Computational & Statistical Physics Group
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Matrix Algebra

Applied Photonics

Computational & Statistical Physics Group

Nanoscale Physics

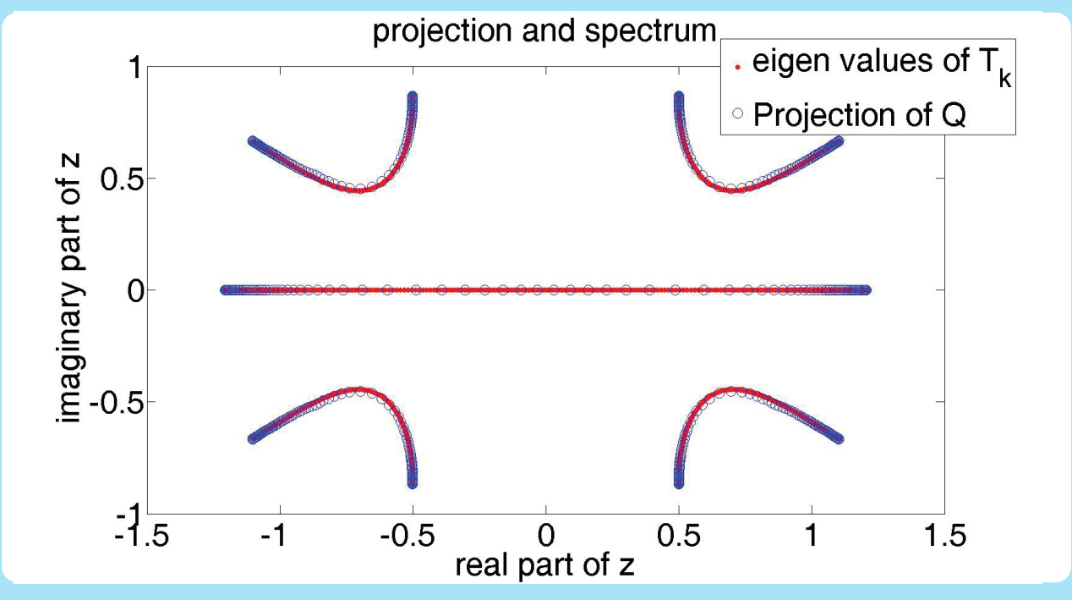
Numerical methods for Physics

Examples

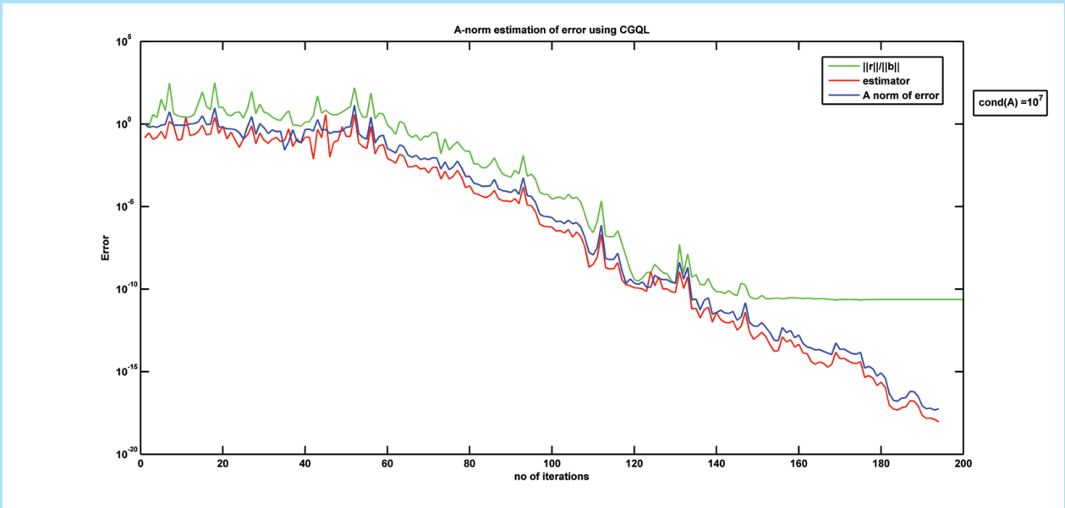
Matrix Algebra

Matrices occur in many kinds of problems across disciplines. Our work can be broadly classified into (a) Study of matrices with periodic or random entries, (b) linear algebra solvers and their error estimators. Many problems in physics, economics, biology and engineering are modelled as one dimensional chains. These models result in tridiagonal k-Toeplitz matrices with periodicity along the three diagonals (figure 1a). Analysis of chain models and their eigen modes involve the spectral analysis of such matrices to derive useful theorems.

