# Haldane-gapped spin chains: Exact low-temperature expansions of correlation functions

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We study both the static and dynamic properties of gapped, one-dimensional, Heisenberg, antiferromagnetic, spin chains at finite temperature through an analysis of the O(3) nonlinear sigma model. Exploiting the integrability of this theory, we are able to compute an exact low-temperature expansion of the finite temperature correlators. We do so using a truncated ''form-factor'' expansion and so provide evidence that this technique can be successfully extended to finite temperature. As a direct test, we compute the static zero-field susceptibility and obtain an exact match to the susceptibility derived from the low-temperature expansion of the exact free energy. We also study transport properties, computing both the spin conductance and the NMR-relaxation rate, $1/T_1$. We find these quantities to show ballistic behavior. In particular, the computed spin conductance exhibits a nonzero Drude weight at finite temperature and zero applied field. The physics thus described differs from the spin diffusion reported by Takigawa *et al.* [Phys. Rev. Lett. **76**, 2173 (1996)] from experiments on the Haldane gap material, $AgVP_2S_6$.

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## I. INTRODUCTION

The realization that one-dimensional, integer spin, antiferromagnets possess an energy gap[1] has made these systems the object of intense study. The model perhaps most commonly used to explore their properties is the field theoretic O(3) nonlinear sigma model (NLSM).[2–7] Although the model has the virtue of being integrable,[8,9] its properties are nonetheless only partially understood. It is possible to access static, thermodynamic quantities while dynamic properties, in particular, transport properties, are in general, unavailable. These latter quantities depend upon knowledge of correlation functions which are generically not exactly computable in integrable models. There are, of course, perturbative techniques by which correlators in the O(3) NLSM may be analyzed. But in strongly coupled models, of which the O(3) NLSM is one, perturbative techniques present a host of difficulties and so can miss qualitative (never mind quantitative) features in the physics.

The inability to completely understand correlation functions in the fully quantum O(3) NLSM has been at the root of a recent controversy in the literature. Takigawa *et al.*[10] demonstrated through measurements of the NMR relaxation rate, $1/T_1$, of the Haldane gap compound, $AgVP_2S_6$, that at long wavelengths, the spin–spin correlation functions are diffusive in nature. In an elegant series of papers, Sachdev and Damle[6,7] developed a semi-classical treatment to attack the problem and subsequently were able to describe this diffusive behavior. Nonetheless their computation was semiclassical leaving open the possibility that a fully quantum treatment of the O(3) NLSM would lead to different physics. This possibility was hinted at in the work of Fujimoto.[11] There the spin conductance was computed using exact thermodynamic considerations. Upon subsequent work,[12] it became clear that the two treatments produced qualitatively different results. In particular, the Drude weight of the spin conductance, $D$, of the O(3) NLSM was found to be nonvanishing in the zero field limit[11], whereas the corresponding semi-classical treatment sees $D(H=0)=0$. This qualitative difference opens up the possibility that diffusive physics is not present in the O(3) NLSM itself but requires some additional mechanism. Such mechanisms might include a spin-phonon coupling (as suggested by Ref. 11), spin anisotropy, inter-chain coupling (the spin-chains in $AgVP_2S_6$ are only quasi 1-D; there do exist weak couplings in between chains although the weakness of these couplings seems to preclude this possibility), or perhaps small generic integrable-breaking perturbations.[13]

In this paper we attempt to address this problem by demonstrating a technique to compute exactly a low-temperature expansion of correlators in the O(3) NLSM. This expansion is based upon a ''form-factor'' expansion. Form-factor expansions have a long history in the computation of correlators.[14–19] However these expansions have been used almost exclusively at zero temperature. When they have been used at finite temperature, they have been used either in the computation of expectation values lacking dynamical properties[20–23] or in the development of distinct nonperturbative representations (i.e., Fredholm determinants) of correlators[24,25] where all the terms in the expansion were kept. In this article we show that *truncated* form-factor expansions can be used to sensibly describe correlation functions at finite temperature. This is distinct from the program proposed in[26,27] where form-factor expansions were employed but the form factors themselves were recomputed to take direct account of thermal fluctuations. Here we employ the same form factors used in zero temperature computations.

A form-factor expansion of a correlation function is predicated upon some generic properties of integrable models. Most importantly, the exact eigenfunctions of the model's fully interacting Hamiltonian are known. With this knowledge comes a well-defined notion of ''particles'' or elementary excitations in the system. The scattering of these particles is completely described by two-body S-matrices. In particular, particle nonconserving processes are disallowed. Ultimately this feature is a consequence of a series of nontrivial conservation laws possessed by the integrable model.

 

In some sense, an integrable model is a superior version of a Fermi liquid: a particle's lifetime is infinite regardless of distance from the Fermi surface.

In order to understand these features of the O(3) NLSM, we begin by providing an overview of the model. The O(3) NLSM is described by the action,

$$S=\frac{1}{2g}\int dx\,dt(\partial^{\mu}\mathbf{n}\,\partial_{\mu}\mathbf{n}), \tag{1.1}$$

where $\mathbf{n}=(n_x,n_y,n_z)$ is a bosonic vector field constrained to live on the unit sphere. This action is arrived at from the Hamiltonian of the spin chain,

$$H=J\sum_i S_i\cdot S_{i+1}. \tag{1.2}$$

In the continuum, large s, limit, the spin operator, $S_i$, is related to the field, $\mathbf{n}$, via

$$S_i=(-1)^i s\mathbf{n}_i+M_i,$$

that is, $\mathbf{n}(x,t)$ is the sub-lattice or Néel order parameter. $M$ on the other hand describes the uniform (i.e., wave vector $k\sim 0$) magnetization. M is related to $\mathbf{n}$ via

$$M=\frac{1}{g}\mathbf{n}\times\partial_t\mathbf{n},$$

and so is given in terms of the momentum conjugate to $\mathbf{n}$.

The low energy excitations in the O(3) NLSM take the form of a triplet of bosons. The bosons have a relativistic dispersion relation given by

$$E(p)=(p^2+\Delta^2)^{1/2}.$$

Here $\Delta$ is the energy gap or mass of the bosons related to the bare coupling, $g$, via $\Delta\sim Je^{-2\pi/g}$. The dispersion relation of all three bosons is identical as the model has a global SU(2) symmetry. The exact eigenfunctions of the O(3) NLSM Hamiltonian are then multi-particle states made up of mixtures of the three bosons. Scattering between the bosons is described by the S-matrix[8]

$$S_{a_1a_2}^{a_3a_4}(\theta)=\delta_{a_1a_2}\delta_{a_3a_4}\sigma_1(\theta)+\delta_{a_1a_3}\delta_{a_2a_4}\sigma_2(\theta)+\delta_{a_1a_4}\delta_{a_2a_3}\sigma_3(\theta);$$

$$\sigma_1(\theta)=\frac{2\pi i\theta}{(\theta+i\pi)(\theta-i2\pi)};$$

$$\sigma_2(\theta)=\frac{\theta(\theta-i\pi)}{(\theta+i\pi)(\theta-i2\pi)};$$

$$\sigma_3(\theta)=\frac{2\pi i(i\pi-\theta)}{(\theta+i\pi)(\theta-i2\pi)}. \tag{1.3}$$

Here $\theta$ parameterizes a particle's energy/momentum via $E=\Delta\cosh(\theta)$, $P=\Delta\sinh(\theta)$. The primary advantage of this parameterization is the implementation of Lorentz boosts. Under such a boost, $\theta\to\theta+\alpha$. As such Lorentz invariant quantities are invariably functions of differences of rapidities. We stress that this relativistic invariance is a natural feature of the low energy structure of the spin chain. (However we do point out for spin 1 chains, $\Delta\sim .4J$. As $J$ serves as the cutoff for the theory, the low energy sector of the theory is not unambiguously defined.)

With the excitation spectrum of the O(3) NLSM in hand, we return to the form-factor expansion. A finite temperature expansion of correlators is given in terms of a trace over the Boltzmann density matrix:

$$G^{\mathcal{O}}(x,t)=\frac{1}{\mathcal{Z}}\mathrm{Tr}(e^{-\beta H}\mathcal{O}(x,t)\mathcal{O}(0,0))=\frac{\sum_{ns_n}e^{-\beta E_{s_n}}\langle n,s_n|\mathcal{O}(x,t)\mathcal{O}(0,0)|n,s_n\rangle}{\sum_{ns_n}e^{-\beta E_{s_n}}\langle n,s_n|n,s_n\rangle}. \tag{1.4}$$

Here the state, $|n,s_n\rangle$, denotes a set of n-particles carrying spin quantum numbers $\{s_n\}$. Inserting a resolution of the identity between the two field then leads us to a double sum,

$$G^{\mathcal{O}}(x,t)=\frac{\sum_{ns_n}\sum_{ms_m}e^{-\beta E_{s_n}}\langle n,s_n|\mathcal{O}(x,t)|m,s_m\rangle\langle m,s_m|\mathcal{O}(0,0)|n,s_n\rangle}{\sum_{ns_n}e^{-\beta E_{s_n}}\langle n,s_n|n,s_n\rangle}. \tag{1.5}$$

We thus have reduced the evaluation of the correlator to the evaluation of a series of matrix elements (known as ''form factors''). In an integrable model like the O(3) NLSM, these matrix elements are in principle exactly computable. However as the number of excitations involved increases, the functional forms of the matrix elements become increasingly unwieldy. This, together with the difficultly in evaluating the sums, $\Sigma_{(n,s_n),(m,s_m)}$, ensure in all but a few special cases the correlators do not admit a closed form expression.

To surmount this we adapt an idea from zero temperature form-factor expansions. Rather than look at the correlator in real space and time, we examine the (more relevant) related spectral function, $G^{\mathcal{O}}(k,\omega)$. In computing $G^{\mathcal{O}}(k,\omega)$, only terms in the form factor sum with a given energy, $\omega$, and momentum, $k$, contribute to the sum,

$$G^{\mathcal{O}}(k,\omega)=\frac{1}{\mathcal{Z}}\sum_{\substack{ns_n\\ms_m}}\delta(\omega-E_{s_n}+E_{s_m})\,\delta(k-p_{s_n}+p_{s_m})\times e^{-\beta E_{s_n}}\langle n,s_n|\mathcal{O}(0,0)|m,s_m\rangle\times\langle m,s_m|\mathcal{O}(0,0)|n,s_n\rangle, \tag{1.6}$$

as enforced by the presence of the two delta functions. For any $\omega,k$, this dramatically reduces the number of matrix el-

ements one must compute. [Here $G^{\mathcal{O}}$ is simply the Fourier transform of $G^{\mathcal{O}}(x,t)$, but similar considerations also apply to the corresponding retarded correlator.] This reduction nonetheless leaves a difficult computation. However we can exploit the gapped nature of the spin chain to make the problem more tractable. Because the theory is gapped (with gap, $\Delta$), the correlator admits a low-temperature expansion of the form,

$$G^{\mathcal{O}}(k,\omega)=\sum_n \alpha_n(k,\omega)e^{-n\beta\Delta}. \tag{1.7}$$

For the particular correlators of concern in this paper and for the range of $\omega$ and $k$ in which we are interested, each $\alpha_n$ is determined by a single matrix element. Because we can compute these matrix elements, we obtain an *exact* low-temperature expansion.

Our ability to compute such an expansion bears upon another controversy in the literature. LeClair and Mussardo[20] argued that it was possible to use the same form-factors we employ here to compute finite temperature correlators. However rather than directly evaluate individual terms in the sum (1.5), they first conjectured an ansatz involving a resummation of terms in the sum. This is described in more detail in Sec. III. This procedure was criticized in Ref. 21. There it was argued that while this worked for the computation of one-point functions, it was problematic for two-point functions. Rather it was argued it was better in general to attack such problems through the use of form factors computed against a thermalized vacuum.[26–28] However the counterexample cited in Ref. 21, a computation involving interacting quantum Hall edge states, involved a gapless theory, and so is in a different class than the model considered in this paper. (Without a gap, the low-temperature expansion we consider above ceases to make sense.) This work here shows that it is possible, at least in certain cases, to make sense of the form-factor expansion of two point functions at finite temperature. But while we can make sense of this expansion, we cannot compare our computations directly to the ansatz posited in Ref. 20. Their ansatz as is applies only to diagonal theories where scattering does not permute internal quantum numbers, contrary to the case here.

The outline of the paper is as follows. In Sec. II we summarize the results of the form-factor computations for three quantities: the magnetic susceptibility, and two transport properties, the spin conductance and the NMR relaxation rate, $1/T_1$. The details of these computations are found in later sections or in appendices if the reader is so interested. The first quantity, the susceptibility, is compared to the susceptibility as derived from a low-temperature expansion of the exact free energy. We see that they match verifying our claim that the form factor expansion can yield an exact low-temperature expansion.

We compare our transport calculations to the semi-classical computations in Refs. 6 and 7. The essence of this method lies in treating the spin-chain as a Maxwell-Boltzmann gas of spins which interact with one another through the low energy limit of the scattering of the O(3) NLSM,

$$S_{ab}^{cd}(\theta=0)=-\delta_{ad}\delta_{cb}. \tag{1.8}$$

While static properties computed in the two treatments agree (for the susceptibility, we find that up to temperatures on the order of the gap, $T\sim\Delta$, the two computations agree), we see differences in transport properties. For the spin conductance we find, in contradistinction to the semi-classical computation, that the Drude weight of the spin conductance is finite in the limit of zero external field. Our results for the NMR relaxation rate, $1/T_1$, indicate a similar discrepancy. We, like Ref. 5, find that $1/T_1$ is characterized by ballistic logarithms. These logarithms are relatively robust: they continue to appear at higher orders in the low temperature expansion. We do not, however, see diffusive behavior in the relaxation rate, i.e., $1/T_1\sim 1/\sqrt{H}$, nor does our low-temperature expansion match the low-temperature expansion of the semi-classical computation of the correlator.

We consider two possibilities in explaining these discrepancies. We argue that the structure of the conserved quantities or charges differs between the O(3) NLSM and its semi-classical variant and that these differences lead to ballistic behavior on the one hand and diffusive behavior on the other. The other explanation we forward to explain this discrepancy lies in the supra-universality of the low energy S-matrix (1.8). The low energy limit of this S-matrix is shared by generic integer spin chains. Indeed it is shown in Ref. 7 that a two-leg spin-1/2 ladder, expected to share the low energy behavior of a spin-1 chain, has this exact low-energy S-matrix. However rather than the supra-universality being a virtue, it may be that it under-specifies the physics. In this way the semi-classical treatment, valid in and of itself (particularly in light of its ability to reproduce experimental data), may capture different physics than that of the O(3) NLSM. In Sec. II we consider this further in the light of the sine-Gordon model where a similar phenomena may be argued to occur.

In the first part of Sec. III we explain in some detail how the form-factor expansion is to be understood. In particular we consider the various technical details of the expansion, including how to regulate the infinities that appear generically in the form factors of the double expansion. In second part of Sec. III we review the specific form factors of the O(3) NLSM. And finally in Sec. IV, we review the low-temperature expansion of the exact free energy, necessary for comparison with the form-factor computation of the susceptibility.

## II. SUMMARY AND DISCUSSION OF RESULTS

### A. Zero field, finite temperature susceptibility

In this subsection we present results for the magnetic susceptibility arising from several methods of computation: a form-factor evaluation of the magnetization–magnetization correlator in the context of a Kubo formula, an exact computation of the system's free energy, and finally, treating the excitations of the O(3) sigma model as noninteracting particles obeying both a Fermi-Dirac distribution and a Maxwell-Boltzmann distribution in the spirit of the semi-classical approximation of Sachdev and Damle.[6,7] We thus

will be able to determine the temperature regime over which our truncation of the form-factor expansion applies as well as comparing with other computational techniques.

#### *1. Kubo formula and form factors*

The susceptibility, $\chi$, at $H=0$ can be computed from the magnetization-magnetization operator using a Kubo formula:

$$\chi(H=0)=C(\omega=0,k=0),$$

$$C(\omega=0,k=0)=\left[\int_{-\infty}^{\infty}dx\int_0^{\beta}d\tau e^{iw_n\tau}e^{ikx}\times\langle T(M_0^3(x,\tau)M_0^3(0,0))\rangle\right]_{\omega_n\to -i\omega+\delta}. \tag{2.1}$$

To evaluate this correlator we employ an expansion in terms of the exact eigenfunctions of the theory, i.e., a form-factor expansion. In particular we write

$$\langle M_0^3(x,\tau)M_0^3(0,0)\rangle=\frac{1}{\mathcal{Z}}\mathrm{Tr}(e^{-\beta H}\mathcal{O}(x,\tau)\mathcal{O}(0,0))=\frac{\sum_{ns_n}e^{-\beta E_{s_n}}\langle n,S_n|\mathcal{O}(x,\tau)\mathcal{O}(0,0)|n,S_n\rangle}{\sum_{nS_n}e^{-\beta E_{s_n}}\langle n,S_n|n,S_n\rangle}. \tag{2.2}$$

Here $|n,S_n\rangle$ is a state of n excitations with spins described by $S_n=\{s_1,\cdots,s_n\}$. In writing the above we have suppressed sums over the energy and momenta of the excitations. A term in the thermal trace with n excitations is weighted by a factor of $e^{-n\beta\Delta}$. At low temperatures it is thus a good approximation to truncate this trace. For this computation we keep only terms with one and two excitations, i.e., $n=1,2$. To evaluate the matrix elements appearing in Eq. (2.2) we insert a resolution of the identity in between the two fields. As we only consider matrix elements involving one and two excitations from the thermal trace, we thus have

$$\begin{aligned}\langle s_1|M_0^3(x,\tau)M_0^3(0,0)|s_1\rangle&=\sum_{mS_m}\langle s_1|M_0^3(x,\tau)|mS_m\rangle\times\langle mS_m|M_0^3(0,0)|s_1\rangle\\&=\sum_{s_1'}\langle s_1|M_0^3(x,\tau)|s_1'\rangle\times\langle s_1'|M_0^3(0,0)|s_1\rangle+\cdots;\end{aligned}$$

$$\begin{aligned}\langle s_1s_2|M_0^3(x,\tau)M_0^3(0,0)|s_2s_1\rangle&=\sum_{mS_m}\langle s_1s_2|M_0^3(x,\tau)|mS_m\rangle\times\langle mS_m|M_0^3(0,0)|s_2s_1\rangle\\&=\sum_{s_1's_2'}\langle s_1s_2|M_0^3(x,\tau)|s_1's_2'\rangle\times\langle s_2's_1'|M_0^3(0,0)|s_2s_1\rangle+\cdots.\end{aligned} \tag{2.3}$$

In the above we have truncated the sum arising from the resolution of the identity. With the first matrix element of the thermal trace, we only keep terms from the resolution of identity with one excitation. We are interested in the behavior of the susceptibility at $\omega=0$ and this term provides the only contribution. Similarly, the only term arising from the second matrix element of the thermal trace contributing to the dc susceptibility comes from keeping the term from the resolution of the identity involving two excitations. Further details surrounding the methodology of this expansion and the explicit exact evaluation of the matrix elements are found in Sec. III and Appendix A. With such details we can evaluate $C(\omega=0,k=0)$ with the result

$$C(\omega=0,k=0)=C_1(\omega=0,k=0)+C_2(\omega=0,k=0), \tag{2.4}$$

where $C_1$ and $C_2$ are given by

$$C_1(\omega=0,k=0)=\frac{2\beta\Delta}{\pi}K_1(\beta\Delta);$$

$$\begin{aligned}C_2(\omega=0,k=0)&=-\frac{6\beta\Delta}{\pi}K_1(2\beta\Delta)+\frac{2\beta\Delta}{\pi}\int d\theta_1 d\theta_2\times e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}\cosh(\theta_1)\\&\quad\times\frac{11\pi^2+2\theta_{12}^2}{\theta_{12}^4+5\pi^2\theta_{12}^2+4\pi^4}\\&=-\frac{6\beta\Delta}{\pi}K_1(2\beta\Delta)+\frac{22\beta\Delta}{\pi^3}K_0(\beta\Delta)K_1(\beta\Delta)\\&\quad+\mathcal{O}\left(\frac{T}{\Delta}e^{-2\beta\Delta}\right),\end{aligned} \tag{2.5}$$

where $\theta_{12}=\theta_1-\theta_2$ and $K_n$ are standard modified Bessel functions. The first term in $C_2$ is a ''disconnected'' contribution related to $C_1$. The second term is a connected contribution and as such is genuinely distinct from $C_1$. We now consider such disconnected contributions further.

