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# Derivation of The Laser Gain Profile Equation by The Quantum Mechanics' Approach

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## Abstract

*An exact equation of atomic resonance has been derived and modified by the quantum mechanics' approach. Exact solution of this equation is given. It produces a complex line shape with asymmetric, skewed, shifted, and broadened characteristics. This exact equation of atomic resonance is compared with the standard model of the Lorentzian-Voigt equation (See Figures 1 to 4.). This exact equation is essential in many areas of study.*

**Keywords:** Laser Gain, Quantum Mechanics' Approach, Exact Solution, Emission-laser

## 1. Introduction

An equation for atomic resonance was derived using a quantum-mechanical approach and is proposed here. The complex refractive index is a function of the complex error function. (It's the complex conjugate of the complex error function, to be exact.) Lorentzian Line shapes (1) and the Voigt profile (1) did not change over time. Modern concepts, such as energy levels and population inversion, are necessary for the derivation. Schrödinger's equations had been used twice. The advantage of quantum mechanics' approach is that it is uniquely capable of explaining laser emission. There are no other ways, nor classical Lorentzian equations.

The atomic resonance equation can be derived using a quantum-mechanical approach. The complex refractive index is also a function of the complex conjugate of the complex error function, with each variable defined quantum-mechanically. This equation is modified here, and its derivation is presented below. Last but not least, the solution of this atomic resonance equation by the quantum mechanics' approach is given along with the solution of the complex error function, which is a convolution integral.

The derivation, whether using a classical or quantum mechanics' approach, involves three steps (1). Get the polarizability equation, (2). Link the complex index of refraction to the polarizability, and (3). Incorporate the Doppler effect into the equation.

An external electric field is considered a small perturbation to the system's Hamiltonian. Accurate wave functions for the ground and excited states of the system are required to calculate polarizability.

The perturbation theory was used to solve the time-independent Schrödinger's equations for the perturbed wave function $\psi'$, (2), $\psi_m'$- $\psi_m$ *is small,where* $\psi_m$ *is the unperturbed wavefunction*. Then the integral of the perturbed wave function, ex, and the complex conjugate of the perturbed wave function $\psi'^*$ gives induced dipole moment, $p_i$, then electronic polarizability, $\alpha$,(2-4).

$$p_i = \int_{-\infty}^{\infty} \psi' ex \psi'^* d\tau$$

Where $x$ is the induced displacement due to the external electric field.

$$\alpha = \frac{e^2/m}{\omega_r{}^2 - \omega^2 + i\omega\gamma_r}$$

The classical model for obtaining polarizability is straightforward. It's based on Newton's law and the force balance of an atom's electronic harmonic oscillator. The quantum-mechanical approach, which involves solving Schrödinger's equation, is based on the energy balance of a quantum harmonic oscillator. Both methods, originating from either solving Schrödinger's equations or solving Newton-Lorentz's formula, are equivalent, and the equations derived for atomic resonance are almost identical. The difference is that all variables are defined quantum-mechanically in the quantum-mechanical approach.

Maxwell's equations and some constitutive relations were used to link the complex index of refraction with electronic polarizability. It is the Lorenz-Lorentz theory of electronic dispersion. This equation is also known as the Clausius-Mossotti equation. It is the second step of derivation.

The equation of atomic resonance line shape for stationary atoms is therefore given, either by the classical approach or the quantum mechanics' approach:

$$\frac{\tilde{n}^2-1}{\tilde{n}^2+2}=\frac{Ne^2}{3\varepsilon_0 m}\sum_r \frac{f_r}{{\omega_r}^2-\omega^2+i\omega\gamma_r} \qquad (1)$$

The third step of the derivation involves incorporating the Doppler effect for atoms in a crystalline structure within a quantum-mechanical framework.

The general momentum distribution applies to solid-state systems, specifically crystal media, because the Maxwellian distribution of Brownian motion is not a valid mathematical model. This general momentum distribution can be modified for various cases, including laser-cooled atoms.

