Unphysical and Physical Solutions in Many-Body Theories: from Weak to Strong Correlation

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The noninteracting Green’s function $Z_0$ as a function of the interaction $V$ obtained in a simple one-point model using two different iteration schemes (A and B). Squares (red): $Z_0^-$, the solution of scheme A; circles (blue): $Z_0^+$, the solution of scheme B; continuous line (orange): $Y_0$, the physical noninteracting Green’s function.

Many-body theory is largely based on self-consistent equations that are constructed in terms of the physical quantity of interest itself, for example the density or the one-body Green’s function. Therefore, the calculation of important properties such as total energies or photoemission spectra requires the solution of non-linear equations that have unphysical and physical solutions \cite{1,2}. In this work we show using a simple model in which circumstances one runs into an unphysical solution (see the figure for an example), we illustrate the dramatic consequence that many-body theories become unpredictive, and we indicate how one can overcome this problem \cite{3}. Our findings point out that currently used strategies to develop approximations are only valid in a regime of weak to moderate interaction strength, and that they have to be completely changed in the strong-correlation regime. We propose a new strategy for strong correlation.

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