Iterative methods are more computationally efficient requiring O(n^2) operations than direct solvers which require O(n^3) operations, where 'n' is the number of equations in a linear system of equations. An accurate criteria for stopping and restarting is needed when we deal with iterative solvers. These estimators need to work for any matrix with minimal computation added to the iterative method used (figure 1b).



1a.
Spectrum of 5 Toeplitz matrix approximated by polynomial projection.

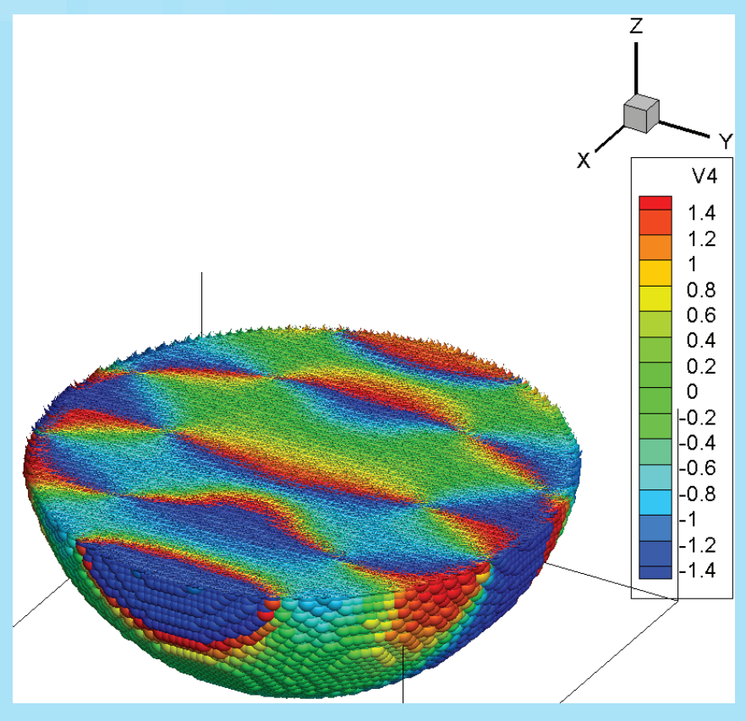


1b.
A-norm estimation using CGQL algorithm.

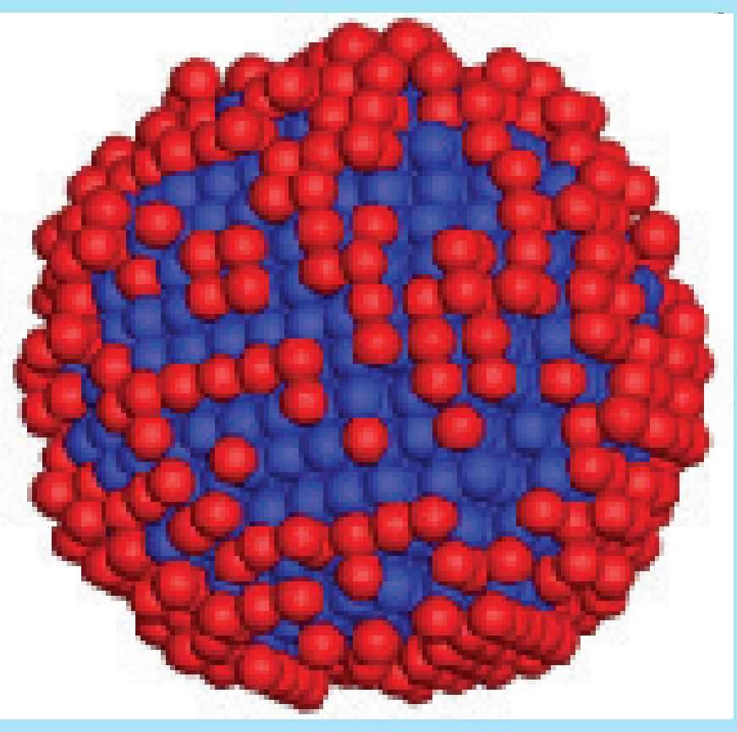
Applied Photonics

Controlling optical properties of nanoparticles is required in applications like optical antennas, photocatalysis, optical sensing and energy conversion. Composite particles like nanoshells (figure 2a), are studied to realize such properties.

Increase in absorption efficiency of nanoshells by large factors by the use of incomplete nanoshells was shown by us a few years ago (figure 2b). These have applications in photocatalysis and UV-protection.



2a.
Phase oscillations of the polarization in coreshell particle.

