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(I) Dynamic response and correlation exchange kernel of the electron gas from algorithmic computational tools.

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The general computation of dynamic properties of materials remains a longstanding, difficult problem within computational physics. Surprisingly, simple models such as the homogeneous electron gas (jellium) play critical roles in application of Density Functional Theory and its time-dependent extensions. Those calculations are impeded by the difficulty of evaluating Feynman diagrams on the real frequency axis that are required to describe screening processes. In this talk I will introduce a diagrammatic Monte Carlo technique based on a partially symbolic computational tool, algorithmic Matsubara integration, that allows us to compute frequency and momentum resolved finite temperature response functions directly in the real frequency domain. Using the obtained data for charge response at moderate electron density we, for the first time, compute the exchange-correlation kernel for jellium by a controlled method and revealed unexpected features in its frequency dependence. To emphasize the wide applicability of the approach I will also summarize other applications of the methodology for computation of diagrammatic expansions in model systems.

Keyword-1

Correlated Electrons

Keyword-2

Free electron Gas

Keyword-3

Numerical Methods

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