Atoms in a fluid or a crystal (3) are executing harmonic oscillations about certain equilibrium positions. The Fourier Transform of the position-space wavefunction($\psi(x,t)$) is calculated, and the resulting wavefunction is the momentum-space wavefunction($\psi(p,t)$). The squared modulus of the momentum-space wavefunction $|\psi_m(p,t)|^2$ is the quantum probability distribution for the momenta $p$, at time $t$, of an oscillator in the $m^{th}$ state, and the distribution $\eta_p$ is the probability of finding the oscillator in the $m^{th}$ state. Multiplying ${\psi_m}^2$ *by the* $\eta_p$, and then summing over all possible states, the required momentum distribution $d\eta_p$ is given, after normalization, in SI units:(given by F. Bloch (5,6), (1932))

$$d\eta_p=(\xi/2\pi kMT)^{1/2}[exp(-\xi p^2/2kMT)]dp \qquad (2)$$

$$where\ \xi=\left(\frac{2kT}{h\nu_a}\right)tanh\left(\frac{h\nu_a}{2kT}\right)=\left(\frac{2T}{T_E}\right)tanh\left(\frac{T_E}{2T}\right)$$

*M,* $\nu_a$ *= mass and oscillation frequency of an atom,*
*h,k = Planck' s and Boltzmann's constants,*
$T_E$ *= Debye or Einstein temperature =* $\frac{h\nu_a}{k}$

*T = Temperature of the dielectric crystal,or liquid.*

Three dimensionless parameters,
$u_r$, $y_r$, *and* $a_r$, *now modified based on Voigt' s parameters are introduced:*

Let

$$u_r=\frac{2(\xi ln2)^{1/2}[\nu-\nu_{u(r)l}]}{\gamma_D}$$

$$y_r=2(\xi ln2)^{1/2}[\nu^*-\nu_{u(r)l}]/\gamma_D$$

$$a_r=(\xi ln2)^{1/2}\gamma_L/\gamma_D$$

$$where\ \nu=frequency\ of\ electronic\ oscillation,$$

$$\nu_{u(r)l}=transition\ frequency,$$

*The quantity v*=resonant frequency with respect to a moving atom, and is used to replace* $\nu_o$ *the resonant frequency for stationary atom resonant frequency,*
*The quantities* $\gamma_L$, $\gamma_D$, $\gamma_c$, *and* $\gamma_n$ *are the Lorentzian,Doppler,collision and natural widths,respectively.*

The atomic resonance equation, derived by the quantum mechanics' approach, under the condition of the quantum Doppler effect, is modified in this form:

$$\frac{\tilde{n}^2-1}{\tilde{n}^2+2}=-i\sum_r C_r\,\bar{W}_r \qquad (3)$$

*where the subscript r =* 2, *and r=* 1, are for doublets. (such as for sodium atoms' *D*2 *and D*1 *lines*)

$$\tilde{n}=n-i\kappa$$

Where *n* = the index of refraction, $\kappa$ *= an extinction coefficient.* The negative extinction coefficient is the emission coefficient.

$\bar{W}_r$ *= complex conjugate of complex error function*

$$\bar{W}_r=\frac{a_r}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y_r^2}}{(u_r-y_r)^2+(a_r)^2}\,dy_r-\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{(u_r-y_r)\,e^{-y_r^2}}{(u_r-y_r)^2+(a_r)^2}\,dy_r$$

$$C_r=\frac{\pi^{1/2}N_l e^2 f_r a_r}{12\pi^2 m^*\epsilon_0\gamma_L\nu_{u(r)l}}\left[1-\frac{N_{u(r)}g_l}{N_l g_{u(r)}}\right]$$

*The first term in* $\bar{W}_r$ *is the real part of the complex error function, and the second term in* $\bar{W}_r$

is the imaginary part of the complex error function.

Where *m* = reduced mass of electron in atom,*

$f_r$ *= the fraction of all oscillators having the resonant frequency* $\nu_{u(r)l}$,

g = statistical weight
where the subscript u = upper energy level, and the subscript l = lower energy level.

For atoms, either in a gaseous state, a liquid, or a solid state, their interaction forces are considered; their momentum distribution is given by (6), (pages 98 to 104, L.D. Landau and E.M. Lifshitz)

Let $\xi$ = 1, *equation* (2) *becomes a Maxwellian momentum distribution, and*

T is replaced by $T_{eff}$, Effective temperature:

$$T_{eff} = T + \frac{\hbar^2}{12(kT)^2 m_i}\overline{\left(\frac{\delta U}{\delta q_l}\right)^2}$$

Where $\overline{\left(\frac{\delta U}{\delta q_l}\right)^2}$ = *mean squares of the interaction forces,* $\frac{\delta U}{\delta q}$, *acting on the atoms.*

Either the quantity ξ or T,is a key factor to incorporate the quantum

Doppler effect into equation (3).
*The quantity ξ or T also affects the width and amplitude of the laser gain profile.*
(See Conclusions— "light squeezing" and "sensitivity".).