#### *2. Resummed form factors*

In computing the susceptibility, we are able to go beyond the approximation introduced in truncating the form-factor sum arising from the thermal trace. It is possible to include ''disconnected'' terms arising from higher particle contributions. Such disconnected terms appear when higher particle

matrix elements are evaluated. For example when we evaluate the four excitation matrix element $\langle s_2' s_1' | M_0^3(0,0) | s_2 s_1 \rangle$, we obtain a term of the form

$$\langle s_2' s_1' | M_0^3(0,0) | s_2 s_1 \rangle = \cdots + \delta_{s_2' s_1} \langle s_1' | M_0^3(0,0) | s_2 \rangle + \cdots .$$

This term is "disconnected" in that it is directly related to a matrix element involving a lesser number (two) of excitations. It arises from the annihilation of $s_2'$ with $s_1$. Such a term is responsible, as we just indicated, for the first term of $C_2$ above.

What is remarkable is that we are able to sum up over *all* possible disconnected pieces arising from arbitrarily high particle form factors which are proportional to the connected lower particle matrix elements already computed. This resummation amounts to the evaluation of a geometric series. For example, including all disconnected terms involving the matrix element going into the evaluation of $C_1$ modifies it as follows

$$\begin{aligned} C_1 &= \frac{\beta\Delta}{\pi} \int d\theta e^{-\beta\Delta \cosh(\theta)} \cosh(\theta) \\ &\to \frac{\beta\Delta}{\pi} \int d\theta e^{-\beta\Delta \cosh(\theta)} \cosh(\theta) \sum_{n=0} (-3)^n e^{-n\beta\Delta \cosh(\theta)} \\ &= \frac{\beta\Delta}{\pi} \int d\theta \frac{e^{-\beta\Delta \cosh(\theta)} \cosh(\theta)}{1+3e^{-\beta\Delta \cosh(\theta)}} = \frac{2\beta\Delta}{\pi} K_1(\beta\Delta) \\ &\quad - \frac{6\beta\Delta}{\pi} K_1(2\beta\Delta) + \mathcal{O}(e^{-3\beta\Delta}). \end{aligned} \tag{2.6}$$

We see resumming the disconnected pieces thus reproduces both $C_1$ and the first term in $C_2$ plus additional terms higher order in $e^{-\beta\Delta}$. The appearance of the factors $e^{-\beta\Delta \cosh(\theta)}$ in the geometric series is natural and arises from the Boltzmann weighting of the higher particle terms. The combinatorial factor of 3 reflects the three bosons in the system.

In collecting all the disconnected pieces related to the *connected* term in $C_2$, we find something similar

$$\begin{aligned} &\text{connected } C_2 + \text{disconnected terms} \\ &= \frac{\beta\Delta}{\pi} \int d\theta_1 \, d\theta_2 \frac{e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}}{1+3e^{-\beta\Delta \cosh(\theta_1)}} (\cosh(\theta_1) \\ &\quad + \cosh(\theta_2)) \frac{11\pi^2 + 2\theta_{12}^2}{\theta_{12}^4 + 5\pi^2\theta_{12}^2 + 4\pi^4}. \end{aligned} \tag{2.7}$$

One expects in general that the inclusion of disconnected terms from arbitrarily high particle number will improve the accuracy of the calculation. In the case of the susceptibility, the agreement between the form-factor computation and the exact numerical analysis actually becomes slightly worse. However, this should not be taken as indicative of the resummation in general. We will comment on this further at the end of this section.

#### *3. Gases of free particles*

For the purposes of comparison, we compute the susceptibility of both a free electron gas (or equivalently, a system of hard-core bosons) as well as a Maxwell-Boltzmann gas. At sufficiently low temperatures both of these quantities should be close to the exact value of $\chi$ for the O(3) sigma model. How the susceptibility of the free electron gas deviates from the exact value of $\chi$ gives us an understanding of the temperature at which interactions become important. And how the susceptibility of the Maxwellian gas deviates from the exact answer marks the temperature at which the semiclassical approximation found in Damle and Sachdev[6,7] must begin to breakdown.

These two susceptibilities are given by

$$\begin{aligned} \chi_{\text{free el.}} &= \frac{\beta\Delta}{\pi} \int d\theta \frac{\cosh(\theta) e^{-\beta\Delta \cosh(\theta)}}{(1+e^{-\beta\Delta \cosh(\theta)})^2} = \frac{2\beta\Delta}{\pi} K_1(\beta\Delta) \\ &\quad + \mathcal{O}(e^{-\beta\Delta}) = \sqrt{\frac{2\beta\Delta}{\pi}} e^{-\beta\Delta} + \mathcal{O}\left(\frac{T}{\Delta} e^{-\beta\Delta}\right); \\ \chi_{\text{MB}} &= \sqrt{\frac{2\beta\Delta}{\pi}} e^{-\beta\Delta}. \end{aligned} \tag{2.8}$$

We see that at low temperatures ($\beta\Delta \ll 1$) both of these expressions coincide with the low temperature limit of the form factor computation of $\chi$. In particular, the terms of $\mathcal{O}(e^{-\beta\Delta})$ are identical.

#### *4. Thermodynamic Bethe Ansatz*

It is possible in the case of the O(3) sigma model to arrive at exact expressions (in the form of coupled integral equations) for the zero-field susceptibility.[29,30] These equations, in their most compact form, appear as

$$\begin{aligned} \chi(H=0) &= -\frac{\Delta}{2\pi} \int d\theta \cosh(\theta) \frac{\partial_H^2 \epsilon(\theta)|_{H=0}}{1+e^{\beta\epsilon(\theta)}}; \\ \epsilon(\theta) &= \Delta \cosh(\theta) - T \int d\theta' \log(1+e^{\beta\epsilon_2(\theta')}) s(\theta-\theta'); \\ \epsilon_n(\theta) &= T \int d\theta' s(\theta-\theta') \{\log(1+e^{\beta\epsilon_{n-1}(\theta')}) \\ &\quad + \log(1+e^{\beta\epsilon_{n+1}(\theta')}) + \delta_{2n} \log(1+e^{\beta\epsilon(\theta')})\} \\ H &= \lim_{n\to\infty} \frac{\epsilon_n(\lambda)}{n} \end{aligned} \tag{2.9}$$

We will show results from the exact numerical evaluation of these equations in the next section. However these equations admit a closed form low-temperature expansion. The details of this expansion may be found in Sec. IV. Here we just give the final results

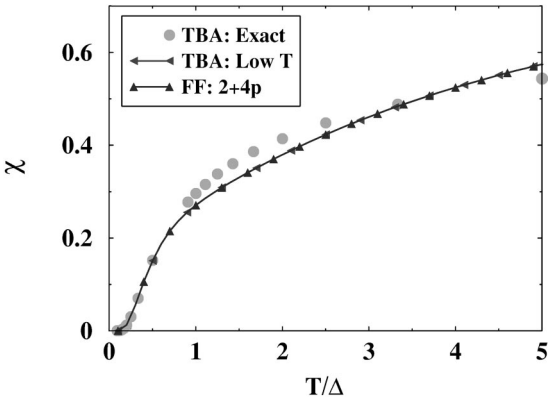


FIG. 1. Plots of the zero-field susceptibility computed both from the TBA equations and from the form-factor expansions. The first of these is an exact numerical solution of the TBA equations for the O(3) sigma model. The second is arrived from a small temperature expansion in powers of $e^{-\beta\Delta}$ of these same equations. The final plot gives the form-factor computation of the susceptibility. We have truncated the form-factor expansion at the four particle level.

$$\chi = \frac{2\beta\Delta}{\pi} K_1(\beta\Delta) - \frac{6\beta\Delta}{\pi} K_1(2\beta\Delta) + \frac{2\beta\Delta}{\pi} \int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \cosh(\theta_1) \times \frac{11\pi^2 + 2\theta_{12}^2}{\theta_{12}^4 + 5\pi^2\theta_{12}^2 + 4\pi^4}. \quad (2.10)$$

Remarkably, we see this expansion agrees exactly with the corresponding expression derived with the aid of form factors. Thus the form-factor expansion at finite temperature passes an important test.

#### *5. Comparison of methodologies*

In this section we compare the various methods of computing the susceptibility of the O(3) sigma model. In Fig. 1 are plotted the susceptibilities computed via an exact numerical analysis of the TBA equations, a low-temperature expansion of the same equations, and a computation based upon the two and four particle form factors. We see that as indicated previously that the form-factor computation and the low-temperature expansion match exactly. Moreover these two computations track the exact susceptibility over a considerable range of temperatures despite the fact these computations are truncated low-temperature expansions.

In Fig. 2 we compare both the exact TBA susceptibility and the form-factor computation of $\chi$ with the susceptibility of a classical Maxwellian gas. We see the results track one another for temperatures, $T \leqslant \Delta$. For temperatures beyond $\Delta$, however, the Maxwellian susceptibility differs markedly. This is then roughly the temperature at which the semiclassical approximation found in Refs. 6 and 7 should be expected to break down.

In Fig. 3 are plotted the exact results for the susceptibility together with the susceptibility from the resummed form factors. We see that the resummed susceptibility is somewhat

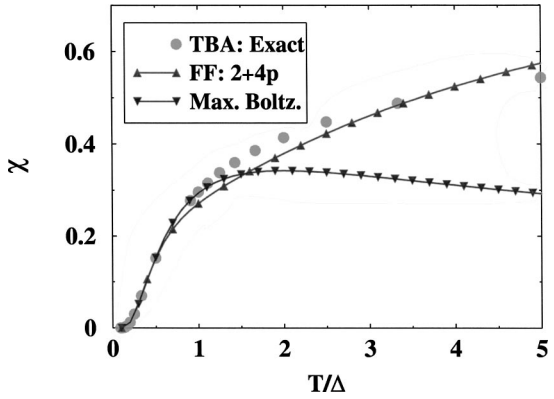


FIG. 2. The zero-field susceptibility of a Maxwellian gas is compared here to both the exact susceptibility of the O(3) NLSM and the susceptibility of the O(3) NLSM computed via a form-factor expansion.

higher that the exact numerics at $T \sim 5\Delta$ and disagrees at roughly the 10% level whereas the susceptibility computed using the unresummed form factors sees better agreement at these same temperatures. At lower temperatures ($T \sim 2$–$3\Delta$) the disagreement between the exact numerics and the two form-factor computations is roughly the same. In general then, the resummation does not improve the accuracy of the computation of the susceptibility.

### B. Spin conductance

In this section we compute the spin conductivity, $\sigma_s$. The spin conductivity gives the response of the spin chain to a spatially varying magnetic field. It is defined via

$$j_1(x,t) = \sigma_s \nabla H, \quad (2.11)$$

and so can be expressed in terms of a Kubo formula,

$$\mathrm{Re}\,\sigma_s(k,\omega) = -\frac{1}{k}\int dx\, dt e^{ikx+i\omega t}\, \mathrm{Im}\langle j_0(x,t) j_1(0,0)\rangle_{\mathrm{retarded}}. \quad (2.12)$$

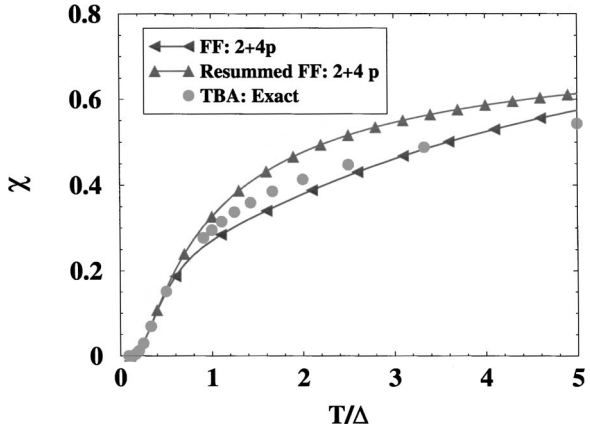


FIG. 3. The zero-field susceptibility of the O(3) NLSM as computed using a resummed form-factor expansion is compared both with the exact result coming from the TBA equations and the unresummed form-factor susceptibility.

In the notation used in this paper the spin current $j_1$ is synonymous with $M_1$, the Lorentz current counterpart of the uniform magnetization, $M_0 \equiv j_0$. We will focus primarily on computing the Drude weight, D, of $\mathrm{Re}\,\sigma_s$, i.e., computing the term in $\sigma_s(k,\omega)$ of the form

$$\sigma_s(k=0,\omega) = D\,\delta(\omega). \tag{2.13}$$

However we are able to compute $\sigma_s$ for general $k,\omega$. We find that for $\omega \ll 2\Delta$, $k=0$, the spin conductivity is described solely by the Drude weight. In particular, we find no indication of a regular contribution to $\sigma_s(k=0,\omega)$.

To evaluate $\sigma_s$, we employ the identical form-factor expansion to that used in computing the susceptibility. And like the susceptibility, our result is an exact low-temperature expansion of $D$,

$$D = \sum_n D_n e^{-n\beta\Delta}.$$

Here we will compute $D_1$ and $D_2$ exactly. As the details of the computation are nearly identical to that of the susceptibility, we merely write down the results:

$$\begin{aligned} D(H=0) &= \beta\Delta \int d\theta e^{-\beta\Delta\cosh(\theta)} \frac{\sinh^2(\theta)}{\cosh(\theta)} (1 - 3e^{-\beta\Delta\cosh(\theta)}) \\ &\quad + 2\beta\Delta \int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ &\quad \times \frac{\sinh^2(\theta_2)}{\cosh(\theta_2)} \frac{11\pi^2 + 2\theta_{12}^2}{\theta_{12}^4 + 5\pi^2\theta_{12}^2 + 4\pi^4} + \mathcal{O}(e^{-3\beta\Delta}) \\ &= e^{-\beta\Delta}\sqrt{\frac{2\pi}{\beta\Delta}}\left(1 + \mathcal{O}\left(\frac{T}{\Delta}\right)\right) - e^{-2\beta\Delta}\sqrt{\frac{1}{\beta\Delta}} \\ &\quad \times \left(\frac{3}{2}\sqrt{\pi} - \frac{11}{\pi}\sqrt{\frac{T}{\Delta}} + \mathcal{O}\left(\frac{T}{\Delta}\right)\right) + \mathcal{O}(e^{-3\beta\Delta}). \end{aligned} \tag{2.14}$$

This expression involves only the two and four particle form factors. If we also include all higher order disconnected terms related to those above we find instead (akin to the susceptibility),

$$\begin{aligned} D(H=0) &= \beta\Delta \int d\theta e^{-\beta\Delta\cosh(\theta)} \frac{\sinh^2(\theta)}{\cosh(\theta)} \frac{1}{1+3e^{\beta\Delta\cosh(\theta)}} \\ &\quad + 2\beta\Delta \int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ &\quad \times \frac{\sinh^2(\theta_2)}{\cosh(\theta_2)} \frac{11\pi^2 + 2\theta_{12}^2}{\theta_{12}^4 + 5\pi^2\theta_{12}^2 + 4\pi^4} \\ &\quad \times \frac{1}{2}\left(\frac{1}{1+3e^{\beta\Delta\cosh(\theta_1)}} + \frac{1}{1+3e^{\beta\Delta\cosh(\theta_2)}}\right). \end{aligned} \tag{2.15}$$

We plot these two results in Fig. 4 as a function of $T/\Delta$. Akin to the susceptibility, the result does not differ greatly if the resummed disconnected terms are included.

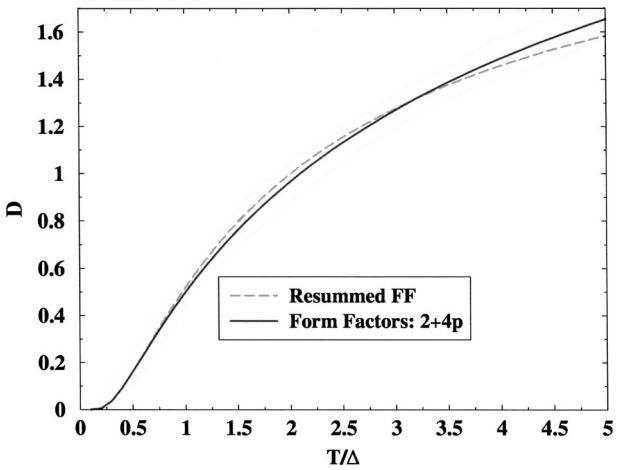


FIG. 4. In this plot we present the form-factor computation of the Drude weight, $D$, of the spin conductance. As with the susceptibility, both the unresummed and resummed computation give roughly the same answer.

We observe that $D(H=0) \neq 0$. This is in accordance with Ref. 11 where $D$ is computed using an argument involving the finite size scaling of the thermodynamic Bethe ansatz equations. (We do note that the computation of $D$ at $H=0$ in Ref. 11 appears only as a note added in proof and so is decidedly sketchy. However, the equations governing $D$ developed in Ref. 11 are manifestly positive with the consequence $D$ cannot vanish.) But our results do differ from the semi-classical computation of Ref. 12 where it was found that $D$ vanishes at $H=0$. We find as well no additional regular contributions to $\sigma_s(\omega,k=0)$ near $\omega=0$—only the Drude term is present in contrast to Refs. 6 and 7. (There will, however, be regular contributions at higher frequencies, in particular for $\omega > 2\Delta$, which persist even in the zero temperature limit).

