Quantum emitter dipole-dipole interactions in nanoplasmonic arrays

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(Dated: September 24, 2015)

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PACS numbers: ...

INTRODUCTION

- Our focus: the effects of dipole-dipole interactions between the emitters in the nanoplasmonic array system. What could we see in our systems, i.e. nanoparticle arrays?
- Mention Salomon's (slit array; FDTD/Bloch equations) and Delga's (single sphere; Wubs's frequency domain quantum multiple scattering model) results. Salomon's parameters are probably bit unrealistic in our context.

SINGLE FIELD MODE MODEL

This has been done.

Model description

$$H = \omega b^\dagger b + \sum_{i=1}^{K} \epsilon_i S_i^z + \sum_{i=1}^{K} V_i \left(b^\dagger S_i^- + S_i^+ b \right) + \sum_{i<j=1}^{K} g_{ij} \left(S_i^+ S_j^- + S_j^+ S_i^- \right). \quad (1)$$

- Description: only one field mode, no losses, several dipoles, ...
  - How we calculate couplings for real configurations.
- Excitation number conserved in RWA.

Exact diagonalisation results

- Spectra for $N \lesssim 16$, single excitation subspace
- Coupling strength effects

Randomness effects

Effects of disorder on "band" width and position.

- Directional randomness.
- Positional randomness.

Scaling effects

- Nearest neighbour approximation shows no qualitative effects at this tiny scale. This does not necessarily mean that they are negligible in large systems.
- Realistic concentrations and dipole moments.
  - What are the quantities for our systems.
  - How do the effects compare to e.g. thermal energy.

Interpretation

- Model does not show anything about experimental observables in the real systems.
- On the other hand, we can exactly see in the energy spectrum what can be attributed to the direct d-d interaction and what is mediated.
- Probably no important effects for realistic concentrations.

MULTIPLE SCATTERING MODEL

In progress / not done. Cf. timetable.

Model description

- Brief model description with references to Wubs and Delga
- The advantage of this model is that it should give an actual observable light spectrum.

Single nanoparticle case

- Custom nanoparticle geometry: description, BEM modelling, classical scattering properties. *Timetable item 3.*
- Results: observable spectra for some realistic parameters (QE concentration, dipole moment). Far field / near field. *Timetable item 6.*

Arrays

- Similar as in the previous subsection, but now with multiple nanoparticles in array. *Timetable item 5.*
- Results: spectra for array geometries. *Timetable item 6.*

CONCLUSIONS

Not done.

- What do the results from the two models tell us about how the dipole-dipole interactions affect the system. At which parameter regions do we get some interesting effects.
- Compare the shape of spectra from the scattering models to the "simple" exactly diagonalised model.

Timetable

Items 1, 2, 3, 6 are in my opinion necessary in order to answer the original question "can we see the dipole-dipole effects in our systems"? Item 4 would be nice because I have not seen any paper doing that, but it is the main candidate to be postponed. Item 5 might be circumvented by using BEM for several nanoparticles, but I am not completely sure about the time complexity in this case. But if it works, item 5 will become nice-to-have only.

Note: I have recently found a code[1] for classical multiple-sphere scattering. It could save me a lot of time, especially on item 5, if I link it to my code.

1. (7 days) Reproducing Delga's results (getting the spherical wave solution right).
   - (1 week) Case of 1 source atom + 1 spherical NP.
     - Debugging.
   - (2 days) Case of N source atoms + 1 spherical NP.
     - Debugging, but there should not be much work beyond the single source case.
2. (3 days) Learning (by doing) to use the grid infrastructure.
   - Some of the following tasks will probably need more computational power in order to be finished in some reasonable time, and they can be easily parallelised (e.g. BEM scattering calculations at different frequencies).
3. (10 days) Custom nanoparticle geometry.
   - (3 days) Learning to define gmsh geometries for BEM calculations and creating geometry files for our (single) nanoparticles.
   - (4 days) Single NP calculations as in 1., but with custom geometry.
     - Writing a wrapper to integrate scuff-EM BEM solver to my calculations.
     - Getting actual numerical results.
   - (3 days) Consistency check (needed for most of the following steps): T-matrix and direct BEM scattering calculations must yield the same results.
4. (25 days) "Coherent" sources. In Delga's papers, the initial states are always single excited atom. I would like to try different initial states, e.g. a plane wave. One drawback is that some of the "simple" formulae from Wubs's and Delga's papers will no longer be applicable and there will appear at least one more dimension for numerical integration. On the other hand, I am not aware that anyone else has done something like this yet, so it could give quite original results.

[1] `http://eng.auburn.edu/users/dmckwski/scatcodes/`

- (8 days) Theory, numerical methodology and algorithmisation.
- (17 days) Implementation and debugging.

5. (25 days) Nanoparticle arrays. It should be possible to use the single-particle T-matrix and multipole reexpansion to solve the scattering problem in the multiple nanoparticle configuration. However, the translation operators are complicated, hence very error-prone.

   - (5 days) Theoretical and numerical considerations.
   - (5 days) Implementation.
   - (15 days) Debugging.

6. (5 days) Parameter sweep (concentrations, configurations, dipole moments, frequencies, etc.).