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# QUANTUM DYNAMICS OF A TWO-LEVEL ATOM NEAR GOLD NANOSTRUCTURES

Somayeh Mohammad Ali Mirzaee  
*University of Windsor*

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QUANTUM DYNAMICS OF A TWO-LEVEL ATOM NEAR  
GOLD NANOSTRUCTURES

by

Somayeh Mohammad Ali Mirzaee

A Thesis

Submitted to the Faculty of Graduate Studies  
through Department of Physics  
in Partial Fulfillment of the Requirements for  
the Degree of Master of Science at the  
University of Windsor

Windsor, Ontario, Canada

2012

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# **“Quantum Dynamics of a Two-Level Atom Near Gold Nanostructures ”**

by

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## Abstract

When an atomic/molecular system controlled by an external field (to imprint information on it, such as preparing a qubit), is brought near a plasmonic nanostructure, the control problem changes. On one hand, the field experienced by the atom is modified due to the plasmon effects of the nanostructure. On the other hand, due to atom-nanostructure interactions the quantum state spontaneous emission is increased. Purification of states is fundamental to the implementation of quantum technologies. My approach for state purification is based on the interplay of control fields and spontaneous emission from a two-level quantum system in presence of a gold nanoparticle (GNP). For a specific location of the system around the GNP, I can find a control field that increases the purity of the system more than without the GNP. Unlike previous efforts of state purification that involve cooling to the ground state, here the excited state population remains significant.

## Dedication

*For My Parents and My Husband For Their Love and Endless Support*

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I apologize to those I've inadvertently left out. Lastly, thank God!



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## List of Abbreviations

DDA	Discrete Dipole Approximation
EIT	Electromagnetically Induced Transparency
FDTD	Finite Difference Time Domain
GNP	Gold Nano Particle
HOMO	Highest Occupied Molecular Orbital
LSP	Localized Surface Plasmon
LSPR	Localized Surface Plasmon Resonance
LUMO	Lowest Unoccupied Molecular Orbital
LVN	Liouville-Von Neumann
SEF	Surface Enhanced Fluorescence
SERS	Surface Enhanced Raman Scattering
SPR	Surface Plasmon Resonance
TDSE	Time Domain Schrödinger Equation
TFSF	Total-Field Scattered-Field
UV	Ultra Violet
Vis	Visible
2LS	Two-Level System
3LS	Three-Level System

# Chapter 1

## Introduction

Quantum dynamics is studied in many fields such as quantum information processing, coherent control, quantum optics, quantum state engineering etc. Even with a few-level model of the quantum system, there is a rich variety of phenomena that can be observed including:  $N$ -level atomic and molecular systems that are near-resonantly coupled to monochromatic radiation fields [1], quantum optics problems which can be treated using the two-level system as a standard model [2], and Electromagnetically Induced Transparency [3] phenomena. In this study, my goal is to understand the temporal evolution of a quantum system interacting with the electromagnetic field in proximity to a Gold Nanoparticle (GNP) over the interaction time period.

Metallic nanoparticles have fascinated scientists for over a century and are now heavily utilized in biomedical sciences [4] and engineering [5]. Nanoplasmonics deals with the conduction-electron oscillations in metallic nanostructures and nanoparticles, and the excitation of those oscillations with light [6]. These oscillations cause an enhanced electric field intensity around the nanoparticle, and a “localized surface plasmon resonance” (LSPR) peak in the absorption spectrum that is measured as a function of wavelength [7]. The shape of the nanoparticle absorption (and scattering) spectrum, and its maximum wavelength  $\lambda_{max}$ , depend on the nanoparticle

composition, size, shape, orientation and dielectric environment [8]. The LSPR is theoretically possible in any metal with a large negative real dielectric constant and small imaginary dielectric constant, however experimentally the most common materials are silver and gold with their LSPR characteristics in the visible spectrum[7]. The local electric field depends on the incident light polarization, and the distance from the surface of the metal nanoparticle where the electric field is measured [9]. The ability to increase the emission of nearby fluorophores in proximity to the metal nanoparticles is another interesting phenomenon[10]. The mechanism contributing to spontaneous emission enhancement is the nanoparticle modification of the molecule radiative and nonradiative decay rates [11]. This enables molecule-nanoplasmonic structures to serve as promising configurations for many applications including biochemical sensors [12], surface enhanced spectroscopies [13], and nanophotonics [14].

In this thesis, I am interested in another application of controlling a two-level system (2LS) that is in proximity to a noble-metal nanosurface (typically gold nanoparticle). I investigate the possibility of increasing the purity (or quantum coherence) of the atomic or molecular state by coupling the atomic excitation to the plasmon modes of a gold nanoparticle. Using the interplay of control fields and spontaneous emission in quantum state purification by laser cooling is not a new idea [15]. In this study, I employ the control of the electric field and spontaneous emission rates to purify the quantum state *without* cooling the population to the ground state.

In order to understand this topic, one must understand the interactions between different systems as: (1) 2LS-light interaction (2) The GNP-light interactions (3)

The GNP-2LS interactions. Each of these being fairly large topics, these topics are presented in separate chapters, each of which have a literature review of that topic. The quantum dynamics of a single qubit interacting with an electromagnetic field in the presence of an environment is modelled by the Lindblad equations; and their solutions are described in chapter 2. Chapter 3 presents the gold nanoparticle and light interactions. Maxwell's equations are solved for the nanoplasmonic structure using the three-dimensional Finite Difference Time Domain (FDTD) method [16]. The results show that the field modification pattern around the GNP differ at different orientations and distances from the GNP surface. Chapter 4 contains a brief explanation about the mechanism of quantum decay rate modification in proximity to a GNP. The results show the connection between the radiative (and nonradiative) decay rate enhancement and position of the molecule around the GNP. Moreover, they confirm that the orientation of the molecule dipole with respect to the GNP surface affects the decay rate.

In chapter 5, the combined structure of a two-level system interacting with the control field in presence of a GNP is investigated. Preparation of the 2LS state without cooling the population to the ground state is presented. The effects of competition between the field enhancement and spontaneous emission modification on the state purification process, versus position around the GNP is studied in this chapter. It is shown that there are some possibilities to improve the quantum state preparation specifications such as required time, essential light intensity, and state purity in presence of a GNP.



## Chapter 2

### Atom - Light Interaction

#### 2.1 Introduction

A main interest in laser driven atomic media is the study of their coherence properties. Coherent excitation occurs when an atom interacts with a monochromatic radiation field [17]. Coherent effects like electromagnetically induced transparency (EIT) [18, 19], coherent population trapping [20, 21], lasing without inversion [22], and others [23, 24] are examples where the optical properties of an atomic medium are influenced by coherent fields.

The atom-field interaction is one of the most fundamental problems of quantum optics [23, 25, 26, 27]. To gain an accurate description of the interaction, one must solve the time-dependent Schrödinger equation with an appropriate Hamiltonian [28]. In the presence of interactions with the environment, one must solve the Master equation with appropriate Lindblad terms [29]. First, let us consider a single source of incident radiation, which interacts with a simple two-state quantum system. The other levels of the system can be neglected, as they are far off resonance with the applied field. The knowledge that we gain from this simple two-level quantum system will form the foundations of more complex, multi level systems.

## 2.2 Semiclassical Approach

A fully quantum mechanical description of the atom-laser interaction is not straightforward. The equations of motion for the atomic states are treated in the semiclassical approximation, meaning that the electromagnetic field is considered to be classical (non-quantized), but the atom is described by a quantum model. This approximation is appropriate when the fields contain many photons. The semiclassical theory, when extended to take into account both the effect of the molecules on the field and the effect of the field on the molecules, reproduces almost quantitatively the same laws of energy exchange and coherence properties as the quantized field theory, even in the limit of one or a few quanta in the field cavity mode. In particular, the semiclassical theory is shown to lead to a prediction of spontaneous emission, with exactly the same decay rate as given by quantum electrodynamics for the low orders of  $\alpha$  in the Fermi golden-rule transition rate (see chapter 4), as described by the Einstein A coefficients[30].

The interaction between light and an atom is modelled using the electric dipole approximation. The electric field of the radiation is assumed to interact with the atom through its electric dipole moment. In addition, we neglect the spatial variation of the electric field, as its wavelength is much greater than the atomic dimensions. These approximations allow us model the atom-field interaction as  $\hat{H}_a - \hat{\boldsymbol{\mu}} \cdot \mathbf{E}(t)$  [31].

How can a two-level system (2LS) be a good approximation for atomic or molecular structures? The reason lies in two factors: 1) Near-resonant excitation and 2)

Selection rules. The absorption cross section of an atom absorbing an off-resonant photon is generally of the order of  $1 A^{\circ 2}$ . But when the frequency of the photon matches with that of transition frequency from the initial state to some final state, the cross section can be enhanced by many orders of magnitude. Under the resonance condition, many levels lying far away from the resonance can be simply ignored. In addition, the dipole selection rules dictate only certain transitions are allowed. In most cases, the field therefore only causes transitions between a small number of discrete states, in the simplest of which only two states are involved. The states for a two-level system are labelled  $|g\rangle$  and  $|e\rangle$ . Their energies are separated by  $\hbar\omega_{ge}$ , the transition energy. It is assumed that a dipole transition is allowed between the two states, and that the two states are orthogonal to each other. A schematic diagram of a quantum system with two non-degenerate states

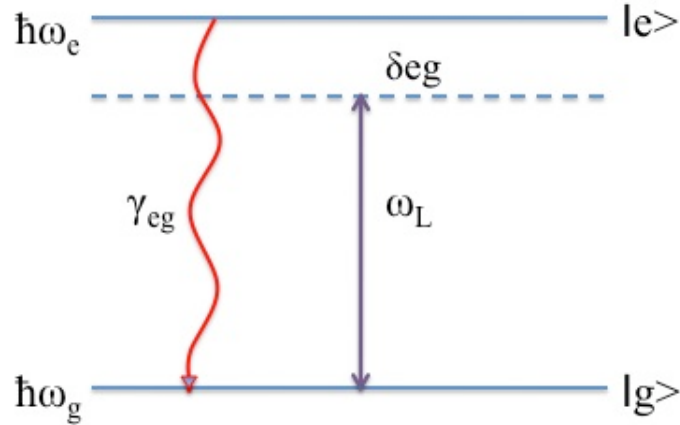


Figure 2.1: Schematic diagram of a quantum system with two non-degenerate states.

is shown by Fig. 2.1. The ground state  $|g\rangle$  with energy  $\hbar\omega_g$  is coupled to the excited state  $|e\rangle$  with energy  $\hbar\omega_e$  by a laser radiation field with frequency  $\omega_L$ . The

laser is detuned from resonance by  $\delta_0 = \omega_L - \omega_{ge}$  where the transition frequency is  $\omega_{ge} = \omega_e - \omega_g$ . The excited state  $|e\rangle$  decays by spontaneous emission with rate  $\gamma_{eg}$  to the ground state  $|g\rangle$ .

The interaction between a two-level system and light field is given by

$$\hat{H} = \hat{H}_a + \hat{H}_i, \quad (2.1)$$

where the total Hamiltonian  $H$  is given by the sum of the field-free Hamiltonian,  $H_a$  and the light field interaction  $H_i$ . The light-matter interaction of the system is treated in the electric dipole approximation, thus the interaction Hamiltonian is given by

$$\hat{H} = \hat{H}_a - \hat{\boldsymbol{\mu}} \cdot \mathbf{E}(t), \quad (2.2)$$

where  $\hat{H}_a|i\rangle = E_i|i\rangle$ , where  $E_i$  is the energy of the eigenstate for  $i = g, e$ . The dipole moment is given by

$$\hat{\boldsymbol{\mu}} \equiv -e\hat{\mathbf{r}} = -e \sum_{i,j} |i\rangle\langle i|\hat{\mathbf{r}}|j\rangle\langle j| = -e(|g\rangle\langle e|\langle g|\hat{\mathbf{r}}|e\rangle + h.c.) = |g\rangle\langle e|\boldsymbol{\mu}_{ge} + h.a., \quad (2.3)$$

where  $\boldsymbol{\mu}_{ge}$  is the transition dipole moment, which in general is a complex-valued vector, and h.a. stands for Hermitian adjoint. However, the dipole moment has an imaginary part; this can be absorbed into the basis vectors, i.e.,

$$|g\rangle\langle e|(|\boldsymbol{\mu}_{ge}|e^{i.arg(\boldsymbol{\mu}_{ge})}) = |g\rangle\langle e|e^{i.arg(\boldsymbol{\mu}_{ge})}|\boldsymbol{\mu}_{ge}| = |g\rangle\langle e|\boldsymbol{\mu}'_{ge}, \quad (2.4)$$

where  $\boldsymbol{\mu}'_{ge} \equiv |\boldsymbol{\mu}_{ge}|$ . Therefore, without loss of generality, we can write

$$\hat{\boldsymbol{\mu}} = \boldsymbol{\mu}_{ge}(|g\rangle\langle e| + |e\rangle\langle g|), \quad (2.5)$$

where we suppress the prime. Now, the Hamiltonian is given by

$$\hat{H} = \hat{H}_a - [\boldsymbol{\mu}_{ge}(|g\rangle\langle e| + |e\rangle\langle g|)] \cdot \mathbf{E}(t), \quad (2.6)$$

It is therefore the product of the electric field and the transition dipole moments that dictate the strength of the interaction. To see this, we can consider the field component which is parallel to the transition dipole moment. Thus Eq.(2.6) becomes

$$\hat{H} = \hat{H}_a - \mu_{ge}E(t)(|g\rangle\langle e| + |e\rangle\langle g|), \quad (2.7)$$

where  $\mu_{ge} = |\boldsymbol{\mu}_{ge}|$ . The equation of motion is given by the Schrödinger equation  $i\hbar\dot{\psi} = \hat{H}\psi$ .

It is convenient to view this expression in an interaction picture or a rotating frame [32].

The transformation operator that takes us to rotating frame is given by,  $\hat{U} = \exp(-i\hbar\omega_L t)$ . Where  $\omega_L$  is the optical frequency of the electric field. This unitary operator rotates the basis to a new basis that rotates with the optical frequencies. The Hamiltonian in the new frame is given by [33]

$$\tilde{H} = \hat{U}^\dagger \hat{H} \hat{U} - i\hbar \dot{\hat{U}} \hat{U}^\dagger = \hbar(\delta_0 |e\rangle\langle e|) - \mu_{ge}E(t)|g\rangle\langle e|e^{i(\omega_L t)} + h.a., \quad (2.8)$$

Suppose that the field is monochromatic, then, in complex representation, for a real field

$$E_L(t) = E_L \cos(\omega_L t) = \frac{E_L}{2}(e^{-i(\omega_L t)} + e^{i(\omega_L t)}). \quad (2.9)$$

If this is substituted into Eq.(2.8 ) one can identify one term that oscillates with twice the optical frequency. This oscillation is extremely fast and does not contribute much to the important physics as the mean value of this fast variation is very close to zero [23]. Thus we perform the rotating wave approximation (RWA) by throwing away these terms. Under this approximation, and at resonance, the dynamics of the

system can be solved analytically [30]. The basic assumptions in the RWA are as follows [34]:

- 1) The electromagnetic field and the quantum system should be in near resonance, that is  $\delta_0 \ll \omega_{ge}$ .
- 2) There should be relatively weak coupling between the exciting laser and the quantum system that is  $\Omega_{ge} = \frac{\mu_{ge} E_L}{\hbar} \ll \omega_L$ .
- 3) There are no quantum levels with energies close to those of the counter rotating terms.

After performing the transformation to a rotating frame and the RWA, the Hamiltonian is given by

$$\tilde{H}_{RWA} = -\hbar(\delta_0|e\rangle\langle e|) - \frac{\hbar\Omega_{ge}}{2}|g\rangle\langle e| + h.a., \quad (2.10)$$

where the strength of the interaction is given by the Rabi frequency

$$\Omega_{ge} = \frac{\mu_{ge} E_L}{\hbar}. \quad (2.11)$$

The Rabi frequency is a parameter that depends on the amplitude on the electric field, not the the intensity. It is denoted a frequency since it corresponds to the angular frequency of the Rabi oscillation of a two-level atom in a coherent resonant field. In an appropriate matrix representation we write the corresponding Hamiltonian matrix,

$$\tilde{H}_{RWA} = \begin{pmatrix} 0 & -\frac{\hbar\Omega_{ge}}{2} \\ -\frac{\hbar\Omega_{ge}^*}{2} & -\hbar\delta_0 \end{pmatrix}, \quad (2.12)$$

where  $\Omega_{ge}$  is equal to  $\Omega_{ge}^*$  in the case of linear polarized light. This matrix is often a convenient starting point when considering the coherent effects associated with

the two level system. The evolution of the quantum state vector  $|\psi(t)\rangle$ , is given by solving the Schrödinger equation using the (2.12) Hamiltonian.

Until now, our discussion has primarily been about closed quantum systems, which evolve unitarily. However, in real systems, we often want to be able to disregard certain microscopic dynamics, or do not have access to certain parts of a system. For example, we may want to cool an atom, but will not keep track of the microscopic state of the cooling laser beam after it has interacted with the atom, or an atom may interact with the vacuum, emitting a photon which we do not track. The study of such topics is the subject of open quantum system dynamics. The next section begins our investigation of open quantum systems, with the goal of developing a fully quantum-mechanical model of an atom undergoing spontaneous emission, while interacting with a classical electromagnetic field.

### 2.3 Master Equation

The master equation [23] is an equation of motion for a density matrix describing an open quantum system, much like the Schrödinger equation describes the evolution of a closed quantum system. This section provides a derivation of the master equation for a spontaneously emitting quantum system, driven by a classical field.

Is there a straightforward quantum analogue of this? We might be tempted to simply add a damping term to the Schrödinger equation, like

$$i\partial_t|\psi\rangle = \hat{H}|\psi\rangle - i\hat{\Gamma}|\psi\rangle, \quad (2.13)$$

but this model is not include the decoherence terms. How, then, can we construct a fully quantum-mechanical description of open system dynamics? The key concept is that we must properly account for noise.