We have only given the spin conductivity at $H=0$. However, it is extremely straightforward to generalize the form factor computation to finite H. As H couples to the total spin, a conserved quantity, the form factors, $f^{\mathcal{O}}(x,t)$, of an operator, $\mathcal{O}(x,t)$, carrying spin s, are altered via the rule

$$f^{\mathcal{O}}(t) \to e^{iHst} f^{\mathcal{O}}(t).$$

(In the case of the spin conductance, the spin currents, $j_\mu = M_\mu^3$, carry no spin and so are not altered at all.) The only remaining change induced by a finite field is to the Boltzmann factor appearing in the thermal trace. If an excitation with rapidity, $\theta$, carries spin s, its Boltzmann factor becomes

$$e^{-\beta(\Delta\cosh(\theta) - sH)}.$$

For example, we find $D$ as a function of $H$ (to $\mathcal{O}(e^{-\beta\Delta})$) to be

$$D(H) = \beta\Delta\cosh(\beta H) \int d\theta e^{-\beta\Delta\cosh(\theta)} \frac{\sinh^2(\theta)}{\cosh(\theta)}. \tag{2.16}$$

Again this in agreement with Ref. 11. Indeed Ref. 11 computes $D(H)$ at large $H/T$ (but $H \ll \Delta$) to be

$$D=\frac{\beta\Delta}{4\pi}e^{\beta H}\int d\theta\frac{\sinh^2(\theta)}{\cosh(\theta)}e^{-\beta\Delta\cosh(\theta)}+\mathcal{O}(e^{-2\beta\Delta}). \tag{2.17}$$

Up to a factor of $2\pi$, this expression is in exact agreement with Eq. (2.16). In this particular case our derivation of $D(H)$ agrees with the semi-classical computation[12] (provided $T\ll H\ll\Delta$). The symmetries in the semi-classical model that lead $D(H=0)$ to vanish are broken for finite H.

### C. NMR correlators

In this section we compute the NMR relaxation rate, $1/T_1$. We are interested in computing this rate in order to compare it to the experimental data found in Ref. 10 on the relaxation rate of the quasi one-dimensional spin chain, $AgVP_2S_6$. For temperatures in excess of 100 K (the gap, $\Delta$, in this compound is on the order of 320 K), the experimental data[10] shows the relaxation rate to have an inverse dependence upon $\sqrt{H}$:

$$1/T_1\propto\frac{1}{\sqrt{H}}.$$

This dependence is nicely reproduced by the semi-classical methodology in Refs. 6 and 7. Moreover, the semi-classical computation reproduces the activated behavior of $1/T_1$ in this same temperature regime:

$$1/T_1\propto e^{-3\beta\Delta/2}.$$

We are interested in determining whether a calculation in the fully quantum O(3) NLSM can reproduce these results. To this end we compute $1/T_1$ using a form factor expansion. Sagi and Affleck[5] have already done such a computation to lowest order in $e^{-\beta\Delta}$. But they do not find the above behavior. Rather they see

$$1/T_1\propto\log(H);\quad 1/T_1\propto e^{-\beta\Delta}.$$

We continue this computation one further step, computing to $\mathcal{O}(e^{-2\beta\Delta})$. Given the behavior, $1/T_1\sim H^{-1/2}$, appears only as T is increased beyond 100 K (i.e., $T/\Delta\sim 1/3$), it is not unreasonable to suppose higher order terms in a low-temperature expansion of $1/T_1$ are needed to see this singularity.

To proceed with the computation of $1/T_1$, we review its constituent elements. $1/T_1$ can be expressed in terms of the spin–spin correlation function:[5]

$$1/T_1=\sum_{\substack{\alpha=1,2\\ \beta=1,2,3}}\int\frac{dk}{2\pi}A_{\alpha\beta}(k)A_{\alpha\gamma}(-k)\langle M_0^\beta M_0^\gamma\rangle(k,\omega_N), \tag{2.18}$$

where $\omega_N=\gamma_N H$ is the nuclear Lamour frequency with $\gamma_N$ the nuclear gyromagnetic ratio and the $A_{\alpha\beta}$ are the hyperfine coupling constants. In the above we assume H is aligned in the 3-direction. The above integral is dominated by values of $k$ near 0.[5] Moreover in the relevant experiment, the hyperfine couplings are such that only $\langle M_0^1M_0^1\rangle$ contributes. Hence

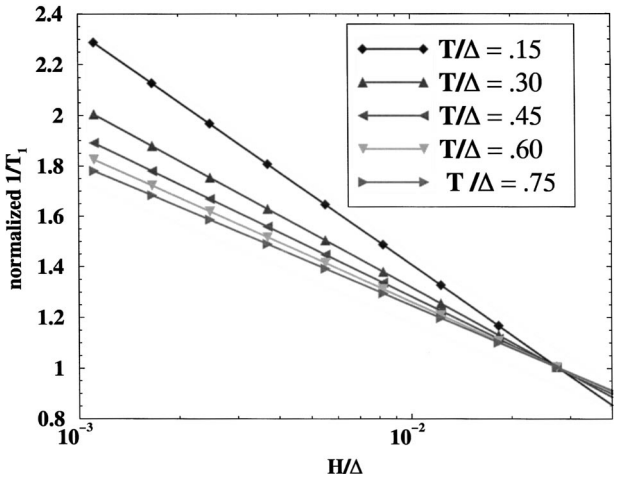


FIG. 5. In this log-linear plot we present the form factor computation of the NMR relaxation rate, $1/T_1$, as a function of H for a variety of temperatures. We plot a normalized rate, the ratio of $1/T_1(H)$ with $1/T_1(H=\Delta/36)$.

$$1/T_1\propto\langle M_0^1M_0^1\rangle(x=0,\omega_N\sim 0). \tag{2.19}$$

We now proceed to compute $\langle M_0^1M_0^1\rangle$.

To compute $\langle M_0^1M_0^1\rangle$, we again employ a form-factor expansion. Akin to the computation of the susceptibility and the spin conductance, this computation amounts to a low-temperature expansion of $\langle M_0^1M_0^1\rangle$,

$$\langle M_0^1M_0^1\rangle=a_1e^{-\beta\Delta}+a_2e^{-2\beta\Delta}+\cdots,$$

where we are able to compute $a_1$ and $a_2$. We place the details of this computations in Appendix B, here merely quoting results:

$$\begin{aligned}\langle M_0^1M_0^1\rangle(x=0,\omega=0)=&\left(\frac{2\Delta}{\pi}e^{-\beta\Delta}\left(\log\left(\frac{4T}{H}\right)-\gamma\right)\right.\\&-\frac{6\Delta}{\pi}e^{-2\beta\Delta}\left(\log\left(\frac{2T}{H}\right)-\gamma\right)\\&\left.+\Delta e^{-2\beta\Delta}\left(\log\left(\frac{4T}{H}\right)-\gamma\right)\sqrt{\frac{2\pi}{\beta\Delta}}\left(24\pi+\frac{17}{\pi^3}\right)\right)\\&\times(1+\mathcal{O}(H/T)+\mathcal{O}(T/\Delta)),\end{aligned} \tag{2.20}$$

where $\gamma=0.577\ldots$ is Euler's constant. We are interested in the regime $H\ll T\ll\Delta$ (the regime where it is expected spin diffusion produces singular behavior in $1/T_1$). The terms that we have dropped do not affect this behavior. In principle there is no difficulty in writing down the exact expression [to $\mathcal{O}(e^{-2\beta\Delta})$]; it is merely unwieldy. This expression for $1/T_1$ is plotted in Fig. 5 for a variety of values of the ratio $T/\Delta$.

We see that we do not obtain the same behavior as found in Refs. 6 and 7. Going to the next order in $\mathcal{O}(e^{-2\beta\Delta})$ produces a behavior in $1/T_1$ as $H\to 0$ identical to the lower order computation of $\mathcal{O}(e^{-\beta\Delta})$: we again find a logarithmic behavior consistent with ballistic transport. An alternative comparison we might make to the results of Refs. 6 and 7 is to perform a low-temperature expansion (in $\mathcal{O}(e^{-\beta\Delta})$) of the

semi-classical computation of $\langle M_0^1 M_0^1\rangle(x=0,\omega=0)$. Doing so by treating $Te^{-\beta\Delta}/H$ as a small parameter, we find

$$\langle M_0^1 M_0^1\rangle(x=0,\omega=0)\propto \Delta e^{-\beta\Delta}\left(\log\left(\frac{4T}{H}\right)-\gamma+\left(\frac{\pi}{4}-\frac{1}{2}\right)\frac{T^2}{\pi H^2}e^{-2\beta\Delta}+\mathcal{O}(e^{-3\beta\Delta})\right). \tag{2.21}$$

We see that the low-temperature expansion of the semi-classical result agrees to leading order with our computation but afterward differs. (We have already seen that this occurs with the computation of the susceptibility.) It possesses no term of $\mathcal{O}(e^{-2\beta\Delta})$. The next term rather appears at $\mathcal{O}(e^{-3\beta\Delta})$ and possesses a $1/H^2$ divergence. That the small $H$ behavior should be $1/\sqrt{H}$ does suggest the importance of summing up terms. But the lack of a term of $\mathcal{O}(e^{-2\beta\Delta})$ in the semi-classical result nonetheless hints that the two results are genuinely different.

### D. Discussion

We have demonstrated that it is possible to compute exact low-temperature expansions of correlators using form factors. Moreover, we have done so in a nontrivial theory where particle scattering sees the exchange of quantum numbers. An important question to answer concerns the breadth of the applicability of our techniques. Our ability to carry out these computations was partially predicated upon the particular correlators we studied. For example, the fact that only a single matrix element contributes at $\mathcal{O}(e^{-\beta\Delta})$ and $\mathcal{O}(e^{-2\beta\Delta})$ in the computation of the susceptibility is related to the magnetization operator in the O(3) NLSM model being a Lorentz current density. Because of these particular details, we thus expect that exact low-temperature expansions of correlators will not be available in all theories.

The computation of correlators is done in the context of a grand canonical partition function. Specifically, we do not work at fixed particle number but include matrix elements involving an arbitrary number of particles or excitations [see Eq. (1.5) for example]. This differs from the treatment found in Ref. 28. There correlators are computed in a canonical ensemble using form factors at some fixed particle number, $N$. A thermodynamic limit is then taken, $N,L\to\infty$ holding $N/L$ (i.e., the particle density) fixed. On a technical level these methods may seem ostensibly different. In particular in this paper we end up computing correlators using form factors involving a small finite number of particles whereas Ref. 28 computes correlators using form factors involving a diverging number of particles. It might appear then that we are somehow missing information that arises in working at a finite particle density. This would seem crucial in computing transport properties where a finite particle density is necessarily determinant.

However, this difference is only apparent. The N particle form factors used by Ref. 28 include disconnected terms. These disconnected terms are equivalent to form factors involving small numbers of particles. The (large) N-particle form factors then contain the same information we use in our representation of the correlators. Moreover, we can make this identification precise. Our use of form factors in the grand canonical ensemble involving some few number of particles, $n$, is predicated upon the small parameter, $e^{-n\Delta\beta}$. But the disconnected terms of an N-particle form factor involving $n$ particles (with $n<N$) are similarly weighted by the same small parameter, $e^{-\beta\Delta n}$. More generally, the presence of a gap, $\Delta$, thus means we can in principle create an explicit map between the two approaches.

The semi-classical method found in Refs. 6 and 7 is similar to the approach taken in Ref. 28 in that it uses a canonical ensemble. It is an interesting question whether a grand canonical ensemble approach can be developed in this same semi-classical approach. The answer is not obvious. Our method works (at least at the technical level) because we can readily identify disconnected terms. It is not clear whether a similar identification can be made semi-classically.

We do want to emphasize a caveat to our methodology as discussed in some detail in Sec. III. It is unclear whether it is possible to compute quantities that show nonanalyticities as $T\to 0$. For example, it is not obvious how to compute the thermal broadening present in the single particle spectral function. At $T=0$ it takes the form

$$\langle nn\rangle(\omega,k)\sim\delta(\omega-\sqrt{k^2+\Delta^2}), \tag{2.22}$$

but is expected to broaden into a Gaussian-like peak at finite T. To see this in a form-factor expansion would likely require a resummation of terms. However, it may well be feasible to deduce the necessary resummation from the lower order terms in the form-factor expansion.

We have also discussed using a resummation of higher order ''disconnected'' terms to improve the form-factor computation. For the quantities considered, it turned out the resummation did not provide a real improvement to the original computation. Nevertheless we would guess that in general, the resummed form factors will provide a more reliable answer as the temperature is increased. It is an artifact of the above cases that they do not do so here. For example, we see that at extremely high temperatures, the susceptibility as computed by either of the form-factors methods saturates to a constant. As such, errors in either method are cutoff—as these expressions at $T=\infty$ do not differ greatly from their low $T$ values, any potential error is bounded. If instead we computed the finite field magnetization (where at lowest order we would expect a linear $T$ dependence—provided $\beta H$ is kept constant), the differences between the two form-factor computations would be comparatively magnified.

To come to some sort of judgement between the form-factor and the semi-classical approaches, an understanding is needed of the differences between our computations of the spin conductance and the NMR relaxation rate. In the case of the first quantity, it is likely this difference is real and not an artifact of our methodology. The data that go into the spin conductance is identical to that needed to compute the susceptibility and we know that we can match the low-temperature expansion of the susceptibility with a similar expansion coming from the exact free energy. Moreover, we

know that the Drude weight of $\sigma_s(H=0)$ has been found to be finite from an approach[11] independent of ours.

In generic systems the Drude weight, $D$, of a conductivity at finite temperatures will be zero. It is then the integrability of the O(3) NLSM and the attendant existence of an infinite number of conserved quantities that leads to a finite weight. The existence of these quantities can be directly related to a finite $D$. As discussed in Ref. 31, $D$ is bounded from below via an inequality developed by Mazur:

$$D \geqslant c \sum_n \frac{\langle JQ_n \rangle}{\langle Q_n^2 \rangle}, \tag{2.23}$$

where $J$ is the relevant current operator, $Q_n$ are a set of orthogonal conserved quantities, i.e., $\langle Q_n Q_m \rangle = \delta_{nm} \langle Q_n^2 \rangle$, and $c$ is some constant. For a finite Drude weight we then require that at least one matrix element, $\langle JQ_n \rangle$, does not vanish. While we do no direct computations, we can obtain an indication of whether the matrix elements vanish by examining the symmetries of the model. Under the discrete ($Z_2$) symmetries of the O(3) NLSM, the spin current, $J$, transforms via

$$Z_2(J) \rightarrow \pm J.$$

In order that the matrix element, $\langle JQ_n \rangle$, not vanish we require that

$$Z_2(Q_n) \rightarrow \pm Q_n.$$

The $Z_2$ symmetries in the O(3) NLSM include $n_a \rightarrow -n_a$, $a=1,2,3$, parity, and time reversal. The spin current we are interested in transforms under rotations as a pseudo-vector. Thus any charge, $Q_n$, coupling to the current must also transform as such. From the work by Lüscher,[32] there is at least one conserved pseudo-vectorial quantity such that $\langle JQ_n \rangle$ does not vanish due to the action of one of the above $Z_2$ symmetries. For the sake of completeness we exhibit it. Rewriting the magnetization and spin current, $M_{0,1}$, explicitly as antisymmetric tensors,

$$M_\mu^{ab} = n^a \partial_\mu n^b - n^b \partial_\mu n^a, \quad \mu = 0,1;$$

the conserved quantity, takes the form,

$$Q^{ab}(t) = \sum_c \int dx_1\, dx_2\, \mathrm{sgn}(x_1 - x_2) M_0^{ac}(t,x_1) M_0^{cb}(t,x_2) - \int dx M_1^{ab}(t,x).$$

While the first term of $Q^{ab}$ does not contribute to the matrix element, $\langle JQ^{ab} \rangle$, as it is bilinear in the currents, $M^{ab}$, the second term does. We point out that $Q^{ab}$ is an exotic object inasmuch as it is a *nonlocal* conserved quantity. As pointed out in Ref. 32, it is the first in a series of nonlocal charges.

While the structure of the conserved quantities in the O(3) NLSM seem to be consistent with the existence of a finite Drude weight, this is not the case in the semi-classical approach. The dynamics of the semi-classical approximation used in Refs. 6 and 7 also admit an infinite number of conserved quantities. Importantly, however, these are different than those appearing in the fully quantum model. In particular, the semi-classical approximation does not admit nonlocal conserved quantities. As shown in Refs. 6 and 7, the structure of the $Z_2$ symmetries in the semi-classical approach is such that all matrix elements, $\langle JQ_n \rangle$, vanish. It would thus seem the absence of a Drude weight in the semi-classical case is a consequence of differences in the symmetries between the semi-classical and fully quantum models.

To understand the discrepancies in the case of the NMR relaxation rate, $1/T_1$, is not as simple. However, if we believe that the spin conductance demonstrates finite temperature ballistic behavior, it is hardly surprising to find the NMR relaxation rate characterized by ballistic logarithms. Again the difference between the fully quantum treatment and the semi-classical approach will lie in the differences between the models' conserved quantities. Nonetheless one possibility that we must consider is that merely going to $\mathcal{O}(e^{-2\beta\Delta})$ in the computation of $1/T_1$ is insufficient. It is possible that we need to perform some resummation of contributions from all orders to see the desired singular behavior, $1/T_1 \sim 1/\sqrt{H}$. While this would belie our experience with computing the susceptibility and the spin conductance via the correlators, the data that goes into the two computations is not exactly identical. Thus the possibility that the low-temperature expansion of $1/T_1$ is not well controlled cannot be entirely ruled out.

The differences in the nature of the conserved quantities between the O(3) NLSM and the semi-classical model of Refs. 6 and 7 suggest the latter is not equivalent to the O(3) NLSM, even at low energies. An indication of this lack of equivalency may lie in the universal nature of the ultra low energy S-matrix. This quantity is the primary input of the semi-classical model. The semi-classical model imagines a set of classical spins interacting via

$$S_{ab}^{cd}(\theta = 0) = -\delta_{ad}\delta_{cb},$$

i.e., in the scattering of two spins, the spins exchange their quantum numbers. However this specification may be insufficient to adequately describe the O(3) NLSM. Even beyond the quantum interference effects which are neglected by the semi-classical treatment, it is not clear that the zero-momentum S-matrix is enough to determine the model.

In this light it is instructive to consider the sine-Gordon model in its repulsive regime. The sine-Gordon model is given by the action

$$S = \frac{1}{8\pi} \int dx\, dt (\partial_\mu \Phi\, \partial^\mu \Phi + \lambda \cos(\hat{\beta}\Phi)), \tag{2.24}$$

where $\hat{\beta} = \beta/\sqrt{4\pi}$. The model is generically gapped. Its repulsive regime occurs in the range, $4\pi < \beta^2 < 8\pi$. The model's spectrum then consists solely of a doublet of solitons carrying U(1) charge. It is repulsive in the sense that the solitons have no bound states. The sine-Gordon model has a similar low energy S-matrix to the O(3) NLSM,

$$S_{ab}^{cd}(\theta = 0) = -\delta_{ad}\delta_{cb},$$

where here the particle indices range over $\pm$, the two solitons in the theory. Thus we might expect that sine-Gordon model to possess identical low energy behavior over its entire repulsive regime.

