Poster-1-31

Calculating the complete spectral functions of quantum magnetic models and materials

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We report on the development of systematic cylinder matrix-product-state (MPS) methods to perform unbiased calculations of the full spectral function, $S(\mathbf{q}, \omega)$, of any spin model with local interactions. By applying these methods to different systems in all applied magnetic fields up to saturation, we show how spectral fingerprints reveal novel phenomena. In unfrustrated Heisenberg antiferromagnets, we examine the presence of field-induced shadow modes, which are found experimentally in the square-lattice material $(CuF_2(H_2O)_2)2pyz$ [1] and the honeycomb-lattice compound $YbBr_3$ [2]. In the ideally frustrated "Shastry-Sutherland material," $SrCu_2(BO_3)_2$, we reveal the presence of the spin-nematic phase, which is a low-field $S = 2$ condensate [3]. In the triangular-lattice Heisenberg system $CsYbSe_2$, we benchmark and offer an explanation for the extensive scattering continua [4]. While a quantitative calculation of excitation spectra constitutes an evolution in the understanding of unfrustrated models, it is a veritable revolution for frustrated ones. The provision of unbiased MPS spectral functions allows the problem of understanding to be factorised into the two separate stages of expression and interpretation, thereby sharpening the focus on the latter step. We conclude that there is still plenty of new physics to be found in the spectral response.

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