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Critical behavior of an impurity at the boson superfluid-Mott insulator transition

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Abstract

We present a universal theory for the critical behavior of an impurity at the two-dimensional superfluid-Mott insulator transition. Our analysis is motivated by a numerical study of the Bose-Hubbard model with an impurity site by Huang *et al.* (Phys. Rev. B **94**, 220502 (2016)); they found an impurity phase transition as a function of the trapping potential, while the bulk was critical. The bulk theory is described by the $O(2)$ symmetric Wilson-Fisher conformal field theory, and we model the impurity by a localized spin-1/2 degree of freedom. We also consider a generalized model by considering an $O(N)$ symmetric bulk theory coupled to a spin-S degree of freedom. We study this field theory using the $\epsilon = 3-d$ expansion, where the impurity-bulk interaction flows to an infrared stable fixed point at the critical trapping potential. We determine the scaling dimensions of the impurity degree of freedom and the associated critical exponents near the critical point. We also determine the universal contribution of the impurity to the finite temperature compressibility of the system at criticality. Our results are compared with numerical simulations.

I. INTRODUCTION

The quantum phase transition between a superfluid and a Mott insulator in two dimensions represents one of the best studied examples of quantum critical matter, both theoretically and experimentally. The critical properties of this transition are described by a strongly interacting relativistic quantum field theory whose properties have been well-studied in the literature [1, 2]. This phase transition can be realized experimentally using cold atoms trapped in optical lattices, providing greater access to its properties [3–5].

In this paper, we study the superfluid-insulator transition in the presence of an impurity degree of freedom, motivated by recent numerical work by Huang *et al.* [6] of the lattice Bose-Hubbard model. Their study models the presence of an impurity in terms of a trapping potential, representing the attachment of charge to the impurity. With the bulk taken to be at the superfluid-insulator quantum critical point, they found a remarkable quantum transition at the impurity, where the total boson number trapped by the impurity jumped by unity. Despite the jump in the boson number, the transition is second order because it is associated with divergence in the size of the screening cloud. They find the emergence of scale-invariant behavior for a critical value of the trapping potential, suggesting the emergence of a new universality class associated with the impurity degree of freedom.

Models of impurities coupled to an interacting bulk critical theory were considered in References 7 and 8. Furthermore, a model of impurities coupled to a bulk interacting critical theory was investigated in Refs. 9–11. The latter model describes the effect of impurities coupled to quantum antiferromagnets close to their critical point. In that work, the impurities are represented by a localized spin degree of freedom which coupled to the bulk quantum field theory, and a stable interacting fixed point was found perturbatively in the $\epsilon = 3 - d$ expansion. This novel impurity-driven critical behavior led to new observables associated with the impurity degree of freedom.

Here we take a similar approach in studying the superfluid-insulator transition coupled to impurities. We will argue for the particular form of an impurity-bulk interaction to model the critical behavior, and study the resulting theory in the ϵ expansion. Working with a slightly generalized model, we will find an interacting fixed point, and calculate the new critical exponents associated with the theory. Unlike the case with the antiferromagnet, this impurity fixed point has a single relevant perturbation which does not break any symmetries:

this relevant direction corresponds to the tuning of the magnitude of the trapping potential. We will also determine the universal dependence of the finite temperature compressibility on the impurity degree of freedom at the fixed point. The exponents and the compressibility can be related to those calculated numerically in Refs. 6 and 12.

Our paper is arranged as follows. In Section II we discuss the microscopic model of Ref. 6, and argue for the form of the universal quantum field theory describing its universal properties. We set up the form of the ϵ expansion of a generalized form of the theory. Section III describes how the diagrammatic expansion of the model is constructed, and gives the expansion to two-loop order. We give a summary of the renormalization group equations in Section IV, and give our predictions for the critical exponents of the model. In Section V, we determine the universal contribution of the impurity to the finite temperature compressibility of the model, and we conclude in Section VI.