The main tool we shall use to model open quantum systems is the density matrix representation for quantum states, so it is helpful to begin with a review of density matrices and how they evolve under Hamiltonian dynamics. In general, a density matrix  $\rho$  may always be written as a statistical mixture of pure states,  $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ , where  $p_k$  are probabilities, such that  $\sum_k p_k = 1$ . A matrix  $\rho$  is a valid density matrix if and only if the eigenvalues of  $\rho$  are non-negative, and sum to one, such that  $Tr(\rho) = 1$ .  $\rho$  represents a pure state if and only if  $Tr(\rho^2) = 1$ . How does a density matrix evolve in a closed system? From the Schrödinger equation,

$$i\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle, \quad (2.14)$$

it follows that a pure state density matrix  $\rho = |\psi\rangle\langle\psi|$  evolves as

$$\dot{\rho} = |\dot{\psi}\rangle\langle\psi| + |\psi\rangle\langle\dot{\psi}| = -\frac{i}{\hbar}[\hat{H}, \rho]. \quad (2.15)$$

This governs the evolution of the density matrix. However loss out of this system has not been accounted for, namely decay due to spontaneous emission. This is included by adding a decay term [35],  $\Gamma$ ;

$$\hat{\Gamma} = \sum_d \frac{\gamma_d}{2} (\hat{\sigma}_d^\dagger \hat{\sigma}_d \hat{\rho} + \hat{\rho} \hat{\sigma}_d^\dagger \hat{\sigma}_d - 2\hat{\sigma}_d \hat{\rho} \hat{\sigma}_d^\dagger), \quad (2.16)$$

where  $\sigma_d$  are the Lindblad operators that model a decoherence process“ $d$ ”. In this



model, we assumed that the only relaxation mechanism is spontaneous emission and therefore we take  $\hat{\sigma}_d^\dagger = |n\rangle\langle m|$  and  $\gamma_d$  represents the decay rate from state  $n, m \in \{|g\rangle, |e\rangle\}$ . Thus a more complete description of the system is,

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] - \hat{\Gamma}, \quad (2.17)$$

the so called Lindblad master equation.

## 2.4 Lindblad Master Equation

The phenomenological decay matrix is inserted into the equation and contains the decay rates for each of the states and their coherences. In the case of a two-level atom, the decay matrix  $\hat{\Gamma}$  is given by [36].

$$\hat{\Gamma} = \begin{pmatrix} -\gamma_{eg}\rho_{ee} & \frac{\gamma_{eg}}{2}\rho_{ge} \\ \frac{\gamma_{eg}}{2}\rho_{eg} & \gamma_{eg}\rho_{ee} \end{pmatrix}. \quad (2.18)$$

Calculating the Lindblad term and density matrix in the rotating frame, and inserting into the Eq.(2.18), one obtains four first order coupled differential equations:

$$\begin{aligned} \dot{\tilde{\rho}}_{gg} &= \frac{i\Omega_{ge}}{2}(\tilde{\rho}_{ge} - \tilde{\rho}_{eg}) + \gamma_{eg}\tilde{\rho}_{ee} \\ \dot{\tilde{\rho}}_{ee} &= \frac{i\Omega_{ge}}{2}(\tilde{\rho}_{eg} - \tilde{\rho}_{ge}) - \gamma_{eg}\tilde{\rho}_{ee} \\ \dot{\tilde{\rho}}_{ge} &= \frac{i\Omega_{ge}}{2}(\tilde{\rho}_{gg} - \tilde{\rho}_{ee}) + \tilde{\rho}_{ge}(-i\delta_0 - \frac{\gamma_{eg}}{2}) \\ \dot{\tilde{\rho}}_{eg} &= \frac{i\Omega_{ge}}{2}(\tilde{\rho}_{ee} - \tilde{\rho}_{gg}) + \tilde{\rho}_{eg}(i\delta_0 - \frac{\gamma_{eg}}{2}), \end{aligned} \quad (2.19)$$

where new variables are introduced to suppress the time dependence of the density matrix components in the coupled differential equations [25].

$$\hat{\rho} = \begin{pmatrix} \tilde{\rho}_{gg} & \tilde{\rho}_{ge} \\ \tilde{\rho}_{eg} & \tilde{\rho}_{ee} \end{pmatrix} = \begin{pmatrix} \rho_{gg} & \rho_{ge}e^{-i\omega_L t} \\ \rho_{eg}e^{i\omega_L t} & \rho_{ee} \end{pmatrix}, \quad (2.20)$$

it is helpful to mention that, in a two level system, the atomic population just decays to the internal ground state, i.e., the atomic population is conserved,  $\rho_{gg} + \rho_{ee} = 1$ . This system of equations has an analytic solution in two limits; 1) when the laser is in resonance,  $\delta_0 = 0$ , the analytical solution is given by S.K. Lee and et al.[37] as:

$$\rho_{ee}(t) = \frac{4|\frac{\Omega_{ge}}{2}|^2}{8|\frac{\Omega_{ge}}{2}|^2 + \gamma_{eg}^2} [1 - (\cos \lambda t + \frac{3\gamma_{eg}}{4\lambda} \sin \lambda t) e^{-(\frac{3}{4})\gamma t}], \quad (2.21)$$

where,  $\lambda = \sqrt{4|\frac{\Omega_{ge}}{2}|^2 - \frac{\gamma_{eg}^2}{16}}$ . 2) At steady state condition or  $\dot{\rho}_{gg} = 0$ , the analytical solution is given by Käll and et al.[29].

We are interested in the dynamical solution of Eq. 2.19 even when the exciting field is off resonance. Therefore, the coupled first-order differential equations 2.19 are solved numerically using the MATLAB computer software. Solving the equations without further approximations is advantageous as it allows an analysis of the density matrix elements throughout the interaction time period.

The numerical solution is bench marked against the analytical solution for zero detuning [37] and agree to within 0.093%. In the general problem that we solve, we have nonzero detuning as well as arbitrary pulse envelopes for the electromagnetic fields.

## Chapter 3

### Light and Gold Nanoparticle (GNP) Interaction

#### 3.1 Introduction

When a metal is exposed to light, a number of processes occur: (1) The light can be absorbed, (2) The light can be scattered at the same frequency as the incoming light (Rayleigh scattering), (3) The absorbed light can be re-scattered (i.e., Mie scattering [38]), (4) The local electromagnetic field of the incoming light can be enhanced, thus enhancing any spectroscopic signals from the molecules at the material surface, that is, Surface-Enhanced spectroscopy, such as surface-enhanced Raman Scattering (SERS) and Surface-Enhanced Fluorescence (SEF).

Noble-metal nanostructures show very complex and interesting properties when interacting with light. The history of using colloidal gold to generate beautifully colored glass for decorative purposes dates back to Roman times [39]. Faraday in 1850s, observed that the optical properties of nanogold particles are different from bulk gold [40]. Gold nanospheres have a characteristic red color, while the large particles show yellowish color. The special color of nanoparticles is caused by the collective oscillation of the electrons in the conduction band, known as the surface plasmon oscillation. A description of the origin of this plasmon resonance will be described in next section. Plasmon modes exist in a number of geometries and in various metals. Under certain circumstances plasmons are excited by light, which

leads to strong light scattering and absorption and an enhancement of the local electromagnetic field [41].

Depending on the boundary conditions, one can distinguish between bulk plasmons (3D plasmon), surface propagating plasmons (2D films), and localized surface plasmons (nanoparticles) [4]. The physics of surface-plasmon excitations occurring at metal/dielectric interfaces has been studied for the possibility of using such excitations for the localization of electromagnetic energy in one, two, and three dimensions, in the context of applications such as sensing and waveguiding for functional photonic devices [42].

The optical properties of metal nanoparticles are found to depend on the shape and size of the nanoparticle [43] and the dielectric constant of the surrounding medium [44]. Due to these unique optical properties, the noble metal nanoparticles are the subject of many recent studies, with a large number of applications including biological applications [45], biosensing [46], nanospectroscopy [47] and optoelectronics [48]. In the case of gold nanoparticles, all the surface-enhanced processes are enhanced strongly owing to the unique interaction of light with the free electrons in the metal particles, and the resonance occurs in the visible spectral region [49]. Gold nanoparticles become very good candidates for implementing biosensing methods due to their sensitive localized surface plasmon resonance spectra [50]. The effect of size [51], shape [52] and environment refractive index [53] on enhancement wavelength have been well investigated.

In this chapter, the focus will be mostly on particle plasmons, which is the most interesting phenomenon in light - gold nanoparticle (GNP) interactions.

## 3.2 Background

During the interaction between light and a gold nanoparticle (GNP), the oscillating electromagnetic field of the light causes the oscillation of the free electrons in the GNP with respect to the metal lattice [54]. When the wavelength of light is much larger than the nanoparticle size, the interaction with the surface is dominant. Therefore, as shown in Fig. 3.1, the traveling light wave causes the electron density in the particle to be polarized to one surface and oscillates in resonance with the light frequency creating a standing oscillation. The unique characteristics of such oscillations originate from the confined spatial distribution of the polarization charges over the surface of the nanostructure [55]. This process is resonant at a particular frequency of the light and is termed the localized surface plasmon resonance (LSPR). The negative – positive charge separation can be controlled by the size and the shape of nanoparticles that will change the frequency and the intensity of the LSPR in the visible and infrared region [56].

This interaction of gold nanoparticles and light can be discussed in the classical regime and a complete definition for this problem will be derived by solving Maxwell's equations. In 1908, Gustav Mie calculated the surface plasmon resonance by solving Maxwell's equations that define the extinction efficiency  $Q_{ext}$  (where extinction efficiency ( $Q_{ext}$ ) = scattering efficiency ( $Q_{sca}$ ) + absorption efficiency ( $Q_{abs}$ )) of spherical particles of arbitrary size [38] interacting with the electromagnetic field. Later Richard Gans extended Mie's solutions to Au spherical particles [57]. In some literature, Mie's solutions to Maxwell's equation are referred to as Mie theory,

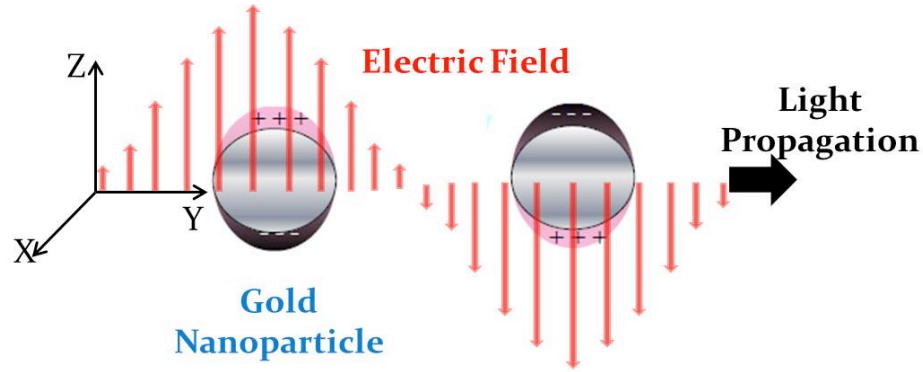


Figure 3.1: Schematic diagram for Localized Surface Plasmon Resonance (LSPR).

although they do not investigate an independent physical phenomenon.

The basic concepts of solid state theory and electrodynamics that are needed to investigate the optical properties of metal nanostructures are described completely in the textbooks, *Electrodynamics* by J.D. Jackson [58] and *Solid State Physics* by Ashcroft and Mermin [59], and will not reproduce here.

### 3.3 Mie's Solution of Maxwell's Equations

Electromagnetics is governed by Maxwell-Ampere's law, Faraday's law, and Gauss' laws, collectively known as Maxwell's equations. In differential form, these equations are [58]:

$$\begin{aligned}
(1) \quad & \epsilon \frac{\partial}{\partial t} E = \nabla \times H - J \\
(2) \quad & \mu \frac{\partial}{\partial t} H = -\nabla \times E \\
(3) \quad & \nabla \cdot (\epsilon E) = \rho \\
(4) \quad & \nabla \cdot (\mu H) = 0
\end{aligned} \tag{3.1}$$

The conditions used in Mie theory to solve Maxwell's equations for the electromagnetic field outside the particle are as follows. The particle under consideration is spherical, with radius  $r$ , and is irradiated by  $\hat{z}$ -polarized light with the wavelength  $\lambda$ . In this case,  $r$  is much smaller than the wavelength of light (i.e.,  $\frac{r}{\lambda} \ll 0.1$ ). The electric field is approximated as constant (or static) around the nanoparticle. The Mie solution for these limitations is discussed in detail in the Handbook of Nanoscale Optics and electronics by Gary P. Wiederrecht [49]. In this approach, the quasi static approximation is employed. The dielectric function of a metallic particle is complex and changes with wavelength. Mie's solutions showed that the electric field outside a particle can be described by [49]:

$$E_{out}(x, y, z) = E_0 \hat{z} - \left[ \frac{\epsilon_{in} - \epsilon_{out}}{\epsilon_{in} + 2\epsilon_{out}} \right] \alpha^3 \cdot E_0 \left[ \frac{\hat{z}}{r^3} - \frac{3z}{r^5} (x\hat{x} + y\hat{y} + z\hat{z}) \right], \tag{3.2}$$

In Eq. 3.2,  $\alpha$  is the polarizability,  $r$  is the distance from the center of the particle, and  $\hat{x}$ ,  $\hat{y}$  and  $\hat{z}$  are unit vectors. The first part in Eq. 3.2 depicts the incident field. The metal particle's dielectric function and the ambient dielectric constant are described by  $(\epsilon_{in})$  and  $(\epsilon_{out})$  respectively. It is obvious from Eq. 3.2, that the dipole resonance condition of the particle in which the electric field is enhanced compared

to the incident field, is related to the  $(\epsilon_{in})$  and  $(\epsilon_{out})$ . Mie's solution to Maxwell's equations results in the general equation describing the extinction spectrum [49]:

$$E(\lambda) = \frac{24\pi^2 N r^3 \epsilon_{out}^{\frac{3}{2}}}{\lambda \ln(10)} \left[ \frac{\epsilon_{in}''(\lambda)}{(\epsilon_{in}'(\lambda) + \chi \epsilon_{out})^2 + \epsilon_{in}''(\lambda)^2} \right], \quad (3.3)$$

in Eq. 3.3,  $E(\lambda)$  is the wavelength-dependent extinction for spherical metallic nanoparticles, where  $r$  is the sphere radius,  $\chi$  is a shape factor ( $\chi = 2$  for a sphere), and  $N$  is the number of particles.  $\epsilon_{out}$  is the dielectric constant of the environment and the  $\epsilon_{in}'$  and  $\epsilon_{in}''$  are the real and imaginary components of the metal dielectric constant. As is shown by Eq. 3.3, when  $\epsilon_{in}' = -2\epsilon_{out}$  and  $\epsilon_{in}''$  is small and positive, the extinction is maximized. This solution shows that the extinction spectrum of a small nanoparticle depends on its size, shape, and composition.

### 3.4 Numerical solution of Maxwell's equations

Mie's exact solutions to Maxwell's equations are known for spherical particles and infinite cylinders. Because it is usually not possible to solve Maxwell's equations for nonspherical particles analytically, developing numerical methods is important. The discrete dipole approximation (DDA) is a numerically exact method used to describe nonspherical metal nanoparticles and was originally proposed in 1973 [60]. Another popular technique to model nanoplasmonic systems is Finite Difference Time Domain (FDTD) [61].

The advantages and disadvantages of each method can be found in a recent review [4]. In this study, the FDTD method was employed to solve the Maxwell's equations



around a GNP. The FDTD Solutions (version 7.5.3) from Lumerical Solution, Inc. is used to numerically solve the Maxwell's equations for the interaction of light with a GNP.

### 3.4.1 The Finite-Difference Time-Domain (FDTD) Method

The FDTD method explicitly solves Maxwell-Ampere's law and Faradays law in differential form, equations 3.1-1 and 3.1-2, by approximating the partial derivatives using central finite-difference expressions (derived using Taylor expansions) over a grid-based domain, which has second-order accuracy (i.e., the truncation errors are of higher order than 2). In the next step, special care must be taken in order to satisfy Gauss' laws, equations 3.1-3 and 3.1-4. One way to do this, suggested by Yee, is to use a Cartesian spatial grid with all of the field components shifted by half a grid spacing relative to each other, known as the Yee spatial lattice. For a proof of his results see Ref. [62]. To calculate the field enhancement and electric field vector around a GNP, three-dimensional FDTD calculations were performed.

## 3.5 Simulation setup

A GNP with radius equal to 20nm is used. The field source is a total-field scattered-field source (TFSF) that surrounds a gold nanoparticle. The light source is linearly polarized in the  $\hat{z}$ -direction, and propagates in the  $\hat{y}$ -direction. There are two analysis groups, each of which consist of a box of power monitors: one in the total field region and one in the scattered field region. These analysis groups can be used to

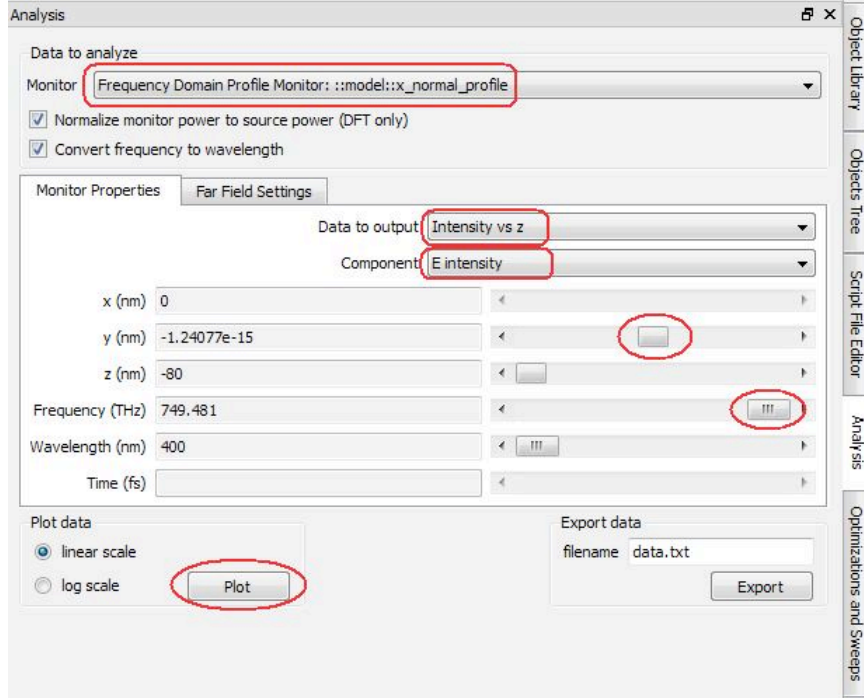


Figure 3.2: Screenshot of the FDTD Solutions to find the maximum field enhancement direction around the GNP. The pertinent results are highlighted.

calculate the absorption and scattering cross sections, as well as the angular distribution of scattered radiation. In addition, three 2D frequency profile monitors are added in the total field region to calculate the electric field enhancement. The total scattered field source covers a wavelength range of 400 to 700 nm. In addition, several point frequency profile monitors are located on each of the main Cartesian axes at different distances from the GNP surface to find the exact value of the electric field enhancement at those specific points.

I used the 2D monitors (the screenshot of related monitors is shown by Fig. 3.2) to determine the maximum field enhancement direction.

