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# Numerical Modeling of the Finite Well with Implications for Observing Quantum Interference Between Coherent Electron Wave Packets

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**Abstract:** We use numerical modeling in Fortran to investigate the claims of Wollenhaupt et al. (2006) and Hommelhoff et al. (2002) regarding ultra-short electron pulses ionized via laser excitation of a tungsten nanotip. We assume that the nanotip acts as a finite one-dimensional potential well with the depth equal to the work function of tungsten and the width of the order of the radius of curvature of the nanotip. The interactions of propagating Gaussian wave packets are modeled in order to give insight into the temporal and spatial evolution of the generated electron wave packets. Furthermore we hope to demonstrate the transference of the temporal coherence of the light pulse to the free electron wave packets generated.

## 1. Introduction

Ultra-short laser pulses have been developed to provide insight into the quantum world of nanostructures and electrons. These pulses are capable of providing time-resolved imaging of matter by observing the interference pattern of the waves with the matter itself. By studying the interference patterns, an ultrahigh sensitivity can be obtained when compared to previous methods. According to Wollenhaupt et al. [1] "a pair of ultra-short laser pulses can be used to generate wave packet interferences in bound states of an atomic or molecular system." However, they extend the technique to the theoretical generation of free electron wave packets. In order to provide accurate experimental values, we follow the conventions of Hommelhoff et al. [2] which use an 8 fs laser pulse to emit electrons from a sharp field emission tip. Electron emission is assumed to be set by the laser period and is therefore much shorter than the laser pulse itself. The electron wave packets can then be used as a source of optical accelerators, new interferometers, ultrafast electron microscopy or even to probe the exciting laser electric field [2]. Upon generation of the wave packets, the interference pattern of the waves can be observed to test whether or not the wave packets are coherent. If the two wave packets are coherent their probability amplitudes rather than probabilities add together. In order to numerically model this phenomenon, we created the program Laserfield in Fortran which uses the Numerov algorithm in order to solve the boundary value conditions of the Schrödinger equation.

# 2. Methods

## 2.1 General Approach

We begin by first considering the tungsten nanotip to act as a finite well with the depth determined by the work function of tungsten or 0.1587570143 Hartree (Atmoic units were used in order to decrease rounding errors in Fortran, note one Hartree=27.211 eV). The width of the well was set equal to the average radius of curvature of a tungsten nanotip or 1511.780791 Bohr radii (160 nm) [3]. The numerical model should hopefully mimic the conditions required for the excitation of an electron from a nanotip in the real world.

## 2.2 Analytical Solution

The accepted eigenvalues for a given well of width 2α and depth Vo (Figure 1) can be calculated by a combination of analytical and numerical or graphical methods. Ψ(x) is considered to be composed of three different regions; exponential growth to the left of the well, cosines and sines inside the well, and exponential decay to the right of the well. Eigenvalues of energy are obtained when these three equations and their derivatives are matched at the boundaries of the well. With some substitution and manipulation a transcendental equation in E can be solved to find the eigenvalue. This approach was undertaken in Maple 15 to generate the accepted eigenvalues.

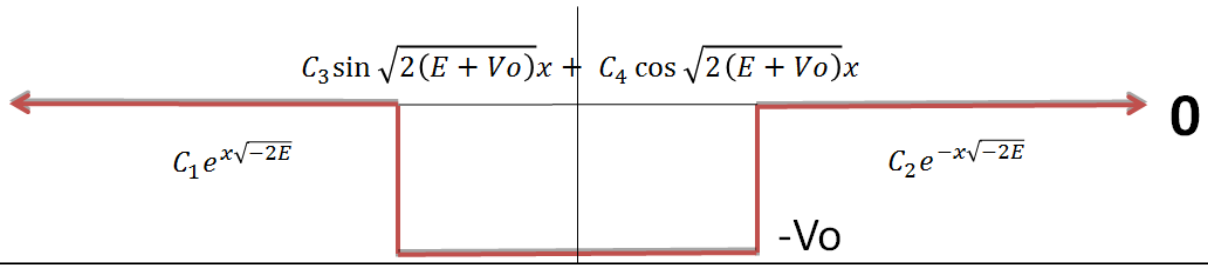


Figure 1: Schematic of the finite well with width 2α and depth Vo. Each regions equation is also shown above or below the given region with C corresponding to a given constant and E the energy.

