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Perturbation theory on the ESR shift and its applications

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Electron Spin Resonance (ESR) has been studied extensively for both its experimental and theoretical interests for a long time. Much of the foundation of the widely used theoretical frameworks, most notably those by Kubo and Tomita, by Mori and Kawasaki and by Nagata and Tazuke, were developed more than 30 years ago. However, the range of validity of assumptions and approximations utilized in these theories remain unclear, especially in the systems with strong quantum fluctuations. In fact, recently, it has been pointed out that a straightforward application of the Kubo-Tomita theory to the Dzyaloshinskii-Moriya interaction yields an incorrect result. Recently, on the other hand, a field theory approach and a direct numerical approach opened new directions of the ESR theory. However, the former works only in one dimension and in the low energy (low temperature, low frequency) regime, and the latter approach can handle only small systems.

Motivated by this situation, we develop a new direct perturbation scheme for the ESR resonance frequency shift in order to circumvent the previous non-trivial assumptions; in Ref.[1,2]. We then exactly evaluate the first order of it for the $S = 1/2$ antiferromagnetic chain for arbitrary temperature and magnetic field by using Quantum Transfer Matrix method. The resonance shift can be expressed as the quit simple form: $\delta\omega_m = f(\theta,\phi)Y(T,H)$, where $f(\theta,\phi)$ is determined by the anisotropy in Hamiltonian and $Y(T,H)$ is

$$Y(T,H) = \frac{1}{2} - \frac{T}{2\pi J}\oint_\Gamma \ln(1+\eta(x+i))dx.$$

Here $\eta(x)$ is determined by a following single integral equation

$$\ln\eta(x) = \frac{2\pi J}{T}a_1(x) - \frac{H}{T} - \oint_\Gamma a_2(x-y-i)\ln(1+\eta(y+i))dy, \qquad a_n(x) = n/(\pi(x^2+n^2))$$

This is solved numerically with a very high precision. The obtained result shows a quite different behavior from the Nagata-Tazuke theory, which is based on the classical spin approximation, especially at low temperature. In low temperature regime, logarithmic and subleading correction terms are analytically obtained. Combing our results with the field theoretical results, we can obtain the logarithmic corrections also in the ESR linewidth. We also compare ours result with experimental data on $LiCuVO_4$.

We show our recent numerical calculations of the ESR shift for $S = 1$ Haldane chain when time permits.

[1] Y. Maeda, M. Oshikawa, J. Phys. Soc. Jpn. **74**, (2005) 283.

[2] Y. Maeda, K. Sakai, and M. Oshikawa, Phys. Rev. Lett. **95** (2005) 037602.