For laser-cooled atoms, as the temperature decreases, the momentum distribution approaches and becomes a delta function, and equation (1) is recovered.

The quantum Doppler broadening is negligibly small; therefore, equation (3) is reduced to the Lorentzian form, where atoms are stationary.

A brief discussion of the slight Doppler shift, the Lorentzian term, and the delta function was given by A. E. Siegman (7) (1971)

$$\int_{-\infty}^{\infty} dx\delta(x-a)f(x) = f(a)$$

*Where δ(x-a) is a Dirac delta function.*

*Equation (3)and it's exact solution, inevitably contains two intrinsic relations between*
*n and κ.Let the right hand side of equation (3) be represented by a complex number:*
*b–id,*

$$where\ b = -C_{r1}W_{img1} - C_{r2}W_{img2}$$

$$d = C_{r1}W_{real1} + C_{r2}W_{real2}$$

The result of algebraic development gave a pair of *n and κ new relationship*:

$$n^2 - \kappa^2 + \frac{4}{j_3}n\kappa - 1 = 0 \qquad (4)\ \text{(real part of equation (3))}$$

$$n^2 - \kappa^2 - j_3 n\kappa + 2 = 0 \qquad (5)\ \text{(imaginary part of equation (3))}$$

*Let equation* (5) − (4),

$$n\kappa = \frac{3}{j_3 + \frac{4}{j_3}} \qquad (6)$$

Where $j_3 = \frac{2(1-b)}{d}$

Substitute the expression κ of (6)into (5),and compare it to standard quadratic

$$equation: A(n^2)^2 + Bn^2 + C = 0$$

Where A = 1, B = $j_4$, C=$\frac{-9}{\left(j_3+\frac{4}{j_3}\right)^2}$

$$j_5 = (B^2 - 4AC)^{1/2}$$

$$j_4 = \frac{3(1-b)}{d^2 + (1-b)^2}$$

$$j_5 = \left\{j_4{}^2 + \frac{9d^2}{[d^2+(1-b)^2]^2}\right\}^{1/2} = \left\{\frac{9}{d^2+(1-b)^2}\right\}^{1/2}$$

*Equations (4)and (5) are equations of two hyperbolas of oblique axis.*
*Their locus intersections give a set of solutions of n and κ:*
*That is,solve n and κ from equations (4)and (6);or (5)and (6).*

*Solve (5) and (6):*

$n^2 = \frac{-B \pm (B^2-4AC)^{1/2}}{2A}$ Similarly, solve for $\kappa^2$, and therefore,

$$\kappa = [(j_5 + j_4)/2]^{1/2}$$

$$n = [(j_5 - j_4)/2]^{1/2}$$

$n^2 + \kappa^2 = f(j_3) = j_5$ (7) (a circle)
*From (4) and (6),another set of n and κ can be solved similarly.*

*Substitute κ of* (6) *into equation* (4), *and solve* $n^2$ from "quadratic equation."
*Same procedure for solving* $\kappa^2$ by substituting n of (6) into equation (4).

## 2. Conclusions

The rational approximation for the calculation of the complex error function, a convolution integral, given by Hui, Armstrong, and Wray (8-9), was used. It involves only two arithmetic statements.

*Equation (3) has been progrommed and gives a laser gain profile*
*and it' s full width at half maximum.*

(-κ = *emission index*.) The program has been modified and used for simulation. The full width at half maximum (FWHM)

can be reduced, and its amplitude increased for different ξ and $T$. Therefore, the "light squeezing" can be achieved.

The sensitivity (10) of the Laser Interferometer Gravitational-wave Observatory (LIGO) can be enhanced by increasing the amplitude of the laser gain profile.

Equation (3) yields an exact complex line shape characterized by an asymmetric, skewed, shifted, and broadened nature. These complex line shapes were shown in Figures 1 to 4. Figures 1 and 2 gave the absorption profile and its corresponding positive dispersion. Figures 3 and 4 gave the gain profile and its corresponding negative dispersion. Series 1, in blue, was calculated from Equation (3), the exact formulation and solution. Series 2, the orange color, was calculated using the standard model equations for comparison. The line of symmetry for the standard model is at 5889.963 Armstrong (number 6 data from 5889.958 A in Figure 1). This line is the sodium D2 resonant line.

