The Model Periodic Coulomb interaction in k-space: modelling the spherically averaged structure factor RENE GAUDOIN, Donostia International Physics Center (DIPC), Manuel de Lardizabal Pasealekua, E-20018 Donostia, Basque Country, Spain, IDOIA GURTUBAY, Materia Kondentsatuaren Fisika Saila, Zientzia eta Teknologia Fakultatea, Euskal Herriko Unibertsitatea, PO 644, E-48080 Bilbo, Basque Country, Spain, TXEMA PITARKE, CIC nanoGUNE Consolider, Mikeletegi Pasealekua 56, E-2009 Donostia, Basque Country, Spain — Within Quantum Monte Carlo (QMC) calculations the Model Periodic Coulomb (MPC) interaction is a well know method to reduce finite size effects related to the long range nature of the Coulomb interaction. Recently we presented a method based on modelling the continuous-k spherically averaged structure factor (SF) to understand and reduce Coulomb finite size effects. Here we show that our SF based method can be viewed as k-resolved MPC. This allows us to analyse the implicit assumptions that underlie MPC and what to do when these assumptions are not justified, i.e. in non-interaction Hartree-Fock systems or even surfaces. While we present data for the homogeneous electron gas the method itself is general.

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