Atomic resonances above the total ionization energy*

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A rigorous result obtained using the theory associated with dilatation analytic potentials is that by performing a complex coordinate rotation, $r_j \rightarrow r_j e^{i\theta}$, on a Hamiltonian whose potential involves only pairwise Coulombic interactions, one can show that when $\theta = \pi/2$, no complex eigenvalues (resonances) appear whose energies have a real part greater than the total ionization energy of the atomic system. This appears to conflict with the experimental results of Walton, Peart, and Dolder, who find resonance behavior above the total ionization energy of the H^{--} system and also the theoretical stabilization results of Taylor and Thomas for the same system. A possible resolution of this apparent conflict is discussed and a calculation to check its validity is proposed.

Among others, Simon[1] has derived a very restrictive theorem concerning positive-energy resonances. This theorem appears to prohibit positive-energy resonances, indications of which have been observed in the H^{--} system experimentally by Walton, Peart, and Dolder[2] and Peart and Dolder[3] and theoretically by Taylor and Thomas[4] and Thomas.[5] We shall examine the theorem, propose a possible resolution to the apparent conflict, and then outline a calculation which can determine the validity of the proposed resolution.

The theorem states "Let H be the Hamiltonian of an N-body system with $V_{ij}(\vec{r}_{ij}) = C_{ij}/|\vec{r}_{ij}|$. Then H has no bound states of energy $E > 0$ and no positive-energy resonances, in the sense that for θ with $0 < \mathrm{Im}\,\theta < \pi/2$, $H(\theta)$ has no eigenvalues λ, where $-2\,\mathrm{Im}\,\theta < \arg\lambda < 0$." Here $E = 0$ is the energy at which the atom becomes totally ionized. θ is a parameter used to analytically continue the Hamiltonian by the replacement $\vec{r}_i \rightarrow \vec{r}_i e^{\theta}$. $H(\theta)$ is the Hamiltonian obtained by this analytic continuation. This analytic continuation procedure is similar to the complex coordinate rotation method.[6,7,8] The following statements can be made concerning the spectrum of $H(\theta)$:

The real eigenvalues and thresholds of $H(\theta)$ are the same as those of H. All complex eigenvalues (resonances) of $H(\theta)$ lie below the real axis. These complex eigenvalues can appear or disappear when a ray of the continuous spectrum crosses the eigenvalue location in the complex energy plane. When exposed (between crossings of rays of the continuous spectrum) the complex eigenvalue location is independent of θ. To illustrate these statements, Fig. 1 shows the location of some of the continuous and discrete spectra of $H(\theta)$ for the H^{--} system, consisting of a proton and three electrons for $\theta = \frac{1}{4}$ rad. What the theorem states is that there are no eigenvalues between the real axis and the ray emanating from the ionization threshold.

It is still possible that a complex eigenvalue (resonance) exists with $E > 0$. This eigenvalue would have to be exposed as one of the denumerable infinity of rays crosses it as $\mathrm{Im}\,\theta$ is increased. It would then be covered up as another ray crosses it. It is also possible that such an eigenvalue could cause the behavior noted experimentally and theoretically.

In order to check the validity of this possibility, it is proposed that a configuration-interaction calculation be carried out for the H^{--} system. If a sufficient number of appropriate basis functions are included, one of the eigenvalues of the Hamiltonian in the configuration-interaction basis set will be associated with a wave function which simulates the resonance. The Hamiltonian can be rotated by multiplying the kinetic energy by $e^{-2\theta}$ and the potential by $e^{-\theta}$. If the complex eigenvalue exists as proposed, the associated eigenvalue
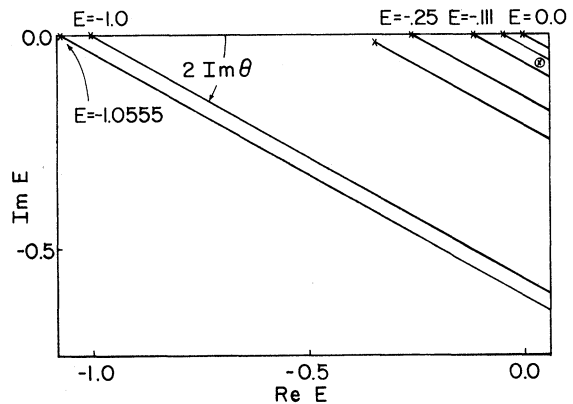

FIG. 1. Part of the spectra of $H(\theta)$ are indicated in the complex energy plane for the H^{--} system for $\mathrm{Im}\,\theta = \frac{1}{4}$ rad. The branch points on the real axis lie at the H^- binding energy and the infinity of H binding energies. Complex branch points occur at the resonant energies for the H^- system. A possible uncovered H^{--} resonance eigenvalue location is indicated by ⊗. The units are rydbergs.

should rotate away from the real axis along with the ray which will uncover it as $\text{Im}\,\theta$ is varied. When the eigenvalue reaches its uncovered location, it will remain stationary as $\text{Im}\,\theta$ is varied until the ray which covers it up crosses it. The eigenvalue will then attach itself to this ray and continue to follow it as $\text{Im}\,\theta$ is varied. Hence one would diagonalize $H(\theta)$ for several values of θ in the configuration-interaction basis. If one of the eigenvalue trajectories exhibits the characteristic behavior described above, then the theorem could be shown to be consistent with the experiment and stabilization calculation.

The above comments apply for a complete basis set. In practice, one must choose a finite basis set. Only if the basis set is capable of providing an adequate description of the resonance wave function can the above behavior be observed.

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