Numerical studies on fractional excitations in strongly correlated electron systems

Youhei YAMAJI
Department of Applied Physics, the University of Tokyo
Hongo, Bunkyo-ku, Tokyo 113-8656

Fractionalized excitations have been actively studied in strongly correlated electron systems over the last several decades. The exploration of the fractionalized particles initiated by the discovery of the fractional quantum Hall effect has flourished and led to findings of exactly solvable many-body quantum systems such as the Kitaev model [1], which has been proposed to capture low-energy spin degrees of freedom in honeycomb networks of heavy transition metal ions typified by an iridium oxide Na_2IrO_3 and α-$RuCl_3$ [2].

Although these *relativistic* Mott insulators, Na_2IrO_3 and α-$RuCl_3$, exhibit spontaneous time-reversal symmetry breakings at low temperatures, their finite-temperature behaviors have been explained by assuming fractionalized Majorana excitations. The most characteristic signature of the fractionalization is the continuous spin excitation spectrum of α-$RuCl_3$ [3], in addition to the recent observation of the quantized thermal Hall effect [4].

Estimates of exchange couplings among ruthenium ions in α-$RuCl_3$ by using the density functional theory reveal that the dominant couplings are the Kitaev interaction and off-diagonal symmetric exchange coupling [5]. The off-diagonal symmetric coupling among $S = 1/2$ quantum spins on the honeycomb lattice is given by the following hamiltonian called the Γ model,

$$\hat{H} = \sum_{\gamma=x,y,z} \sum_{\langle i,j\rangle\in\gamma} \Gamma(\hat{S}_i^\alpha \hat{S}_j^\beta + \hat{S}_i^\beta \hat{S}_j^\alpha) \qquad (1)$$

where couplings for the nearest-neighbor bonds depend on the bond direction $\gamma = x, y, z$, (α, β, γ) is a permutation of (x, y, z), and Γ is the coupling constant and set as $\Gamma = 1$. To clarify the origin of the continuum in α-$RuCl_3$ and possible fractionalization, we examine spin dynamics dominated by the Γ model.

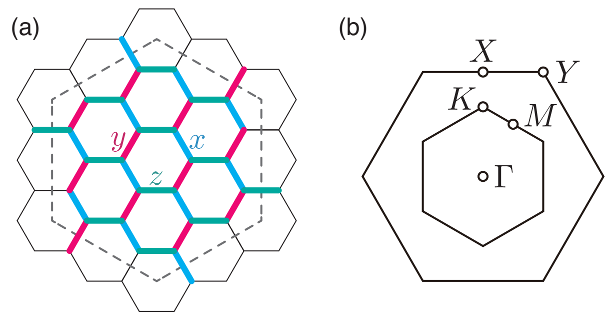

Figure 1: (a) 24 site cluster used in the present report. (b) Brillouin zone and high symmetry points of honeycomb lattices.

By applying the finite-temperature shifted Krylov subspace method [6], we simulate the exact dynamical spin structure factor $S(Q, \omega)$ of the Γ model for a 24 site cluster (see Fig. 1 (a)). At moderate temperatures $T = 0.5$, $S(Q, \omega)$ shows continuum, while suppression of low-energy spectral weight around the Γ and X points, as shown in Fig. 2 (a).

The continuum is interpreted as a combination of relaxational dynamics due to nearly degenerated exponentially degenerated low-energy states [7], which is also valid for the Kitaev model. As temperatures are lowered, the degeneracy is lifted and spin gaps seem to open as shown in Fig. 2 (b), (c), and (d), which also resembles the spin gap opening in the Kitaev model.

The continuous spectra from the common origin in the Kitaev and Γ model indicates the existence of the fractionalized excitations even in the Γ model [7]. Further examination of the thermal Hall effect is desirable to elucidate the fractionalization.

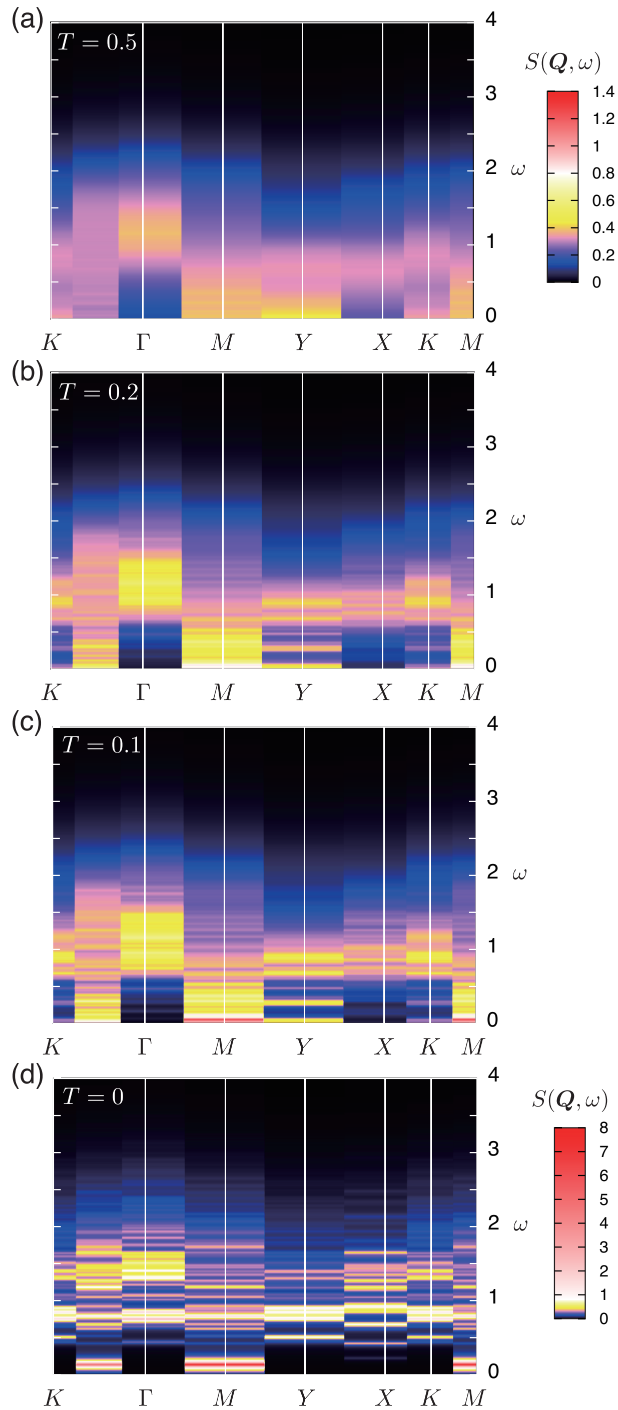

Figure 2: Finite-temperature $S(Q, \omega)$ along a path connecting high symmetry points defined in Fig. 1 (b), at $T = 0.5$ (a), $T = 0.2$ (b), $T = 0.1$ (c), and $S(Q, \omega)$ at $T = 0$ (d).

References

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