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Modelling and computation for nanoparticle reconstruction using Electron Energy Loss Spectroscopy

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Abstract

In Electron Energy Loss Spectroscopy, or EELS, one measures the interaction between a nanoparticle and a probing relativistic electron beam. When the beam is steered to a small but finite distance from the particle surface, the plasmons induced in the particle emit an electromagnetic field that causes a measurable change in the kinetic energy of the beam electrons [1, 2, 3, 4, 5]. The measured electron energy loss spectrum can be used to infer the size, shape and material properties of the nanoparticle [6]. A fast and stable solution of this inverse problem requires a sparse but physically well-justified forward model. In this talk, we shall describe and discuss important issues that arise in the mathematical modelling and the numerical implementation of relevant forward models based on discrete sources. We shall pay special attention to a Generalized Multipole Technique (GMT, [7, 8]) and to the Null-Field Method with Discrete Sources (NFM-DS) of T-Matrix type [9, 10]. The models are constructed around the central equation

$$P(\omega) = \frac{e}{\pi\hbar\omega}\int_{t=-\infty}^{\infty} \Re\left[\mathbf{v}.\mathbf{E}^{\mathrm{sca}}(\mathbf{r}_{\mathrm{e}}(t),\omega)e^{-i\omega t}\right] \qquad (1)$$

that links the probabilistic and the classical aspects of the EELS setup, and describes the electron energy loss probability density P at energy $\hbar\omega$ in terms of the electron beam velocity $\mathbf{v}$ and path $\mathbf{r}_{\mathrm{e}}(t)$, and the near field $\mathbf{E}^{\mathrm{sca}}$ induced by plasmons in the nanoparticle. We shall support our discussion using concrete examples and numerical results.

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