The transcendental equations to be solved are:

$$\sqrt{2(E+Vo)}\tan\sqrt{2(E+Vo)}\alpha = \sqrt{2E} \quad Even\ Solutions \qquad (1)$$

$$\sqrt{2(E+Vo)}\cot\sqrt{2(E+Vo)}\alpha = -\sqrt{-2E} \quad Odd\ Solutions \qquad (2)$$

## 2.3 Numerov Method

The program Laserfield is the Fortran program created in order to calculate the time-independent starting point for the Schrödinger equation. The Numerov method is well suited for solving boundary value problems of second-order, linear differential equations lacking a first derivative. The algorithm can be used to numerically solve for the energy and wave function of the one dimensional Schrödinger equation, where V(x) is the potential at X and ε is the energy.

$$\frac{d^2}{dx^2}\Psi(X) - 2(V(x)-\varepsilon)\Psi(X) = 0 \qquad (3)$$

In order to apply a numerical approach to the Schrödinger equation the interval over which the equation is to be solved is divided into equally spaced steps of length H. It can be shown through discretization, Taylor expansion and difference formulas that Equation 3 can be equated to a 3-point recursive form (where Q =V(x)+E and n is a given step) [4]:

$$\psi_{n+1} = \frac{2\left(1-\frac{5H^2}{12}Q_n\right)\psi_n - \left(1+\frac{H^2}{12}Q_{n-1}\right)\psi_{n-1}}{\left(1+\frac{H^2}{12}Q_{n+1}\right)} \qquad (4)$$

$$\psi_{n-1} = \frac{2\left(1-\frac{5H^2}{12}Q_n\right)\psi_n - \left(1+\frac{H^2}{12}Q_{n+1}\right)\psi_{n+1}}{\left(1+\frac{H^2}{12}Q_{n-1}\right)} \qquad (5)$$

This is the effective Numerov algorithm which can be used to generate a wave function by finding the value of subsequent steps by using two previous steps. The Equation 4 is used to step toward x=0 from x=-∞ and the Equation 5 steps from x=∞ to x=0. Two values that are close to zero are required at each end to give initial values of the first two steps, which should correspond to the exponential decay to zero, without causing rounding errors in Fortran. The parity of the state must also be supplied in order to account for one starting negative. The wave function is accurate when the two equations and their derivatives are continuous and equal at x=0. An intial guess for the energy is applied that is only slightly greater then the bottom of the well. The algorithm is then run to produce the wavefuntion with the derivative being numerically calculated by a 3-point difference formula. If the two derivatives are equal at X=0 for the given energy, the wavefunction Ψ(x) is recorded. If not the energy is then varied until the two equations have the same value and derivative at x=0. This is accomplished by the Bisection method. The energy value which correspond to a match between the derivative Equation 4 and Equation 5 should correspond to d(Eq4)-D(Eq5) and would be zero when they are equal. If there is a low value for the energy ($E_{MIN}$) and a high value ($E_{MAX}$) such that there exist one root between the two, one will return a positive value and the other a negative. Therefore, an energy half-way between the two values ($E_{STEP}$) can also be evaluated. If the value $E_{STEP}$ will then replace the energy with the same sign and the bisection will repeat until it returns a value satisfactoryly close to 0. $E_{STEP}$ can then be recorded as the Eigenvalue of Energy and the wave function will be numerically normalized and recorded as Ψ(x).

## 2.4 Wave Packet Interference

In order to get a better understanding of interference pattern to expect from the completed program, preliminary work was done in Maple to determine the characteristic time period and length over which the electron wave packets will interfere. The two electron wave packets are assumed to be similar Gaussians, as defined by Equation 6.

$$e^{i(k_0 x-\omega_0(t-\tau))}\sqrt{\frac{\pi}{\eta+i\beta(t-\tau)}}\,e^{-\frac{\left(x-Vg(t-\tau)\right)^2}{4\eta+4i\beta(t-\tau)}} \qquad (6)$$

Where Ko=the energy (3.68Hartree), τ is the pulse time, ωo is the frequency, η is a measure of the peakedness given by $\frac{\sqrt{2}}{HWHM}$ (Half Width at Half Maximum),β= $\frac{d^2\omega o}{dko^2}$=1/2, and Vg is the group velocity. As each Gaussian propagates its peak height decreases and its width increases. As the wave packets spread the two begin to interfere causing an interference pattern that occurs both spatially and temporally. The presence of such interference indicates the coherence of the electrons. The graphs produced in Figure 7 are the ultimate goal of the Laserfield program which will show the entire evolution from the bound state to the free state.