The results show that for a GNP with  $r = 20$  nm, the maximum field enhancement

at our desired wavelength  $\lambda_{excit} = 542$  nm (see chapter 5), occurs on  $\hat{z}$ -axis. The dielectric function of gold was chosen to be “Au (gold) - Johnson and Christy” from the material database. With these settings the simulation span is  $1 \times 1 \times 1 \mu\text{m}^3$ . The mesh size is applied using two different mesh regions. The first mesh region will only be used over the sphere region known as override region. The mesh size for the override region is 1 nm, which is applied at the spheres area  $\pm 10$  nm. The second mesh region is the automatically graded meshing that used outside the override region with a mesh accuracy of 3. The mesh accuracy parameter is an integer that defines the number of mesh cells per wavelength. FDTD will automatically generate a mesh based on specified mesh accuracy and the material properties [16]. Note that for simulations with metals, the mesh override region is often used to more accurately resolve the locations of the metal interface, especially with curved surfaces. In this simulation, the mesh override region is large enough to encompass not only the gold sphere, but also the entire TFSS region. This was done intentionally; the TFSS sources work best in uniformly meshed regions. Once the simulation is setup, the FDTD code (Appendix A) will be run to perform the appropriate calculations.

### 3.6 Results

Figures 3.3 and 3.4 show the calculated scattering and absorption cross sections of the GNP with  $r = 20$  nm respectively. In those figures, the Mie efficiency factors for scattering ( $Q_{sca}$ ) and absorption ( $Q_{abs}$ ) are just the corresponding cross sections divided by the geometric cross-sectional area ( $\pi \cdot r^2$ ) to give a dimensionless efficiency

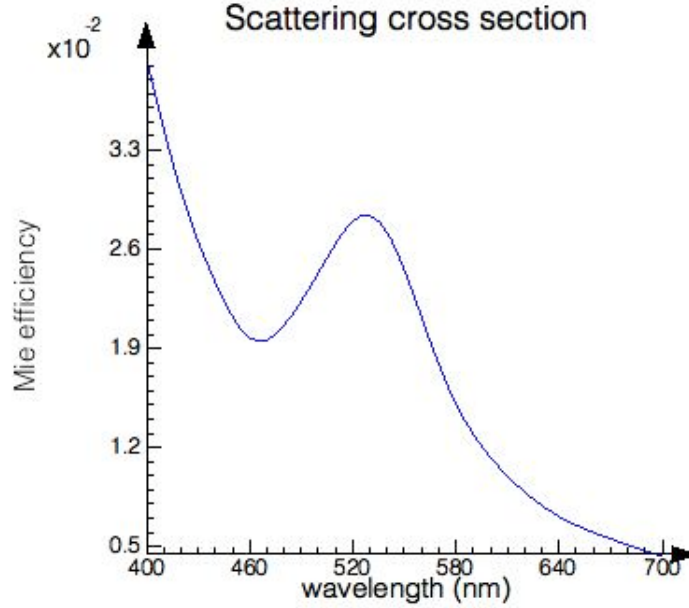


Figure 3.3: Scattering cross section of the GNP with  $r = 20$  nm.

parameters. The results show that the field will be modified around the GNP in different patterns corresponding to the incident light wavelength. Figure 3.5, shows the field modification rates versus wavelength variations at different distances from the GNP surface in four main directions for the GNP with  $r = 20$  nm. The near-field modification is calculated as ratio of the near field intensity to the incident field intensity, that is  $\frac{|E|^2}{|E_{inc}|^2}$ .

As is illustrated in the figure, the maximum field enhancement for the GNP with  $r = 20$  nm is in the  $\hat{z}$ -direction and the resonance wavelength is about  $\lambda = 540$  nm. The total field enhancement profile at the desired wavelength  $\lambda_{excit} = 542$  nm around the GNP is plotted in Fig. 3.6. Figure 3.7 shows the components of the electric field vector around the GNP.

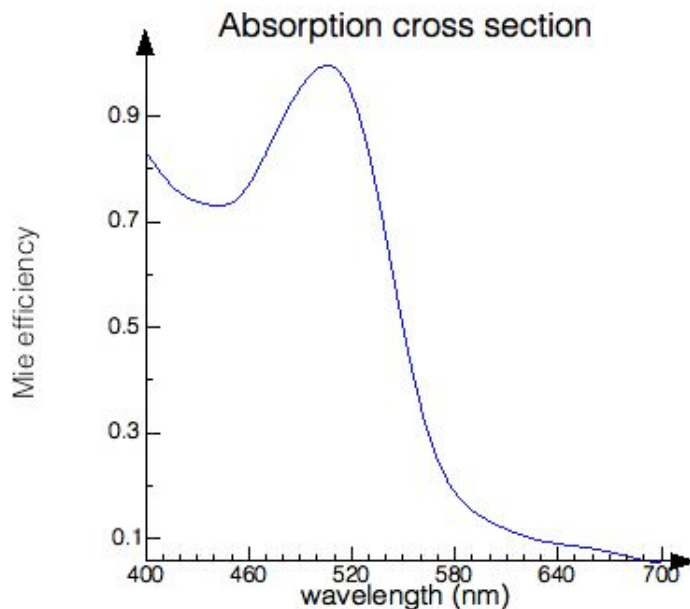
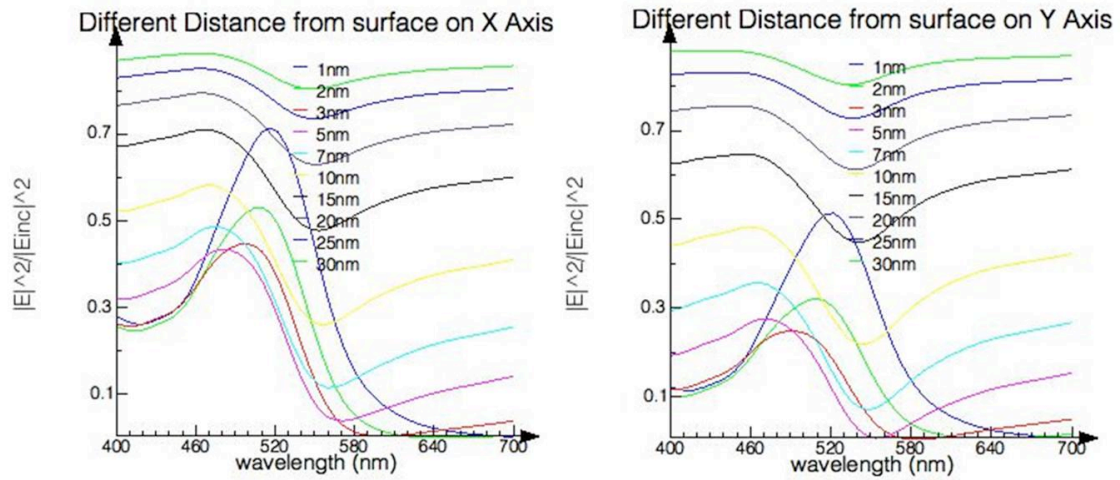


Figure 3.4: Absorption cross section of the GNP with  $r = 20$  nm.

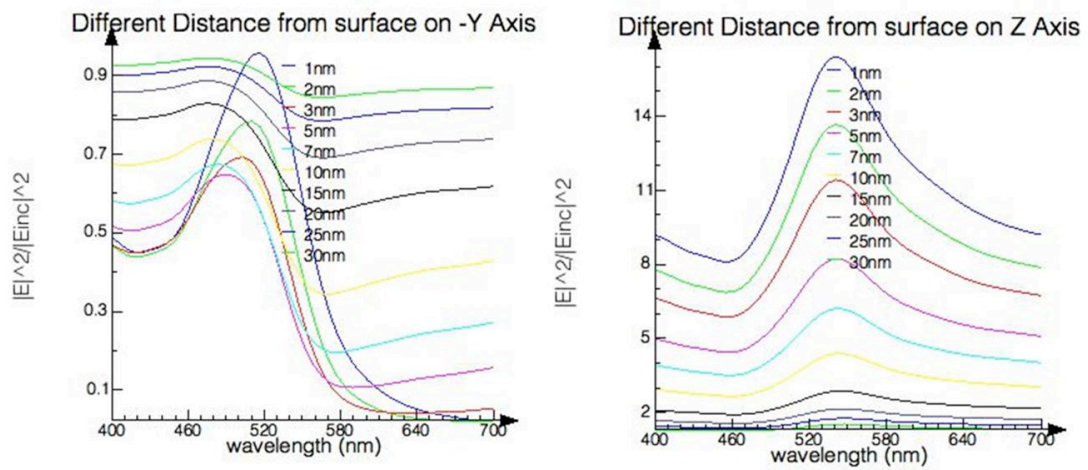
Those results show that, while the dominant plasmon mode is a dipole, plasmonic modes of higher order than the dipolar mode are present, and contribute to the electric field distribution. In particular, we observe a finite  $E_x$  and  $E_y$  component. The electric field vector components values that are calculated through the more accurate point monitors can be found in Appendix B.

Fig. 3.8 shows that as much as the GNP's size getting larger compare to the excitation laser wavelength, these higher-order modes will be dominant and cause the tilt of the electric field maximum in the direction of the light propagation.

Figure 3.9 summarizes the results of Fig. 3.7 for the electric field vector components enhancement, around the GNP versus distance from its surface along the main axes. As shown, the maximum radial component enhancement will occur along the



(a)



(b)

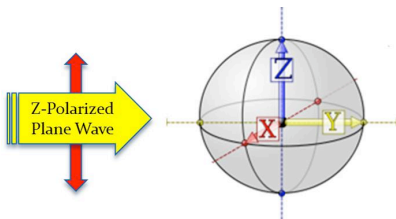


Figure 3.5: Field modification rates around the GNP with  $r = 20$  nm (the bottom cartoon, shows the axes configuration).

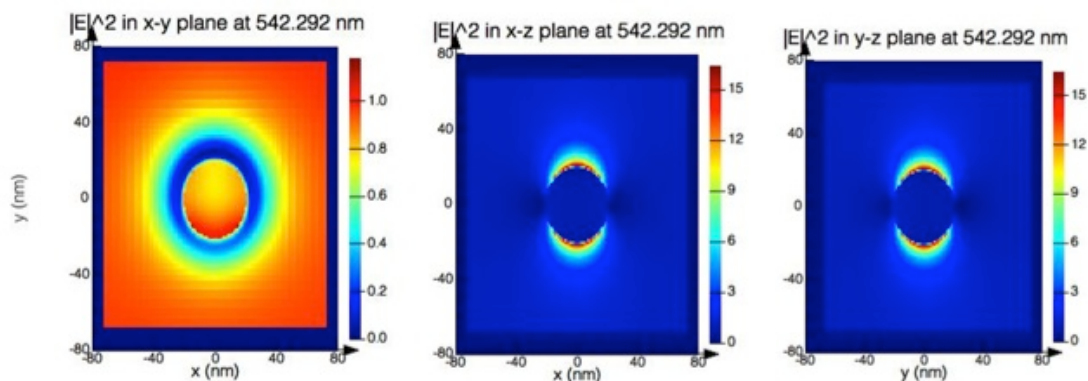
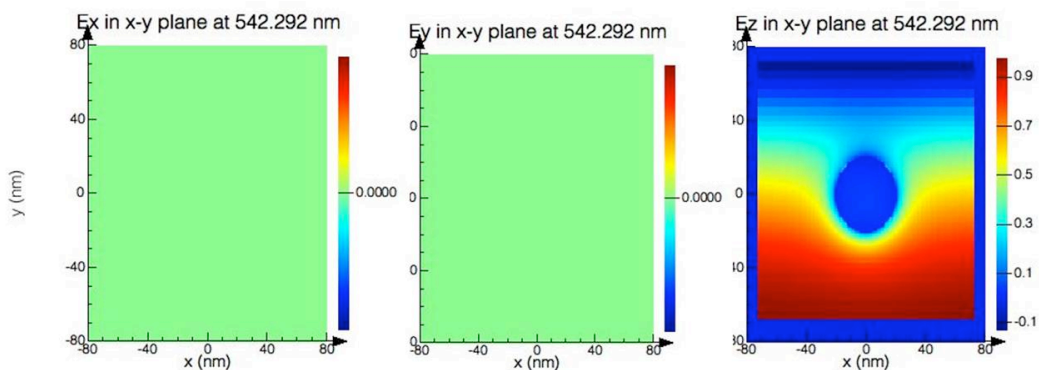
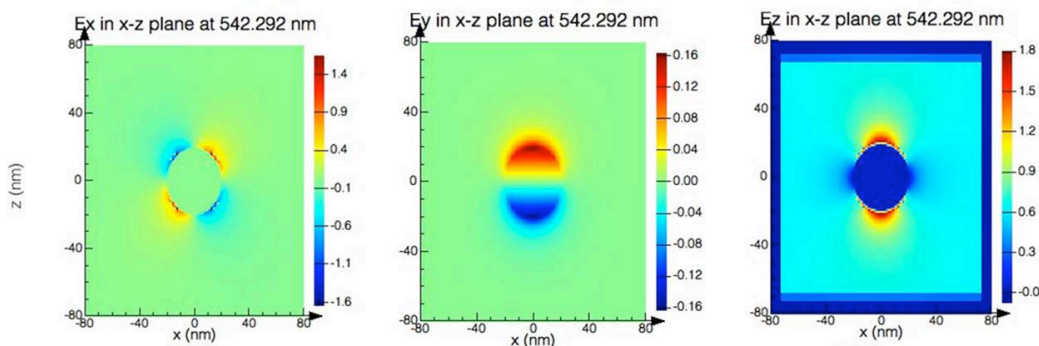


Figure 3.6: Field enhancement around the GNP with  $r = 20$  nm at  $\lambda_{excit} = 542$  nm.

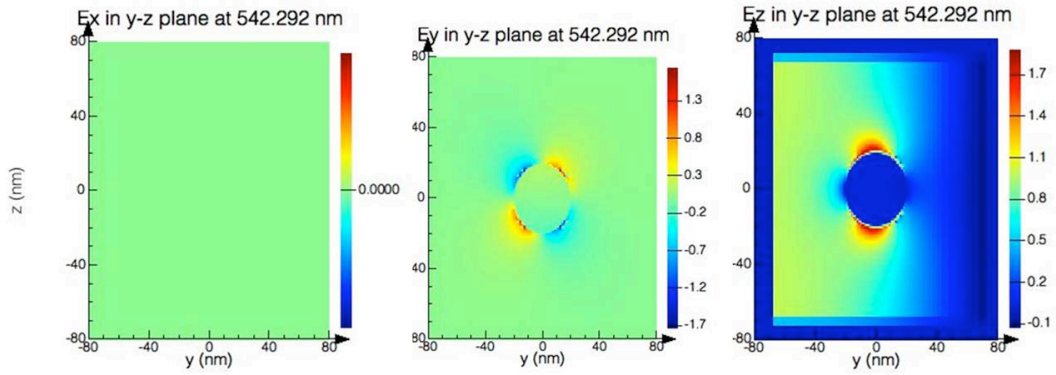


(a)  $\vec{E}$  Components in x-y plane



(b)  $\vec{E}$  Components in x-z plane

Figure 3.7



(c)  $\vec{E}$  Components in y-z plane

Figure 3.7: Calculated  $\vec{E}$  vector components around the GNP with  $r = 20$  nm at  $\lambda_{excit} = 542$  nm.

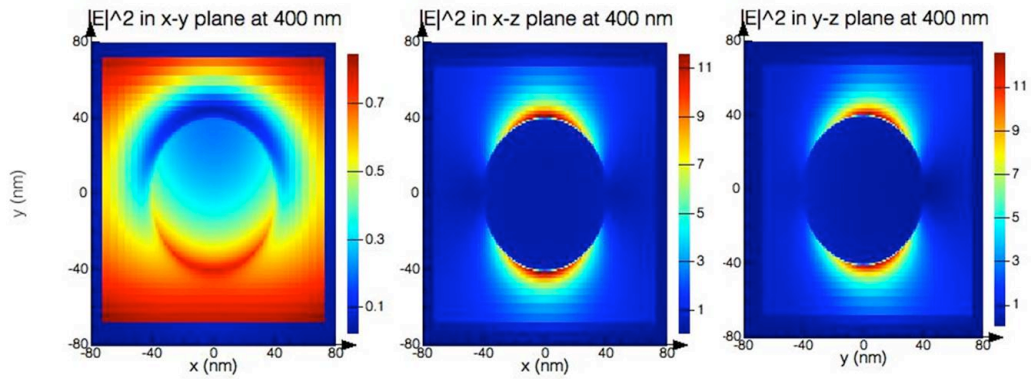


Figure 3.8: Field enhancement around the GNP with  $r = 40$  nm.



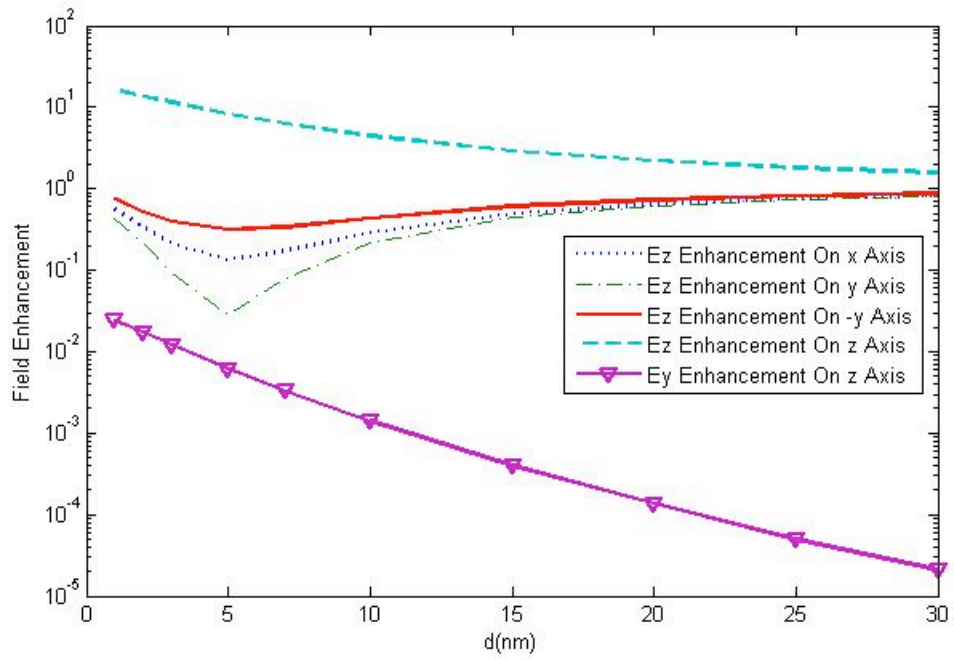


Figure 3.9: Modification of field components around the GNP with  $r = 20$  nm at different positions,  $\frac{|E(d)|^2}{|E_{inc}|^2}$ .

