

# The theoretical study of singly and doubly resonances of photoionization of neon

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## Abstract

For the excitation of a subshell  $2s$  electron of Ne, we investigate the autoionizing spectrum of  $2s^2 2p^5 2P_{1/2} ns, nd$  and  $2s 2p^6 2S_{1/2} np$  Rydberg series by means of R-matrix theory and QB method. We predict the autoionizing energy and width of four Rydberg series.

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## 1. Introduction

With the advent of third-generation synchrotron radiation facilities and recent improvements in their resolution [1], it is now possible to study higher-order photoionization processes in greater experimental detail. Among these are two-electron processes, which require going beyond the single-electron picture and considering further the interaction between atomic electrons.

In a pioneering work of neon excitation, Codling et al. [2] measured the absorption spectrum at photon energies from 44 to 64 eV. Higher-resolution photoionization experiments in VUV energy range have been conducted for rare-gas atom [2–5]; a comprehensive review of many experimental aspects can be found in Ref. [1]. In 1996, Schula et al. reported the experimental and theoretical study of ground-state photoionization of neon in the photon energy range between 44 and 53 eV. In present Letter we use R-matrix theory and combine with the QB method to study the singly and doubly excited resonances

of neon, and predict the energy and autoionizing width of four Rydberg series of neon.

## 2. Theory

We use R-matrix theory [6] to determine the energy variation of the eigenphase analytically rather than numerically, and use QB [7] method to determine the resonance position and resonance widths for doubly excited states of neon.

R-matrix theory starts by partitioning configuration space into two regions by a sphere of radius  $a$  centred on the centre-of-mass and chosen in such a way as to effectively enclose the target electrons. When the colliding electron is within this sphere, a many-body Schrödinger equation must be solved. In the external region the system reduces to a two-body problem. The connection between these two regions is via the R-matrix.

In the internal region the total wavefunction  $\Psi(E)$  at energy  $E$  is expanded in terms of antisymmetrized energy-independent R-matrix basis states  $\psi_k$

$$\Psi(E) = \sum_k A_k(E) \psi_k, \quad r < a. \quad (1)$$

Let  $F_i(r)$  and  $w_{ik}(r)$  be the projections of  $\Psi$  and  $\psi$  respectively onto each channel. Substituting Eq. (1) into the Schrödinger

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equation and evaluating at the boundary  $r = a$  gives the basic equations of R-matrix theory,

$$A(E) = \varepsilon^{-1} w^T R^{-1} F, \quad (2)$$

$$R(E) = w \varepsilon^{-1} w^T + R_{\text{Buttle}}(E), \quad (3)$$

$$F(E, a) = R \dot{F}, \quad \dot{F} \equiv \left( \frac{d}{dr} - \frac{b}{a} \right) F \Big|_{r=a}, \quad (4)$$

where  $\varepsilon(E)$  is a diagonal matrix whose elements are  $(E_k - E)$ , and  $R_{\text{Buttle}}(E)$  is a diagonal matrix containing a correction [8]. The dimension  $R$  is  $n \times n$ , where  $n$  is the total number of channel retained in the clocoupling expansion. The matching equation on the boundary for the scattering electron radial function  $F$  is given by Eq. (4), where the logarithmic derivative  $b$  is fixed.

In the external region the total wavefunction is expanded in terms of the channel functions

$$\Psi(x_1 \cdots x_{N+1}) = \sum_i \bar{\Phi}_i(x_1 \cdots x_N; \hat{r}_{N+1} \sigma_{N+1}) \frac{1}{r_{N+1}} F_i(r_{N+1}), \quad r > a. \quad (5)$$

Substituting into the Schrödinger equation and projecting onto the channel yields a set of coupled differential equations satisfied by  $F_i(r)$ ,

$$\left( \frac{d^2}{dr^2} - \frac{l_i(l_i + 1)}{r^2} + \frac{2z}{r^2} + k_i^2 \right) F_i(r) = \sum_{j=1}^n V_{ij}(r) F_j(r), \quad (6)$$

where  $z = Z - N$  is the residual target charge,  $l_i$  and  $k_i^2$  are the channel angular momenta and energies, and  $V_{ij}(r)$  is the potential matrix. In the external region, there are two independent sets of solutions,  $S(E, r)$  and  $C(E, r)$ , with known asymptotic forms for  $r \rightarrow \infty$ . Quantities such as reactance ( $K$ ) and scattering matrices are obtained on matching the internal region radial functions  $F$  to  $n \times n_0$  linear combinations of the external region radial functions  $S(E, r)$  and  $C(E, r)$ , for  $n_0$  open channels