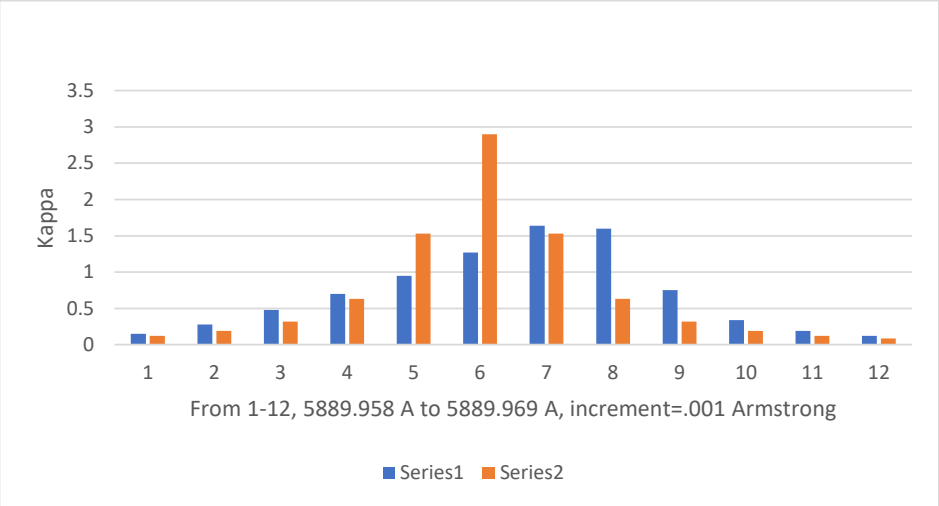


**Figure 1: Kappa, index of Absorption**

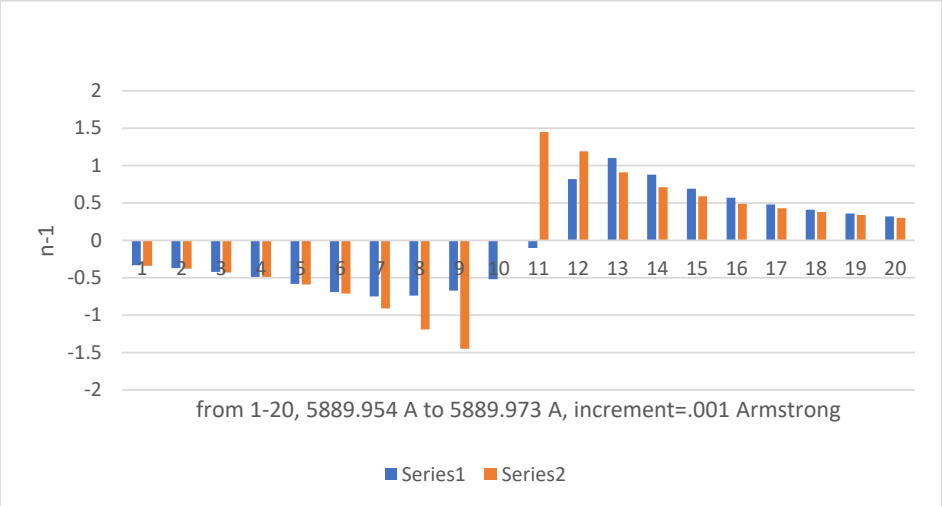


**Figure 2: Index of Refraction, n-1**

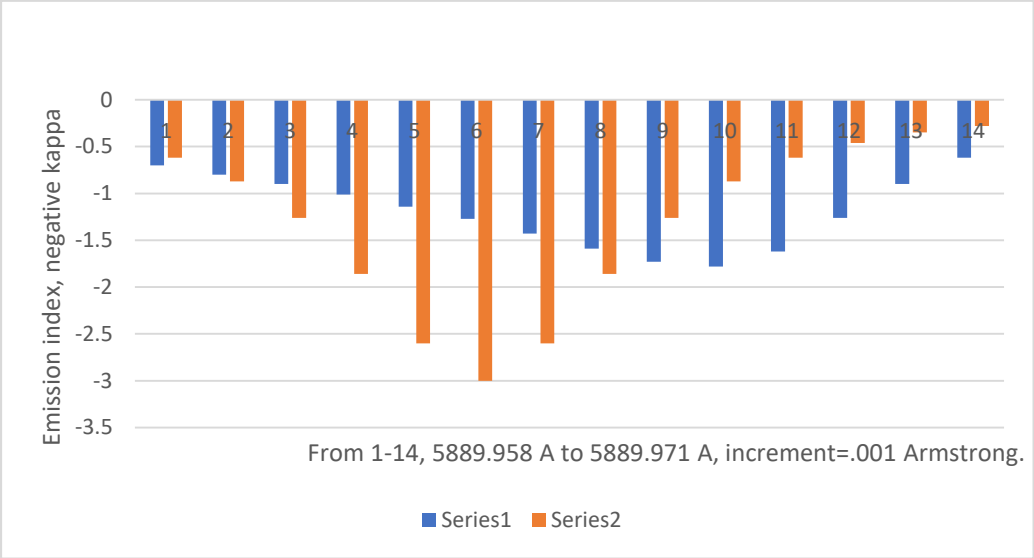


**Figure 3: Gain Profile**

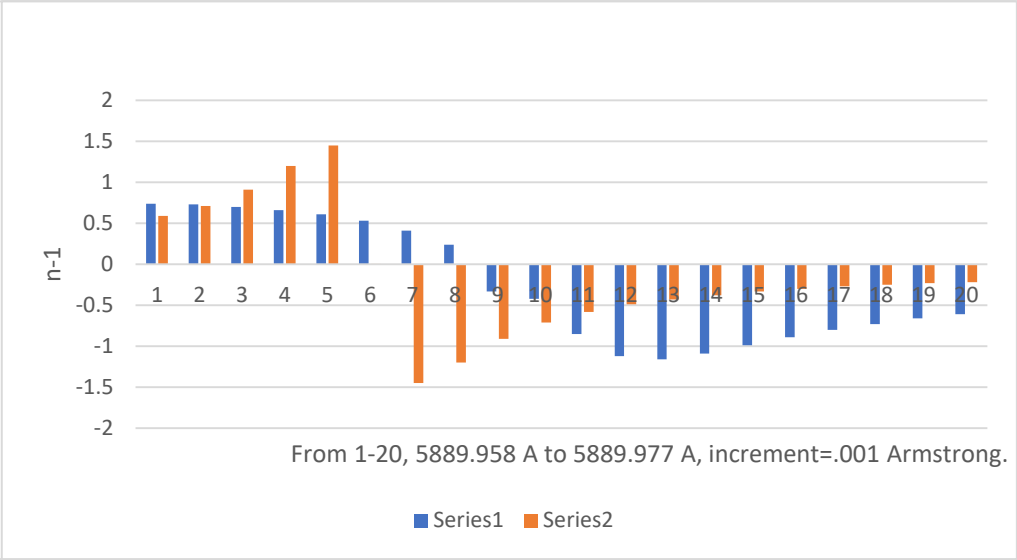


**Figure 4: Negative Dispersion (gain profile)**

From equation (1),

$$\frac{\tilde{n}^2-1}{\tilde{n}^2+2} \cong \frac{2}{3}(\tilde{n}-1) = \frac{2}{3}(n-1-i\kappa)$$

*The left hand side of equation* (1) *had been linearized because*

For gas, n is very close to one, and the extinction index kappa, *κ,is two orders of magnitude less than n,for the resonant wing region.*

Therefore, it had been set $\tilde{n}^2 + 2 = 3$, and $\tilde{n} + 1 = 2$.

The linearization of the left-hand side of equation (1) is the cause of the standard model's symmetric, non-skewness, and non-shifted characteristic line shapes. The exact formulation and exact solution preserved the asymmetric, skewed, shifted, and broadened character of the atomic complex line shapes. Because it is a non-linear equation. After the linearization, equation (1) became a standard model equation by introducing Voigt's parameters.

Two mistakes this approximation made: first, the equation was derived for the resonant core region, whereas the linearization assumed wing-region conditions. Second,
It was clearly illogical to make $\tilde{n}$ = 1, and meanwhile, define $\tilde{n}$ as a complex number. $\tilde{n}$ *is a complex number,at the formulation and solution.*

The derived formula (equation (3)) is unique and follows a quantum-mechanical approach. The wave function of the Schrödinger's equation has been used in the derivations of polarizability and Doppler momentum distributions, and these derivations were well reasoned.

Equation (3) is essential in many areas of study, including

atomic spectroscopy, atomic absorption and emission (using lasers), and enhanced flow visualization (1).

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**Disclosures**
The author declares no conflicts of interest.

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