## 3. Results

The eigenvalues found using the analytical method in Maple 15 are compared to the experimental value determined by the program Laserfield for the first four states in Table1. As evidenced by the table, the two values are in close agreement in each state with only a slight discrepancy, which corresponds to a percent error of less than one hundredth of a percent. The wave function Ψ(X) of each state is presented in Figures 2-5 and show the oscillatory and exponential behavior as would be expected from analytical approaches. Additionally, an image of the exponential tail of the wave function is shown to indicate the behavior of the wave function outside the well which was not clear in the full scale images.

| State | Numerical | Analytical | Difference |
|---|---|---|---|
| Ground State | -0.1587505902 | -0.1587564758 | 5.8856E-6 |
| First Excited | -0.1587313120 | -0.1587376271 | 6.3151E-6 |
| Second Excited | -0.1586991806 | -0.1586918517 | 7.3289E-6 |
| Third Excited | -0.1586541940 | -0.1586514617 | 2.7323E-6 |

Table 1-Comparisons of the Numerical result found using Laserfield and the analytical solutions found using Maple. Also included is the difference between the two. The percent error was less than one hundredth of a percent for all states showing the values are in close agreement.

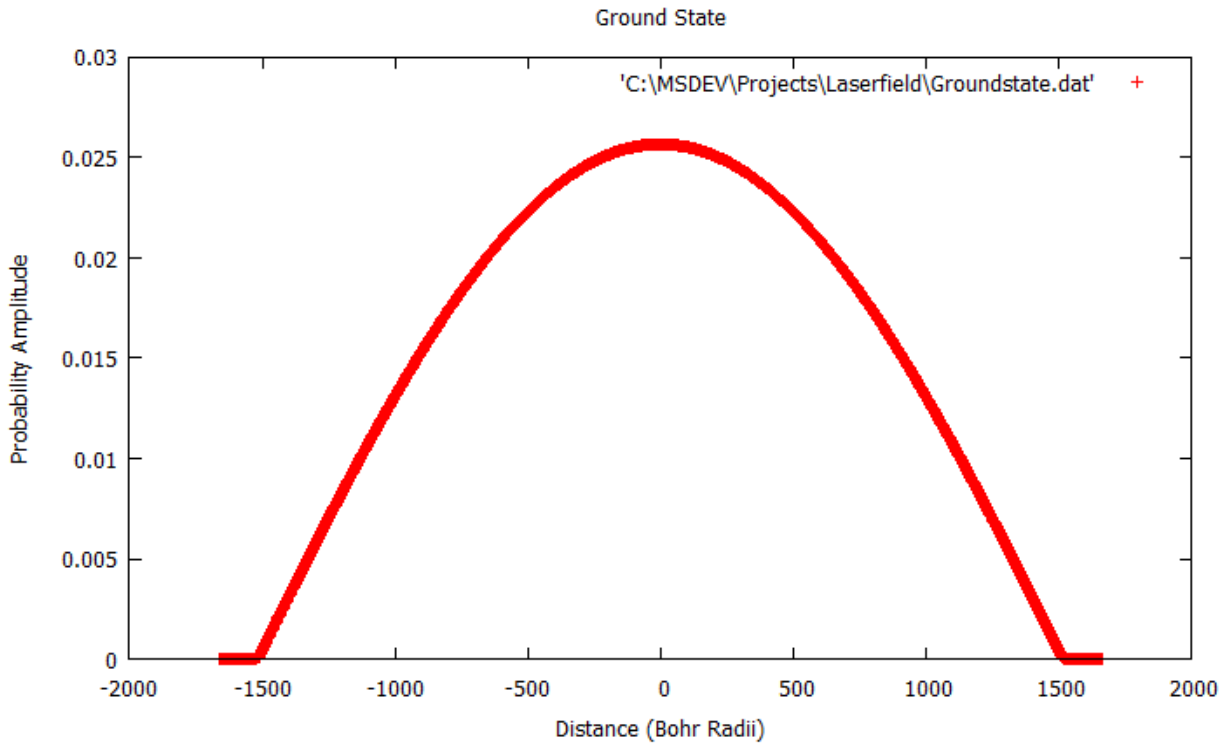


Figure 2-Normalized Ground state of Ψ(x), with X measured in Bohr Radii. The half width of the well is given to be 1511.780791 Bohr radii