$$F(E, r) = S(E, r) + C(E, r)K(E). \quad (7)$$

Differentiating and evaluating at  $r = a$  and substituting into Eq. (4) gives

$$B(E)K(E) = P(E) \Rightarrow K(E) = B^{-1}(E)P(E), \quad (8)$$

where

$$B = +C - R\dot{C}, \quad P = -S + R\dot{S}. \quad (9)$$

Diagonalizing the  $K$ -matrix in the space of the open channels  $n_0$ , i.e. let  $K_{00}$  has eigenvalues  $\lambda_i$ , then

$$K_{00}X = \lambda X, \quad \text{where } X^T X = 1, \quad (10)$$

and  $\lambda$  is diagonal. The eigenphase in each channel is then defined as

$$\delta_i = \tan^{-1} \lambda_i, \quad i = 1, n_0, \quad (11)$$

and the eigenphase sum  $\delta$  is the sum over Eq. (11). The above argument concerning a pole in  $K$  also applies to  $\lambda$ , and so one normally fits the eigenphase to a Breit and Wigner [9] form, as

in Tennyson and Noble [10]

$$\delta = \bar{\delta} + \tan^{-1} \frac{\Gamma/2}{E_r - E}, \quad (12)$$

where  $E_r$  is the resonance energy,  $\Gamma$  is the resonance width and  $\bar{\delta}$  is the background.

A resonance position is the energy at which the eigenphase sum increases most rapidly, i.e. has maximum gradient  $d\delta/dE \equiv \delta'$

$$\delta'(E) = \left[ 1 + \left( \frac{E_r - E}{\Gamma/2} \right)^2 \right]^{-1} \frac{1}{\Gamma/2} \quad (13)$$

and this is used by QB method to locate resonances.

Resonance widths  $\Gamma$  are related to the inverse of the eigenphase derivate at resonance, as can be seen by differentiating Eq. (12) and assuming the background gradient  $\bar{\delta}' < \Gamma^{-1}$  and setting  $E = E_r$

$$\Gamma = 2/\delta'(E_r). \quad (14)$$

Generalizing to the multichannel case (channel  $i$ ), the normalized widths  $\Gamma_i$ , which are related to the autoionization decay rates to each open channel, are

$$\Gamma_i = \frac{\Gamma/\delta'_i}{\sum_{i=1}^{n_0} 1/\delta'_i}. \quad (15)$$

Because Eq. (12) is valid strictly for isolated resonances, we should estimate the perturbation of the width by a nearby resonance. This can be done by introducing a nonconstant background  $\bar{\delta}$ , whose main variation over the width of a resonance at  $E_r$  is due to the ‘tail’ of some perturbing resonance at  $E_p$  of width  $\Gamma_p$  of the form Eq. (13), so that at  $E = E_r$

$$\bar{\delta}'(E_r) = \left[ 1 + \left( \frac{E_p - E_r}{\Gamma_p/2} \right)^2 \right]^{-1} \frac{1}{\Gamma_p/2}. \quad (16)$$

Differentiating Eq. (12) and evaluating at  $E = E_r$

$$\delta'(E_r) = \bar{\delta}'(E_r) + 2/\Gamma \Rightarrow \Gamma = 2/[\delta'(E_r) - \bar{\delta}'(E_r)]. \quad (17)$$

### 3. Resonances in Ne above the first threshold

According to the R-matrix theory and the energy region between 44 and 48.5 eV is dominated by singly excited resonances  $2s2p^6np$ , which are weakly perturbed by the  $n = 3, 4$ , and 5 members of the first doubly excited Rydberg series  $2p^4(1D)3s(2D)np$  [11], the elastic and inelastic scattering of electrons by the three lowest fine-structure levels of the ion  $\text{Ne}^+$  are

$$\text{Ne}^+(1s^22s^22p^5)^2P_{3/2}^0, \quad \text{Ne}^+(1s^22s^22p^5)^2P_{1/2}^0, \\ \text{Ne}^+(1s^22s2p^6)^2S_{1/2}^e,$$

where the total system of electron plus  $\text{Ne}^+$  ion is in the  $0^e$  or  $1^0$  states. The photoionization process corresponds to photoionization from the ground state of Ne leaving the  $\text{Ne}^+$  ion in one

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