $g(E)$ is real, the spectrum of H, as defined by Hermitian quantum mechanics, is enclosed, and two poles (the time-reversed states) contribute to $G(t)$. The same result is obtained if only one part of $g(E)$ is used, namely ${}^dG^+(E)$, and the integration is taken (unphysically) from $E = -\infty$ to $+\infty$ (Nicolaides and Beck, 1978b).

When the constraints $t = 0$ and $E = 0$ are imposed, then the following result is obtained (Nicolaides and Beck, 1977, 1978b).

$$G(t) = \frac{1}{2\pi i}\oint \frac{\exp(-izt)}{z - z_0}dz = \exp(-z_0 t)\left[1 - \frac{1}{2\pi i}E_1(-iz_0 t)\right] \tag{38}$$

where $E_1(x)$, is the exponential function. By taking the first term of the asymptotic form of $E_1(x)$, the result is

$$P_{\mathrm{NED}}(t \rightarrow \infty) \approx \frac{h^2}{\pi^2\left(E^2 + \frac{\Gamma^2}{4}\right)t^2} \tag{39}$$

Objections to this result were raised in Druger and Samuel (1984) and Sluis and Gislason (1991). However, these objections did not consider the fact of the imposed boundary conditions of $t \geq 0$ and $\infty > E > 0$, and therefore the contribution of both poles was included in the analysis of Druger and Samuel (1984) and Sluis and Gislason (1991). (The result of Sluis and Gislason (Gislason, 1991) is obtained from the Lorentzian with $0 < E < \infty$, and therefore it is Eq. (37)). In this respect, it is significant to observe that exactly the same result as Eq. (39) was later obtained by Holstein (Holstein, 1983) in his treatment of a realistic model of alpha particle decay using path integral techniques (Eq. 29 of Holstein, 1983), although his attention was not on the issues discussed here. In the path integral formulation, the direction $(x_1, t_1) \to (x_2, t_2)$, $t_2 > t_1$, comes in naturally, and therefore the corresponding $G(t)$ incorporates only the $t > 0$ contribution. For the path integral treatment of a general tunneling potential, see Douvropoulos and Nicolaides (2002).

Although the results (37) and (39) are specific to the simple pole approximation resulting from the approximation $A(z) \approx A(E_0)$, it is the fact that they are different that has value regarding the understanding of time-asymmetry at the microscopic level. If, in the future, it becomes possible to measure with great accuracy the NED of an isolated unstable state, for which accurate calculations of the same quantity could also exist within the two frameworks discussed in this paper, significant information as to the physical relevance of long-time NED should emerge. A proposal for an experiment in Atomic physics is presented in Mercouris and Nicolaides, 2002.

7. THE SOLUTION OF THE TDSE FROM FIRST PRINCIPLES, FOR ATOMIC RESONANCE STATES

Until the 1990s, the time-dependent problem of decaying states was treated by methods of analysis, via models, and via assumptions or definitions. In a series of papers, Mercouris and Nicolaides (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Mercouris, 1996) demonstrated how the time-evolution of polyelectronic non stationary states decaying into the continuous spectrum of free electrons can be calculated from first principles. By expanding the time-dependent wave function into very large sets of state-specific bound Ψ_n and scattering $U(\epsilon)$ (energy-normalized) wave functions, the TDSE is transformed into a system of coupled integrodifferential equations of the form

$$\begin{aligned} i\frac{d}{dt}\alpha_n(t) + i\int \frac{d}{dt}b(\epsilon, t)S_n(\epsilon)d\epsilon &= E_n\alpha_n(t) \\ &\quad + \int_0^\infty b(\epsilon, t)V_n(\epsilon)d\epsilon \quad n = 0, 1, \ldots, N \\ i\frac{d}{dt}b(\epsilon, t) + i\sum_{m=0}^{N}\frac{d}{dt}\alpha_m(t)S_m(\epsilon)d\epsilon & \\ &= (E_{\text{th}} + \epsilon)b(\epsilon, t) + \sum_{m=0}^{N}\alpha_m(t)V_m(\epsilon) \end{aligned} \tag{40}$$

The overlap, $S_n(\epsilon)$, and interaction, $V_n(\epsilon)$, matrix elements are given by

$$S_n(\epsilon) = \langle \Psi_n | U(\epsilon) \rangle, \quad V_n(\epsilon) = \langle \Psi_n | U(\epsilon) \rangle. \tag{41}$$

The integrals in Eq. (40) are performed by the trapezoidal rule and the solution for the coefficients is tested for convergence with respect to two parameters: The number of scattering states and the extent of the continuous spectrum. The time-dependent coefficients are advanced in time via the Taylor series expansion technique (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Mercouris, 1996) that has proven efficient in solving systems of tens of thousands of coupled equations, regardless of the number of electrons of the initial state.

The results of (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Mercouris, 1996) indicated that indeed there exist states close to threshold where long-time NED is enhanced. Furthermore, a variety of results for the $t \approx 0$ region were obtained and analyzed. The efficiency of other methods for solving the TDSE for such resonance states are discussed in those works (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Mercouris, 1996).

8. CONCLUSION

The conventional development of nonrelativistic quantum mechanics has been based on Hermitian formulations, involving stationary states and transition amplitudes. Both the time-independent and time-dependent formalisms constituting this framework require unitarity and time-reversibility as the parameter of time extends from $-\infty$ to ∞.