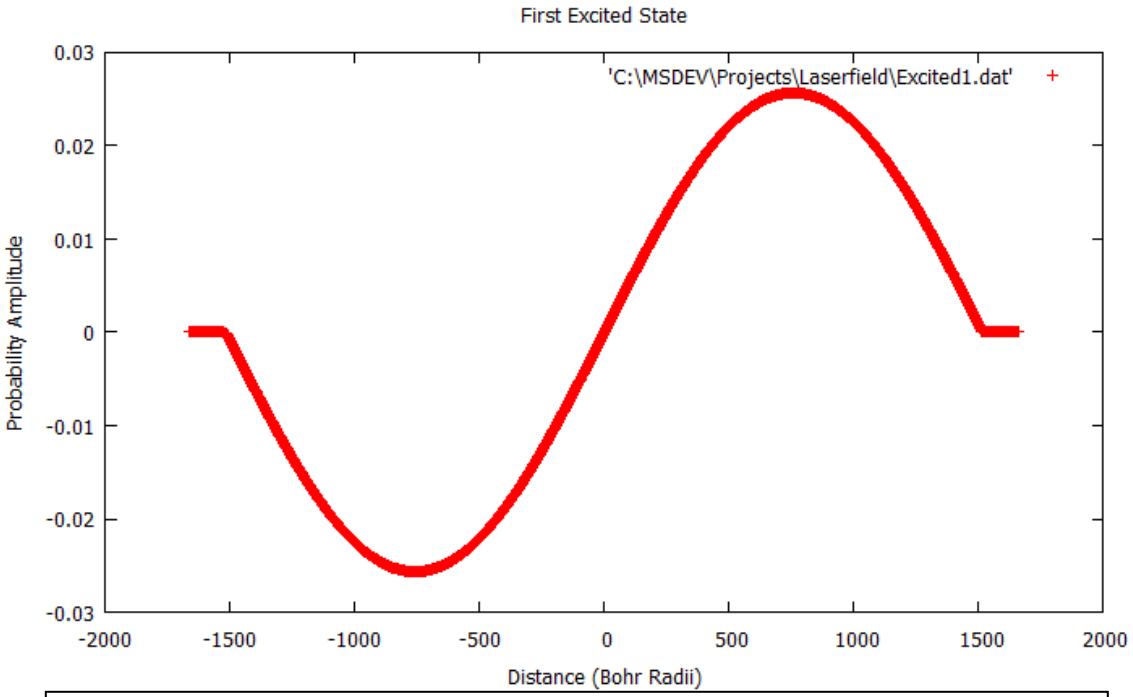


Figure 3-Normalized First Excited state of Ψ(x). The wave function was chosen to be negative as it approached x=0 from -∞ by convention since the positive values are more readily visualized as tunneling through the well barrier.

