# Quantum corrections to the efficiency of solar cells with conductive nanostructured layers

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***Abstract*—It was shown in many experiments that the incorporation of metallic nanostructures into photovoltaic devices results in the enhancement of solar cell efficiency. Most simulations of such devices are based on classical electrodynamics and neglect quantum effects arising from nanosized metallic structures. Here, we look at nonlocal electron-electron interactions, Lorentz friction and strong coupling of plasmon modes with a Si substrate.**

***Index Terms*—photovoltaics, nonclassical electron dynamics, theory and simulation, nanoparticles**

## I. Scope of this work

We investigate plasmon enhanced solar cells [1], [2] including (i) Lorentz friction caused by the oscillation of electrons, (ii) nonlocal electron-electron interactions, and (iii) the microscopic description of the strong interaction between plasmon excitations in metal nanoparticles (MNPs) and semiconductor states. With this, the impact of the resulting corrections on the light absorption and photocurrent gain, and estimate under which conditions those corrections are significant [3], [4].

## II. Quantum Corrections

We combine several semi-classical approaches towards microscopic electron dynamics into a single feasible framework. The advantage lies in the straightforward integration of analytical expressions into standard computational procedures such as modified Mie coefficients and multiple scattering techniques [5] for NP clusters or commercial software such as COMSOL.

### A. Lorentz friction

The microscopic dynamics of electrons inside the MNP leads to energy loss via irradiation of the electromagnetic field due to their accelerated movement during the plasmon oscillation [6], [7]. For NPs much smaller than the incident wavelength, Lorentz friction describes an effective field [8] stemming from the plasmon induced dipole field $\mathbf{D}(t)$ as $\mathbf{E_L} = {}^{2}/_{3c^3}\partial_t^3\mathbf{D}(\mathbf{t})$ .

An analytical form of the exact solution for the damping $\gamma$ and self-frequency $\omega_L$ including Lorentz friction within microscopic RPA leads to an extended, semi-classical damping expression [9]

$$\gamma = \frac{-1}{3l} + \frac{1+6lq}{2^{\frac{2}{3}}3l\mathcal{A}} + \frac{\mathcal{A}}{2^{\frac{1}{3}}6l}, \tag{1}$$

where $\mathcal{A} = \left(\mathcal{B} + \sqrt{4(-1-6lq)^3 + \mathcal{B}^2}\right)^{1/3}$, $\mathcal{B} = 2 + 27l^2 + 18lq$, and $q = \frac{\gamma_p}{\omega_1}$, $l = \frac{2}{3\sqrt{\epsilon_0}}\left(\frac{a\omega_p}{c\sqrt{3}}\right)^3$.

Direct comparison to experimental work for this framework is available within Refs. [1], [3], [6], [9] and good agreement has been found.

### B. Nonlocal electron-electron interaction

Maxwell's equations for external sources result in the following electromagnetic wave-equation (Gauss units)

$$\nabla \times \nabla \times \vec{E} - k^2\epsilon_b\vec{E} = \frac{4\pi i k^2}{\omega}\vec{j}. \tag{2}$$

The induced current density $\vec{j}$ is obtained with the Navier-Stokes equation for a charged electron plasma

$$\vec{j} = \frac{i}{\omega + i\gamma}\left(\frac{Q^2 n_0}{m}\vec{E} - \nabla\beta^2_{\mathrm{GNOR}}\rho\right). \tag{3}$$

The pressure term can be derived from classical gas theory [10]–[12] or from quantum mechanics including Coulomb interaction [13] and accounts in the generalized nonlocal optical response (GNOR [14], [15]) for electron diffusion $D$. This results in $\beta^2_{\mathrm{GNOR}} = \frac{3}{5}v_F^2 + D(\omega + i\gamma)$, where $v_F$ is the Fermi velocity of the material.

Local scattering matrices are extended by a single analytic parameter describing nonlocal behavior of the conduction band electron. This nonlocal parameter vanishes under the assumption of local response ($\beta \to 0$) recovering original Mie or Fresnel coefficients [16], [17].

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### C. Strong coupling

The photon absorption probability $\delta w$ within the Fermi Golden Rule approach for a dipole near-field is

$$\delta w = \frac{2\pi}{\hbar}\left|\langle \vec{k}_1|W|\vec{k}_2\rangle\right|^2 \delta(E_p(\vec{k}_1) - E_n(\vec{k}_2) + \hbar\omega).$$

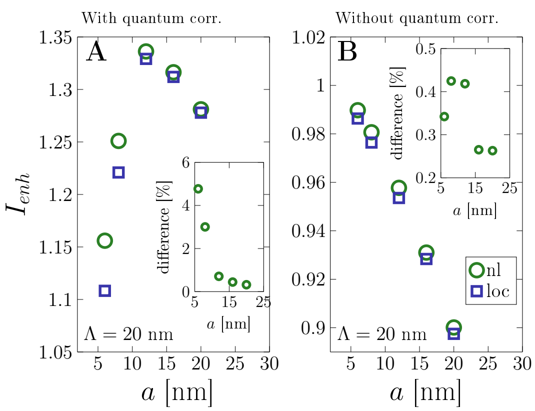


Fig. 1. Impact of strong coupling corrections on the photocurrent. (A) with and (B) without particle–substrate coupling. The lattice period is $\Lambda = 20$ nm and various nanoparticle radii $a$ are used. The insets show the difference between classical and nonlocal theory results.

Hereby, $\vec{k}_1(\vec{k}_2)$ is the momentum of the holes (electrons) and $W$ defines the coupling between the subbands. The coupling matrix $W$ depends on the environment. In the presence of the dipole field of a nanoparticle with radius $a$ and bulk plasma frequency $\omega_p$ it reads

$$W = W^+ e^{i\omega t} + c.c = \frac{e}{4\pi\epsilon_0 R^2}\vec{n}\cdot\vec{D}_0 \sin(\omega t + \phi),$$

where $W^\pm$ correspond to the absorption and emission of photons, respectively, and have the form

$$W^+ = \frac{e}{4\pi R^2 \epsilon_0}\frac{e^{i\phi}}{2i}\vec{n}\cdot\vec{D}_0,$$

where $\phi$ is a phase factor. Hereby, $\epsilon_0$ is the vacuum permittivity, $R$ is the distance form the dipole axis and $\vec{n}$ the surface normal of the substrate. The dipole moment $\vec{D}_0$ is analytic for a spherical nanoparticle and local electron dynamics, namely $\vec{D}_0 = \frac{\omega_p^2}{\omega_1^2}\vec{E}\frac{a^3}{2}$, where $\omega_1 = \omega_p/\sqrt{3}$ is the related Mie frequency of the dipole and $\vec{E} = i\omega\vec{A}_0 e^{i(\omega t - \vec{k}\vec{r})}$ is the incident field at frequency $\omega$ as before. For nonlocal electron dynamics, we determine $\vec{D}_0$ from the nonlocal near-field.

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