This is likely to be in general untrue. For example, we might consider the behavior of the single particle spectral function. We might thus want to compute a correlator of the form

$$\langle \psi_+(x,t)\psi_-(0,0)\rangle,$$

where $\psi_\pm$ are Mandelstam fermions given by

$$\psi_\pm(x,t)=\exp\left(\pm\frac{i}{2}\left(\frac{1}{\hat{\beta}}+\hat{\beta}\right)\phi_L(x,t)\mp\frac{i}{2}\left(\frac{1}{\hat{\beta}}-\hat{\beta}\right)\phi_R(x,t)\right);$$

$$\phi_{L/R}=\frac{1}{2}\left(\Phi(x,t)\pm i\int_{-\infty}^{x}dy\,\partial_t\Phi(y,t)\right). \qquad (2.25)$$

As these fields depend explicitly upon $\hat{\beta}$, it is hard to see how the properties of the above correlator, even at low energies could be independent of this same quantity. More generally, $\hat{\beta}$ determines the compactification radius of the boson in the model and so is related in a fundamental way to the model's properties.

It is useful to point out that Mandelstam fermions are the unique fields that create/destroy solitons that carry Lorentz spin 1/2, i.e., a spin that is independent of $\hat{\beta}$. They would then be the only fields with a chance of matching any semiclassical computation. However there are other soliton creation fields, for example,

$$e^{\pm i\phi_{L,R}/\hat{\beta}},$$

for which one could determine the corresponding spectral density. As these fields carry spin that varies as a function of $\hat{\beta}$, their spectral functions will depend upon more than the ultra low energy soliton S-matrix. In general, the semiclassical treatment of the sine-Gordon model cannot capture its full quantum field content.

As with the O(3) NLSM, the conductance of the fully quantum model differs from that of the semi-classical treatment. If one were to compute the conductance at finite temperature in the sine-Gordon model one would again find a finite Drude weight, $D$, while the semi-classical approach yields $D=0$.[13] The notion of under-specificity appears here again. The semi-classical approach for the sine-Gordon model equally well describes the Hubbard model at half-filling (the solitons are replaced by particle/hole excitations in the half-filled band). But it fails to give the correct Drude weight. An analysis of finite size corrections to the free energy in the presence of an Aharonov–Bohm flux[33] again finds a finite Drude weight in the half-filled Hubbard model at finite temperature.

Interestingly, however, there are certain properties at low energies that seem to be independent of $\hat{\beta}$. For example, if one were to compute the low-temperature static charge susceptibility, the term of $\mathcal{O}(e^{-\beta\Delta})$ would be independent of $\hat{\beta}$. However, at the next order, $\mathcal{O}(e^{-2\beta\Delta})$, this would almost certainly cease to be true. And the energy/temperature ranges we are interested in exploring do not permit dropping terms of $\mathcal{O}(e^{-2\beta\Delta})$.

It is important to stress we do not question the agreement between the semi-classical model and experiment. What we do question is whether the fully quantum O(3) NLSM exhibits spin diffusivity. If we are then to understand spin diffusion in terms of the O(3) NLSM, it is possible we need to include additional physics such as an easy axis spin anisotropy (weakly present in the experimental system, $AgVP_2S_6$), inter-chain couplings, or a spin-phonon coupling (as done in Ref. 11).

Beyond these, another mechanism that might lead to diffusive behavior are small integrable breaking perturbations of the O(3) NLSM. Generically any physical realization of a spin chain will possess such perturbations, even if arbitrarily small. Such perturbations may introduce the necessary ergodicity into the system, ergodicity that is absent in the integrable model because of the presence of nontrivial conserved charges, and so lead to diffusive behavior. As discussed in the semi-classical context by Garst and Rosch,[13] such perturbations introduce an additional time scale, $T$, governing the decay of conserved quantities in the problem. For times, $t<T$, the behavior of the system is ballistic and the original conserved quantities do not decay. For times, $t>T$, the behavior is then diffusive. Consequently the Drude weight in the purely integrable model is transformed into a peak in $\sigma(\omega)$ at $\omega\sim 1/T$.

Now the difference in the physics between the O(3) NLSM and its semi-classical variant is not that of integrable breaking perturbations. As demonstrated in Refs. 6 and 7, their semi-classical model is classically integrable. However, as discussed above the models do possess different conserved charges. It might then seem for certain transport quantities, the semi-classical model cures the lack of ergodicity present in its quantum counterpart.

## III. COMPUTATION OF FINITE TEMPERATURE CORRELATORS

Here we present the general method by which we compute the correlators at low but finite temperature and field: form-factor expansions. In the first part of this section we consider the general form of these expansions and why we expect them to be applicable at finite temperature. In the latter parts of this section, we review the exact expressions for the form factors in the O(3) sigma model together with the necessary regulation of said form factors at finite temperature.

### A. General methodology

To compute two-point correlation functions, we employ a form-factor expansion. At finite temperature, such correlators take the form

$$G^{\mathcal{O}}(x,t)=\frac{1}{\mathcal{Z}}\mathrm{Tr}(e^{-\beta H}\mathcal{O}(x,t)\mathcal{O}(0,0))$$
$$=\frac{\sum_{ns_n} e^{-\beta E_{s_n}}\langle n,s_n|\mathcal{O}(x,t)\mathcal{O}(0,0)|n,s_n\rangle}{\sum_{ns_n} e^{-\beta E_{s_n}}\langle n,s_n|n,s_n\rangle}. \quad (3.1)$$

Here t can be real or imaginary time and the sum $\Sigma_{ns_n}$ is over all possible eigenstates of the Hamiltonian. Each eigenstate is characterized by the number of particles, $n$, in the state together with a set of internal quantum numbers, $\{s_n\}$, in this case the value of $S_z$ carried by each particle. The form factor representation of the correlator is then arrived at by inserting a resolution of the identity between the two fields:

$$G^{\mathcal{O}}(x,t)=\frac{\sum_{ns_n}\sum_{ms_m} e^{-\beta E_{s_n}}\langle n,s_n|\mathcal{O}(x,t)|m,s_m\rangle\langle m,s_m|\mathcal{O}(0,0)|n,s_n\rangle}{\sum_{ns_n} e^{-\beta E_{s_n}}\langle n,s_n|n,s_n\rangle}. \quad (3.2)$$

At zero temperature, the representation of $G^{\mathcal{O}}$ reduces to one involving a single sum, $\Sigma_{m,s_m}$.

Thus the computation of $G^{\mathcal{O}}$ amounts to the evaluation of a set of matrix elements. These matrix elements can be computed in principle for arbitrary $n,m$ from a knowledge of the two-body S-matrix together with various constraints coming from the analytic dependence of the matrix elements upon energy-momentum. However, with increasing $n$ and $m$ the evaluation of these matrix elements and the corresponding evaluation of the sums, $\Sigma_{n,s_n}$, becomes increasingly arduous.

We are, however, in a better position when we consider the spectral function corresponding to $G^{\mathcal{O}}$:

$$G^{\mathcal{O}}(x,\omega)=\frac{\sum_{ns_n}\sum_{ms_m} e^{-\beta E_{s_n}} 2\pi\delta(\omega-E_{s_m}+E_{s_n})\langle n,s_n|\mathcal{O}(x,0)|m,s_m\rangle\langle m,s_m|\mathcal{O}(0,0)|n,s_n\rangle}{\sum_{ns_n} e^{-\beta E_{s_n}}\langle n,s_n|n,s_n\rangle}. \quad (3.3)$$

We see then that only certain terms, those meeting the matching condition, $\omega=E_{s_m}-E_{s_n}$, contribute to the spectral function.

In this paper we are concerned in particular with massive or gapped theories. Gapped theories are particularly amenable to this sort of computation as they admit a notion of thresholds. First imagine fixing $n,s_n$ in the sum above. In a massive theory the intermediate states have a finite energy. In particular in the O(3) sigma model, the energy of an m-particle state has a minimum threshold of $m\Delta$. And so states with $E_{s_m}$ exceeding $\omega+E_{s_n}$ do not contribute to the sum. For example if $\omega+E_{s_n}$ is below the three particle threshold, $3\Delta$, states with $m\geqslant 3$ do not make a contribution.

At zero temperature, i.e., $E_{s_n}=0$, the notion of thresholds leads to a situation where only a finite number of matrix elements needs to be computed in order to obtain an *exact* result at a given energy, $\omega$. In contrast, at finite temperature we in general would need to compute an infinite number of matrix elements in order to arrive at an exact result. However, here the massiveness of the theory again comes to our aid. With increasing $n$, the terms are weighted with the Boltzmann factor, $e^{-\beta E_{s_n}}<e^{-\beta n\Delta}$. Thus at temperatures small relative to the gap, $\Delta$, we expect in general only the first terms to make a significant contribution. We can thus evaluate the correlator in a controlled fashion, expanding it as the sum,

$$G^{\mathcal{O}}(x,\omega)=\sum_n c_n(x,\omega)e^{-n\beta\Delta}.$$

Moreover, while the evaluation of this sum in its entirety would require the evaluation of an infinite number of matrix elements, each individual coefficient, $c_n$, depends only upon a finite number of matrix elements (at least in the cases considered in this paper). As such we are able to compute these coefficients exactly.

While the ability to do so results from each $c_n$ being determined by a small, finite number of matrix elements, this feature will not be found in all theories. However form factor expansions in massive theories have in general found to be strongly convergent.[14,16–18] Specifically, matrix elements, $\langle n,s_n|\mathcal{O}(0,0)|m,s_m\rangle$, where $n$ and $m$ are large have been found to be relatively small. Even in massless theories where there are no explicit thresholds, convergence is good provided the engineering dimension of the operator $\mathcal{O}$ matches its anomalous dimension. Thus even if each $c_n$ were determined by a large (even infinite) number of matrix elements it would be possible nonetheless to arrive at a reasonable approximation for the coefficient.

There are, however, certain situations where we do not expect to be able to truncate the sum, $\Sigma_{n,s_n} e^{-\beta E_{s_n}}$. In certain circumstances, a physical quantity will see a transition as the limit of zero temperature is taken that is non-analytic in nature. To be concrete consider the single particle spectral function of the staggered component of the spin field:

$$S(x,\omega)=\langle n(x,\omega)n(0,0)\rangle. \tag{3.4}$$

At zero temperature, we expect that for energies, $\omega<3\Delta$, $S(x,\omega)$ takes the form of a $\delta$-function:

$$S(x,\omega)=c\,\delta(\omega-\Delta), \quad \omega<3\Delta, \quad T=0. \tag{3.5}$$

However, at finite temperatures this $\delta$-function is broadened. We then do not expect to be able to see this broadening unless we evaluate the sum, $\Sigma_{n,s_n} e^{-\beta E_{s_n}}$, in its entirety. Indeed, computing $S(x,\omega)$ through the truncation of this sum at any finite $n$ leads to

$$S(x,\omega)=c\,\delta(\omega-\Delta)+\cdots, \quad T>0. \tag{3.6}$$

Only through the resummation of the higher order terms is the $\delta$-function replaced by a broadened peak. However, it may well be possible to guess at the resummation on the basis of the first terms in the series.

Rather than consider such situations, we want to focus upon quantities that possess a smooth $T\to 0$ transition. As such consider the behavior of the staggered field spectral function, $S(x,\omega)$, for energies below the gap $\omega<\Delta$. At $T=0$ we have

$$S(x,|\omega|<\Delta)=0, \tag{3.7}$$

while at $T\neq 0$

$$S(x,|\omega|<\Delta)=\mathcal{O}(e^{-\beta\Delta}). \tag{3.8}$$

Thus the $T\to 0$ limit behaves in a smooth fashion.

This method is markedly different than that developed in Refs. 26–28. In our method we employ the basis of eigenstates, $|n,s_n\rangle$, that arises from the zero temperature problem. There a new basis is adopted that takes into direct account the thermalization of the vacuum state. Let $|0_T\rangle$ be the state with a representation of the particle content of the system in equilibrium at finite $T$ and let $|(n,s_n)_T\rangle$ be states that are excitations above this thermalized ground state. (In contrast, $|n,s_n\rangle$ are excitations above the empty vacuum state.) With such a basis, the correlators have the following form factor representation:

$$\langle\mathcal{O}(x,t)\mathcal{O}(0,0)\rangle=\sum_{n,s_n}\langle 0_T|\mathcal{O}(x,t)|(n,s_n)_T\rangle \times\langle(n,s_n)_T|\mathcal{O}(0,0)|0_T\rangle. \tag{3.9}$$

This method involves considerable technical complications. In general, it is a challenge to compute the new vacuum state $|0_T\rangle$ as well as the excitations above $|0_T\rangle$, never mind the form factors $\langle 0_T|\mathcal{O}(x,t)|(n,s_n)_T\rangle$. These difficulties are only enhanced by the nondiagonal scattering present in the O(3) sigma model, i.e., the two-body S-matrix is other than $S_{ab}^{a'b'}=\delta_{aa'}\delta_{bb'}$, where no internal quantum number are exchanged. This method was developed in particular for theories that are massless. However, in our case the theory is gapped. It thus makes sense to exploit the control over the sum, $\Sigma_{n,s_n} e^{-\beta E_{s_n}}$, that the low-temperature regime affords us.

In some sense our approach is similar to that of LeClair and Mussardo.[20] There they begin with the form-factor sum as in Eq. (3.1). However they recast the sum of the thermal trace through introducing a set of hole excitations complementary to the particles. Hole excitations appear naturally in terms of the form factors. A typical form factor that needs to be evaluated for a finite T correlator looks as follows:

$$\langle s_1,\epsilon_{s_1}|\mathcal{O}(x,t)|s_2,\epsilon_{s_2}\rangle, \tag{3.10}$$

where we have explicitly labeled the energy of the state. Using crossing symmetry, this matrix element can be rewritten as

$$\langle\mathcal{O}(x,t)|s_2,\epsilon_{s_2};\overline{s_1},-\epsilon_{s_1}\rangle, \tag{3.11}$$

provided $\epsilon_1=\epsilon_2$, $s_1=s_2$ does not hold. Here $\overline{s_1}$ is the ''charge conjugate'' of $s_1$. The excitation, $(\overline{s_1},-E_{s_1})$, can be thought of as a new type of excitation, a hole. Thus the double sum of a two point correlator was recast in Ref. 20 as

$$\langle\mathcal{O}(x,t)\mathcal{O}(0,0)\rangle=\sum_{m_p,s_p;m_h,s_h}\prod_p f(\epsilon_{s_p})\prod_h f(\epsilon_{s_h}) \times\langle\mathcal{O}(x,t)|m_p,s_p;m_h,s_h\rangle \times\langle m_h,s_h;m_p,s_p|\mathcal{O}(0,0)\rangle. \tag{3.12}$$

Notice that the partition function, $\mathcal{Z}$, is absent from Eq. (3.12) while new factors, $\Pi f$, have been added to the expression. Each $f(\epsilon_s)$ is the occupation number of the excitation (in this case assumed to be fermionic), $s$, with energy $\epsilon$:

$$f(\epsilon_s)=\frac{1}{1+e^{\epsilon_s/T}}.$$

These modifications represent an ansatz put forward in Ref. 20, and are argued to come from the regulation of the matrix elements,

$$\langle s_1,\epsilon_1|\mathcal{O}(x,t)|s_2,\epsilon_2\rangle, \tag{3.13}$$

in the case $s_1=s_2$, $\epsilon_1=\epsilon_2$.

Although this ansatz is supported in the case of one point functions (i.e., expectation values of the energy or spin),[20–22] it has come under criticism for the computation of two-point functions in Ref. 21. There the allied case of current–current correlators in the quantum Hall edge problem at $T=0$ but finite voltage was examined and it was found that their ansatz did not seem to reproduce the correct results.

What relevance does this critique have for our approach? We do not and cannot use the ansatz of LeClair and Mussardo as scattering in our theory is nondiagonal and their ansatz only makes sense in the case of theories that are diagonal. However, might the critique in Ref. 21 still have bearing upon our results? We do not think so. The correlator considered in Ref. 21 is computed in a massless theory whereas our results depend upon the gapped nature of the O(3) sigma model producing a series of thresholds. Moreover, we already expect to run into difficulties whenever there is nonanalytic behavior at $T=0$ near a threshold as in the behavior of the staggered field spectral function near $\omega\sim\Delta$. Thus we do not expect to capture the physics of the conflation of all the thresholds in a massless theory.

### B. Form factors in the O(3) sigma model

#### 1. Constraints upon form factors

The form factors of a field $\mathcal{O}$ are defined as the matrix elements of the field with some number of particles, $A_a(\theta)$:

$$f^{\mathcal{O}}_{a_1\cdots a_n}(\theta_1,\cdots,\theta_n)=\langle\mathcal{O}(0,0)A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)\rangle. \tag{3.14}$$

The $A_a(\theta)$ are Faddeev–Zamolodchikov operators which create and destroy the elementary excitations of the theory. $\theta$ is the rapidity which encodes the energy-momentum carried by the excitation,

$$p=\Delta\sinh(\theta);\quad E=\Delta\cosh(\theta). \tag{3.15}$$

The form of $f^{\mathcal{O}}_{a_1\cdots a_n}$ is determined by a combination of two-body scattering, Lorentz invariance, analyticity, and hermiticity.

The constraint from scattering is derived from the commutation relations of Faddeev–Zamolodchikov operators:

$$\begin{aligned}
A_{a_1}(\theta_1)A_{a_2}(\theta_2)&=S^{a_3a_4}_{a_1a_2}(\theta_1-\theta_2)A_{a_4}(\theta_4)A_{a_3}(\theta_3);\\
A^\dagger_{a_1}(\theta_1)A^\dagger_{a_2}(\theta_2)&=S^{a_3a_4}_{a_1a_2}(\theta_1-\theta_2)A^\dagger_{a_4}(\theta_4)A^\dagger_{a_3}(\theta_3);\\
A^\dagger_{a_1}(\theta_1)A_{a_2}(\theta_2)&=\delta_{a_1a_2}\delta(\theta_1-\theta_2)\\
&\quad+S^{a_3a_1}_{a_2a_4}(\theta_1-\theta_2)A_{a_3}(\theta_4)A^\dagger_{a_4}(\theta_3).
\end{aligned} \tag{3.16}$$

S, the two-body S-matrix, gives the amplitude of the process by which particles $\{a_1,a_2\}$ scatter into $\{a_3,a_4\}$. It is solely a function of $\theta_1-\theta_2\equiv\theta_{12}$ by Lorentz invariance. In our case, scattering between magnons in the O(3) model, the S-matrix is given by

$$\begin{aligned}
S^{a_3a_4}_{a_1a_2}(\theta)&=\delta_{a_1a_2}\delta_{a_3a_4}\sigma_1(\theta)+\delta_{a_1a_3}\delta_{a_2a_4}\sigma_2(\theta)\\
&\quad+\delta_{a_1a_4}\delta_{a_2a_3}\sigma_3(\theta);\\
\sigma_1(\theta)&=\frac{2\pi i\theta}{(\theta+i\pi)(\theta-i2\pi)};\\
\sigma_2(\theta)&=\frac{\theta(\theta-i\pi)}{(\theta+i\pi)(\theta-i2\pi)};\\
\sigma_3(\theta)&=\frac{2\pi i(i\pi-\theta)}{(\theta+i\pi)(\theta-i2\pi)}.
\end{aligned} \tag{3.17}$$

As $\theta\to0$, the S-matrix reduces to $S^{a_3a_4}_{a_1a_2}=-\delta_{a_1a_4}\delta_{a_2a_3}$. This is the approximation underlying the semi-classical analysis of Damle and Sachdev.[6,7] For the form factor to be consistent with two body scattering we must then have

$$\begin{aligned}
&f^{\mathcal{O}}_{a_1,\cdots,a_{i+1},a_i,\cdots,a_n}(\theta_1,\cdots,\theta_{i+1},\theta_i,\cdots,\theta_n)\\
&\quad=S^{a_i',a_{i+1}'}_{a_ia_{i+1}}(\theta_i-\theta_{i+1})f^{\mathcal{O}}_{a_1,\cdots,a_i',a_{i+1}',\cdots,a_n}\\
&\qquad\times(\theta_1,\cdots,\theta_i,\theta_{i+1},\cdots,\theta_n).
\end{aligned} \tag{3.18}$$

This relation is arrived at by commuting the $i$th and $i+1$th particle.