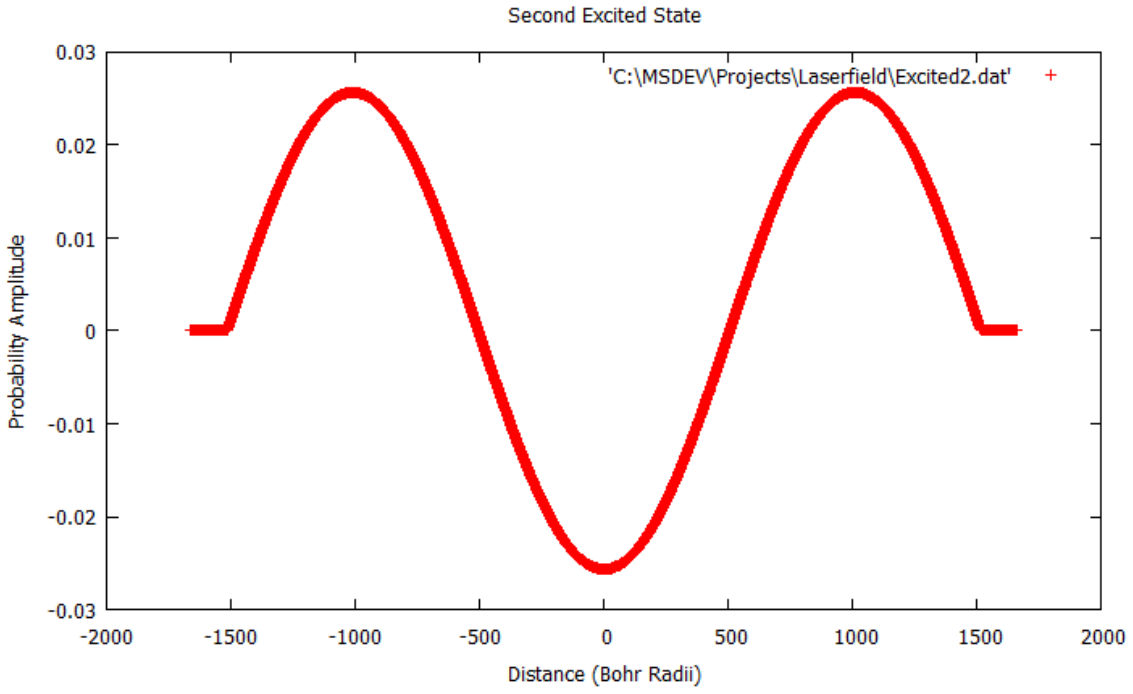


Figure 4-Normalized Second Excited state of Ψ(x).

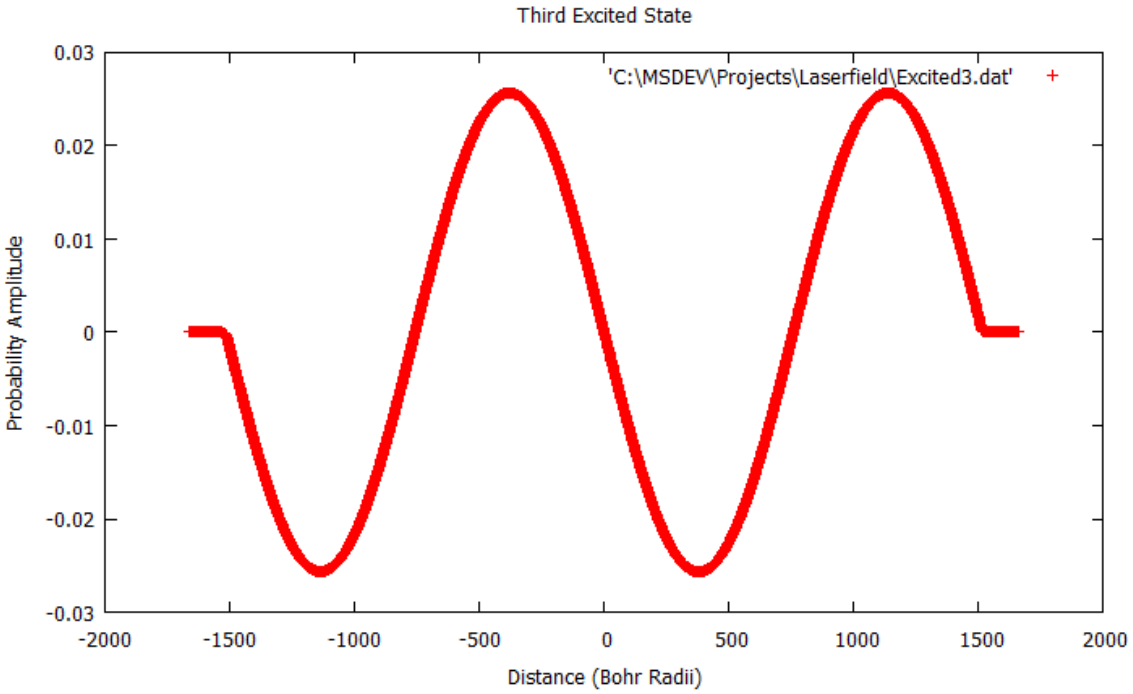


Figure 5-Normalized Third Excited state of Ψ(x).