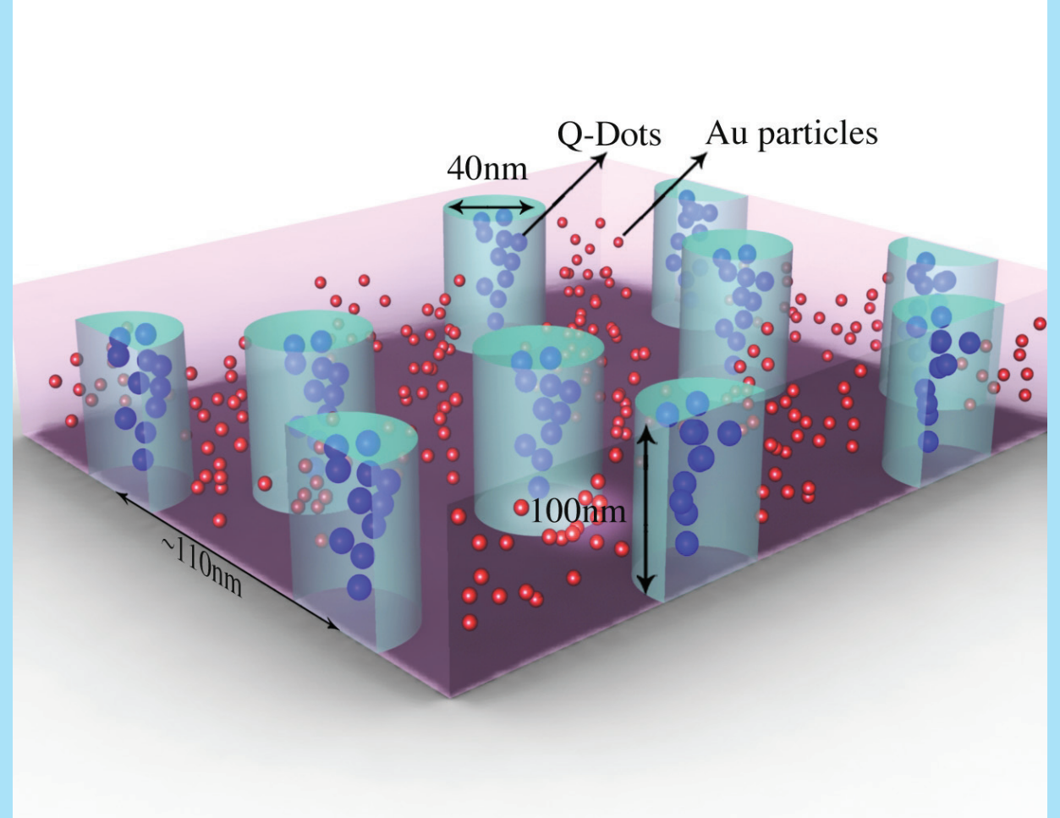


2b.
Incomplete nanoshell particle made of a silica and titania.

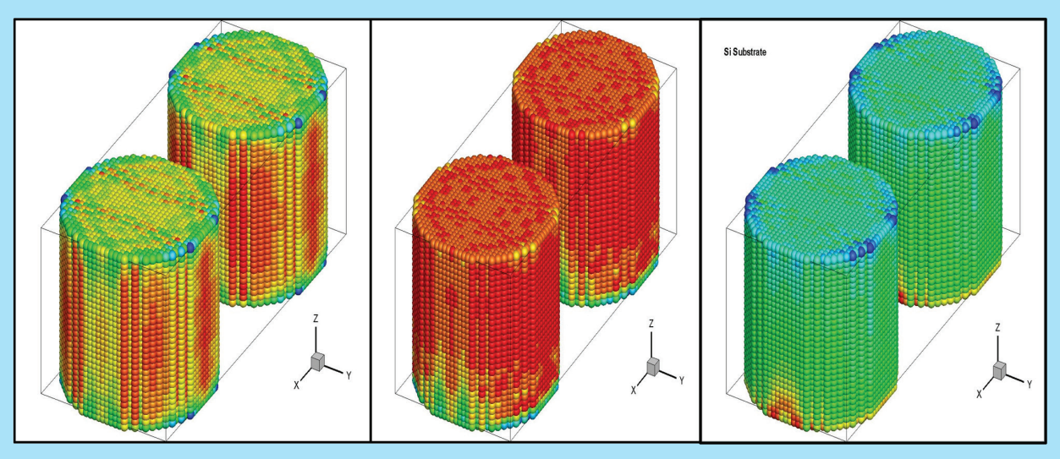
Nanoscale Physics

Quantum dots are a class of novel nanoscale materials which has high tunable properties. Studies of photoluminescence intensity of the quantum dots with metal nanoparticles is significant for applications like sensors, solar cells, LEDs, LCD displays, diode lasers and second-harmonic generation. Quantum dots embedded in an ordered template, using lightly doped small gold nanoparticles (nano-antennae) is shown in the figure 3a, as a representative example. The collective quantum effects in such materials, and the computational tools to model them, is one area of study.

Localized plasmon resonances occurring in metallic nanoparticles both for single particles and particle ensembles on a substrate has range of applications in sensors, biophotonics, photovoltaics etc. Energy distribution in the gold nano-cylinders in free space, on glass and Si substrates respectively (higher from blue to red) shown in the figure 3b, is based on studies on substrate effect through our theoretical and computational models.