A second constraint upon the form factor can be thought of as a periodicity axiom. In continuing the rapidity, $\theta$, of a particle to $\theta-2\pi i$, the particle's energy-momentum is unchanged. However, the form factor is not so invariant. We instead have

$$\begin{aligned}
f^{\mathcal{O}}_{a_1,\cdots,a_n}(\theta_1,\cdots,\theta_n)&=f^{\mathcal{O}}_{a_n,a_1,\cdots,a_{n-1}}\\
&\quad\times(\theta_n-2\pi i,\theta_1,\cdots,\theta_{n-1}).
\end{aligned} \tag{3.19}$$

This constraint is derived from crossing symmetry.[20] It implicitly assumes that the field $\mathcal{O}$ is local: if $\mathcal{O}$ is nonlocal additional braiding phases appear in the above relation.[34–36]

Another condition related to analyticity that a form factor must satisfy is the annihilation pole axiom. This condition arises in form factors involving a particle and its antiparticle. Under the appropriate analytical continuation, such a combination of particles are able to annihilate one another. As such this condition relates form factors with $n$ particles to those with $n-2$ particles. In the case of the O(3) sigma model it takes the form

$$\begin{aligned}
&i\,\mathrm{res}_{\theta_n=\theta_{n-1}+\pi i}f(\theta_1,\cdots,\theta_n)_{a_1,\cdots,a_n}\\
&\quad=f(\theta_1,\cdots,\theta_{n-2})_{a_1',\cdots,a_{n-2}'}\delta_{a_na_{n-1}'}\\
&\qquad\times(\delta^{a_1'}_{a_1}\delta^{a_2'}_{a_2}\cdots\delta^{a_{n-2}'}_{a_{n-2}}\delta^{a_{n-1}'}_{a_{n-1}}\\
&\qquad-S^{a_{n-1}'a_1'}_{\tau_1a_1}(\theta_{n-11})S^{\tau_1a_2'}_{\tau_2a_2}(\theta_{n-12})\cdots S^{\tau_{n-4}a_{n-3}'}_{\tau_{n-3}a_{n-3}}(\theta_{n-1n-3})\\
&\qquad\times S^{\tau_{n-3}a_{n-2}'}_{a_{n-1}a_{n-2}}(\theta_{n-1n-2})).
\end{aligned} \tag{3.20}$$

Here res refers to the residue of the pole in the form factor when two particles are allowed to annihilate, i.e. $\theta_n$ is taken

to $\theta_{n-1}+i\pi$.This relation as written assumes that we are normalizing our particle states as $\langle\theta|\theta'\rangle=2\pi\delta(\theta-\theta')$.

The form factor must also satisfy constraints coming from Lorentz invariance. In general, the form factor of a field, $\mathcal{O}$, carrying Lorentz spin, s, must transform under a Lorentz boost, $\theta_i\to\theta_i+\alpha$, via

$$f^{\mathcal{O}}_{a_1\cdots a_n}(\theta_1+\alpha,\cdots,\theta_n+\alpha)=e^{s\alpha}f^{\mathcal{O}}_{a_1\cdots a_n}(\theta_1,\cdots,\theta_n). \tag{3.21}$$

The particular fields we will be interested in are the magnetization density, $M_0(x,t)$, as well its corresponding conserved current, $M_1(x,t)$. Together they form a Lorentz two-current. (Here 0,1 are Lorentz indices. Spin indices have been suppressed.) As this current is topological we may rewrite it in terms of a Lorentz scalar field, $m(x,t)$:

$$M_\mu(x,t)=\epsilon_{\mu\nu}\partial^\nu m(x,t) \tag{3.22}$$

The form factors are then determined for the field $m(x,t)$ which obeys Eq. (3.21) with $s=0$ while the corresponding form factors of $M_\mu(x,t)$ are related to those of $m(x,t)$ by

$$f^{M_\mu}_{a_1\cdots a_n}(\theta_1,\cdots,\theta_n)=\epsilon_{\mu\nu}P^\nu(\theta_i)f^{m}_{a_1\cdots a_n}(\theta_1,\cdots,\theta_n), \tag{3.23}$$

where $P^0=\Sigma_i\Delta\cosh(\theta_i)$ and $P^1=\Sigma_i\Delta\sinh(\theta_i)$.

These conditions do not uniquely specify the form factors. It is easily seen that if $f(\theta_1,\cdots,\theta_n)_{a_1,\cdots,a_n}$ satisfies these axioms then so does

$$f(\theta_1,\cdots,\theta_n)_{a_1,\cdots,a_n}\frac{P_n(\cosh(\theta_{ij}))}{Q_n(\cosh(\theta_{ij}))}, \tag{3.24}$$

where $P_n$ and $Q_n$ are symmetric polynomials in $\cosh(\theta_{ij})$, $1\leqslant i,j\leqslant n$, and are such that

$$P_n|_{\theta_n=\theta_{n-1}+\pi i}=P_{n-2};\quad Q_n|_{\theta_n=\theta_{n-1}+\pi i}=Q_{n-2}. \tag{3.25}$$

To deal with this ambiguity, we employ a minimalist axiom. We choose $P_n$ and $Q_n$ such that $P_n/Q_n$ has the minimal number of poles and zeros in the physical strip, $\mathrm{Re}\,(\theta)=0$, $0<\mathrm{Im}\,\theta<2\pi$. Additional poles are only added in accordance with the theory's bound state structure, an unnecessary complication in our case as the O(3) sigma model has no bound states. Using this minimalist ansatz, one can determine $P_n/Q_n$ up to a constant.

To determine this constant we rely upon the action of the conserved charge

$$S_z=\int dx M^3_0(x,0),$$

upon the single particle states. We expect

$$\langle\theta,S_z=1|S_z|\theta',S_z=1\rangle=2\pi\delta(\theta-\theta'). \tag{3.26}$$

Thus from the knowledge of the two particle form factor, we can fix the overall normalization. To check this normalization we will compare the form-factor computations with the results of other techniques. For example we will compute the magnetic susceptibility using both form factors and the thermodynamic Bethe ansatz. Through comparing the $T\to0$, $H\to0$ results, we see that the normalization has indeed been consistently computed.

As yet another check we can fix the phase of this constant using hermiticity. For this purpose it is sufficient to consider 2-particle form factors. Hermiticity then gives us

$$\begin{aligned}\langle\mathcal{O}(0,0)A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle^*&=\langle A^\dagger_{a_1}(\theta_1)A^\dagger_{a_2}(\theta_2)\mathcal{O}^\dagger(0,0)\rangle\\&=\langle\mathcal{O}^\dagger(0,0)A^-_{a_1}(\theta_1-i\pi)\\&\quad\times A^-_{a_2}(\theta_2-i\pi)\rangle,\end{aligned} \tag{3.27}$$

where the last line follows from crossing and so

$$f^{\mathcal{O}}_{a_1a_2}(\theta_1,\theta_2)^*=f^{\mathcal{O}^\dagger}_{\bar{a}_2\bar{a}_1}(\theta_2-i\pi,\theta_1-i\pi). \tag{3.28}$$

### C. Review of O(3) sigma model form factors

From Eqs. (3.22) and (3.23) it is sufficient to give the form factors for the scalar operator, $m(x,t)$. These have been computed by both Smirnov[15] and Balog and Niedermaier.[37] However, Ref. 37 presents them in a more amenable form, possible in this particular case because of the simple structure of the S-matrix of the O(3) sigma model.

Using the axioms as presented in the previous section, Ref. 37 thus finds for the two and four particle form factors

$$f^{m_a}_{a_1a_2}(\theta_1,\theta_2)=i\frac{\Delta\pi^2}{4}\epsilon^{aa_1a_2}\psi(\theta_{12}),$$

$$\psi(\theta)=\frac{\tanh^2(\theta/2)}{\theta}\,\frac{i\pi+\theta}{2\pi i+\theta};$$

$$\begin{aligned}&f^{m_a}_{a_1a_2a_3a_4}(\theta_1,\theta_2,\theta_3,\theta_4)\\&\quad=-\frac{\pi^5\Delta}{8}\prod_{i<j}\psi(\theta_{ij})G^{m_a}_{a_1a_2a_3a_4}\\&\quad=-\frac{\pi^5\Delta}{8}\prod_{i<j}\psi(\theta_{ij})(\delta^{a_4a_3}\epsilon^{aa_2a_1}g_1(\theta_i)\\&\quad+\delta^{a_4a_2}\epsilon^{aa_3a_1}g_2(\theta_i)+\delta^{a_4a_1}\epsilon^{aa_3a_2}g_3(\theta_i)\\&\quad+\delta^{a_3a_2}\epsilon^{aa_4a_1}g_4(\theta_i)+\delta^{a_3a_1}\epsilon^{aa_4a_2}g_5(\theta_i)\\&\quad+\delta^{a_2a_1}\epsilon^{aa_4a_3}g_6(\theta_i));\end{aligned}$$

$$\begin{pmatrix} g_1(\theta_i) \\ g_2(\theta_i) \\ g_3(\theta_i) \\ g_4(\theta_i) \\ g_5(\theta_i) \\ g_6(\theta_i) \end{pmatrix} = i \begin{pmatrix} -i\pi(\theta_{32}^2+\theta_{31}^2-i\pi\theta_{32}-i\pi\theta_{31}+2\pi^2) \\ (\theta_{32}-i\pi)\theta_{31}(\theta_{31}-i\pi) \\ (\theta_{32}-i\pi)(\theta_{32}+i2\pi)(i\pi-\theta_{31}) \\ \theta_{32}\theta_{31}(3\pi i-\theta_{31}) \\ \theta_{32}(\theta_{32}-i\pi)\theta_{31} \\ 2\pi i(i\pi-\theta_{32})\theta_{31} \end{pmatrix}$$
$$+ i(\theta_{43}-i\pi) \times \begin{pmatrix} -4\pi^2-i\pi(\theta_{32}+\theta_{31})-(\theta_{32}-\theta_{31})^2 \\ -2\pi^2-3\pi i\theta_{31}+\theta_{31}^2 \\ -4\pi^2+i\pi(\theta_{32}-2\theta_{31})-\theta_{32}^2 \\ 2\pi^2+i\pi(\theta_{32}+2\theta_{31})-2\theta_{32}\theta_{31} \\ -i\pi(2\theta_{32}+\theta_{31})+2\theta_{32}\theta_{31} \\ -2\pi^2+i\pi(\theta_{32}-3\theta_{31}) \end{pmatrix}$$
$$+ i(\theta_{43}-i\pi)^2 \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\theta_{32} \\ \theta_{31}-2\pi i \\ \theta_{32}-\theta_{31} \end{pmatrix}. \quad (3.29)$$

We have checked that these form factors do indeed satisfy the necessary axioms and found that the results of Ref. 37 are without typographical error. The reader should note however that we use a different particle normalization than Ref. 37 and so the results differ by an overall multiplicative constant.

The two particle form factor differs from that appearing in Affleck and Weston's work[3] on the O(3) sigma model. The two particle form factor Affleck and Weston use is given by

$$f^{M_0^3}_{a_1a_2}(\theta_1,\theta_2) \propto (\cosh(\theta_1) - \cosh(\theta_2))\epsilon^{3a_1a_2}\frac{\tanh(\theta_{12}/2)}{\theta_{12}}\frac{i\pi+\theta_{12}}{2\pi i+\theta_{12}}.$$

This differs from our form in that it has a different Lorentz structure and lacks an extra factor of $\tanh(\theta_{12}/2)$. The different structure of the two particle form factor is a result of the constraint the annihilation pole axiom places on form factors of different particle numbers. If one only computes the two particle form factor, as done in Ref. 38, this constraint can go unsatisfied. However, in terms of the low energy behavior (i.e., $\theta_1,\theta_2\to 0$), the two forms for $f^{m_a}_{a_1a_2}$ are nearly identical.

### D. Regularization of form factors

We end this section with a discussion of the regularization of form factors that appear in the evaluation of thermal correlators. Form factors with all particles either to the right or the left of the field such as

$$f^{\mathcal{O}}_{a_1,\cdots,a_n}(\theta_1,\cdots,\theta_n) = \langle \mathcal{O}(0,0) A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)\rangle$$

do not pose any such problems. However, the form factors encountered in the evaluation of finite temperature correlators are of the form

$$\langle A_{b_m}(\tilde{\theta}_m)\cdots A_{b_1}(\tilde{\theta}_1)\mathcal{O}(0,0)A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)\rangle.$$

To understand such an object we must contend with the possibility that $\tilde{\theta}_i=\theta_j$, $a_i=b_j$ for some $i,j$. From the algebra of the Fadeev–Zamolodchikov operators (3.16), we know the commutation relations involve $\delta$-functions, i.e.,

$$A^\dagger_{a_i}(\tilde{\theta}_i)A_{b_j}(\theta_j) = 2\pi\delta(\tilde{\theta}_i-\theta_j)\delta_{a_ib_j}+\cdots. \quad (3.30)$$

It is crucial to include the contributions of the $\delta$-functions to the correlators. In particular they contribute pieces which cancel off otherwise ill-defined terms arising from the partition function. To do so we must understand the above form factor to equal

$$\langle A_{b_m}(\tilde{\theta}_m)\cdots A_{b_1}(\tilde{\theta}_1)\mathcal{O}(0,0)A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)\rangle = \sum_{\substack{\{a_i\}=A_1\cup A_2 \\ \{b_i\}=B_1\cup B_2}} S_{A,A_1}S_{B,B_1}\langle B_1|A_1\rangle\langle B_2|\mathcal{O}(0,0)|A_2\rangle_{\text{connected}}. \quad (3.31)$$

The sum in the above is over all possible subsets of $\{a_i\}$ and $\{b_i\}$. The S-matrix $S_{A,A_1}$ arises from the commutations necessary to rewrite $A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)|0\rangle$ as $A_2A_1|0\rangle$ and similarly for $S_{B,B_1}$. The matrix element $\langle B_1|A_1\rangle$ is evaluated using the Fadeev–Zamolodchikov algebra. In this way (ill-defined) terms proportional to $\delta(0)$ are produced but which cancel similarly ill-defined terms arising from the evaluation of the partition function.

The ''connected'' form factor appearing in the above expression is to be understood as follows. Using crossing symmetry, the form factor can be rewritten as

$$\begin{aligned}\langle B_2|\mathcal{O}(0,0)|A_2\rangle_{\text{connected}} &= \langle A_{b'_{i_k}}(\tilde{\theta}_{i_k})\cdots A_{b'_{i_1}}(\tilde{\theta}_{i_1})\mathcal{O}(0,0) \\ &\quad \times A_{a'_{j_q}}(\theta_{j_q})\cdots A_{a'_{j_1}}(\theta_{j_1})\rangle_{\text{connected}} \\ &= \langle \mathcal{O}(0,0)A_{a'_{j_q}}(\theta_{j_q})\cdots A_{a'_{j_1}}(\theta_{j_1})A_{\overline{b'_{i_k}}} \\ &\quad \times(\tilde{\theta}_{i_k}-i\pi)\cdots A_{\overline{b'_{i_1}}}(\tilde{\theta}_{i_1} \\ &\quad -i\pi)\rangle_{\text{connected}} \\ &= f^{\mathcal{O}}_{\overline{b'_{i_1}}\cdots\overline{b'_{i_k}}a'_{j_1}\cdots a'_{j_q}}(\tilde{\theta}_{i_1}-i\pi,\cdots,\tilde{\theta}_{i_k} \\ &\quad -i\pi,\theta_{j_1},\cdots,\theta_{j_q})_{\text{connected}}, \quad (3.32)\end{aligned}$$

where the last relation holds provided we do not have $\theta_i = \tilde{\theta}_j$, $a_i = b_j$ for any $i,j$. If this does occur we see from the annihilation pole axiom that the form factor is not well defined, having a pole at $\theta_i = \tilde{\theta}_j$. In such cases the form factor requires regulation.

To regulate the form factor, we employ a scheme suggested by Balog[39] and used by LeClair and Mussardo[20]. We define

$$\begin{aligned} f^{\mathcal{O}}_{\bar{b}'_{i_1}\cdots\bar{b}'_{i_k}a'_{j_1}\cdots a'_{j_q}}&(\tilde{\theta}_{i_1}-i\pi+i\eta_1,\cdots,\tilde{\theta}_{i_k}-i\pi \\ &+i\eta_k,\theta_{j_1},\cdots,\theta_{j_q})_{\text{connected}} \\ &=\text{finite piece of}\lim_{\eta_i\to 0} f^{\mathcal{O}}_{\bar{b}'_{i_1}\cdots\bar{b}'_{i_k}a'_{j_1}\cdots a'_{j_q}}(\tilde{\theta}_{i_1}-i\pi \\ &+i\eta_1,\cdots,\tilde{\theta}_{i_k}-i\pi+i\eta_k,\theta_{j_1},\cdots,\theta_{j_q}). \end{aligned} \tag{3.33}$$

In taking the finite piece of $f^{\mathcal{O}}$, we discard terms proportional to $\eta_i^{-p}$ as well as terms proportional to $\eta_i/\eta_j$. In this way the connected piece is independent of the way the various limits $\eta_i \to 0$ are taken. Balog[39] has already used this prescription to compute one point functions and successfully compare them to TBA calculations. In Ref. 39 it was argued that the delta functions leading to such terms arise from the use of infinite volume wave functions. If such wavefunctions are replaced instead with finite volume counterparts, the delta functions are regulated. For example, a pole in $\eta$ is changed as follows:

$$\frac{1}{i\eta}=\int d\theta\frac{\delta(\theta)}{\theta+i\eta}\to\int d\theta\frac{f(\theta)}{\theta+i\eta}, \tag{3.34}$$

where $f(\theta)$ is some sharply peaked function about $\theta=0$ which in the infinite volume limit evolves into a $\delta$-function. However, the principal value of this regularized integral is zero. Thus discarding the pole terms is justified in this sense. For terms that are ratios of infinitesimals, Balog also demonstrates that such terms, once regularized, disappear in the infinite volume limit.