$\hat{z}$ -direction and the maximum tangential component of electric field is along the  $-\hat{y}$ -direction.

## Chapter 4

### Two-Level System near a Gold Nanoparticle

#### 4.1 Surface modification of spontaneous emission

Before Purcell's analysis in 1946, spontaneous emission was considered as a radiative intrinsic property of atoms or molecules [63]. His works established that the spontaneous decay rate of a magnetic dipole placed in a resonant electronic device, can be enhanced in compared to the free-space decay rate. That is, the environment surrounding an atom modifies the radiative properties of the atom. Since the pioneering work of Purcell, amplified and inhibited spontaneous emission have been observed from single atoms coupled to resonant cavities [64], semiconductor quantum wells integrated into microstructures [65], photonic crystals [66], and fluorophores near metal surfaces or nanoparticles [67, 68]. During past decades there are many efforts to establish applicable devices based on modified spontaneous emission, including single-photon sources for quantum cryptography [69], surface plasmon enhanced LEDs [70] and photonic crystal lasers [71].

Theoretical methods have also been presented to calculate the lifetime of an excited molecule near a nanoparticle [72, 73] which show the radiative and nonradiative decay rate modifications. Both are expected to be vary based on size and shape of the nanoparticle, the molecule - nanoparticle distance, the orientation of the molecular dipole with respect to the surface of the nanoparticle, and the connection

of the nanoparticle absorption spectrum and molecular emission wavelength [68]. It is shown that the fluorescence of single molecules will be enhanced in presence of sharp metallic tips [74]. This happens due to an enhancement of the exciting local intensity (see chapter 3), and a modification of the radiative emission rate. However, the absorption cross section of the metallic nanostructure will also create additional nonradiative channels, which will compete with the radiative process in fluorescence enhancement phenomena [75, 76].

In this chapter, we investigate the spontaneous decay rate of a single dipole emitter close to a gold nanoparticle. This issue has already been addressed numerically in various configurations, involving particles [77] or using theoretical methods [78] beside experimental demonstrations involving tips [79] and/or surfaces [80]. Our focus is on the distance and orientation dependence of the radiative and non-radiative decay rates. Our objective here is not to discuss the fluorescence enhancement factor, but to get a better understanding of the radiative and nonradiative decay rate enhancement near a gold nanoparticle.

## 4.2 Damping mechanisms of Gold Nanoparticle(GNP) plasmons

Plasmon excitations in a quasi particle picture, dissipate their energy as population decay which can be either through radiative [81] or nonradiative decay [82], as shown schematically in Fig. 4.1.

Plasmons, which are the collective oscillation of the conduction electrons, can radiate their energy back by emitting a photon under specific conditions known as radia-

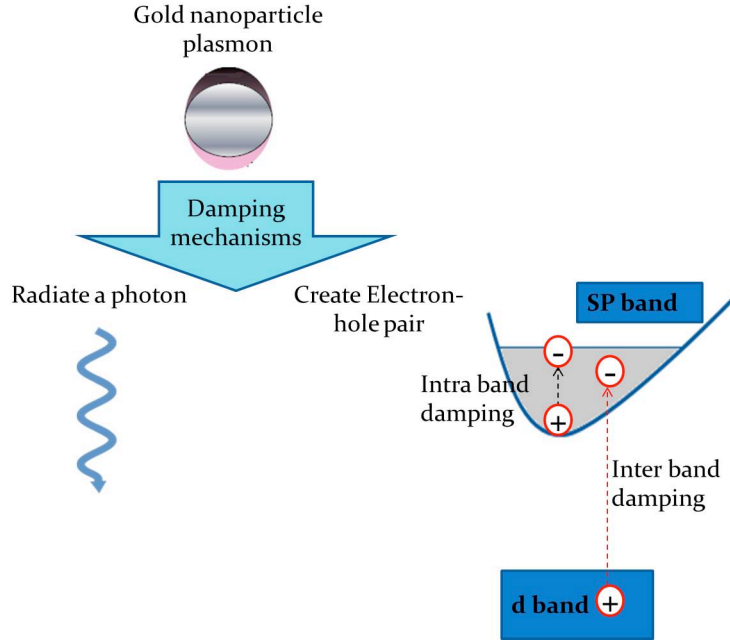


Figure 4.1: Gold Nanoparticle(GNP) plasmons decay either radiatively (left) or non-radiatively by creation of electron-hole pairs (right). (Based on Fig.4.5 of Ref.[83])

tive damping. Unlike radiative damping, the nonradiative damping phenomenon involves a process named electron-hole pair creation [29]. Through this process, the electron-hole pairs are excited, even within the conduction band known as intra-band excitations, or between the inner lying d-band electrons and the conduction band (sp-band for noble metals). The energy dissipated through these nonradiative channels is transferred ultimately into heat. There is a connection between the gold nanoparticle cross sections discussed in chapter 3 and time constant of decay processes. The decay time constants as  $T_{tot}$ ,  $T_{rad}$  and  $T_{nonrad}$  (total, radiative and nonradiative decay, respectively) are connected with extinction, scattering and absorption cross sections, respectively [83].

### 4.3 Molecule/atom near a gold nanoparticle

The spontaneous emission rate of a molecule in free space can be calculated using the Fermi golden-rule transition rate [11]:

$$\gamma_{gn,em} = \frac{\omega^3}{3\pi\hbar\epsilon_0c^3}|p_0|^2|F(n,m)|^2, \quad (4.1)$$

where  $\gamma_{gn,em}$  is decay rate from state  $|e; m\rangle$  to  $|g; n\rangle$  ( $m$  and  $n$  correspond to vibrational levels), and  $\omega$  is the angular frequency corresponding to the transition energy. For a two-level system without any vibrational levels, the decay rate and the angular frequency are equal to  $\gamma_{ge}$  and  $\omega_{ge}$ , respectively.  $p_0$  is the transition dipole moment between the electronic states and expressed as the product of elementary charge  $e_e$  and a dipole length  $l_{dip}$ . In our model we assume  $l_{dip} = 1\text{\AA}$ .  $F(n, m)$  is a Franck Condon factor, i.e., the overlap between state  $|n\rangle$  in the ground state oscillator potential and state  $|m\rangle$  in the excited state potential. By including this factor, we can model molecular electronic levels, as well as atomic levels. The simplest Franck Condon factor for the transition between state 0 of the ground state (no vibrational state) to 0 of the excited state (no vibrational state) is given by  $F(0, 0) = e^{-\frac{\alpha^2}{2}}$  [11], where  $\alpha$  is equal to 0.5 in the model for molecular system [29]. For modelling an atomic system, we can set the displacement between the two potentials to be zero. The GNP can enhance the excited state decay rate of any proximate atomic system by offering the nonradiative decay channels for the dipole, and by coupling radiative emission to a radiative localized surface plasmon mode. Therefore the transition rate is modified when the molecule is placed near the GNP by the factor  $M_d(\omega)$  known

as dissipation enhancement factor. The enhancement of decay rate will cause some interesting phenomena as quenched fluorescence, enhanced fluorescence, and surface enhanced Raman scattering [84].

There are many efforts to understand and model the molecule-molecule and molecule-nanoparticle interaction mechanisms. Theoretical models including Drexhage's work in 1970 [85] to investigate the molecule in proximity to the planar metal interfaces, consider the reflected field of the image dipole. In 1981, Gresten and Nitzan [72] investigated the optical properties of the molecules adsorbed on or enclosed in a dielectric particle. They calculated the dipole moment induced on the metal nanoparticle by the excited molecule. In their model, the expression of the normalized decay rate can be obtained by treating the emitter as a classical harmonic damped dipole oscillating at frequency ( $\omega_{ge}$ ).

#### 4.3.1 Decay rate modification calculations

To calculate the decay rate enhancement factor in the presence of a gold nanoparticle, the same model as Gresten-Nitzan model was employed. The system of radiating dipole interacting with an isolated GNP is solved using the finite-difference time-domain (FDTD) method. The quantum system is simulated by a point radiating dipole source in the near field of the nanoparticle. Parallel and normal orientations of the radiating dipole moment relative to the nanoparticle surface are also examined. The analysis of the FDTD results relies on the fact that, for an atomic dipole transition, the normalized quantum mechanical decay rate can be related to the

normalized classical power radiated by the dipole. The relation is as follows:

$$\frac{\gamma}{\gamma_0} = \frac{P}{P_0}, \quad (4.2)$$

where  $\gamma$  and  $P$  are the decay rate and radiated power in the presence of the environment, while  $\gamma_0$  and  $P_0$  are the decay rate and power emitted by the same dipole in free-space. In the presence of absorption, this classical approach allows one to calculate separately the radiative decay rate  $\gamma_R$  (proportional to the farfield radiated power) and the nonradiative decay rate  $\gamma_{NR}$  (proportional to the power absorbed by the environment) [86].

Three-dimensional FDTD simulations [61, 87] were performed using the program FDTD Solutions (version 7.5.3) from Lumerical Solution, Inc. (Vancouver, Canada). A time-windowed dipole source, radiating at a fixed wavelength, was used to mimic the emission of a two-level quantum system.

In our FDTD simulation, a set of six frequency-domain surface monitors has been used to create a box around the system. The total power radiated by the system is measured by integrating the real part of the Poynting vector over all six surfaces. To calculate the relative change in radiated power, the measured power was normalized to the analytic expression for the power radiated by a dipole source in a homogeneous environment (in this case, air) that is well-known [58]. In our calculations, the spacing of the GNP from the two-level system is varied to get the variation of decay enhancement versus distance from the GNP surface. The decay rate modifications have been calculated using the above method for the proposed system (see chapter

5) of a gold nanoparticle with radius  $r = 20$  nm, and an emitter with emission wavelength  $\lambda = 520$  nm corresponding to the  $\hbar\omega_{ge} = 2.38$  eV of the atomic system. The mesh size equal to 1 nm is applied in the mesh override region over the sphere and dipole region. Outside this region, automatic graded meshing was used with mesh accuracy 3.

We calculate and plot the radiative and nonradiative decay rate enhancements of the atomic system versus its distance to the GNP surface. Figures 4.2 and 4.3 show the results of the parallel and perpendicular orientations of dipole emitter to the GNP surface, respectively. The decay rates are normalized to the decay rates in free space.

As shown in Fig. 4.2, the normalized radiative decay rate for the parallel dipoles are less than one near the GNP, however Fig. 4.3 shows an enhancement for the radiative decay rate of the perpendicular dipoles around the GNP. These results are in agreement with the idea that the perpendicular dipoles exhibit in general larger fluorescence enhancement [88] around the metal nanoparticles. As the dipole goes farther from the GNP surface, the normalized radiative decay rate reaches 1, that it is approaches free-space conditions. Moreover, figures 4.2 and 4.3 show that, for both the parallel and perpendicular dipoles, nonradiative decays are enhanced as the dipole is positioned closer to the GNP. Their values also reach 0 as the dipole goes far from the GNP (this is the free space situation without any nonradiative channel). The appropriate calculated decay rates around the GNP at specific points can be found in Appendix C.



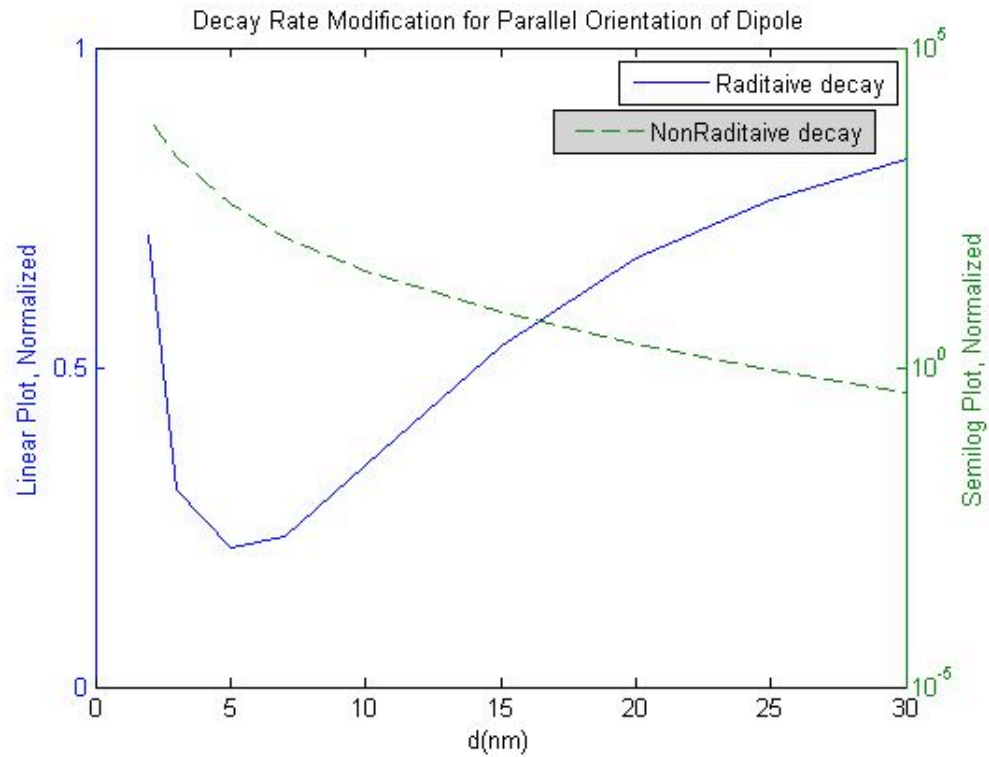


Figure 4.2: Radiative and nonradiative decay rate modification of a radiating point-dipole oriented parallel to a GNP surface at different distances between the dipole and GNP surface.

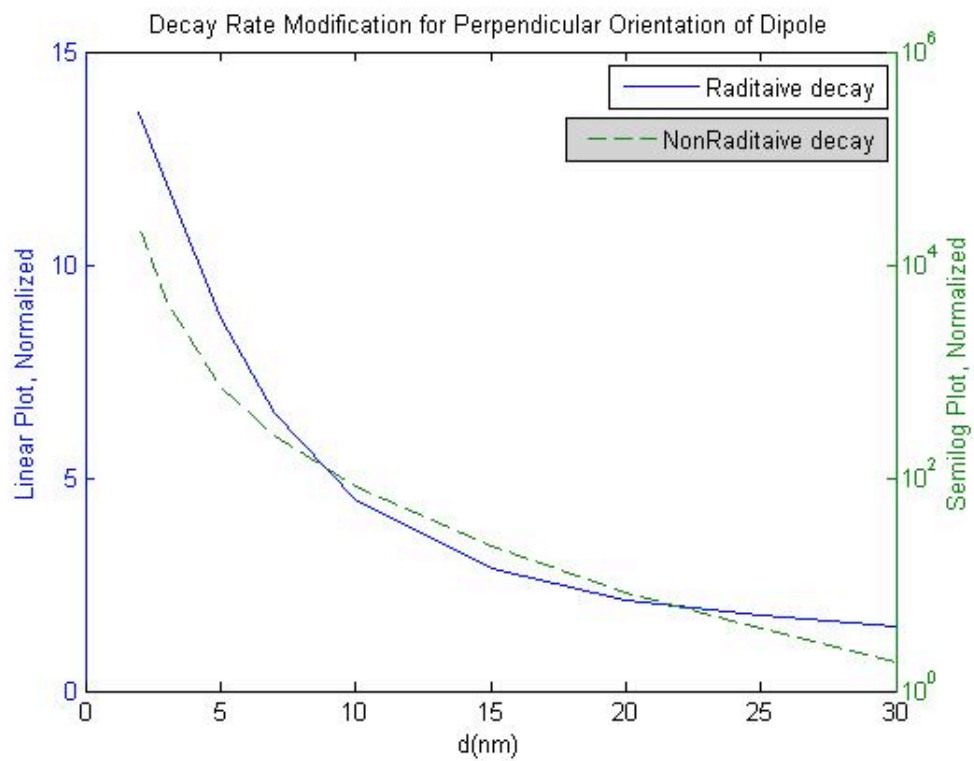


Figure 4.3: Radiative and nonradiative decay rate modification of a radiating point-dipole oriented perpendicular to a GNP surface at different distances between the dipole and GNP surface.

## Chapter 5

# Interplay of Control Field and Spontaneous Emission in Purification of a Qubit near a GNP

### 5.1 Introduction

Manipulating quantum systems by using time-dependent electromagnetic fields remains one of the primary interests in different physical processes ranging from the control of chemical reactions [89, 90, 91] to quantum computing [92]. In recent years, the interaction of the system with the environment has been actively considered [93]. This represents more realistic situations, but also more challenging control scenarios than for closed quantum systems [94].

Decoherence of quantum systems [95] due to the interaction with the environment causes reduction of state purity and loss of coherence. This results in leakage of system information to the environment. Preservation of state purity and the retention of quantum information is of primary importance in quantum information processing [92] and quantum coherent control [96]. Furthermore, quantum cryptography, teleportation or computation [97], rely on an ample supply of qubits in nearly pure quantum states. However, maintaining unknown and uncorrupted entanglement or superpositions in the presence of the coupling to the environment is usually a difficult task. A great deal of recent research has been devoted to issues such as

entanglement purification [98]. To fight against decoherence by the environment, it is fundamental to decouple as much as possible the system from it [99], or to study methods for preserving (or restoring) the entanglement and the purity of the states. So the study of the purification of a quantum system has attracted much attention [100, 101, 102, 103, 104, 105]. Various methods have been developed for this goal, such as quantum error-correcting codes [106, 107] decoherence-free subspaces or noiseless subsystems [108, 109, 110], strategies based on feedback [111] or stochastic control [112, 10], and dynamical decoupling [113, 114, 115].

Although under most circumstances, dissipation leads to an increase in entropy (or a decrease in purity) of the system, there is an important class of problems for which dissipation with external control can decrease the entropy (or increase the purity) of the system [116]. In such systems, there is an interplay of the Hamiltonian part of the dynamics, which is controllable, and the dissipative part of the dynamics, which can be modified in controllable way. The strategy is to control the Hamiltonian portion of the evolution in such a way that the dissipation causes the purity of the system to increase rather than decrease.

The goal of this work is to find the strategy that leads to maximal purity at the steady state time. We propose a scheme to enhance the purity of a single qubit which interacts with its environment through an amplitude-damping quantum channel in presence of a gold nanoparticle (GNP). We present a framework solving the Liouville-von Neumann (LVN) equation [117] that describes the dynamics of a two-level atom interacting with coherent field in a dissipative environment (see Chapter 2). Our calculation shows that by driving a two-level system in proximity to a GNP, we can

prepare a supply of qubits in nearly pure quantum states without cooling to the ground state, and on timescales much faster than typical spontaneous decay times.

