Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

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CFEL Seminar room III (Bldg. 99)

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Application of Time-Dependent Many-Body Perturbation Theory to Excitation Spectra of Selected Finite Model Systems

Many-Body Perturbation Theory (MBPT) is a methodology routinely employed in computational spectroscopy to calculate photoemission and absorption spectra. However, usually these computational experiments are only possible for real nanostructures, solids, etc. by resorting to simple approximations in which, e.g., self-consistency is neglected.

In this talk, by considering only small, finite lattice systems, I instead summarize some of the properties of simple, but self-consistent, many-body approximations in obtaining excitation spectra [1, 3]. In particular, I focus on density response functions from which, e.g., absorption spectra are calculated. Our method of choice for evaluating these functions is time-dependent many-body perturbation theory. What makes this an interesting application is that the used method is equivalent to the traditional approach based on the Bethe-Salpeter Equation (BSE) but the accessible approximations are diagrammatically more sophisticated.

In addition, I summarize the main steps enabling one to take vibrational effects into account, e.g., in such applications. I do this by presenting the Kadanoff-Baym Equations (KBE) for systems of interacting electrons and phonons for which the initial preparation to an equilibrium state is taken into account [2, 3]. The correlated many-body approximations to be discussed in this context are the partially and fully self-consistent Born approximations.

[1] Säkkinen N, Manninen M, and van Leeuwen R, NJP, 14:013032 (2012)

[2] Säkkinen N, Peng Y, Appel H, and van Leeuwen R, JCP, 143:234101 (2015)

[3] Säkkinen N, Peng Y, Appel H, and van Leeuwen R, JCP, 143:234102 (2015)

Host: Angel Rubio

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