## IV. THERMODYNAMIC BETHE ANSATZ AT FINITE TEMPERATURE AND FINITE FIELD

In this section we review the derivation of the equations describing the exact free energy (and hence the susceptibility) of the O(3) sigma model together with its low-temperature expansion. The exact description of the thermodynamics of the O(3) sigma model takes the form of a set of quantization conditions for the momenta, $p_\alpha$, of the excitations in the ground state. With $p_\alpha = \Delta\sinh(\theta_\alpha)$, we have the following condition:[30]

$$\begin{aligned} e^{i\Delta\sinh(\theta_\alpha)}&=\prod_{\beta=1}^{N}\frac{\theta_\alpha-\theta_\beta+i\pi}{\theta_\alpha-\theta_\beta-i\pi}\prod_{\gamma=1}^{M}\frac{\theta_\alpha-\lambda_\gamma-i\pi}{\theta_\alpha-\lambda_\gamma+i\pi}; \\ \prod_{\beta=1}^{N}\frac{\theta_\beta-\lambda_\alpha+i\pi}{\theta_\beta-\lambda_\alpha-i\pi}&=-\prod_{\gamma=1}^{M}\frac{\lambda_\gamma-\lambda_\alpha+i\pi}{\lambda_\gamma-\lambda_\alpha-i\pi}. \end{aligned} \tag{4.1}$$

Here $\theta_\beta$ are the rapidities of the other excitations in the ground state while the $\lambda$'s mark out spin excitations above an originally polarized ground state. (The Bethe ansatz construction begins with a completely polarized ground state of spin 1 excitations above which one then creates spin excitations—marked out by the $\lambda$'s—in order to give the ground state the desired spin polarization.) $N$ is the total number of excitations in the ground state while $M$ is the number of spin excitations. The quantum number, $S_z$, is then given by $S_z = N-M$. The total energy of the ground state in a magnetic field is then equal to

$$E=\Delta\sum_{\alpha=1}^{N}\cosh(\theta_\alpha)-H(N-M).$$

Analysis of these equations proceeds using the string hypothesis. The solutions of the above equations take the form

$$\begin{aligned} &\theta_\alpha \text{ are real;} \\ &\lambda_\alpha^{n,k}=\lambda_\alpha^n+i\pi(n+1-2k)/2,\quad k=1,2,\ldots,n; \end{aligned} \tag{4.2}$$

that is the $\lambda$'s are organized into ''complexes'' which share a real part, $\lambda_\alpha^n$, the center of the complex.

In computing the free energy, we are interested in the continuum limit of the above equations. To arrive at this limit, we introduce densities per unit length, $\rho(\theta)$ and $\sigma_n(\lambda)$, of, respectively, the $\theta_\alpha$'s, and the centers, $\lambda_\alpha^n$, of the complexes. We further introduce particle and hole densities by writing $\rho=\rho_h+\rho_p$ and $\sigma_n=\sigma_{nh}+\sigma_{np}$. A particle density gives the probability that the ground state contains an excitation at a given rapidity, $\theta/\lambda$, while the hole density gives the converse probability that the excitation at the rapidity is not found in the ground state. Equations describing these densities can be arrived at in a standard fashion (see Section 8.3 of Ref. 40 for an analogous derivation in the case of the Anderson model):

$$\begin{aligned} &\rho_p(\theta)+\rho_h(\theta)=\frac{\Delta}{2\pi}\cosh(\theta)+(s*\sigma_{2h})(\theta); \\ &\sigma_{mp}(\lambda)+\sigma_{mh}(\lambda)=\delta_{2m}s*\rho_p(\lambda)+s*(\sigma_{m+1,h}+\sigma_{m-1,h})(\lambda), \end{aligned} \tag{4.3}$$

where $s(x)=[\pi\cosh(x)]^{-1}$ and $f*g$ denotes the convolution of these two functions:

$$f*g=\int d\lambda' f(\lambda-\lambda')g(\lambda').$$

From these equations the free energy per unit length, $\Omega$, can be derived (again see Ref. 40 for details of an analogous derivation):

$$\begin{aligned} &\Omega=-\frac{T\Delta}{2\pi}\int d\theta\cosh(\theta)\log(1+e^{-\beta\epsilon(\theta)}); \\ &\epsilon(\theta)=\Delta\cosh(\theta)-Ts*\log(1+e^{\beta\epsilon_2})(\theta); \end{aligned}$$

$$\epsilon_n(\lambda) = Ts * \log(1+e^{\beta\epsilon_{n-1}})(1+e^{\beta\epsilon_{n+1}})(\lambda) + \delta_{2n} Ts * \log(1+e^{-\beta\epsilon})(\lambda);$$

$$\lim_{n\to\infty} \frac{\epsilon_n}{n} = H. \tag{4.4}$$

Here we have expressed the free energy of the system in terms of the dressed energies (or pseudo-energies), $\epsilon/\epsilon_n$, of the excitations. These functions give the energetic cost of making an excitation at a given rapidity taking into account the excitation's interactions with the other particles in the ground state. These equations are in agreement with Ref. 29 where they were first written down and correct typos found in Ref. 11.

To derive the low temperature expansion of the free energy, we follow Ref. 29. We solve the above Eqs. (4.4) through iteration. We write for each pseudo-energy, $\epsilon_n$

$$1+e^{\beta\epsilon_n(\theta)} = \sum_{m=0}^{\infty} r_{nm}(T,\theta). \tag{4.5}$$

This expansion is such that $r_{nm}$ is of $\mathcal{O}(e^{-m\beta\Delta})$. On the basis of Eq. (4.5) we can write the free energy as a series in $e^{-m\beta\Delta}$:

$$\Omega = \sum_{m=1}^{\infty} c_m(T) e^{-m\beta\Delta}. \tag{4.6}$$

We will compute the $m=1,2$ terms of this expansion.

The $m=0$ term of Eq. (4.5) is arrived at by neglecting the term involving $\log(1+e^{-\beta\epsilon})$ in the equation for $\epsilon_n$. If this is done, these equations reduce to

$$\epsilon_n(\lambda) = \frac{T}{2}\log(1+e^{\beta\epsilon_{n-1}})(1+e^{\beta\epsilon_{n+1}});$$

$$\lim_{n\to\infty} \frac{\epsilon_n}{n} = H. \tag{4.7}$$

They are then algebraic in nature and admit the following solution:

$$1+e^{\beta\epsilon_n} = r_{n0} = \phi^2(n);$$

$$\phi(n) = \frac{\sinh\left(\frac{H}{2T}(n+1)\right)}{\sinh\left(\frac{H}{2T}\right)}. \tag{4.8}$$

At this order of the iteration, $\epsilon(\theta)$ becomes

$$\epsilon(\theta) = \Delta\cosh(\theta) - T\log\phi(2), \tag{4.9}$$

and so

$$\Omega = -\frac{T\Delta}{2\pi}\int d\theta \cosh(\theta)\log(1+3e^{-\beta\Delta\cosh(\theta)}). \tag{4.10}$$

Clearly $\Omega$ is of $\mathcal{O}(e^{-\beta\Delta})$.

The next coefficient in the series (4.5), $r_{n1}$, is found by substituting Eq. (4.9) into the equations for $\epsilon_n$:

$$\epsilon_n = Ts * \log(1+e^{\beta\epsilon_{n-1}})(1+e^{\beta\epsilon_{n+1}}) + \delta_{2n} Ts * \log(1+\phi(2)e^{-\beta\Delta\cosh(\theta)});$$

$$\lim_{n\to\infty} \frac{\epsilon_n}{n} = H. \tag{4.11}$$

To the order in $e^{-\beta\Delta}$ to which we are working, these equations reduce to

$$\frac{\phi^2(n)}{\phi(n-1)\phi(n+1)} r_{n1} = (r_{n-1,1}+r_{n+1,1}) * s + \delta_{2n}\log(1+e^{-\beta\Delta\cosh(\theta)}) * s. \tag{4.12}$$

As can be directly checked, they admit the solution

$$r_{n1} = \frac{\phi(1)}{\phi(2)\phi(n)}(\phi(n+1)a_n - \phi(n-1)a_{n+2}) * s^{-1} * \times \log(1+\phi(2)e^{-\beta\Delta\cosh(\theta)});$$

$$a_n(x) = \frac{2n}{4x^2+n^2\pi^2}. \tag{4.13}$$

With this, $\epsilon(\theta)$ to $\mathcal{O}(e^{-\beta\Delta})$ takes the form

$$\epsilon(\theta) = \Delta\cosh(\theta) - T\log\phi(2) - T\frac{\phi(1)}{\phi(2)}(\phi(3)a_2 - \phi(1)a_4) * e^{-\beta\Delta\cosh(\theta)} + \mathcal{O}(e^{-2\beta\Delta}). \tag{4.14}$$

We can continue this procedure, obtaining $r_{nm}, m \geqslant 2$. Indeed Ref. 29 goes on to compute $r_{n2}$ and so corrections of $\mathcal{O}(e^{-2\beta\Delta})$ to $\epsilon(\theta)$.

The zero field susceptibility is given by

$$\chi(H=0) = -\partial_H^2\Omega\Big|_{H=0} = -\frac{\Delta}{2\pi}\int d\theta\cosh(\theta)\frac{\partial_H^2\epsilon(\theta)}{1+e^{\beta\epsilon(\theta)}}\Big|_{H=0}. \tag{4.15}$$

Using $\epsilon(\theta)$ in Eq. (4.14) and expanding the above expression to $\mathcal{O}(e^{-2\beta\Delta})$, we find

$$\chi(H=0) = \frac{\beta\Delta}{\pi T}\int d\theta\cosh(\theta)e^{-\beta\Delta\cosh(\theta)}(1-3e^{-\beta\Delta\cosh(\theta)}) + \frac{2\beta\Delta}{\pi}\int d\theta_1 d\theta_2\cosh(\theta_1) \times e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \times \frac{2\theta_{12}+11\pi^2}{\theta_{12}^4+5\pi^2\theta_{12}^2+4\pi^4} + \mathcal{O}(e^{-3\beta\Delta}), \tag{4.16}$$

where $\theta_{12} = \theta_1 - \theta_2$. This agrees exactly with the derivation of $\chi$ coming from the computation of the two and four particle form factors.

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## APPENDIX A: COMPUTATION OF MAGNETIC SUSCEPTIBILITY USING FORM FACTORS

To compute the correlator, $\langle M_0^3(x,\tau)M_0^3(0,0)\rangle$, we first consider the action of the thermal trace:

$$C(x,\tau)=\langle M_0^3(x,\tau)M_0^3(0,0)\rangle = \frac{\sum_{s_n,n} e^{-\beta E_{s_n}}\langle n,s_n|M_0^3(x,\tau)M_0^3(0,0)|n,s_n\rangle}{\sum_{s_n,n} e^{-\beta E_{s_n}}\langle n,s_n|n,s_n\rangle}. \tag{A1}$$

Keeping the first two terms leads us to

$$\begin{aligned}\langle M_0^3(x,\tau)M_0^3(0,0)\rangle &= \Bigg( \int \frac{d\theta}{2\pi} e^{-\beta\Delta\cosh(\theta)} \\ &\times \sum_a \langle A_a(\theta)|M_0^3(x,\tau)M_0^3(0,0)|A_a(\theta)\rangle \\ &+ \frac{1}{2}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi} e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ &\times \sum_{a_1 a_2} \langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau) \\ &\times M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle\Bigg) \Bigg/ \\ &\left(1+\sum_a \int \frac{d\theta}{2\pi} e^{-\beta\Delta\cosh(\theta)}\langle A_a(\theta)|A_a(\theta)\rangle\right).\end{aligned} \tag{A2}$$

Expanding the denominator then gives us

$$\begin{aligned}C(x,\tau) &= \int \frac{d\theta}{2\pi} e^{-\beta\Delta\cosh(\theta)} \sum_a \langle A_a(\theta)|M_0^3(x,\tau) \\ &\times M_0^3(0,0)|A_a(\theta)\rangle \times \left(1-\sum_a \int \frac{d\theta}{2\pi} e^{-\beta\Delta\cosh(\theta)} \right. \\ &\left. \times \langle A_a(\theta)|A_a(\theta)\rangle\right) + \frac{1}{2}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi} \\ &\times e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \times \sum_{a_1 a_2} \langle A_{a_1}(\theta_1)A_{a_2}(\theta_2) \\ &\times |M_0^3(x,\tau)M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle.\end{aligned} \tag{A3}$$

The term arising from the partition function is ill-defined as the state normalization is given by $\langle A_a(\theta)|A_{a_1}(\theta_1)\rangle = 2\pi\delta_{aa_1}\delta(\theta-\theta_1)$. However, this term will be canceled by disconnected terms arising from $\langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau)M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle$.

To evaluate this expression we begin by computing the first term of the trace $\langle A_a(\theta)|M_0^3(x,\tau)M_0^3(0,0)|A_a(\theta)\rangle$ by inserting a resolution of the identity between the $M^3$'s:

$$\begin{aligned}&\langle A_a(\theta)|M_0^3(x,\tau)M_0^3(0,0)|A_a(\theta)\rangle \\ &= \sum_{n=1}^{\infty} \sum_{a_1,\cdots,a_n} \frac{1}{n!}\int \frac{d\theta_1}{2\pi}\cdots\int \frac{d\theta_n}{2\pi} \\ &\times \langle A_a(\theta)|M_0^3(x,\tau)|A_{a_n}(\theta_n)\cdots A_{a_1}(\theta_1)\rangle \\ &\times \langle A_{a_1}(\theta_1)\cdots A_{a_n}(\theta_n)|M_0^3(0,0)|A_a(\theta)\rangle.\end{aligned} \tag{A4}$$

We only need to keep the lowest order term, $n=1$, in this expansion; *all other terms make no contribution to the susceptibility*. The terms corresponding to n even are identically zero (by parity); the remaining $n>1$ odd terms vanish in the low energy-low momentum limit of the corresponding spectral function. (We will return to this is a moment.) Given that we can thus compute the entire contribution $\langle A_a(\theta)|M_0^3(x,\tau)M_0^3(0,0)|A_a(\theta)\rangle$ makes to the susceptibility, we will able to find an exact correspondence between the form-factor computation and a low-temperature expansion of the exact free energy. With the $n=1$ term we then have

$$\begin{aligned}&\langle A_a(\theta)|M_0^3(x,\tau)M_0^3(0,0)|A_a(\theta)\rangle \\ &= \sum_{a_1} \int \frac{d\theta_1}{2\pi}\langle A_a(\theta)|M_0^3(x,\tau)|A_{a_1}(\theta_1)\rangle \\ &\times \langle A_{a_1}(\theta_1)|M_0^3(0,0)|A_a(\theta)\rangle; \\ &= \sum_{a_1} \int \frac{d\theta_1}{2\pi} e^{-\tau\Delta(\cosh(\theta_1)-\cosh(\theta))+ix\Delta(\sinh(\theta_1)-\sinh(\theta))} \\ &\times \langle M_0^3(0,0)|A_{a_1}(\theta_1)A_a(\theta-i\pi)\rangle \\ &\times \langle M_0^3(0,0)|A_a(\theta)A_{a_1}(\theta_1-i\pi)\rangle; \\ &= \sum_{a_1} \int \frac{d\theta_1}{2\pi} e^{-\tau\Delta(\cosh(\theta_1)-\cosh(\theta))+ix\Delta(\sinh(\theta_1)-\sinh(\theta))} \\ &\times f_{aa_1}^{M_0^3}(\theta-i\pi,\theta_1) f_{a_1 a}^{M_0^3}(\theta_1-i\pi,\theta).\end{aligned} \tag{A5}$$

We have used crossing symmetry in the second line. From Sec. III C, the form factor $f_{aa_1}^{M_0^3}(\theta,\theta_1)$ is given by

$$f_{aa_1}^{M_0^3}(\theta,\theta_1) = i\frac{\pi^2\Delta}{4}\epsilon^{3aa_1}(\sinh(\theta)+\sinh(\theta_1))\psi(\theta-\theta_1). \tag{A6}$$

Then the lowest order contribution, $C_1(x,\tau)$, to the spin–spin correlator, $C(x,\tau)$, is given by

$$\begin{aligned}C_1(x,\tau) &= -2\int \frac{d\theta}{2\pi}\int \frac{d\theta_1}{2\pi} e^{-\beta\Delta\cosh(\theta)} \\ &\times e^{-\tau\Delta(\cosh(\theta_1)-\cosh(\theta))+ix\Delta(\sinh(\theta_1)-\sinh(\theta))} \\ &\times f_{21}^{M_0^3}(\theta-i\pi,\theta_1) f_{21}^{M_0^3}(\theta_1-i\pi,\theta).\end{aligned} \tag{A7}$$

Fourier transforming in $x$ and $\tau$ and continuing $\omega_n \rightarrow -i\omega + \delta$ yields,

$$C_1(\omega=0,k=0) = \frac{\beta\Delta}{\pi}\int d\theta \cosh(\theta) e^{-\beta\Delta\cosh(\theta)}$$

$$= \frac{2\beta\Delta}{\pi} K_1(\beta\Delta), \tag{A8}$$

where $K_1$ is a modified Bessel function. This has the expected small temperature behavior, $C_1(\omega=0,k=0) \sim T^{-1/2}e^{-\beta\Delta}$.

Let us consider further why the above computation gives the sole contribution to $\langle A_a(\theta)|M_0^3(x)M_0^3(0)|A_a(\theta)\rangle$. The next potential contribution to this matrix element takes the form

$$\int d\theta_1\, d\theta_2\, d\theta_3 \langle A_a(\theta)|M_0^3(x)|A_{a_1}(\theta_1)A_{a_2}(\theta_2)A_{a_3}(\theta_3)\rangle$$
$$\times\langle A_{a_3}(\theta_3)A_{a_2}(\theta_2)A_{a_1}(\theta_1)|M_0^3(0)|A_a(\theta)\rangle. \tag{A9}$$

Upon evaluation this expression produces two types of terms. The first is associated with the disconnected pieces of the matrix elements appearing in the above. An example of this type of term is

$$\int d\theta_1\, d\theta_2 \langle M_0^3(x)|A_{a_1}(\theta_1)A_{a_2}(\theta_2)\rangle$$
$$\times\langle A_a(\theta)A_{a_2}(\theta_2)A_{a_1}(\theta_1)|M_0^3(0)|A_a(\theta)\rangle$$
$$= \int d\theta_1 d\theta_2 e^{i\Delta x(\sinh(\theta_1)+\sinh(\theta_2))}(\sinh(\theta_1)+\sinh(\theta_2))$$
$$\times(\text{term regular in } \theta_1 \text{ and } \theta_2). \tag{A10}$$

As $M_0^3$ is a Lorentz current, the term $(\sinh(\theta_1)+\sinh(\theta_2))$ appears in the above. Thus when the Fourier transform, $\int e^{ikx}$, is taken followed by the limit, $k\rightarrow 0$, this term vanishes identically.

The second type of term we must deal with in evaluating Eq. (A9) takes the form

$$\int d\theta_1 d\theta_2 d\theta_3 e^{ix\Delta(\sinh(\theta_1)+\sinh(\theta_2)+\sinh(\theta_3)-\sinh(\theta))}$$
$$\times f^{M_0^3}_{\overline{a}a_3a_2a_1}(\theta - i\pi + i\epsilon, \theta_3, \theta_2, \theta_1)$$
$$\times f^{M_0^3}_{\overline{a_1a_2a_3}a}(\theta_1 - i\pi + i\epsilon_1, \theta_2 - i\pi + i\epsilon_2, \theta_3 - i\pi + i\epsilon_3, \theta), \tag{A11}$$

and arises from the connected pieces of the matrix elements appearing in Eq. (A9). To evaluate this term we deform the contours $\theta_{1,2,3}$ via

$$\theta_{1,2,3} \rightarrow \theta_{1,2,3} + i\pi.$$

(In doing so we assume that time is real, not imaginary. This does not pose a problem as we could as well directly evaluate the retarded correlators as opposed to evaluating them via an analytical continuation of imaginary time-ordered correlators.) We then deform through a number of poles whose residues we will pick up. Evaluating these residues we again obtain something of the form (A10). As such, Fourier transforming and taking the $k=0$ limit forces the term to vanish and Eq. (A9) ends up making no contribution to the susceptibility. In the same way, it is easy then to convince oneself that terms involving an even greater number of particles similarly do not contribute to the static susceptibility.