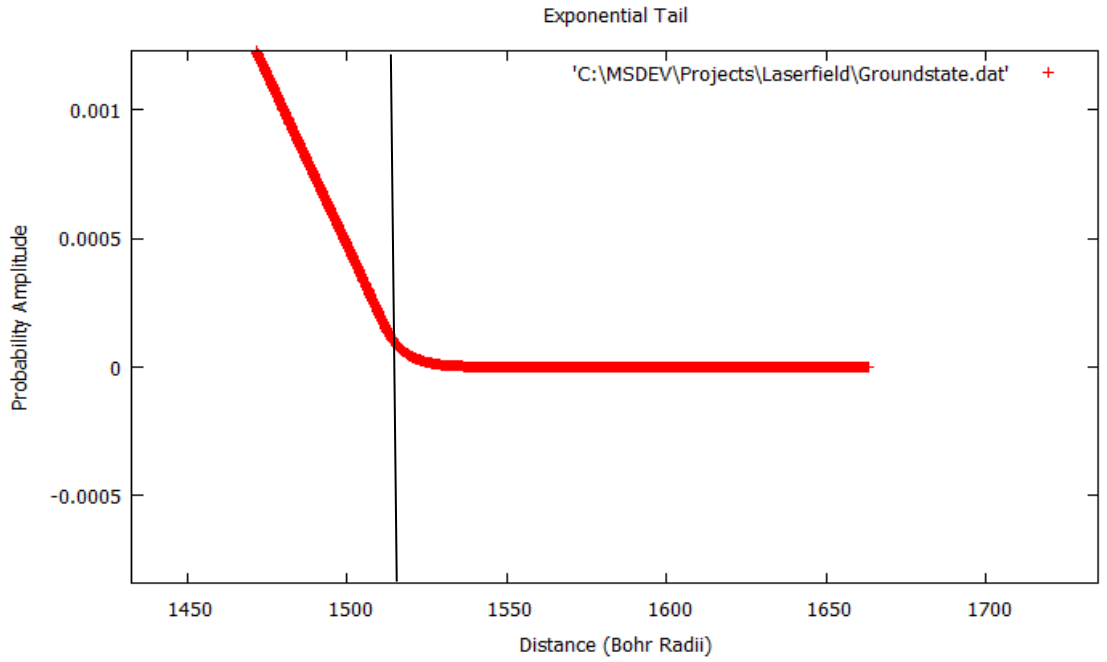


Figure 6-Zoomed in view of the exponentially decaying tail of the ground state showing that there is a smooth transition from inside the well to outside the well. Black line demarcating the boundary of the well

The results from the Gaussian wave packets are shown in compilation Figure 7. The time in atomic units is also displayed next to each plot of the interference figure in order to demonstrate the time evolution of the interference pattern. Any successful application to the Fortran code, must have a time scale equivalent to the time of propagation found from Maple.