## 5.2 Motivations

This work is motivated by the potential for enhanced quantum surface interactions as follows:

### 5.2.1 Quantum Surface Enhanced Purification and Quantum Control of a Qubit

In quantum information processing systems, information is stored in the quantum states of a physical system. Qubits are in general two-level quantum systems such as the ground and excited states of an atom, the vertical and horizontal polarization of a single photon, or the two spin states of a spin  $1/2$  particle. In the real world, however, there are no perfectly isolated systems. Real systems suffer from unwanted interactions with their environments and are hence open. In quantum information processing systems, these interactions manifest themselves as decoherence, which damages the information that the system encodes, thus leading to errors. Coherence plays a vital role in quantum information theory and, in order to understand it, we need to study the properties of states of open quantum systems.

The most general description of open systems is provided by the density matrix formalism (see chapter2). The density matrix formalism also provides a description of a system whose precise state is not known. The density matrix is capable of

describing any mixed state in quantum mechanics, ranging from pure states that are solutions of the time domain Schrödinger equation (TDSE), to completely incoherent states. There are several common ways of characterizing how close an arbitrary mixed state  $\rho$  is to a pure state. These measures can be generally termed purity measures or purities. The most common, and perhaps the simplest measure is  $Tr(\rho^2)$  [118]. For any density matrix,  $0.5 < Tr(\rho^2) \leq 1$ , with equality only for a pure state. Thus, the larger the value of  $Tr(\rho^2)$ , the closer a state is to being pure. Another useful measure is also the von Neumann entropy,  $S_{VN} = -kTr(\rho \ln \rho)$  [119].

Generally, in quantum information, one has to guarantee single- or (coupled) multi-qubit coherence (purity) on the timescales which are required for performing a certain task, which need to be shorter than the timescales on which detrimental effects such as the coupling to uncontrolled degrees of freedom manifest themselves.

### 5.2.1.1 Amplitude Damping Quantum Channel

Consider a single qubit which is initially in a pure state, and which interacts with its environment in an arbitrary manner. A kind of interaction is referred to as an amplitude damping quantum channel and we denote it as  $\Phi$ . The channel acts on an input state  $\rho$ , yielding the output state  $\Phi(\rho)$ . This channel provides a simple model of the decay of the excited state of a 2-level atom due to spontaneous emission of a photon. If the system is in the excited state  $|1\rangle$ , then it has a probability  $\gamma_{eg}$  of decaying to its ground state  $|0\rangle$ , emitting a photon in the process. Consider applying the channel  $n$  times in succession, then the final state of the atom is its

ground state. The amplitude damping channel is an example of a quantum channel which takes a mixed initial state  $\rho = \sum_{i,j=0}^1 \rho_{ij} |i\rangle\langle j|$  to a pure final state  $(\rho_{00} + \rho_{11})|0\rangle\langle 0|$  (asymptotically).

Note that in this case the decrease of entropy should not be looked upon as an information gain. This is because every mixed state decays to the ground state under repeated actions of the amplitude damping channel, and hence we lose the ability to distinguish between different possible preparations of the mixed state. The spontaneous emission is intrinsically uncontrollable, i.e., we cannot induce spontaneous emission.

We can affect the rate of decay by moving around a gold nanoparticle (GNP). As seen in chapter 4, the transition rate is enhanced when the molecule is placed near metallic nanoparticles; i.e. we can control the rate of decay by changing our atom-GNP configuration. According to this effect, we have proposed a method to do the purification without cooling the population to the ground state. We consider a quantum system consisting of a two level atom (qubit) interacting with a coherent field in a dissipative environment. By applying and controlling a classical driving field, we desire to enhance the amount of system purity while at the same time we have the excited state reasonably populated.

## 5.2.2 Modeling of the Surface Enhanced Processes in Dye molecules

The phenomenon of enhancing and quenching of fluorescence as a result of modified dipole decay rates was investigated already more than 30 years ago [72]. The

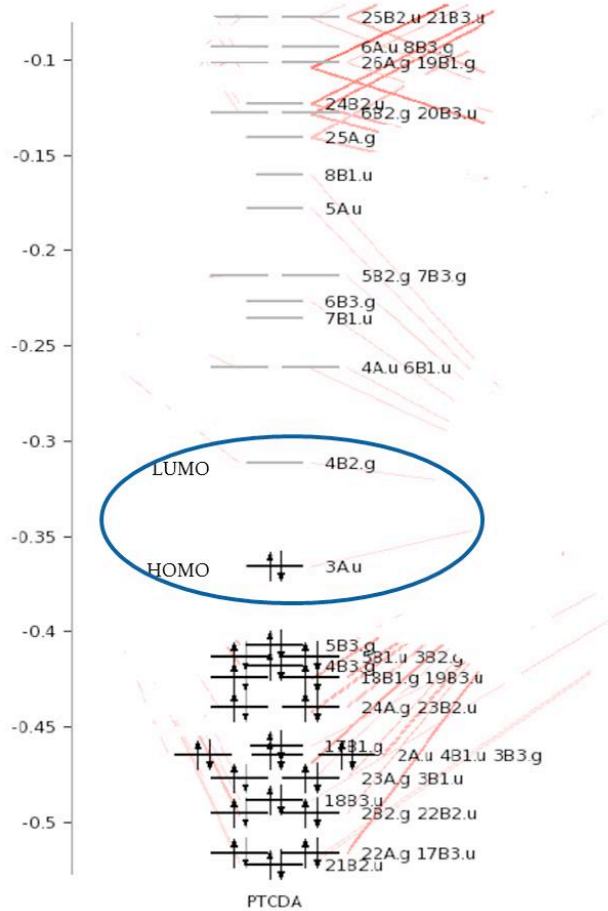


Figure 5.1: Energy-level diagram of PTCDA [121].

modeling of surface enhanced processes such as surface enhanced fluorescence (SEF) at a quantum level provides an additional motivation for this study. We choose to model the SEF of a dye molecule, which has received a great deal of attention in recent years due to its opto-electrical properties and its potential applications in fluorescent spectroscopy [120].

PTCDA (perylene tetracarboxylic dianhydride  $C_{24}H_8O_6$ ), an organic semiconductor dye molecule, is selected as the target. Fig. 5.1 shows the energy levels of the PTCDA and the highest occupied molecular orbital (HOMO) and the lowest unoc-



cupied molecular orbital (LUMO) which are of interest to us as the two-level quantum system. The PTCDA absorption spectrum [122] is dominated by the vibronic progression of the HOMO to LUMO transition with the peak at 2.38 eV (520 nm). It is interesting to note that the HOMO to LUMO transition in all PTCD derivatives is found to be separated quite significantly from the other transitions in the UV/Vis spectrum. This is due to a large gap between the HOMO and (HOMO-1) as well as the LUMO and (LUMO+1). Therefore, a two level model is a very good model for these molecules. Using this model we will continue with the dynamics and the control of a two-level system. The control can be treated theoretically by a classical or a quantized electromagnetic field, but in this work we consider only the classical limit for the field.

### 5.3 Quantum dynamics of a single qubit in interaction with the radiation field in the presence of a GNP

Consider a two-level atom under a periodic force by an oscillating electric field  $E \cos(\omega t)$ , with the linearly polarized field parallel to the  $\hat{z}$ -direction which is emitted in the  $\hat{y}$ -direction. To improve our model, it is worth mentioning that the external control fields, no matter how complicated, can not change the value of the purity of the state in a closed quantum system [15]. Therefore, to achieve a true purification and modify the timescale needed to prepare a qubit in a steady state, we need to add spontaneous emission to the model. We can modify and/or amplify the spontaneous emission of single atoms or molecules using simple nanostructures in a controlled

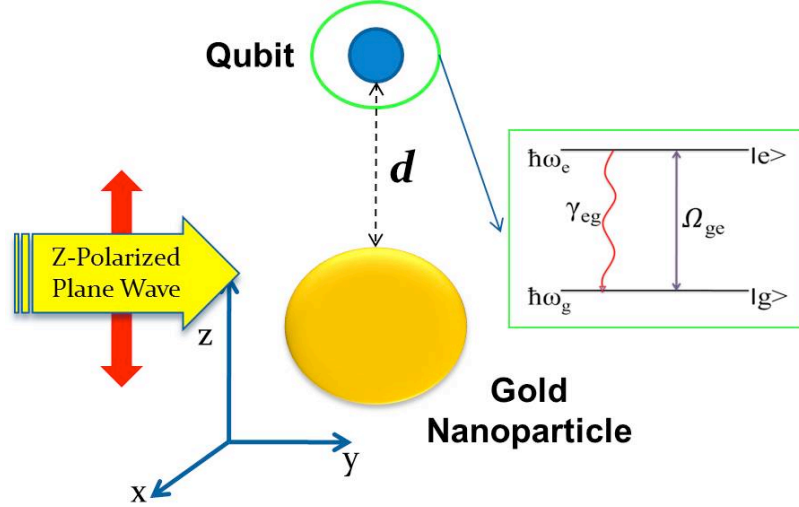


Figure 5.2: Schematic illustration of the model system (Consisting of a qubit placed near a GNP, which are excited by the  $\hat{z}$ -polarized plane wave).

way. Our schematic model for qubit preparation which includes a GNP is presented in Figure 5.2.

As we discussed in Chapter 3, the light incident onto a metal particle can excite localized surface plasmon (LSP) resonances and thus enables the particle to enhance the atomic excitation rate by increasing the local electric field. At the same time the particle can enhance the molecular decay rate by offering the nonradiative decay channels for the molecular dipole, and by coupling radiative molecular emission to a radiative LSP mode (see chapter4).

Here we present a theoretical investigation of how the quantum state preparation is influenced by dipole orientation with respect to both the particle and the exciting field. The calculation was done in a two-step process using a semiclassical model. In the first step, we computed the electric field components at the position of the atom

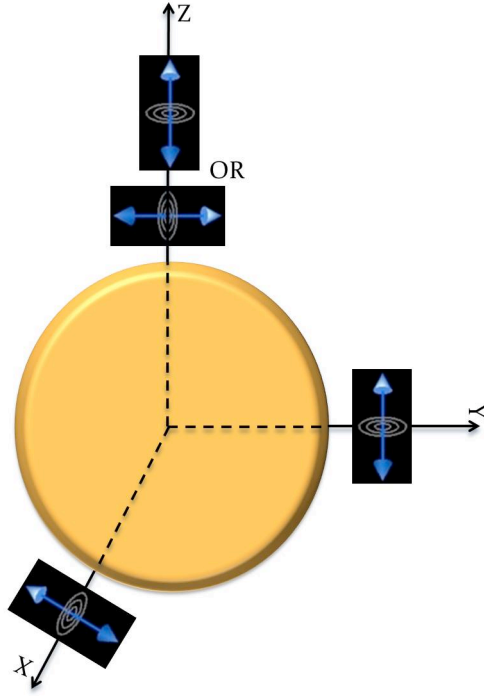


Figure 5.3: Possible dipole-GNP orientations.

using results of chapter 3. In the second step, in order to explore the particle-2LS interaction, a classical dipole emitter was used to model the 2LS and excite the system (see chapter 4). We assumed that the parallel orientation of the dipole moment relative to the nanoparticle surface is excited only by the tangential component of electric field around the GNP, while only the radial component contributes to the dipole with the perpendicular orientation [9]. From chapter 3 investigations, we know that component  $E_z$  exists all around the nanoparticle; however, the  $E_y$  and  $E_x$  components vanish completely in the equatorial plane. The possible nanoparticle and quantum dipole configurations along the X, Y, and Z axes shown in Fig. 5.3.

The two-level system has energy eigenstates  $|g\rangle$  and  $|e\rangle$ . The frequency  $\nu_{ge} = 576 THz$ , defined from the energy-level separation  $E_e - E_g$  as ( $\hbar\omega_{ge} = E_e - E_g =$

2.38eV). These values approximate the HOMO and LUMO levels of a single PTCDA molecule fairly well . The system is illuminated by a  $\hat{z}$ -polarized plane wave incident from the left along the  $-\hat{y}$ -axis. For a GNP with  $r = 20$  nm, the maximum electromagnetic enhancement corresponds to a laser photon energy around 2.29 eV with  $\lambda = 540$  nm (see chapter 3). We choose the same specifications for our incident light, that is also near-resonant with the two-level system transition frequency. The surrounding medium of the system is considered to be air (dielectric constant = 1).

### 5.3.1 Method

We obtain the evolution equation for the statistical operator of our two-level system ( $\rho = |\psi\rangle\langle\psi|$ ) by solving the Lindblad master Eq. 2.17 that will result in the system of equations shown in Eq. 5.1. These equations are derived by the same method as our analysis in Section 2.4.

$$\begin{aligned}
\dot{\rho}_{gg} &= \frac{i\Omega_{ge}}{2}(\rho_{ge} - \rho_{eg}) + \gamma_{eg}\rho_{ee} \\
\dot{\rho}_{ee} &= \frac{i\Omega_{ge}}{2}(\rho_{eg} - \rho_{ge}) - \gamma_{eg}\rho_{ee} \\
\dot{\rho}_{ge} &= \frac{i\Omega_{ge}}{2}(\tilde{\rho}_{gg} - \rho_{ee}) + \rho_{ge}(-i\delta_0 - \frac{\gamma_{eg}}{2}) \\
\dot{\rho}_{eg} &= \frac{i\Omega_{ge}}{2}(\rho_{ee} - \rho_{gg}) + \rho_{ge}(i\delta_0 - \frac{\gamma_{eg}}{2}), \tag{5.1}
\end{aligned}$$

where the  $\Omega_{ge}$  is calculated using Eq. 2.11 , including an electric field enhancement parameter  $M(\omega_L)$  at the position of the molecule. According to the position and orientation of the quantum system dipole, the relation of the enhancement factor to the appropriate electric field component can be seen in Fig. 3.9.

The transition dipole moment between the ground state and the excited state will be calculated using the general formula as follows [29]:

$$\mu_{nm} = p_0 \cdot F(n, m), \quad (5.2)$$

where  $p_0$  is the transition dipole moment between the electronic states and  $F(n, m)$  is a Franck Condon factor, both are calculated as discussed in chapter 4.

The next important parameter  $\gamma_{eg}$  (that includes the enhanced dissipation factor caused by the GNP proximity to the two-level quantum system, see chapter 4) has been calculated using the Eq. 4.1. Different dissipation factors  $M_d(\omega)$  related to a variety of dipole moment orientations and distances from the GNP surface can be found in figures 4.2 and 4.2, and appendix C.

## 5.4 Results

As mentioned in section 2.4, the system of equations 5.1 is solved numerically using a MATLAB code. The code solves the coupled differential equations using an in-built solver function known as ODE45. ODE45 is based on an explicit Runge-Kutta (4,5) formula, the Dormand-Prince pair. It is a one-step solver; in computing  $y(t_n)$ , it needs only the solution at the immediately preceding time point,  $y(t_{n-1})$ . This function requires (i) the initial boundary conditions (the density matrix at  $t=0$ ) (ii) the variables which appear in the system of equations (time-dependent Rabi frequency, its associated detuning and the decay rate of the states in the system) and (iii) the time for which the simulation must run. After the ODE45 function has been called, the program outputs the value of the density matrix elements at

each time step in the simulation time period.  $\rho_{gg}$  and  $\rho_{ee}$  correspond to the state populations and  $\rho_{ge}$  and  $\rho_{eg}$  show the system coherence.

#### 5.4.1 Comparison of analytical and numerical solutions

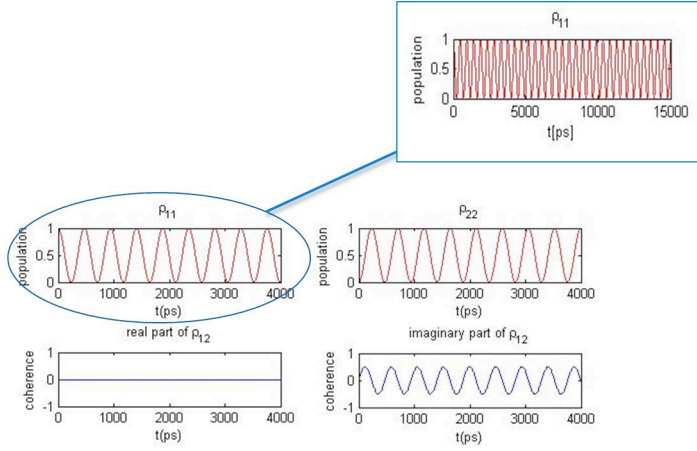
To evaluate the accuracy of the numerical solutions, the system of Eq. 5.1 is solved analytically for some special cases with further approximations using Equ. 2.21 , and the results are compared to the numerical ones in Figures 5.4 and 5.5. As the analytical solution is used, the detuning between the excitation field energy and the two level system transition energy is equal to 0 ( $\delta_0 = 0$ ) in both examples.

Figures 5.4 and 5.5 illustrate the results corresponding to cases with and without any decay rate from the excited state to the ground state. As is shown, there is a perfect correlation between the results of numerical and analytical solutions. The  $\rho_{11}$  mean percent error between analytical and numerical solutions averaged over  $t = 15000 ps$ , is approximately 0.093%.

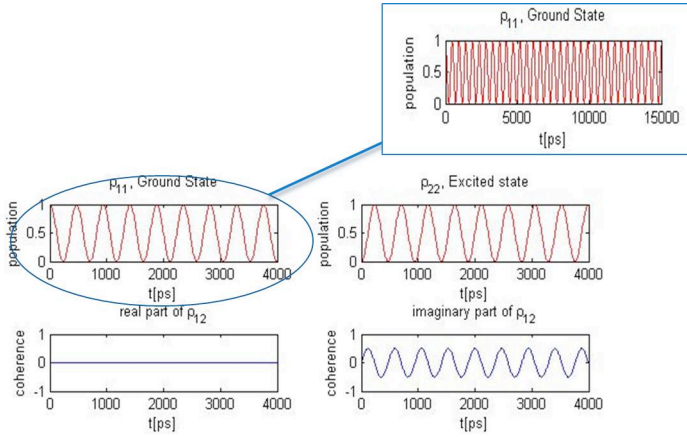
Now let us examine the numerical codes to solve the general problem that includes a field in near resonance conditions and the GNP effects.