We now go ahead and compute the second term arising from performing the thermal trace, $\langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau)M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle$. We evaluate it as before by inserting a resolution of the identity between the two fields. In this case the only term that contributes is the $n=2$ term:

$$\langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau)M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle$$
$$= \frac{1}{2}\sum_{a_3a_4}\int \frac{d\theta_3}{2\pi}\frac{d\theta_4}{2\pi}$$
$$\times\langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau)|A_{a_3}(\theta_3)A_{a_4}(\theta_4)\rangle$$
$$\times\langle A_{a_4}(\theta_4)A_{a_3}(\theta_3)|M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle. \tag{A12}$$

Allowing for the presence of disconnected terms, the matrix elements in the above expression take the form

$$\langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau)|A_{a_3}(\theta_3)A_{a_4}(\theta_4)\rangle$$
$$= \delta_{a_1a_4}2\pi\delta(\theta_1-\theta_4)f^{M_0^3}_{\overline{a_2,a_3}}(\theta_2 - i\pi, \theta_3) + \delta_{a_3'a_2'}2\pi$$
$$\times\delta(\theta_3-\theta_2)S^{a_1'a_2'}_{a_1a_2}(\theta_{12})S^{a_3'a_4'}_{a_3a_4}(\theta_{34})f^{M_0^3}_{\overline{a_1',a_4'}}(\theta_1 - i\pi, \theta_4)$$
$$+ \delta_{a_2'a_4}2\pi\delta(\theta_2-\theta_4)S^{a_1'a_2'}_{a_1a_2}(\theta_{12})f^{M_0^3}_{\overline{a_1',a_3}}(\theta_1 - i\pi, \theta_3)$$
$$+ \delta_{a_1a_3'}2\pi\delta(\theta_1-\theta_3)S^{a_3'a_4'}_{a_3a_4}(\theta_{34})f^{M_0^3}_{\overline{a_2,a_4'}}(\theta_2 - i\pi, \theta_4)$$
$$+ f^{M_0^3}_{\overline{a_2,a_1,a_4,a_3}}(\theta_2 - i\pi, \theta_1 - i\pi, \theta_4, \theta_3)_c, \tag{A13}$$

where $f_c$ refers to a connected form factor. We now substitute Eq. (A13) into Eq. (A12) and obtain the following after some lengthy but straightforward algebra:

$$\frac{1}{4}\sum_{a_1a_2a_3a_4}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\frac{d\theta_4}{2\pi}$$
$$\times\langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^3(x,\tau)|A_{a_3}(\theta_3)A_{a_4}(\theta_4)\rangle$$
$$\times\langle A_{a_4}(\theta_4)A_{a_3}(\theta_3)|M_0^3(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle$$
$$\equiv C_{21}+C_{22}+C_{23}+C_{24}+C_{25}+C_{26};$$

$$C_{21}=2\pi\delta(0)\sum_{a_1a_2a_3}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}$$
$$\times e^{-\tau\Delta(\cosh(\theta_3)-\cosh(\theta_2))-ix\Delta(\sinh(\theta_3)-\sinh(\theta_2))}f^{M_0^3}_{\overline{a_3},a_2}(\theta_3-i\pi,\theta_2)f^{M_0^3}_{\overline{a_2},a_3}(\theta_2-i\pi,\theta_3);$$

$$C_{22}=-3\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}e^{-2\beta\Delta\cosh(\theta_1)}e^{-\tau\Delta(\cosh(\theta_2)-\cosh(\theta_1))-ix\Delta(\sinh(\theta_2)-\sinh(\theta_1))}$$
$$\times\sum_{a_1a_2}f^{M_0^3}_{\overline{a_1},a_2}(\theta_2-i\pi,\theta_1)f^{M_0^3}_{\overline{a_2},a_1}(\theta_1-i\pi,\theta_2);$$

$$C_{23}=-3\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}e^{-\tau\Delta(\cosh(\theta_1)-\cosh(\theta_2))-ix\Delta(\sinh(\theta_1)-\sinh(\theta_2))}$$
$$\times\sum_{a_1a_2}f^{M_0^3}_{\overline{a_1},a_2}(\theta_1-i\pi,\theta_2)f^{M_0^3}_{\overline{a_2},a_1}(\theta_2-i\pi,\theta_1);$$

$$C_{24}=\frac{1}{4}\sum_{a_1a_2a_3}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}e^{-\tau\Delta(\cosh(\theta_3)-\cosh(\theta_2))-ix\Delta(\sinh(\theta_3)-\sinh(\theta_2))}$$
$$\times\Bigg\{f^{M_0^3}_{\overline{a_3},a_1,a_1,a_2}(\theta_3-i\pi,\theta_1-i\pi,\theta_1,\theta_2)_c f^{M_0^3}_{\overline{a_2},a_3}(\theta_2-i\pi,\theta_3)+\sum_{a_4a_1'a_2'a_4'}S^{a_4'a_2'}_{a_4a_3}(\theta_{21})S^{a_2'a_1'}_{a_2a_1}(\theta_{13})$$
$$\times f^{M_0^3}_{\overline{a_2},a_1,a_4,a_3}(\theta_1-i\pi,\theta_3-i\pi,\theta_2,\theta_1)_c f^{M_0^3}_{\overline{a_4'},a_1'}(\theta_2-i\pi,\theta_3)+(\theta_2\leftrightarrow\theta_3)\Bigg\};$$

$$C_{25}=\frac{1}{4}\sum_{a_1a_2a_3}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}e^{-\tau\Delta(\cosh(\theta_3)-\cosh(\theta_2))-ix\Delta(\sinh(\theta_3)-\sinh(\theta_2))}$$
$$\times\Bigg\{\sum_{a_4a_4'}S^{a_4'a_1}_{a_4a_3}(\theta_{21})f^{M_0^3}_{\overline{a_2},a_1,a_4,a_3}(\theta_3-i\pi,\theta_1-i\pi,\theta_2,\theta_1)_c f^{M_0^3}_{\overline{a_4'},a_2}(\theta_2-i\pi,\theta_3)+\sum_{a_4a_1'}S^{a_4a_1'}_{a_2a_1}(\theta_{13})$$
$$\times f^{M_0^3}_{\overline{a_2},a_1,a_4,a_3}(\theta_1-i\pi,\theta_3-i\pi,\theta_1,\theta_2)_c f^{M_0^3}_{\overline{a_3},a_1'}(\theta_2-i\pi,\theta_3)+(\theta_2\leftrightarrow\theta_3)\Bigg\};$$

$$C_{26}=\frac{1}{4}\sum_{a_1a_2a_3a_4}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\frac{d\theta_4}{2\pi}e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}$$
$$\times e^{-\tau\Delta(\cosh(\theta_3)+\cosh(\theta_4)-\cosh(\theta_1)-\cosh(\theta_2))-ix\Delta(\sinh(\theta_3)+\sinh(\theta_4)-\sinh(\theta_1)-\sinh(\theta_2))}f^{M_0^3}_{\overline{a_3},a_4,a_1,a_2}(\theta_3-i\pi,\theta_4-i\pi,\theta_1,\theta_2)_c$$
$$\times f^{M_0^3}_{\overline{a_2},a_1,a_4,a_3}(\theta_2-i\pi,\theta_1-i\pi,\theta_4,\theta_3)_c. \tag{A14}$$

Although appearing exceedingly complicated, these terms dramatically simplify once we Fourier transform.

The first term, $C_{21}$, on the r.h.s. of Eq.(A14) involves $\delta(0)$ and so is ill-defined. However it precisely cancels the term arising from the evaluation of the partition function in Eq. (A3),

$$\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\sum_{a_1a_2}e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}\langle A_{a_1}(\theta)|M_0^3(x,\tau)M_0^3(0,0)|A_{a_1}(\theta)\rangle\langle A_{a_2}(\theta)|A_{a_2}(\theta)\rangle \tag{A15}$$

as is evident if a resolution of the identity is inserted between the two fields, $M_0^3$, in the above and then truncated at the one-particle level.

Having canceled off the $\delta(0)$-terms we now look at terms that make a genuine contribution to the spin–spin correlator. We first consider the completely disconnected terms. Fourier transforming $C_{22}$ and $C_{23}$ in time and space and then analytically continuing, $\omega_n \to -i\omega+\delta$, leads to

$$\begin{aligned} C_{22}(\omega=0,k=0)+C_{23}(\omega=0,k=0) &= -3\frac{\beta\Delta}{\pi}\int_{-\infty}^{\infty} d\theta \cosh(\theta) e^{-2\beta\Delta\cosh(\theta)} \\ &= -6\frac{\beta\Delta}{\pi}K_1(2\beta\Delta), \end{aligned} \tag{A16}$$

where again $K_1$ is a standard Bessel function.

To compute $C_{24}$ we need to evaluate the connected four-particle form factor. To do so we add small imaginary pieces to the rapidities where potential poles lurk and take only the finite piece. For example, the first term of $C_{24}$ upon Fourier transforming reduces to

$$\begin{aligned} C_{24}(\omega=0,k=0) = &-\frac{\beta}{8\pi^2\Delta}\int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ &\times \cosh^{-1}(\theta_2)\times f_{21}^{M_0^3}(\theta_2-i\pi,\theta_2) \\ &\times \sum_{a_1} f_{\overline{1}a_1a_12}^{M_0^3}(\theta_2-i\pi,\theta_1-i\pi,\theta_1,\theta_2)_{\rm c} \\ &+ \text{three other terms}. \end{aligned} \tag{A17}$$

Then to evaluate the connected form factor in this expression we write

$$\begin{aligned} f_{\overline{1}a_1a_12}^{M_0^3}(\theta_2-i\pi,\theta_1-i\pi,\theta_1,\theta_2)_{\rm c} = &\text{ finite part of} \\ &\times f_{\overline{1}a_1a_12}^{M_0^3}(\theta_2-i\pi,\theta_1-i\pi,\theta_1-i\eta,\theta_2-i\delta) \end{aligned} \tag{A18}$$

We evaluate this matrix element using the discussion in Sec. III D, throwing away any poles in $\eta$ or $\delta$ together with terms of the form $\eta/\delta$. Expanding the form factor on the r.h.s. of Eq. (A18) in $\eta$ and $\delta$ by using Eq. (3.29) leads to

$$\begin{aligned} \sum_{a_1} f_{\overline{1}a_1a_12}^{M_0^3}(\theta_2-i\pi,\theta_1-i\pi,\theta_1-i\eta,\theta_2-i\delta) &= -\frac{\Delta\pi^5}{8}\frac{16}{\pi^4}\left(\frac{\cosh(\theta_1)}{i\delta}+\frac{\cosh(\theta_2)}{i\eta}\right) \\ &\times\left(\prod \psi\Big|_{\delta=0,\eta=0}\right) G_{\overline{1}a_1a_12}^{m_{\overline{3}}}(\theta_2-i\pi,\theta_1-i\pi,\theta_1,\theta_2) \\ &-\frac{\Delta\pi^5}{8}\frac{16}{\pi^4}\Bigg\{\cosh(\theta_1)\partial_{-i\delta}\left(\left(\prod \psi\right)\right. \\ &\left.\times G_{\overline{1}a_1a_12}^{m_{\overline{3}}}(\theta_2-i\pi,\theta_1-i\pi,\theta_1-i\eta,\theta_2-i\delta)\right)\Big|_{\substack{\eta=0\\ \delta=0}} \\ &+\cosh(\theta_2)\partial_{-i\eta}\left(\left(\prod \psi\right)\right. \\ &\left.\times G_{\overline{1}a_1a_12}^{m_{\overline{3}}}(\theta_2-i\pi,\theta_1-i\pi,\theta_1-i\eta,\theta_2-i\delta)\right)\Big|_{\substack{\eta=0\\ \delta=0}}\Bigg\}, \end{aligned} \tag{A19}$$

where $\Pi\psi$ is given in this case by

$$\begin{aligned} \prod \psi = &\psi(\theta_{21})\psi(\theta_{21}-i\pi+i\eta)\psi(\theta_{12}-i\pi+i\delta) \\ &\times\psi(\theta_{12}-i\eta+i\delta). \end{aligned}$$

Discarding the pole terms [the first set of terms on the r.h.s. of Eq. (A19)] and evaluating the remainder leaves us with the desired connected form factor

$$\sum_{a_1} f_{\overline{1}a_1a_12}^{M_0^3}(\theta_2-i\pi,\theta_1-i\pi,\theta_1,\theta_2)_{\rm c} = i2\pi\Delta\frac{6\pi^2\cosh(\theta_1)+(5\pi^2+2\theta_{12}^2)\cosh(\theta_2)}{(4\pi^2+\theta_{12}^2)(\pi^2+\theta_{12}^2)}. \tag{A20}$$

Combining Eqs. (A20) and (A6) with (A17) we find

$$\begin{aligned} C_{24}(\omega=0,k=0) = &\frac{\beta\Delta}{4\pi}\int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ &\times\frac{6\pi^2\cosh(\theta_1)+(5\pi^2+2\theta_{12}^2)\cosh(\theta_2)}{(4\pi^2+\theta_{12}^2)(\pi^2+\theta_{12}^2)} \\ &+ \text{ three other terms} = \frac{11\Delta\beta}{4\pi^3}K_0(\beta\Delta)K_1(\beta\Delta) \\ &+\mathcal{O}\left(\frac{T}{\Delta}e^{-\beta\Delta}\right)+\text{three other terms}. \end{aligned} \tag{A21}$$

To arrive at the last line we have dropped terms polynomial in $\theta_{12}$. This leads to errors of $\mathcal{O}((T/\Delta)e^{-\beta\Delta})$. The remaining three terms make equal contributions to $C_{24}$. We thus finally have

$$\begin{aligned} C_{24}(\omega=0,k=0) = &\frac{\beta\Delta}{\pi}\int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ &\times\frac{6\pi^2\cosh(\theta_1)+(5\pi^2+2\theta_{12}^2)\cosh(\theta_2)}{(4\pi^2+\theta_{12}^2)(\pi^2+\theta_{12}^2)}. \end{aligned} \tag{A22}$$

We note that in regulating the form factor for $C_{24}$ we do not allow the infinitesimal imaginary pieces to affect the spatial dependence of the form factor, i.e., we do not write

$$f_{\overline{1}a_1a_12}^{M_0^3}(\theta_2-i\pi,\theta_1-i\pi,\theta_1+i\eta,\theta_2+i\delta,x) = e^{i\Delta x(i\delta\cosh(\theta_2)+i\eta\cosh(\theta_1))}(\cdots)$$

If we were to do so we would find an additional term coming from expanding $\exp(i\Delta x\cdots)$ in $\eta$ and $\delta$. However, generically such terms lead to a violation of translation invariance and as such should not be included. We moreover know that such terms would violate the equivalence of the form-factor computation with the expression for the susceptibility coming the thermodynamic Bethe ansatz.

We go through a similar procedure with $C_{25}$ and find an identical result: $C_{25}(\omega=0,k=0)=C_{24}(\omega=0,k=0)$. That we do so is significant. We might have approached the calculation equally validly by ordering the in and out states in the thermal trace and resolution of identity such that $\theta_1<\theta_2$ and $\theta_4<\theta_3$ [and correspondingly multiplying the expressions in Eq. (A14) by 4]. If we had done so we would find that in this case $C_{25}=0$ and $C_{24}$ is twice its current value. Of course both approaches must yield the same answer. But to do so we need $C_{25}(\omega=0,k=0)=C_{24}(\omega=0,k=0)$. Given the regularization of the form factors one must do to compute $C_{25}$, it is not a priori that this will be the case. That it is is a nontrivial check of our regularization procedure.

The final term we must evaluate is $C_{26}$. Fourier transforming as before we find

$$C_{26}(\omega=0,k=0)=\frac{1}{4\Delta^2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\frac{d\theta_4}{2\pi}\times 2\pi\delta(\sinh(\theta_3)+\sinh(\theta_4)-\sinh(\theta_2)-\sinh(\theta_1))$$
$$\times\frac{e^{-\beta\Delta(\cosh(\theta_3)+\cosh(\theta_4))}(1-e^{-\beta\Delta(\cosh(\theta_3)+\cosh(\theta_4)-\cosh(\theta_1)-\cosh(\theta_2))})}{\cosh(\theta_1)+\cosh(\theta_2)-\cosh(\theta_3)-\cosh(\theta_4)}$$
$$\times\sum_{a_1a_2a_3a_4}f^{M_0^3}_{a_3a_4a_1a_2}(\theta_3-i\pi,\theta_4-i\pi,\theta_1,\theta_2)_{\rm c}\times f^{M_0^3}_{a_2a_1a_4a_3}(\theta_2-i\pi,\theta_1-i\pi,\theta_4,\theta_3)_{\rm c}. \quad \text{(A23)}$$

As the 4-particle form factors are proportional to $(\sinh(\theta_3)+\sinh(\theta_4)-\sinh(\theta_2)-\sinh(\theta_1))$—the Lorentz pre-factor for the matrix element—one might believe it is immediate that this expression vanishes once the Fourier transform, $\lim_{k\to0}\int dx e^{ikx}$, is taken and so makes no contribution to the susceptibility. However the need to regulate the form factor leaves this ambiguous. Nevertheless, after the regulation $C_{26}$ ends up making no contribution to the susceptibility. It will, however, make a contribution to the NMR relaxation rate. Hence some of the details needed to compute $C_{26}$ will be dealt with in the context of that computation (see Appendix B and Sec. II C).