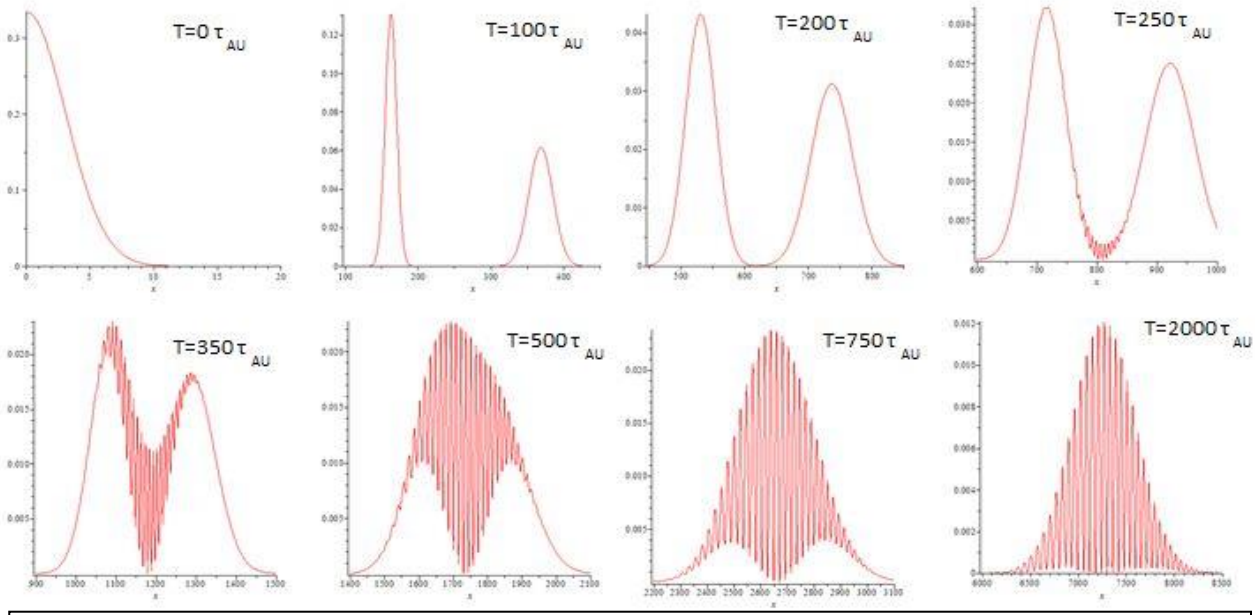


Figure 7-Interference figures generated from Maple showing the time evolution of the interference patterns of two Gaussian waves generated using the parameters given in Section 2.4. The amplitude is given on the Y-axis, with the position on the X-axis.

## 4. Discussion

As can be seen from the table, the values are in close agreement, but are not the same. This can be described from a number of perspectives. First, because Fortran has a greater limitation on the amount of data stored in a variable the Laserfield has obvious pitfalls in terms of rounding error. The discrepancy is also manifested due to the limitations of the initial assumptions. Because the Numerov equation is an approximation, the equations are not infinitely away from

the well with infinitesimally small values, but rather close to the well with two assumed values. Therefore the Numerov method will always be slightly off.

The generation of the interference patterns fits with the expectations of Wollenhaupt et al. Where the temporal evolution of the Gaussian wave packets leads to the tails of the packets first beginning to interact and then after enough time has passed generate an interference pattern that begins to move with a single velocity. The model provides the correct time scale and distance over which the wave packets will interact. This evolution must be incorporated into Laserfield to show that the Gaussians are both generated from same initial probability amplitude. By combining Laserfield with the observed behavior of the Gaussian wave packet interference a single coherent model can be created to accurately model the wave functions evolution.

## 5. Future Work

Laserfield has not yet reached the science goals desired and requires future additions to the code to accurately model the desired behavior. The next steps are currently being implemented, although the code has not yet produced the desired results. The first upgrade merely involved expanding the wave function out further in space. Due to rounding errors, the more extreme values were given a constant value one order of magnitude less than the initial starting points. The next upgrades include developing the proper skills to determine the time-dependent solution under the influence of an electric field. This will be accomplished using the same code used to generate the initial states of the finite well with the exception that the

electric field potential of Equation 6 with Eo equal to the strength of the field, ω the frequency and τ the delay included:

$$V(x,t)_E = eEo\cos(\omega t)\, e^{-\left(\frac{t}{\tau}\right)^2} \quad (6)$$

The same 3-point derivative will again be used to find the derivative of the function and then applied a second time to get the second derivative. The influence of the electrical field could be thought of as lowering one wall of the potential well and allowing the electron to tunnel through it and emerge as a free particle electron wave, mirroring the results found in the wave packet interference section. The time derivative will be constructed in a similar fashion with the initial value being the ground state and the next step in time being a slight increase in the absolute value of the ground state. The final solution for Ψ(x,t) would then satisfy the equation:

$$\frac{-d^2\Psi}{dx^2} + V(x,t)\Psi = i\frac{d\Psi}{dt} \quad (7)$$

The interference pattern should then fall from the Equation 7 with the wave packets probability amplitude adding, not the probability.

## 6. Conclusion

Laserfield is still currently under construction, but initial results have shown its ability to produce an accurate ground state wave function as well as higher excited states. These can then be used for application to the time-dependent electric field and the solution to the time-dependent Schrödinger equation. Although the numerical method does have shortcomings related to the limitations of the variables and size constraints it can nonetheless serve as a close

approximation to the assumed real world experiment. Preliminary testing on the coherence of electron wave packets also showed good results. The modeled electron wave packets clearly show the dispersion and overlap that eventually leads to the interference pattern seen in the graphs. With enough time they combine to form one interference pattern propagating and moving as one. This demonstrates the coherence using the assumed values of the parameters. If the probability amplitudes of the numerical solution once complete do indeed show the coherent nature of the electron packets we can show that we are indeed seeing one electron interacting with itself.

*Laserfield Code available on Request

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