#### 5.4.2 Preparing a single qubit in the superposition of the two states

The goal is to prepare a single qubit in the superposition of the two states as  $|\psi\rangle = (\frac{\sqrt{3}}{2})|0\rangle + (\frac{1}{2})|1\rangle$ , starting from an initial pure state, where all the population is in the ground state. As we have seen in chapter 3, the maximum field enhancement around a GNP is in the  $\hat{z}$ -direction. Moreover, the radial field component that will

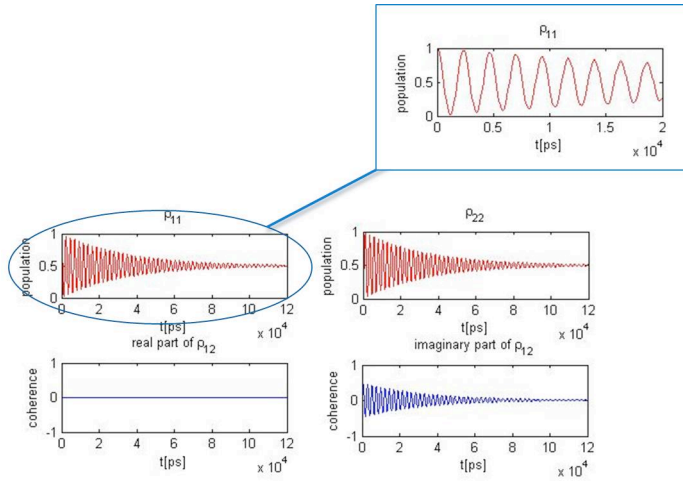


(a) Analytical solution

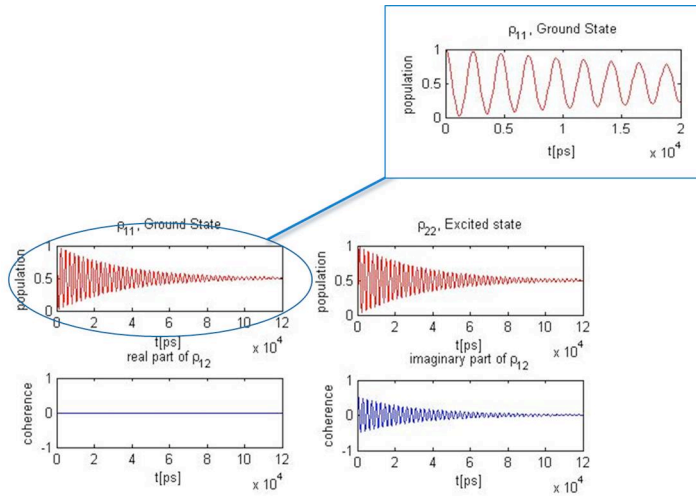


(b) Numerical solution

Figure 5.4: Calculated population and coherence of the two-level system vs. time, with  $\hbar\omega_L = 2.38 \text{ eV} (\delta_0 = 0)$ ,  $E_L = 10^5 \text{ V/m}$ ,  $\gamma_{eg} = 0$ . Initially prepared state was in a pure state with all population in the ground state (a) Analytical solution (b) Numerical solution.



(a) Analytical solution



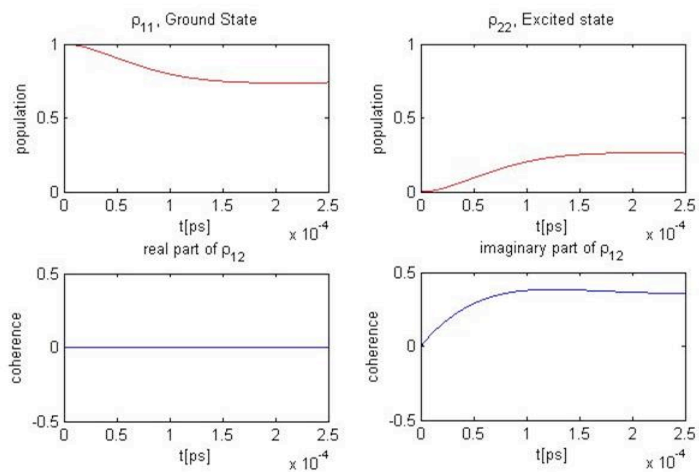
(b) Numerical solution

Figure 5.5: Calculated population and coherence of the two-level system vs. time, with  $\hbar\omega_L = 2.38 \text{ eV} (\delta_0 = 0)$ ,  $E_L = 2 \times 10^4 \text{ V/m}$ ,  $\gamma_{eg} = 3.93e7 \text{ s}^{-1}$  (decay rate for a molecule in free space). Initially prepared state was in a pure state with all population in ground state (a) Analytical solution (b) Numerical solution.

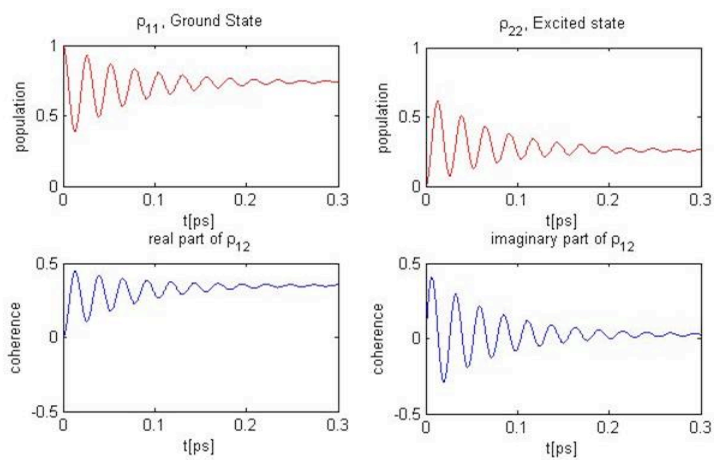


excite the perpendicular atomic dipole moment will have the maximum enhancement in the same  $\hat{z}$ -direction (see Fig 3.9), and the tangential component that will excite the parallel atomic dipole moment will have the maximum enhancement in the  $-\hat{y}$ -direction (see Fig 3.9). Therefore, we will start by putting our two level system near a GNP, first in the  $\hat{z}$ -direction and secondly in the  $-\hat{y}$ -direction at different distances. To prepare the qubit in the intended superposition, it is necessary to use different laser amplitudes corresponding to the position of the qubit according to the GNP. Figures 5.6 and 5.7, display a number of qubits evolving in time according to the different qubit-particle separations,  $d$ , in the  $\hat{z}$  and  $-\hat{y}$  directions.

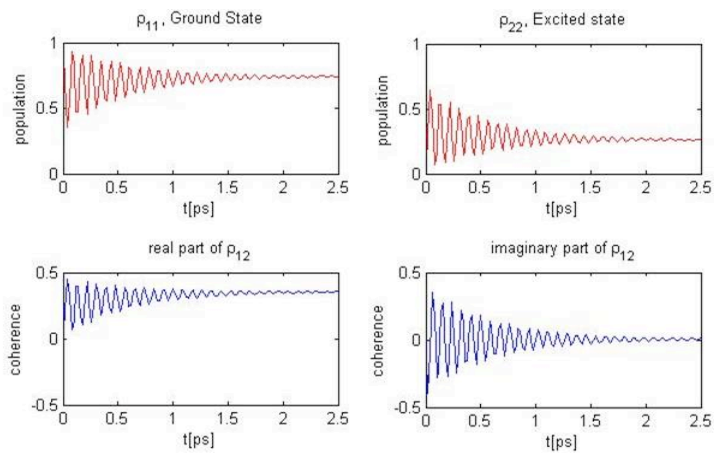
The results presented in Figures 5.6 and 5.7, show the influence of dissipation on the collapse and revival of the Rabi oscillation amplitudes. As is well known, the amplitude of the Rabi oscillation decreases progressively at each successive revival due to decays such as spontaneous emission [123]. Furthermore, it is shown that as the strength of the applied field and decay rate changes at each point, the system approaches a steady state even in the monotonic regime (subplot (a)) or in an oscillatory fashion (subplot (b) and (c)). It is worth noting that, for spaces smaller than 2 nm, we will not see any significant results, due to rapid quenching of the excitation via LSP channels for small  $d$  [29, 84]. The main feature of these results, which of importance to the experimentalist, is to determine how fast the system reaches the steady state and how intense the laser should be to lead the system to that point. According to Figures 5.6 and 5.7, the lowest laser amplitude needed to prepare the intended qubit is  $E_L = 1.8 \times 10^8 \text{ V/m}$ , for  $\vec{d} = 5 \text{ nm}$  in the  $\hat{z}$ -direction. At this position the system will reach the steady state much faster than



(a)  $\vec{d} = 2\hat{z}$  nm,  $E_0 = 9 \times 10^9$  V/m

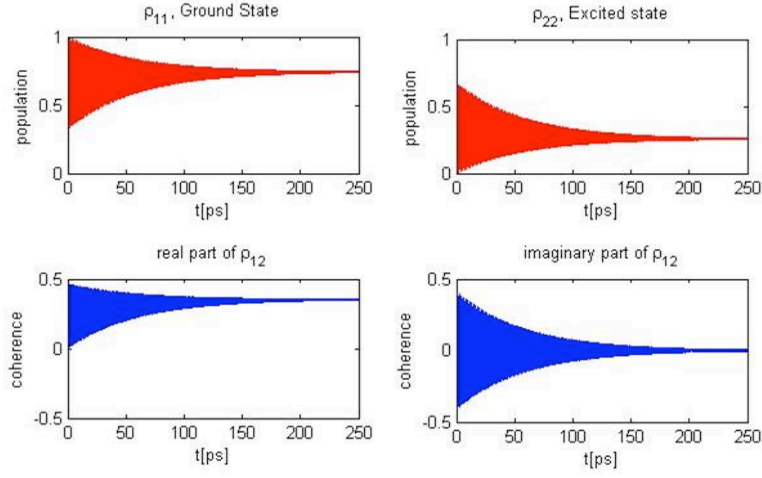


(b)  $\vec{d} = 5\hat{z}$  nm,  $E_0 = 1.8 \times 10^8$  V/m

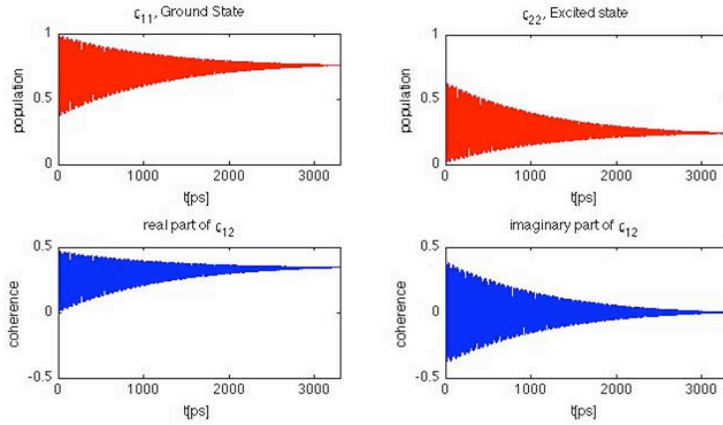


(c)  $\vec{d} = 7\hat{z}$  nm,  $E_0 = 2.4 \times 10^8$  V/m

Figure 5.6

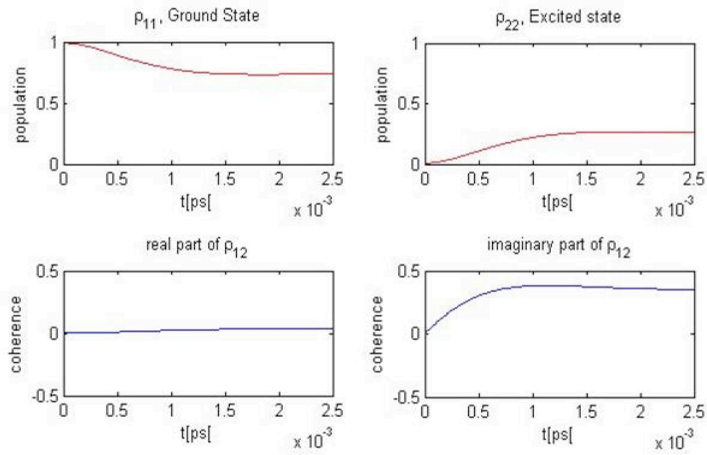


(d)  $\vec{d} = 15\hat{z}$  nm,  $E_0 = 5.1 \times 10^8$  V/m

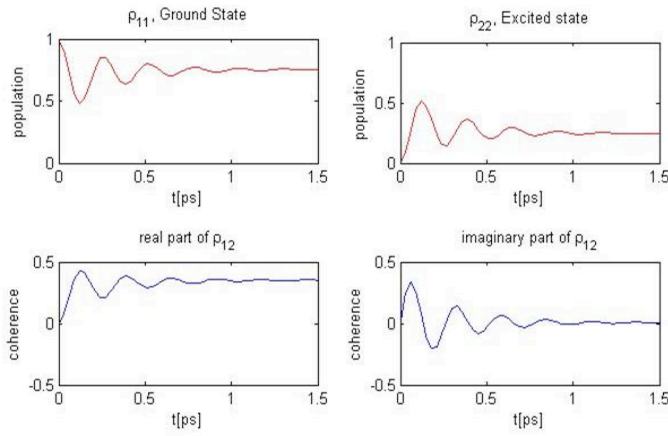


(e)  $\vec{d} = 25\hat{z}$  nm,  $E_0 = 8.2 \times 10^8$  V/m

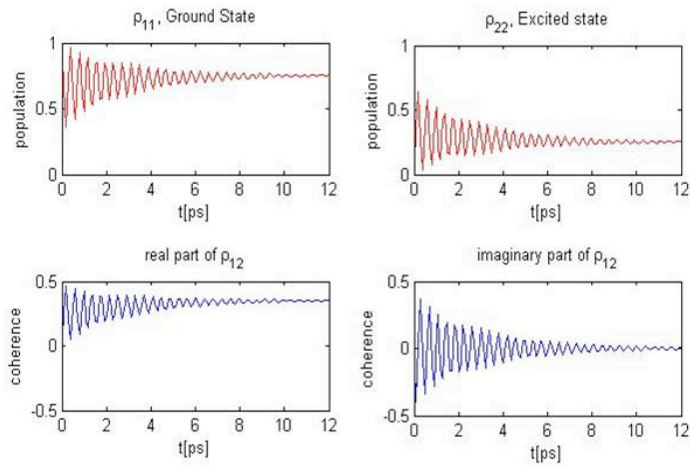
Figure 5.6: Calculated state evolution for a qubit placed near a spherical ( $r=20$  nm) gold nanoparticle. Different plots correspond to different particle-qubit separations along the  $\hat{z}$ -axis, with  $\hbar\omega_L = 2.29$  eV,  $\hbar\omega_{ge} = 2.38$  eV, and perpendicular dipole orientation.



(a)  $\vec{d} = -2\hat{y}$  nm,  $E_0 = 3.9 \times 10^{10}$  V/m

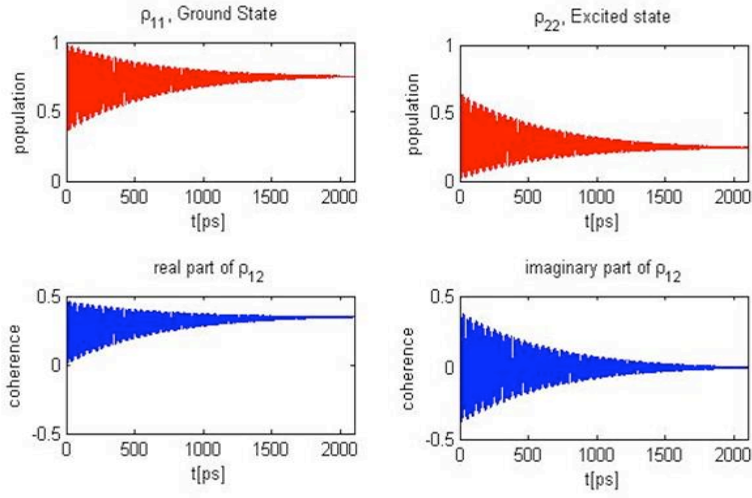


(b)  $\vec{d} = -5\hat{y}$  nm,  $E_0 = 4.7 \times 10^9$  V/m

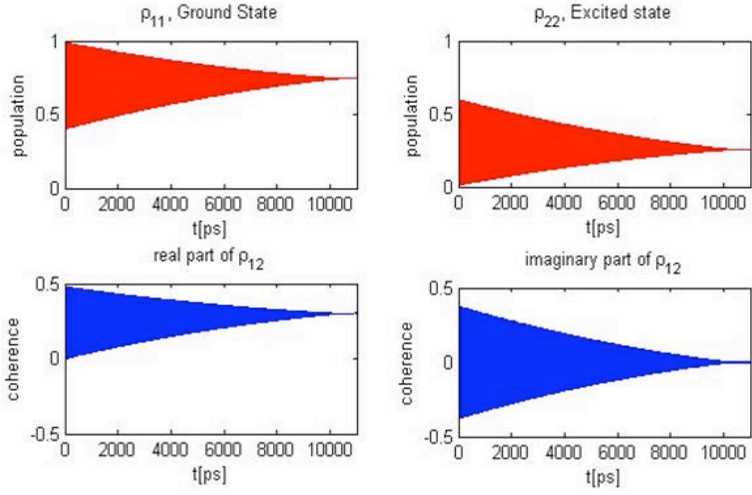


(c)  $\vec{d} = -7\hat{y}$  nm,  $E_0 = 4.3 \times 10^9$  V/m

Figure 5.7



(d)  $\vec{d} = -15\hat{y}$  nm,  $E_0 = 2.9 \times 10^9$  V/m



(e)  $\vec{d} = -25\hat{y}$  nm,  $E_0 = 1.6 \times 10^9$  V/m

Figure 5.7: Calculated state evolution for a qubit placed near a spherical ( $r=20$  nm) gold nanoparticle. Different plots correspond to different particle-qubit separations along the  $-\hat{y}$ -axis, with  $\hbar\omega_L = 2.29eV$ ,  $\hbar\omega_{ge} = 2.38eV$ , and parallel dipole orientation.