On the other hand, when a particular process evolves through an excited (unstable) state, this state must be thought of as a mixture of a localized wave function with some type of a purely continuous spectrum. For example, this occurs when excited states interact with the electromagnetic field and decay spontaneously, or when unstable states are mixed with states of the continuous spectrum of their own, field-free Hamiltonian, as do auto-detaching states of Atomic Physics. If the lifetime (Eq. 34) of the nonstationary state is much larger than the duration of excitation, the concept of a decaying state as a physical entity independent of the excitation mechanism becomes valid. Prerequisite to the formation of a decaying state, regardless of the formalism used for the determination of its properties, is the creation at $t = 0$ of a localized nonstationary wave packet, Ψ_0, inside the continuous spectrum. (Obviously, there must be cases where the borderline of the decoupling of the nonstationary state from the excitation dynamics is fuzzy.) For real polyelectronic systems, once this Ψ_0 has been computed it is possible to solve the time-dependent Schrödinger equation (TDSE) using state-specific wave functions (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Mercouris, 1996).

Decaying states give rise to resonance phenomena inside the continuous spectrum. A rigorous and computationally implementable approach to the description of such phenomena on the real axis is the theory of Fano (1961), which is based on time-independent Hermitian quantum mechanics and standing waves (i.e. real functions), expressing the mixing of Ψ_0 with the scattering states $\varphi(E)$. As regards ab initio calculations of observable quantities, these can be done in terms of well-defined matrix elements and the related basic quantity which is needed is the multichannel K-matrix. In fact, its proper use and the implementation of methods based on polyelectronic wave functions have provided a unified treatment of the discrete and the continuous spectrum.[6]

On the other hand, aspects of resonance phenomena can also be understood within a time-independent framework in terms of states represented by complex eigenfunctions of a complex eigenvalue Schrödinger equation (CESE). This equation and these eigenfunctions (Eq. (16)) were derived here and in (Nicolaides *et al.*, 1981; Nicolaides and Themelis, 1992), by considering the mixing of Ψ_0 with $\varphi(E)$ under boundary conditions either of outgoing or of incoming waves. Their explicit forms and the possibility of normalization by expressions such as Eqs. (26) and (27) have been used for the calculation of various types of field-free and field-dressed resonance states in terms of non Hermitian construction (Bylicki and Nicolaides, 2002; Haritos *et al.*, 2001; Mercouris *et al.*, 2001; Mercouris and Nicolaides, 1990, 2001; Nicolaides *et al.*, 1981, 1990; Nicolaides and Beck, 1977a,b, 1978a,b; Nicolaides and Gotsis, 1992; Nicolaides and Mercouris, 1985; Nicolaids and Themelis, 1992; Themelis and Nicolaides, 2000, 2001).

The dichotomy of one real-energy Schrödinger equation, with the boundary conditions of a standing wave with real energies and real wave functions, to two CESEs, one with outgoing and one with incoming wave as boundary conditions, is equivalent to the extraction of two complex eigenvalues and corresponding eigenvectors from the diagonalization of the non Hermitian matrix $H_0 + A(z)$, defined in Section 4. It also expresses the fact that the creation of the decaying state implies a singularity in the solution of the TDSE at $t = 0$. Only if both solutions, representing time-reversed states, are considered together, does one obtain results equivalent to the Hermitian treatment with real energy distribution functions, $g(E)$. If, however, one imposes the physical restriction of keeping only one solution corresponding to $t \geq 0$, i.e., the complex vector with the complex eigenvalue z_0, representing the decaying state, then the time-dependence at the microscopic level is driven by a complex energy distribution, namely by the Green's function

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[6] Even though in the discussions on resonance states the emphasis has been on S-matrix-type theories, the use of K-matrix type formalism, with its Hermitian structure, can have advantages. For example, for real multiparticle systems, such as the polyelectronic atoms, where scattering theory must be combined with the particularities of the many-body problem, it is possible to unite, formally and computationally, within the K-matrix formalism, properties of the discrete and of the continuous spectrum, using basis sets of bound and scattering functions. (Komninos *et al.*, 1995; Komninos and Nicolaides, 1987; Sinanis *et al.*, 1998).

${}^dG^+(E)$, whose main feature, upon analytic continuation through the cut, is the pole at z_0. This pole is the same as the one of the corresponding $g(E)$, and so there is no difference if the state is defined exclusively by its exponential decay. However, the contribution to the survival probability from the path along the imaginary axis is different in the two cases, leading to different long-time nonexponential decays, (Nicolaides and Beck, 1977, 1978b) and Eqs. (37) and (39). In other words, one of the arguments of this paper is that for time-asymmetry to be accounted for at the quantum level it is necessary to utilize complex functions. Furthermore, for isolated states, the difference between the mathematics of time-symmetric evolution and of time-asymmetric one is detectable in the regime of long-time NED, which is where the results using a real energy distribution differ from those of the corresponding complex distribution with the same pole. Such NED has its origin in the lower energy bound of the continuous spectrum and, therefore, becomes physically significant only in special cases, namely for unstable states that are very close to threshold (Mercouris and Nicolaides, 1997, 2002; Nicolaides and Beck, 1977, 1978b; Nicolaides and Mercouris, 1996).

I close by pointing out that the issues of complex functions and eigenvalues, time-asymmetry and microscopic irreversibility have been, and are being discussed by a number of researchers. For example, such discussions have been given in recent years by research groups at the Universities of Brussels, Belgium, and of Austin, USA. Characteristic review articles can be found in the 1997 volume edited by Prigogine and Rice (1997). Additional relevant articles in the same spirit are by Bohm and Gadella (1993) on mathematical aspects of Gamow states and on time asymmetric quantum mechanics - see also Bohm's book (Bohm, 1993) -, and by Antoniou and Tasaki with their coworkers (Antoniou *et al.*, 1997; Antoniou and Tasaki, 1993).

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