3a.
Representative image of Q-Dots in an ordered template.

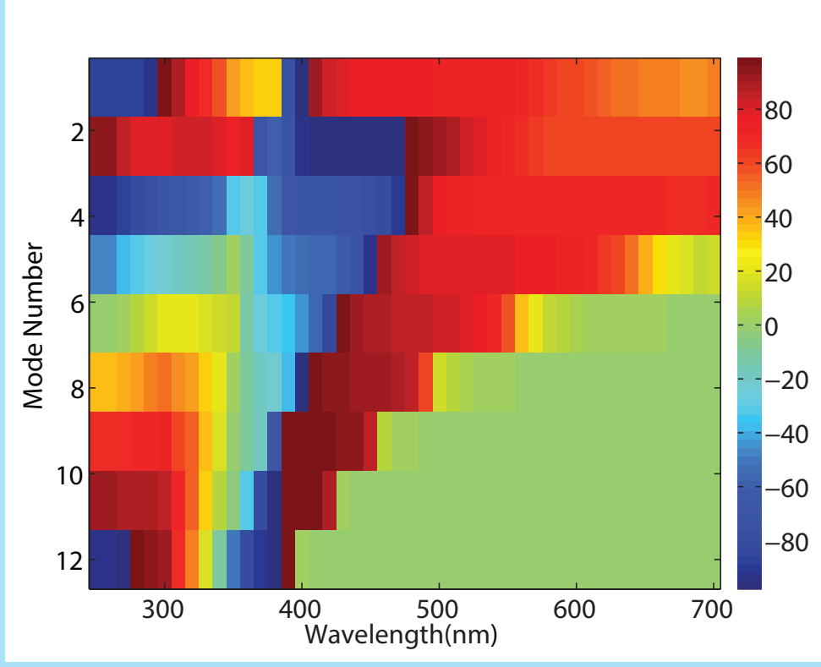


3b.
Energy Distribution in the Gold nano-cylinders on different substrates.

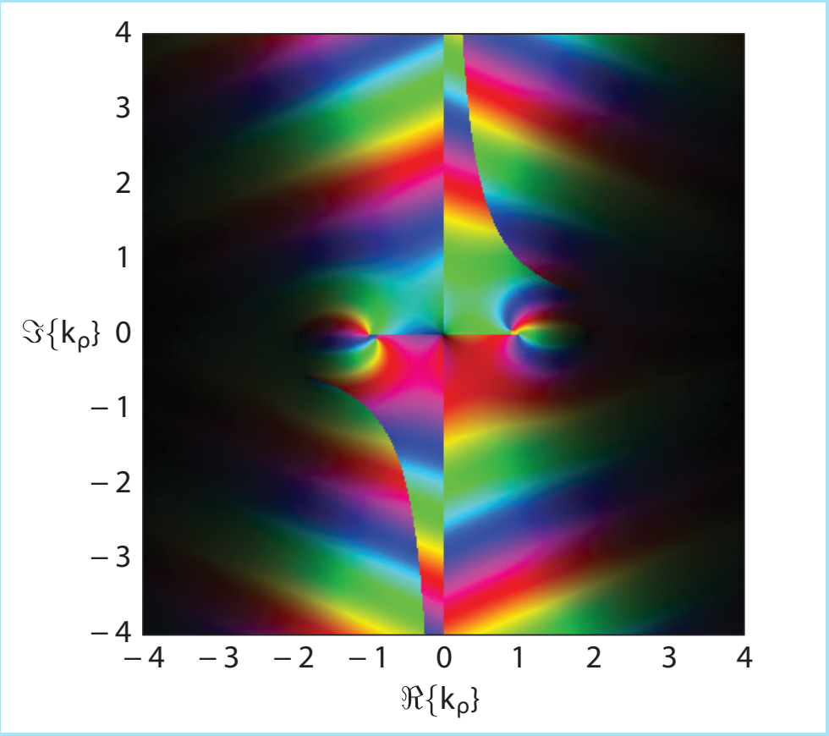
Numerical Methods for Physics

Spectral properties of all-dielectric nanoparticles is significant for lossless applications in optical circuits, photovoltaics etc. Engineering non-trivial interference effects in higher order modes of dielectric particles (figure 4a), is an example where we use computational models.

Numerical techniques and approximations for the evaluation of singular and oscillatory integrals arises in many physical problems - for example, the Sommerfeld integral, in scattering problems involving an infinite planar interface (figure 4b). Efficient evaluation of these integrals is important for computational scalability of the solution.



4a.
Phase distribution (in degrees) of coreshell nanoparticles.



4b.
Represents domain coloring visualization of the Sommerfeld integrand in the complex plane

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