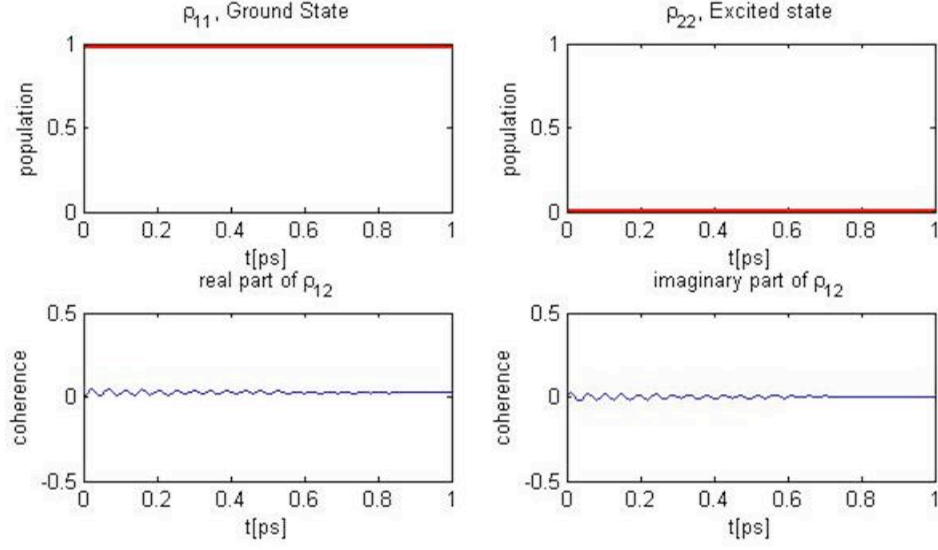


Figure 5.8: Calculated state evolution for a qubit placed at  $\vec{d} = 5\hat{z}$  nm near a GNP. With  $\hbar\omega_{ge} = 2.38$  eV,  $\hbar\omega_L = 2.29$  eV,  $E_L = 1.8 \times 10^8$  V/m and parallel dipole orientation.

the typical spontaneous decay time. Furthermore, with this field magnitude, we are confident that just one of the possible atomic dipole modes in the  $\hat{z}$ -direction would be excited. Figure 5.8 illustrates the parallel dipole excitation contribution in the atomic population inversion positioned at the  $\vec{d} = 5\hat{z}$  nm excited with the laser amplitude valued at  $E_L = 1.8 \times 10^8$  V/m.

In order to prove our method efficient for single qubit preparation, the same qubit was prepared using only a coherent field in absence of any GNP in proximity to the qubit. Figure 5.9 shows a bare qubit preparation in free space in the superposition of two states as  $|\psi\rangle = (\frac{\sqrt{3}}{2})|0\rangle + (\frac{1}{2})|1\rangle$  like in the previous example, starting from an initial pure state with all population in the ground state.

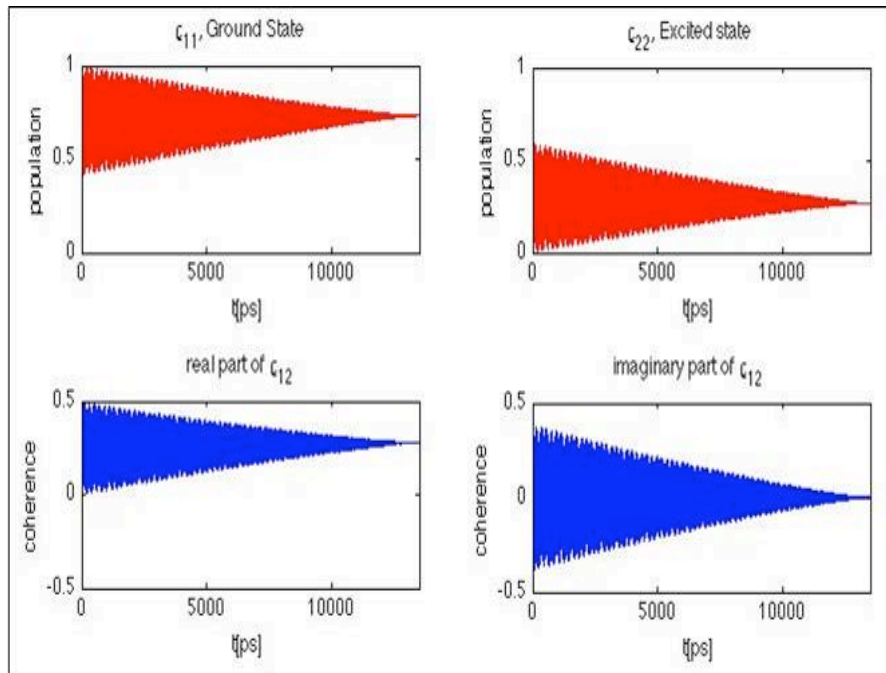


Figure 5.9: Calculated state evolution for a qubit excited by a classical field (i.e. without a proximate GNP).  $\hbar\omega_{ge} = 2.38 \text{ eV}$ ,  $\hbar\omega_L = 2.29 \text{ eV}$ ,  $E_L = 1.22 \times 10^9 \text{ V/m}$ .

Based on the results for the qubit in free space that is just controlled by a near-resonant field, and for the qubit subject to a near-resonant driving field in presence of a gold nanoparticle, it is obvious that preparing a qubit with a GNP needs less laser intensity (100 times) and is faster ( $1ps$  versus  $140ns$ ) compare to without a GNP, which is very important in quantum control and quantum information applications. In the next step, the purity of the prepared qubit will be investigated using the following calculations:

$$Purity = Tr(\rho^2) = \rho_{gg}^2 + \rho_{ee}^2 + 2|\rho_{ge}|^2. \quad (5.3)$$

The purity is calculated for the two-level system discussed in Fig. 5.6-b, which was placed near a GNP at  $\vec{d} = 5\hat{z}$  nm and excited with the laser field to transfer part of its atomic population to the excited state. The purity results are displayed in Fig. 5.10-a. Furthermore, to investigate the purity improvement, the same purity calculation has been done for the bare two-level system excited by the laser to have the same excited state population (Fig. 5.9) and the purity results are illustrated in Fig. 5.10-b. Note that the plots are shown until the steady state time.

Comparing the results in plots (a) and (b) of Fig. 5.10, we will see although in both attempts we tried to build the same final superposition state, purity of the final state differs from 0.87 with the GNP to 0.67 in the absence of any GNP. The steady state purity is achieved at  $0.3ps$  with a GNP, in contrast to  $14000ps$  with out a GNP.



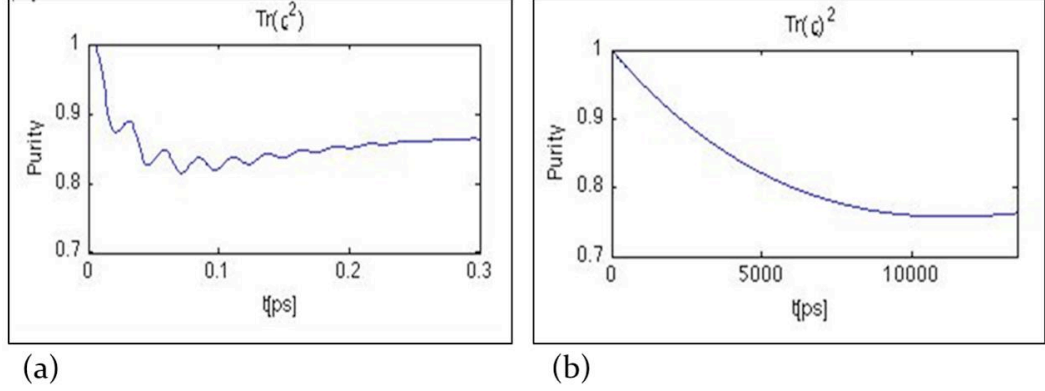


Figure 5.10: Calculated purity of state starting from an initial qubit in the pure state  $|\psi\rangle = |1\rangle$  with  $\hbar\omega_{ge} = 2.38eV$ , and  $\hbar\omega_L = 2.29 eV$ . The target is to produce a final superposition  $|\psi\rangle = (\frac{\sqrt{3}}{2}) |0\rangle + (\frac{1}{2}) |1\rangle$ , (a) The qubit positioned around a GNP at  $\vec{d} = 5\hat{z} \text{ nm}$ , with  $E_L = 1.8 \times 10^8 V/m$ , (b) Bare qubit with  $E_L = 1.22 \times 10^9 V/m$ .

#### 5.4.2.1 State preparation from initially totally mixed state

Now, I would like to investigate if the purity of the state can be increased. In this step, the goal is to prepare a qubit in the superposition  $|\psi\rangle = (\frac{\sqrt{3}}{2}) |0\rangle + (\frac{1}{2}) |1\rangle$ , but starting from a totally mixed initial state as follows:

$$\hat{\rho} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \quad (5.4)$$

Initially, the two-level system is just driven by the near-resonance field without any GNP around it (Fig 5.11).

As is shown in Fig 5.11, the purity will not change over time. However the electric field amplitude was increased, no population transfer was seen. This means that if the quantum system is initially in the totally mixed state, it is impossible to do

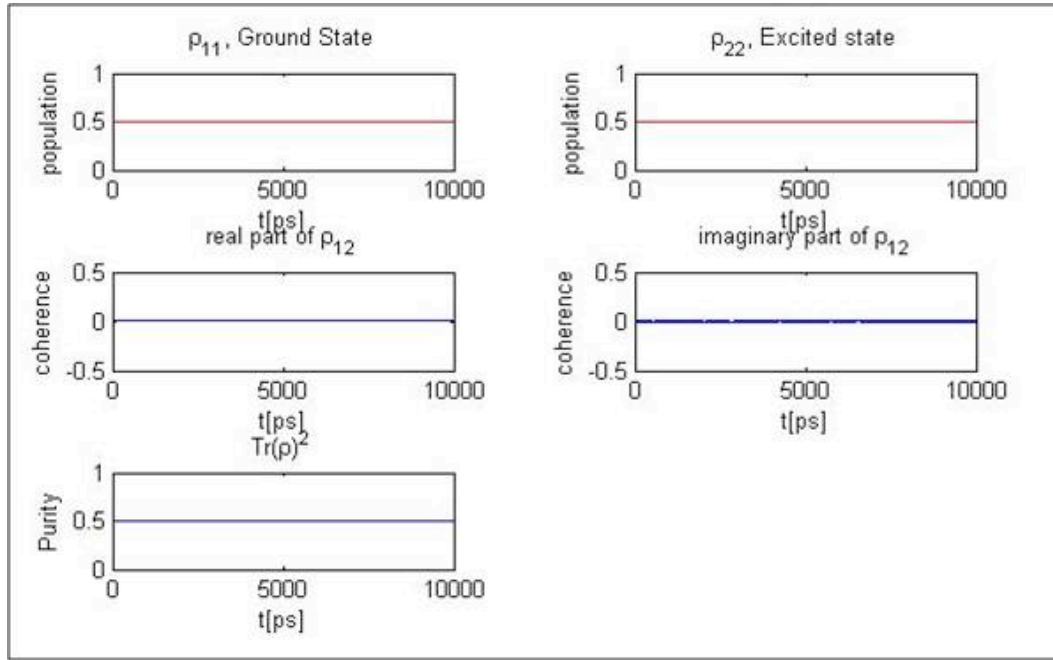


Figure 5.11: Calculated state dynamics and purity evolution for a qubit excited by the classical electromagnetic field with  $\hbar\omega_{ge} = 2.38 \text{ eV}$ ,  $\hbar\omega_L = 2.29 \text{ eV}$ , and  $E_L = 10^{11} \text{ V/m}$ , and initially in a totally mixed state.

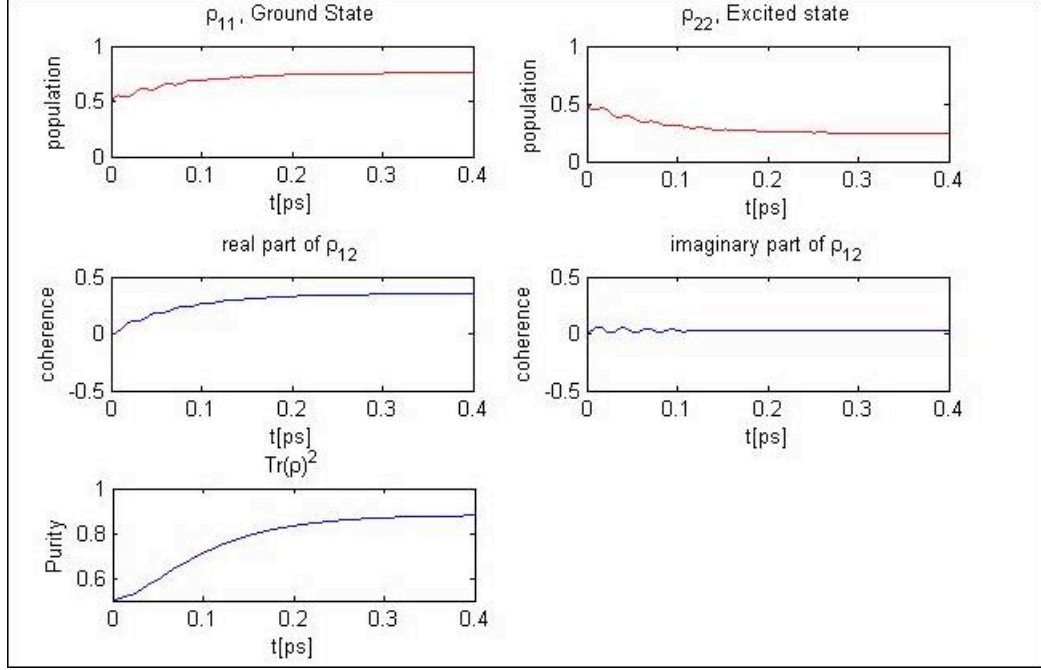


Figure 5.12: Calculated state dynamics and purity evolution for a qubit placed at  $\vec{d} = 5\hat{z}\text{nm}$  near a GNP with  $\hbar\omega_{ge} = 2.38\text{eV}$ ,  $\hbar\omega_L = 2.29\text{eV}$ , and  $E_L = 1.7 \times 10^8\text{V/m}$ , and initially in a totally mixed state.

purification using just the laser field excitation.

Next, the two-level system (qubit) is placed at the same point around the GNP where the lowest field energy is needed to populate the excited state, at  $\vec{d} = 5\hat{z}\text{nm}$ . As seen in Fig. 5.12, in proximity of a GNP, the purity of the system is improved about 30% and reaches 0.9, which is a very interesting result. As the decay rates enhance too much in presence of a GNP, it helps to collect all population in the ground state very fast and then the population will be easily excited by the appropriate excitation field. It is shown that in presence of a nanoplasmonic structure, it is possible to start from a totally mixed state and enhance the amount of system

purity while at the same time we have the excited state reasonably populated. The time needed for the steady state is about  $0.4 \text{ ps}$  which is still much faster than the typical spontaneous decay time.

## 5.5 Conclusion

The motivation for this work is to apply the method proposed by the Kall et al. [29] to investigate the surface-enhanced resonant Raman scattering and fluorescence, focusing on the interplay between electromagnetic (EM) effects and the quantum system dynamics as treated by a density matrix. While focus of their work is on the steady state solution of the equations, in this study, I have employed his model to investigate the dynamical evolution of a resonantly driven two-level system in presence of a gold nanoparticle. To use this method, we need to calculate the electric field enhancement factor as well as the modified decay rate near a GNP. I calculated these two parameters at definite positions around the GNP using FDTD. The Electric field modification calculations demonstrated that, while the corners of nanoparticle on the axis of polarization create the largest electromagnetic enhancements that is very important in LSPR applications, induced electric field components have remarkable values at the other positions around the GNP. As tangential and radial components contribute to the different dipole orientation excitation, their values are important to some applications like state purification. In the case of the GNP with  $r=20 \text{ nm}$  and  $\hat{z}$ -polarized excitation field at  $\lambda = 540 \text{ nm}$ , all three components of the electric field has been seen around the GNP.

A dissipation factor modification also was calculated through the radiative and nonradiative decay channels versus distance variation to the GNP surface. I have shown that for the molecule dipole emission at  $\lambda = 520$  nm , the radiative decay channel for the dipole orientation parallel to the surface, is almost quenched near the GNP with  $r = 20$  nm.

In the last chapter, I proposed a novel idea to use the effects of nanoplasmonics in proximity to a qubit to do state purification without cooling to the ground state. I was able to control the ratio between electric field enhancement and decay rate modification by changing three variables: the position of the two-level system around the GNP, orientation to the GNP surface, and electric field amplitude. Therefore, the time needed to reach to the steady state for a two-level system interacting with the light is improved. Furthermore, by systematically investigating the qubit preparation process, I was able to show that even though Hamiltonian dynamics itself can not increase the purity of a totally mixed state, positioning a nanoplasmonic structure like a gold nanoparticle beside the two-level system, can improve the state purification process.

This result has been presented at two international conferences [124, 125] and a manuscript is in preparation to a peer-reviewed journal.

## 5.6 Further works

There are many possibilities to extend this study. Presently, we have modeled the atomic/molecular system with a two-level system, which is a good approximation; however adding more levels to this system produce a richer problem. For example, using a 3LS with two fields near GNP, one can try to enhance the various three level system effects such as quantum control and electromagnetically induced transparency (EIT).

Furthermore, there are opportunities for optimizing the quantum system-nanoparticle configuration, using a strategy to optimize the number of particles and their size, shape, and arrangements. Aside from the geometry of the system, optimizing the control field specifications including detuning of the exciting field, control field pulse shape, and the number and sequence of control fields will significantly affect the results. It is suggested that an optimization algorithm such as Genetic algorithm to be used to optimize all variables together.

Using the quantum approach to analyze the problem of a quantum system near nanoplasmonic structures may give more accurate data about the system. For example; one may use the Jaynes-Cummings model in which the laser is quantized, which leads to entanglement, and see the results in state purification.

One of the most important problems in quantum information processing which is also the subject of many recent literatures, is doing purification on two coupled quantum states (entanglement purification). Using a nearby nanoplasmonic structure effects to do the entanglement purification is also one of the interesting extension to the

present work.