## APPENDIX B: COMPUTATION OF THE CORRELATOR FOR THE NMR RELAXATION RATE, $1/T_1$

In order to compute $1/T_1$ we must evaluate the correlator,

$$C(x=0,\omega=0)=\int dt e^{i\omega t}\langle M_0^1(0,t)M_0^1(0,0)\rangle. \quad \text{(B1)}$$

The lowest order contribution arising from the evaluation of the thermal trace takes the form

$$\langle M_0^1(0,t)M_0^1(0,0)\rangle_{\text{lowest order}}$$
$$\equiv C_1(t)=\int\frac{d\theta}{2\pi}\frac{d\theta_1}{2\pi}$$
$$\times e^{-\beta\Delta\cosh(\theta)}\sum_{aa_1}e^{-it\Delta(\cosh(\theta_1)-\cosh(\theta))+it(H_{s_{a_1}}-H_{s_a})}$$
$$\times e^{\beta Hs_a}\langle A_a(\theta)|M_0^1(0,0)|A_{a_1}(\theta_1)\rangle$$
$$\times\langle A_{a_1}(\theta_1)|M_0^1(0,0)|A_a(\theta)\rangle, \quad \text{(B2)}$$

where $S_a$ is the spin of particle $a$. We have assumed the field, H, is aligned along the 3-direction. Although we perform the calculation at finite H, the form factors themselves retain their $H=0$ form, a feature of the model's underlying integrability. Finite H merely breaks the degeneracy of the triplet state with the consequent energy shifts seen above. For the purposes of this computation, we are interested in the regime $H\ll T\ll\Delta$. This permits setting $e^{\beta Hs_a}$ to 1, provided we are willing to tolerate errors of $\mathcal{O}(H/T)$. Performing then the sums, $\Sigma_{aa_1}$, over the different types of excitations leaves us with

$$C_1(t)=-2\int\frac{d\theta}{2\pi}\frac{d\theta_1}{2\pi}e^{-\beta\Delta\cosh(\theta)}e^{-it\Delta(\cosh(\theta_1)-\cosh(\theta))}$$
$$\times\cos(Ht)\times f^{M_0^1}_{23}(\theta-i\pi,\theta_1)f^{M_0^1}_{23}(\theta_1-i\pi,\theta)$$
$$\times(1+\mathcal{O}(H/\Delta)). \quad \text{(B3)}$$

Substituting the expression for the form-factors, $f^{M_0^1}_{23}$, from Sec. III into the above, and then performing the necessary Fourier transform, leaves us with

$$C_1(\omega=0)=\frac{2\Delta}{\pi}\int d\theta\frac{e^{-\beta\Delta\cosh(\theta)}\cosh^2(\theta)}{\sqrt{\sinh^2(\theta)+\frac{2H}{\Delta}\cosh(\theta)}}$$
$$\times(1+\mathcal{O}(H/\Delta)+\mathcal{O}(H/T)). \quad \text{(B4)}$$

For $T\ll\Delta$ this reduces to $C_1(\omega=0)\approx 2\Delta/\pi e^{-\beta\Delta}(\log(4T/H)-\gamma)$, where $\gamma$ is Euler's constant.

This is the result found in Ref. 5—a logarithmic dependence on $H$ indicative of ballistic transport.

The next order in the computation, essentially computing terms of $\mathcal{O}(e^{-2\beta\Delta})$, is of the form

$$\begin{aligned} C_2(t) \equiv & \frac{1}{4}\sum_{a_1 a_2 a_3 a_4}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\frac{d\theta_4}{2\pi} \\ & \times \langle A_{a_1}(\theta_1)A_{a_2}(\theta_2)|M_0^1(0,t)|A_{a_3}(\theta_3)A_{a_4}(\theta_4)\rangle \\ & \times \langle A_{a_4}(\theta_4)A_{a_3}(\theta_3)|M_0^1(0,0)|A_{a_2}(\theta_2)A_{a_1}(\theta_1)\rangle \\ \equiv & C_{21}(t)+C_{22}(t)+C_{23}(t)+C_{24}(t)+C_{25}(t)+C_{26}(t). \end{aligned} \tag{B5}$$

Here we have introduced the same notation employed to evaluate the second order contribution to the susceptibility. The definitions of $C_{2i}$ are the same as those in Eq. (A14) but for changing $M_0^3$ to $M_0^1$ and shifting energies by a Zeeman term. As in the susceptibility computation, $C_{21}(t)$ is an ill-defined term proportional to $\delta(0)$, but is cancelled off by similar terms coming from the partition function. Similarly, $C_{22}$ and $C_{23}$ are disconnected terms related to $C_1$. They give a contribution of the form

$$\begin{aligned} & C_{22}(\omega=0)+C_{23}(\omega=0) \\ & = \frac{2\Delta}{\pi}\int d\theta \frac{e^{-\beta\Delta\cosh(\theta)}\cosh^2(\theta)}{\sqrt{\sinh^2(\theta)+\frac{2H}{\Delta}\cosh(\theta)}} \\ & \quad \times(-3e^{-\beta\Delta\cosh(\theta)}) \\ & = -\frac{6}{\pi}\Delta e^{-2\beta\Delta}\sqrt{\frac{2\pi}{\beta\Delta}}\left(\log\left(\frac{2T}{H}\right)-\gamma\right). \end{aligned} \tag{B6}$$

If we were to add similarly disconnected terms coming from matrix elements with a greater number of particle numbers, we would find a resummation of the form:

$$\begin{aligned} & C_{21}(\omega=0)+C_{22}(\omega=0)+C_{23}(\omega=0) \\ & \qquad + \text{higher order disconnected terms} \\ & \quad = \frac{2\Delta}{\pi}\int d\theta \frac{e^{-\beta\Delta\cosh(\theta)}\cosh^2(\theta)}{\sqrt{\sinh^2(\theta)+\frac{2H}{\Delta}\cosh(\theta)}} \\ & \qquad \times \frac{1}{1+3e^{-\beta\Delta\cosh(\theta)}}. \end{aligned} \tag{B7}$$

This type of resummation was discussed in Sec. II A.

The remaining terms are connected. $C_{24}(t)$ is given by (we again set terms of the form $e^{\pm\beta H}$ to 1)

$$\begin{aligned} C_{24}(t) = & \frac{1}{4}\sum_{a_1 a_2 a_3}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi} e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ & \times e^{-it\Delta(\cosh(\theta_3)-\cosh(\theta_2))}\cos(Ht) \\ & \times \Bigg\{ f^{M_0^1}_{\overline{a_3},a_1,a_1,a_2}(\theta_3-i\pi,\theta_1-i\pi,\theta_1,\theta_2)_c \\ & \times f^{M_0^1}_{\overline{a_2},a_3}(\theta_2-i\pi,\theta_3) \\ & + \sum_{a_4 a_1' a_2' a_4'} S^{a_4' a_2'}_{a_4 a_3}(\theta_{21}) S^{a_2' a_1'}_{a_2 a_1}(\theta_{13}) \\ & \times f^{M_0^1}_{\overline{a_2},a_1,a_4,a_3}(\theta_1-i\pi,\theta_3-i\pi,\theta_2,\theta_1)_c \\ & \times f^{M_0^1}_{\overline{a_4'},a_1'}(\theta_2-i\pi,\theta_3)+(\theta_2\leftrightarrow\theta_3)\Bigg\}. \end{aligned} \tag{B8}$$

To evaluate this expression we must again regulate the four particle form factors appearing in the above by removing the singularities arising when two rapidities equal one another. For example, we regulate the first four particle form factor appearing in the above via

$$\begin{aligned} & f^{M_0^1}_{\overline{a_3},a_1,a_1,a_2}(\theta_3-i\pi,\theta_1-i\pi,\theta_1,\theta_2)_c \\ & = \frac{\pi^3}{2}\psi(\theta_{32}-i\pi)\Bigg\{\cosh(\theta_1)\Big(\prod\ \psi\Big) \\ & \quad \times G^{M_0^1}_{\overline{a_3},a_1,a_1,a_2}(\theta_3-i\pi,\theta_1-i\pi,\theta_1,\theta_2) \\ & \quad + (\sinh(\theta_2)-\sinh(\theta_3))\partial_{-i\eta}\Big(\Big(\prod\ \psi\Big) \\ & \quad \times G^{M_0^1}_{\overline{a_3},a_1,a_1,a_2}(\theta_3-i\pi,\theta_1-i\pi,\theta_1-i\eta,\theta_2)\Big)\Bigg\}, \end{aligned} \tag{B9}$$

where $\Pi\psi = \psi(\theta_{31})\psi(\theta_{31}-i\pi+i\eta)\psi(\theta_{12}-i\pi)\psi(\theta_{12}-i\eta)$. Regulating the other form-factors similarly, we find after a long computation

$$\begin{aligned} C_{24}(\omega=0) = & \frac{\Delta\pi}{256}\int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\ & \times\Bigg\{\Bigg(\frac{1}{|\sinh(\theta_3)|}(\sinh(\theta_2)-\sinh(\theta_3)) \\ & \times\left[\frac{\theta_{23}\coth^2(\theta_{23}/2)}{(\theta_{23}^2+\pi^2)}\right]^2\Bigg\{12\theta_{23}\cosh(\theta_1) \\ & +12(\sinh(\theta_2)-\sinh(\theta_3))\left(\frac{\theta_{13}}{\theta_{12}}+\frac{\theta_{12}}{\theta_{13}}-\frac{1}{6}\right)\Bigg\} \\ & \times(1+\mathcal{O}(\theta_{23})^2+\mathcal{O}(\theta_{12})^2+\mathcal{O}(\theta_{13})^2)\Bigg)\Bigg|_{\theta_3=\cosh^{-1}(\cosh(\theta_2)+H)} \end{aligned}$$

$$+(H\leftrightarrow -H)\Big\}$$

$$=\frac{17\Delta}{2\pi^3}e^{-2\beta\Delta}\sqrt{\frac{2\pi}{\beta\Delta}}\left(\log\left(\frac{4T}{H}\right)-\gamma\right)(1+\mathcal{O}(H/T)+\mathcal{O}(T/\Delta)). \tag{B10}$$

We perform a similar procedure on $C_{25}$. As with the susceptibility, $C_{25}$ must and does generate an identical contribution to $C_{24}$.

The remaining term to evaluate is $C_{26}$. This term made no contribution to the susceptibility but does make a contribution to the relaxation rate, $1/T_1$. $C_{26}$ takes the form

$$\begin{aligned}C_{26}(t)=&\frac{1}{4}\sum_{a_1a_2a_3a_4}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\frac{d\theta_4}{2\pi}\\&\times e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}\\&\times e^{-it\Delta(\cosh(\theta_3)+\cosh(\theta_4)-\cosh(\theta_1)-\cosh(\theta_2))}\\&\times e^{itH(S_{a_3}+S_{a_4}-S_{a_1}-S_{a_2})}\\&\times f^{M_0^1}_{\overline{a_2},\overline{a_1},a_4,a_3}(\theta_2-i\pi+i\epsilon_2,\theta_1-i\pi+i\epsilon_1,\theta_4,\theta_3)_c\\&\times f^{M_0^1}_{\overline{a_3},\overline{a_4},a_1,a_2}(\theta_3-i\pi+i\epsilon_3,\theta_4-i\pi+i\epsilon_4,\theta_1,\theta_2)_c.\end{aligned} \tag{B11}$$

Again we must regulate this expression by discarding terms proportional to the $1/\epsilon$'s. To exhibit such terms we deform the contours $\theta_3$ and $\theta_4$ via

$$\theta_3\rightarrow\theta_3+i\pi;$$

$$\theta_4\rightarrow\theta_4+i\pi.$$

In doing so, we deform through a series of poles whose residues we thus pick up. Taking these into account, we end up with

$$C_{26}(t)=-\frac{i}{8\pi^5}\sum_{a_1a_2a_3a_4}\int d\theta_1\,d\theta_2 d\theta_4 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}e^{-i\Delta t\cosh(\theta_4)}\cos(Ht)$$

$$\times\left\{e^{i\Delta t\cosh(\theta_2)}\frac{f^{M_0^1}_{\overline{a_2},\overline{a_1},a_4,a_3}(\theta_2-i\pi+i\epsilon_2,\theta_1-i\pi+i\epsilon_1,\theta_4,\theta_3)}{\psi(\theta_{13}-i\pi+i\epsilon_1)}\Big|_{\theta_3=\theta_1}\right.$$

$$\left.\times f^{M_0^1}_{\overline{a_3},\overline{a_4},a_1,a_2}(\theta_1-i\pi+i\epsilon_3,\theta_4-i\pi+i\epsilon_4,\theta_1,\theta_2)+e^{i\Delta t\cosh(\theta_1)}\frac{f^{M_0^1}_{\overline{a_2},\overline{a_1},a_4,a_3}(\theta_2-i\pi+i\epsilon_2,\theta_1-i\pi+i\epsilon_1,\theta_4,\theta_3)}{\psi(\theta_{23}-i\pi+i\epsilon_2)}\Big|_{\theta_3=\theta_2}\right.$$

$$\left.\times f^{M_0^1}_{\overline{a_3},\overline{a_4},a_1,a_2}(\theta_2-i\pi+i\epsilon_3,\theta_4-i\pi+i\epsilon_4,\theta_1,\theta_2)\right\}-\frac{i}{8\pi^5}\sum_{a_1a_2a_3a_4}\int d\theta_1\,d\theta_2\,d\theta_3 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}e^{it\Delta\cosh(\theta_3)}\cos(Ht)$$

$$\times\left\{e^{i\Delta t\cosh(\theta_2)}\frac{f^{M_0^1}_{\overline{a_2},\overline{a_1},a_4,a_3}(\theta_2-i\pi+i\epsilon_2,\theta_1-i\pi+i\epsilon_1,\theta_4,\theta_3+i\pi-i\epsilon_3)}{\psi(\theta_{14}-i\pi+i\epsilon_1)}\Big|_{\theta_4=\theta_1}\right.$$

$$\left.\times f^{M_0^1}_{\overline{a_3},\overline{a_4},a_1,a_2}(\theta_3,\theta_1-i\pi+i\epsilon_4,\theta_1,\theta_2)+e^{it\Delta\cosh(\theta_1)}\frac{f^{M_0^1}_{\overline{a_2},\overline{a_1},a_4,a_3}(\theta_2-i\pi+i\epsilon_2,\theta_1-i\pi+i\epsilon_1,\theta_4,\theta_3+i\pi-i\epsilon_3)}{\psi(\theta_{24}-i\pi+i\epsilon_2)}\Big|_{\theta_4=\theta_2}\right.$$

$$\left.\times f^{M_0^1}_{\overline{a_3},\overline{a_4},a_1,a_2}(\theta_3,\theta_2-i\pi+i\epsilon_4,\theta_1,\theta_2)\right\}+\frac{1}{64\pi^4}\sum_{a_1a_2a_3a_4}\int d\theta_1\,d\theta_2\,d\theta_3\,d\theta_4 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))}$$

$$\times e^{it\Delta(\cosh(\theta_1)+\cosh(\theta_2)+\cosh(\theta_3)+\cosh(\theta_4))}\cos(Ht)f^{M_0^1}_{\overline{a_2},\overline{a_1},a_4,a_3}(\theta_2-i\pi,\theta_1-i\pi,\theta_4+i\pi,\theta_3+i\pi)f^{M_0^1}_{\overline{a_3},\overline{a_4},a_1,a_2}(\theta_3,\theta_4,\theta_1,\theta_2)$$

$$\equiv\sum_{i=1}^{5}C_{26i}(t). \tag{B12}$$

As we are interested in $C_{26}(\omega\sim 0)$, we immediately see that the last three terms, $C_{263}$ to $C_{265}$, may be neglected as they are only non-zero for frequencies, $\omega$, in excess of $2\Delta$ (provided $H\ll\Delta$).

Focusing then upon $C_{261}$, we obtain upon performing the necessary regulation

$$
\begin{aligned}
C_{261}(t) = i\frac{\Delta^2\pi^3}{128}\int d\theta_1\, d\theta_2\, d\theta_4 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\
\times\cos(Ht)e^{-i\Delta t(\cosh(\theta_4)-\cosh(\theta_2))}\times(\sinh(\theta_4)-\sinh(\theta_2))\left(\prod_1 \psi\right) G^{m_0^1}_{-\,a_2,a_1,a_4,a_3}(\theta_2-i\pi,\theta_1-i\pi,\theta_4,\theta_1) \\
\times\Bigg\{\cosh(\theta_1)\left(\prod_2 \psi\right) G^{m_0^1}_{-\,a_3,a_4,a_1,a_2}(\theta_1-i\pi,\theta_4-i\pi,\theta_1,\theta_2)+(\sinh(\theta_2)-\sinh(\theta_4))\partial_{-i\epsilon}\Bigg(\left(\prod_2 \psi\right) \\
\times G^{m_0^1}_{-\,a_3,a_4,a_1,a_2}(\theta_1-i\pi+i\epsilon,\theta_4-i\pi,\theta_1,\theta_2)\Bigg)\Bigg\}
\end{aligned}
$$

$$
\prod_1 \psi = \psi(\theta_{21})\psi(\theta_{24}-i\pi)\psi(\theta_{21}-i\pi)\psi(\theta_{14}-i\pi)\psi(\theta_{41}),
$$

$$
\prod_2 \psi = \psi(\theta_{14}+i\epsilon)\psi(\theta_{12}-i\pi+i\epsilon)\psi(\theta_{41}-i\pi)\psi(\theta_{42}-i\pi)\psi(\theta_{12}). \tag{B13}
$$

To evaluate the above expression, we first Fourier transform which then leads us to consider the following expressions:

$$
\left(\prod_1 \psi\right)\left(\prod_2 \psi\right) G^{m_0^1}_{-\,a_2,a_1,a_4,a_3} G^{m_0^1}_{-\,a_3,a_4,a_1,a_2} - (\theta_i\leftrightarrow-\theta_i) = 0,
$$

$$
\begin{aligned}
&\left(\prod_1 \psi\right) G^{m_0^1}_{-\,a_2,a_1,a_4,a_3}\partial_{-i\epsilon}\left(\left(\prod_2 \psi\right) G^{m_0^1}_{-\,a_3,a_4,a_1,a_2}\right)+(\theta_i\leftrightarrow-\theta_i) \\
&\quad=\left(\prod_1 \psi\right) G^{m_0^1}_{-\,a_2,a_1,a_4,a_3} G^{m_0^1}_{-\,a_3,a_4,a_1,a_2}\left(\partial_{-i\epsilon}\left(\prod_2 \psi\right)+(\theta_i\leftrightarrow-\theta_i)\right) \\
&\quad= i12\pi\left[\frac{\theta_{24}^2\coth^4(\theta_{24}/2)}{(\theta_{24}^2+\pi^2)}\right]^2(1+\mathcal{O}(\theta_{14}^2)+\mathcal{O}(\theta_{12}^2)+\mathcal{O}(\theta_{24}^2)).
\end{aligned} \tag{B14}
$$

Putting everything together then yields

$$
\begin{aligned}
C_{261}(\omega=0) = \frac{\Delta 3\pi^5}{16}\int d\theta_1\, d\theta_2 e^{-\beta\Delta(\cosh(\theta_1)+\cosh(\theta_2))} \\
\times\Bigg\{\Bigg(\frac{1}{|\sinh(\theta_4)|}(\sinh(\theta_2)-\sinh(\theta_4))^2\times\left[\frac{\theta_{24}^2\coth^4(\theta_{24}/2)}{(\theta_{24}^2+\pi^2)}\right]^2 \\
\times(1+\mathcal{O}(\theta_{24})^2+\mathcal{O}(\theta_{12})^2+\mathcal{O}(\theta_{14})^2)\Bigg)\Bigg|_{\theta_4=\cosh^{-1}(\cosh(\theta_2)+H)}+(H\leftrightarrow-H)\Bigg\} \\
= 12\pi\Delta e^{-2\beta\Delta}\sqrt{\frac{2\pi}{\beta\Delta}}\left(\log\left(\frac{4T}{H}\right)-\gamma\right)(1+\mathcal{O}(H/T)+\mathcal{O}(T/\Delta)).
\end{aligned} \tag{B15}
$$

The evaluation of $C_{262}$ yields an identical contribution to the relaxation time.

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