## Appendix A

FDTD code to analyze the field profile around the GNP (based on code in Ref.[16])

% Description:

% This file shows how to use analysis groups to do 2 types of analysis for 3D Mie scattering

%1) The absorption/scattering cross section

%3) The field enhancement calculation

% Choose which of the 2 possible analysis you want to do

do-cross-sections = 1; % set 0 to not perform this test, 1 to perform the test

do-field-enhancement = 1; % set 0 to not perform this test, 1 to perform the test

select("scat"); runanalysis; ?msg="Starting mie scattering tests";

if(do-cross-sections)

?" Calculating scattering and absorption cross sections";

f=getdata("total","f"); % get frequency data

lambda=c/f; % convert to wavelength

r = getnamed("sphere","radius"); the radius of the mie particle

% Calculate scattering cross-section

sigmascat = getdata("scat","sigma");

Qscat = sigmascat/(pi\*r<sup>2</sup>);



```

% Calculate absorption cross-section

sigmaabs = -getdata("total", "sigma");

Qabs=sigmaabs/(pi*r^2);

% Plot results

plot(lambda*1e9,Qscat,"wavelength (nm)","Mie efficiency","Scattering cross section");

plot(lambda*1e9,Qabs, "wavelength (nm)","Mie efficiency","Absorption cross section");

if(do-field-enhancement)

?" Calculating field enhancement";

% choose one frequency point for the images

% = length(lambda)/2.45;

E1 = getelectric("point x1"); % if you want the field intensity

E2 = getelectric("point x2");

E3 = getelectric("point x3");

E4 = getelectric("point x4");

E5 = getelectric("point x5");

E6 = getelectric("point x6");

E7 = getelectric("point x7");

E8 = getelectric("point x8");

E9 = getelectric("point x9");

E10 = getelectric("point x10");

```

```

f22 = getdata("point x1","f");

plot(c/f22*1e9,E1,E2,E3,E4,E5,E6,E7,E8,E9,E10, "wavelength (nm)", "|E|^2/|Einc|^2",
"Different Distance from surface on X Axis");

legend("1nm", "2nm", "3nm", "5nm", "7nm", "10nm", "15nm", "20nm", "25nm", "30nm");

E1 = getelectric("point y1"); % if you want the field intensity

E2 = getelectric("point y2");

E3 = getelectric("point y3");

E4 = getelectric("point y4");

E5 = getelectric("point y5");

E6 = getelectric("point y6");

E7 = getelectric("point y7");

E8 = getelectric("point y8");

E9 = getelectric("point y9");

E10 = getelectric("point y10");

f22 = getdata("point y1","f");

plot(c/f22*1e9,E1,E2,E3,E4,E5,E6,E7,E8,E9,E10, "wavelength (nm)", "|E|^2/|Einc|^2",
"Different Distance from surface on Y Axis");

legend("1nm", "2nm", "3nm", "5nm", "7nm", "10nm", "15nm", "20nm", "25nm", "30nm");

E1 = getelectric("point -y1"); % if you want the field intensity

E2 = getelectric("point -y2");

E3 = getelectric("point -y3");

E4 = getelectric("point -y4");

E5 = getelectric("point -y5");

```

```

E6 = getelectric("point -y6");
E7 = getelectric("point -y7");
E8 = getelectric("point -y8");
E9 = getelectric("point -y9");
E10 = getelectric("point -y10");
f22 = getdata("point -y1", "f");
plot(c/f22*1e9,E1,E2,E3,E4,E5,E6,E7,E8,E9,E10, "wavelength (nm)", "|E|^2/|Einc|^2",
"Different Distance from surface on -Y Axis");
legend("1nm", "2nm", "3nm", "5nm", "7nm", "10nm", "15nm", "20nm", "25nm", "30nm");
E1 = getelectric("point z1"); % if you want the field intensity
E2 = getelectric("point z2");
E3 = getelectric("point z3");
E4 = getelectric("point z4");
E5 = getelectric("point z5");
E6 = getelectric("point z6");
E7 = getelectric("point z7");
E8 = getelectric("point z8");
E9 = getelectric("point z9");
E10 = getelectric("point z10");
f22 = getdata("point z1", "f");
plot(c/f22*1e9,E1,E2,E3,E4,E5,E6,E7,E8,E9,E10, "wavelength (nm)", "|E|^2/|Einc|^2",
"Different Distance from surface on Z Axis");
legend("1nm", "2nm", "3nm", "5nm", "7nm", "10nm", "15nm", "20nm", "25nm", "30nm");

```

```

% image the total field near the particle

E2 = getelectric("x-normal-profile"); % returns  $|E|^2$ 

E2x = getdata("x-normal-profile","Ex"); % returns Ex

E2y = getdata("x-normal-profile","Ey"); % returns Ey

E2z = getdata("x-normal-profile","Ez"); % returns Ez

y = getdata("x-normal-profile","y");

z = getdata("x-normal-profile","z");

freq=5.55e+14;

f3=getdata("x-normal-profile","f");

fi=find(f3,freq);

fpoint=fi;

lambda3=c/f3;

image(y*1e9,z*1e9,pinch(E2,4,fpoint),"y (nm)","z (nm)"," $|E|^2$  in y-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2x,4,fpoint),"y (nm)","z (nm)","Ex in y-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2y,4,fpoint),"y (nm)","z (nm)","Ey in y-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2z,4,fpoint),"y (nm)","z (nm)","Ez in y-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

?" Maximum field enhancement over all wavelengths ( $|E|^2/|E_{inc}|^2$ ) in y-z plane is:

" + num2str(max(E2));

E2 = getelectric("y-normal-profile"); % returns  $|E|^2$ 

```

```

E2x = getdata("y-normal-profile","Ex"); % returns Ex
E2y = getdata("y-normal-profile","Ey"); % returns Ey
E2z = getdata("y-normal-profile","Ez"); % returns Ez
x = getdata("y-normal-profile","x");
z = getdata("y-normal-profile","z");

freq=5.55e+14;

f3=getdata("y-normal-profile","f");

fi=find(f3,freq);

fpoint=fi;

lambda3=c/f3;

image(x*1e9,z*1e9,pinch(E2,4,fpoint),"x (nm)","z (nm)","|E|^2 in x-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2x,4,fpoint),"x (nm)","z (nm)","Ex in x-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2y,4,fpoint),"x (nm)","z (nm)","Ey in x-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2z,4,fpoint),"x (nm)","z (nm)","Ez in x-z plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

?" Maximum field enhancement over all wavelengths ( $|E|^2/|E_{inc}|^2$ ) in x-z plane is:
" + num2str(max(E2));

E2 = getelectric("z-normal-profile"); % returns|E|^2

E2x = getdata("z-normal-profile","Ex"); % returns Ex

E2y = getdata("z-normal-profile","Ey"); % returns Ey

```

```

E2z = getdata("z-normal-profile","Ez"); % returns Ez

x = getdata("z-normal-profile","x");

y = getdata("z-normal-profile","y");

freq=5.55e+14;

f3=getdata("z-normal-profile","f");

fi=find(f3,freq);

fpoint=fi;

lambda3=c/f3;

image(x*1e9,y*1e9,pinch(E2,4,fpoint),"x (nm)","y (nm)","|E|^2 in x-y plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2x,4,fpoint),"x (nm)","y (nm)","Ex in x-y plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2y,4,fpoint),"x (nm)","y (nm)","Ey in x-y plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

image(y*1e9,z*1e9,pinch(E2z,4,fpoint),"x (nm)","y (nm)","Ez in x-y plane at
"+num2str(lambda3(fpoint)*1e9)+" nm");

?" Maximum field enhancement over all wavelengths ( $|E|^2/|E_{inc}|^2$ ) in x-y plane is:
" + num2str(max(E2));

% X direction

monitorname="point x1";% set the name of your monitor

%freq=5.40e+14; % set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

```

```

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq); % get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "X direction:";

? "At distance=1nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point x2"; % set the name of your monitor

freq=5.40e+14; % set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq); % get index of the frequency point closest to freq

```

```

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=2nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point x3"; % set the name of your monitor

freq=5.40e+14; % set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq); % get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

```



```

? "At distance=3nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point x4"; % set the name of your monitor

%freq=5.40e+14; % set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq); % get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=5nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

```

```

monitorname="point x5"; % set the name of your monitor

freq=5.40e+14; % set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);%get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=7nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point x6";% set the name of your monitor

freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

```

```

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=10nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point x7";% set the name of your monitor

freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

```

```

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=15nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point x8";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=20nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

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```

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point x9";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? "At distance=25nm";
?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point x10";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at

```

```

E-x=getdata(monitormame,"Ex");
E-y=getdata(monitormame,"Ey");
E-z=getdata(monitormame,"Ez");
E-2=getelectric(monitormame);
f=getdata(monitormame,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? "At distance=30nm";
?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);
% Y direction monitormame="point y1";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitormame,"Ex");
E-y=getdata(monitormame,"Ey");
E-z=getdata(monitormame,"Ez");
E-2=getelectric(monitormame);
f=getdata(monitormame,"f");

```

```

fi=find(f,freq);%get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

?"Y direction";

? "At distance=1nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point y2";% set the name of your monitor

%freq=5.40e+14;

% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

```

```

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=2nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point y3";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=3nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

```



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?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point y4";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? "At distance=5nm";
?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point y5";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at

```

```

E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? "At distance=7nm";
?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point y6";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");

```

```

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=10nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point y7";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

```

```

f-freq=f(fi);

? "At distance=15nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point y8";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=20nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

```

```

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point y9";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=25nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point y10";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

```

```

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=30nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

%%%%%%%%%%%%%% % -Y direction monitorname="point -y1";% set the name
of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

```

```

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

?"-Y direction";

? "At distance=1nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point -y2";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

```

```

f-freq=f(fi);

? "At distance=2nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point -y3";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=3nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

```



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?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point -y4";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? " At distance=5nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point -y5";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

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```

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=7nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point -y6";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

```

```

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=10nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point -y7";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=15nm";

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```

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point -y8";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? "At distance=20nm";
?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point -y9";% set the name of your monitor

```

```

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=25nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point -y10";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

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```

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=30nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

%%%%%%%%%% % Z direction monitorname="point z1";% set the name of your
monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

```

```

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

?"Z direction";

? "At distance=1nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point z2";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=2nm";

```

```

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point z3";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? "At distance=3nm";
?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);
monitorname="point z4";% set the name of your monitor

```



```

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitormame,"Ex");

E-y=getdata(monitormame,"Ey");

E-z=getdata(monitormame,"Ez");

E-2=getelectric(monitormame);

f=getdata(monitormame,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=5nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitormame="point z5";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitormame,"Ex");

E-y=getdata(monitormame,"Ey");

E-z=getdata(monitormame,"Ez");

E-2=getelectric(monitormame);

```

```

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? " At distance=7nm";

?"Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

monitorname="point z6";% set the name of your monitor %freq=5.40e+14;% set
frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

```

```

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=10nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point z7";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=15nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

```

```

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point z8";% set the name of your monitor %freq=5.40e+14;% set
frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=20nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point z9";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

```

```

E-y=getdata(monitormame,"Ey");

E-z=getdata(monitormame,"Ez");

E-2=getelectric(monitormame);

f=getdata(monitormame,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? " At distance=25nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitormame="point z10";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitormame,"Ex");

E-y=getdata(monitormame,"Ey");

E-z=getdata(monitormame,"Ez");

E-2=getelectric(monitormame);

f=getdata(monitormame,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

```

```

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=30nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

% m direction

monitorname="point m1";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

```

```

f-freq=f(fi);

?"m direction";

? "At distance=1nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point m2";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=2nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

```

```

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);
monitorname="point m3";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");
E-y=getdata(monitorname,"Ey");
E-z=getdata(monitorname,"Ez");
E-2=getelectric(monitorname);
f=getdata(monitorname,"f");
fi=find(f,freq);% get index of the frequency point closest to freq
Ex-freq=E-x(fi);
Ey-freq=E-y(fi);
Ez-freq=E-z(fi);
E2-freq=E-2(fi);
f-freq=f(fi);
? " At distance=3nm";
?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);
?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);
?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);
?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);
monitorname="point m4";% set the name of your monitor
%freq=5.40e+14;% set frequency that you want to look at
E-x=getdata(monitorname,"Ex");

```



```

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? " At distance=5nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point m5";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

```

```

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=7nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point m6";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

```

```

? "At distance=10nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point m7";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=15nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

```

```

monitorname="point m8";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=20nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point m9";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

```

```

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

Ez-freq=E-z(fi);

E2-freq=E-2(fi);

f-freq=f(fi);

? "At distance=25nm";

?"Ex at " + num2str(f-freq) + "Hz is " + num2str(Ex-freq);

?"Ey at " + num2str(f-freq) + "Hz is " + num2str(Ey-freq);

?"Ez at " + num2str(f-freq) + "Hz is " + num2str(Ez-freq);

?"E2 at " + num2str(f-freq) + "Hz is " + num2str(E2-freq);

monitorname="point m10";% set the name of your monitor

%freq=5.40e+14;% set frequency that you want to look at

E-x=getdata(monitorname,"Ex");

E-y=getdata(monitorname,"Ey");

E-z=getdata(monitorname,"Ez");

E-2=getelectric(monitorname);

f=getdata(monitorname,"f");

fi=find(f,freq);% get index of the frequency point closest to freq

Ex-freq=E-x(fi);

Ey-freq=E-y(fi);

```

$Ez\text{-freq}=E\text{-}z(f_i)$ ;

$E2\text{-freq}=E\text{-}2(f_i)$ ;

$f\text{-freq}=f(f_i)$ ;

? "At distance=30nm";

? "Ex at " + num2str(f-freq) + " Hz is " + num2str(Ex-freq);

? "Ey at " + num2str(f-freq) + " Hz is " + num2str(Ey-freq);

? "Ez at " + num2str(f-freq) + " Hz is " + num2str(Ez-freq);

? "E2 at " + num2str(f-freq) + " Hz is " + num2str(E2-freq);

## Appendix B

Electric field components around a GNP with  $r = 20$  nm

The Electric field components, which are calculated through the more accurate point monitors on the main axes around a GNP with  $r = 20$  nm, are as follows:

X direction:

At distance=1nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.116175-0.736351i

E2 at 5.54333e+14Hz is 0.55571

At distance=2nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.18948-0.547469i

E2 at 5.54333e+14Hz is 0.335625

At distance=3nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.250298-0.383294i

E2 at 5.54333e+14Hz is 0.209563

At distance=5nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.342041-0.124321i

E2 at 5.54333e+14Hz is 0.132448

At distance=7nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.406149+0.0644369i

E2 at 5.54333e+14Hz is 0.169109

At distance=10nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.470892+0.26164i

E2 at 5.54333e+14Hz is 0.290194

At distance=15nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.532626+0.455889i

E2 at 5.54333e+14Hz is 0.491525

At distance=20nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i



Ez at 5.54333e+14Hz is 0.56594+0.562773i

E2 at 5.54333e+14Hz is 0.637001

At distance=25nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.586437+0.628857i

E2 at 5.54333e+14Hz is 0.73937

At distance=30nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.598877+0.668839i

E2 at 5.54333e+14Hz is 0.805999

Y direction

At distance=1nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.0493919-0.654599i

E2 at 5.54333e+14Hz is 0.430939

At distance=2nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.0901668-0.451657i

E2 at 5.54333e+14Hz is 0.212124

At distance=3nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.122574-0.275749i

E2 at 5.54333e+14Hz is 0.091062

At distance=5nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.166589+0.00235288i

E2 at 5.54333e+14Hz is 0.0277574

At distance=7nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.191177+0.206534i

E2 at 5.54333e+14Hz is 0.0792051

At distance=10nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.205789+0.422509i

E2 at 5.54333e+14Hz is 0.220863

At distance=15nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.196758+0.640663i

E2 at 5.54333e+14Hz is 0.449163

At distance=20nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.166317+0.765363i

E2 at 5.54333e+14Hz is 0.613442

At distance=25nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.125673+0.845056i

E2 at 5.54333e+14Hz is 0.729912

At distance=30nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.0782749+0.894488i

E2 at 5.54333e+14Hz is 0.806235

-Y direction

At distance=1nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.152572-0.845772i

E2 at 5.54333e+14Hz is 0.738609

At distance=2nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.252892-0.678877i

E2 at 5.54333e+14Hz is 0.524828

At distance=3nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.337013-0.533729i

E2 at 5.54333e+14Hz is 0.398444

At distance=5nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.466655-0.307421i

E2 at 5.54333e+14Hz is 0.312275

At distance=7nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.560417-0.147038i

E2 at 5.54333e+14Hz is 0.335687

At distance=10nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.659854+0.0119341i

E2 at 5.54333e+14Hz is 0.435549

At distance=15nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.7641+0.147778i

E2 at 5.54333e+14Hz is 0.605687

At distance=20nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.829207+0.198463i

E2 at 5.54333e+14Hz is 0.726971

At distance=25nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.875428+0.208634i

E2 at 5.54333e+14Hz is 0.809903

At distance=30nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is -0+0i

Ez at 5.54333e+14Hz is 0.90842+0.192359i

E2 at 5.54333e+14Hz is 0.862228

Z direction

At distance=1nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.13931-0.0710528i

Ez at 5.54333e+14Hz is 1.75295+3.64929i

E2 at 5.54333e+14Hz is 16.4146

At distance=2nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.117246-0.0585739i

Ez at 5.54333e+14Hz is 1.61044+3.32545i

E2 at 5.54333e+14Hz is 13.6693

At distance=3nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.0987455-0.0482541i

Ez at 5.54333e+14Hz is 1.48249+3.03782i

E2 at 5.54333e+14Hz is 11.4382

At distance=5nm

Ex at 5.54333e+14Hz is -0+0i Ey at 5.54333e+14Hz is 0.0710916-0.0333579i

Ez at 5.54333e+14Hz is 1.28187+2.57079i

E2 at 5.54333e+14Hz is 8.25832

At distance=7nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.0523536-0.0237421i

Ez at 5.54333e+14Hz is 1.14029+2.22235i

E2 at 5.54333e+14Hz is 6.24242

At distance=10nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.0343117-0.0149135i

Ez at 5.54333e+14Hz is 0.997982+1.85212i

E2 at 5.54333e+14Hz is 4.42773

At distance=15nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.0184873-0.00760172i

Ez at 5.54333e+14Hz is 0.861391+1.47437i

E2 at 5.54333e+14Hz is 2.91615

At distance=20nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.0108567-0.00426677i

Ez at 5.54333e+14Hz is 0.785709+1.25425i

E2 at 5.54333e+14Hz is 2.19061

At distance=25nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.00660394-0.00247618i

Ez at 5.54333e+14Hz is 0.741705+1.12191i

E2 at 5.54333e+14Hz is 1.80886

At distance=30nm

Ex at 5.54333e+14Hz is -0+0i

Ey at 5.54333e+14Hz is 0.0042939-0.00154053i

Ez at 5.54333e+14Hz is 0.71286+1.03349i

E2 at 5.54333e+14Hz is 1.57629



## Appendix C.1

Normalized decay rates of a parallel orientation of the dipole moment

The dipole emission wavelength is  $\lambda = 520$  nm near a GNP with  $r = 20$  nm at position  $d$  that is the distance from the surface of the GNP

Distance, $d$ (nm)	Radiative Rate	Nonradiative Rate
2	0.707516	7933.45
3	0.308704	1986.91
5	0.218938	353.752
7	0.236270	110.617
10	0.347838	31.2633
15	0.534883	7.0893
20	0.670623	2.3244
25	0.763161	0.930973
30	0.825202	0.41377

## Appendix C.2

Normalized decay rates of a perpendicular orientation of the dipole moment

The dipole emission wavelength is  $\lambda = 520$  nm near a GNP with  $r = 20$  nm at position  $d$  that is the distance from the surface of the GNP.

Distance, $d$ (nm)	Radiative Rate	Nonradiative Rate
2	13.5832	24027.3
3	11.9110	4517.39
5	8.76144	705.777
7	6.51394	246.539
10	4.50728	82.2694
15	2.89122	22.548
20	2.14984	8.46557
25	1.75678	3.87617
30	1.52544	1.87533

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