II. THE MODEL

A. Continuum field theory

We seek the critical theory describing the microscopic model studied numerically in Ref. 6. This is given by

$$\mathcal{H}_1 = \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i \left(n_i - 1 \right) - \mu \sum_i n_i + V n_0 \tag{1}$$

where $b_i^\dagger$ is a boson creation operator on site i, $\langle \cdots \rangle$ denotes nearest-neigbors, and $n_i \equiv b_i^\dagger b_i$. The model is studied at constant density with unit filling fraction, where a bulk critical point between a superfluid and insulating state is known to exist at the values $U_c = 16.7424(1)$ and $\mu_c = 6.21(2)$ [13, 14]. For $V = 0$, it is known that the bulk transition is described by the relativistically-invariant $O(2)$-symmetric Wilson-Fisher conformal field theory [1], given by the Hamiltonian

$$\mathcal{H}'_\phi = \int d^3x \left\{ \frac{\pi_{\alpha'}^2 + c^2 \left(\nabla \phi_{\alpha'} \right)^2 + s_c \, \phi_{\alpha'}^2}{2} + \frac{u_0}{4!} \left(\phi_{\alpha'}^2 \right)^2 \right\} \tag{2}$$

where the index runs from $\alpha' = 1, 2$. The coupling s_c has been fine-tuned to its critical value, and u_0 flows to a universal value in the infrared. The fields $\phi_{\alpha'}(x,t)$ and $\pi_{\alpha'}(x,t)$ represent

the bulk order parameter and its canonical conjugate respectively, obeying the commutation relation

$$[\phi_{\alpha'}(x,t), \pi_{\beta'}(x',t)] = \delta_{\alpha'\beta'}\delta^d(x-x') \tag{3}$$

The velocity scale c depends on microscopic details of the system, and will henceforth be set to unity.

In Ref. 6, it was found that the addition of the impurity potential V leads to new critical behavior. As the potential is turned on, it is found that charge is either depleted or concentrated at the origin depending on the sign of V. The density profile is characterized by a half-integer charged core, and a half-integer charged halo located at a radius ξ_h from the origin. The sign of the halo charge flips across the critical point.

At a critical value of V, the halo size, ξ_h, diverges to infinity, indicating the onset of scale invariance. If the coupling V continues to increase, the charge of the halo changes sign and contracts back to the origin; so this is a transition between a system with total charge Q and $Q \pm 1$. The radius of the halo is observed to have the universal behavior

$$\xi_h \propto |V - V_c|^{-\nu_z} \tag{4}$$

with $\nu_z = 2.33(5)$ [6].

In seeking the critical theory, we need to couple the bulk Hamiltonian Eq. (2) to a field describing the impurity degree of freedom. This theory retains the $O(2)$ invariance. We claim that the correct impurity coupling is given by

$$\mathcal{H}_{\text{imp}} = -\gamma_0 \left[\phi_1(x=0)\hat{S}_x + \phi_2(x=0)\hat{S}_y\right] + h_z\hat{S}_z \tag{5}$$

where $\hat{S}_\alpha$ represents a spin-1/2 degree of freedom defined at $x = 0$; a spin $S = 1/2$ impurity model has also been proposed and studied independently by Chen *et al.* [12]. The impurity site density n_0, is related to the spin via $\hat{S}_z = n_0 - Q + 1/2$ for a transition between Q and $Q - 1$. We also note that a scalar-spin interaction of this form was studied in a different context by Zaránd and Demler [15]. Here, the two couplings γ_0 and h_z are both relevant in $d = 2$. The $O(2)$ symmetry of the impurity is generated by $\hat{S}_z$, and at $h_z = 0$, there is an exact two-fold degeneracy between the $\hat{S}_z = \pm 1/2$ states, which reproduces the two-fold degeneracy of the microscopic theory at the critical impurity potential $V = V_c$ between the different charge sectors. We will argue below that the coupling γ_0 flows to a universal value which controls the critical behavior of the impurity degree of freedom.

Our analysis will also consider the case where the impurity $\hat{S}_\alpha$ has a generic spin S. This corresponds to possible multicritical points where $2S+1$ states become degenerate at the impurity. In the Bose-Hubbard model, we would have to tune $2S$ couplings to achieve this. In the field theory, the $2S$ relevant couplings correspond to the operators $\hat{S}_z^p$, with $1 \leq p \leq 2S$. We will only consider the scaling dimension of the $p=1$ operator here.

B. Expansion in ϵ

We will work with a generalization of the above theory, given by

$$\mathcal{H} = \mathcal{H}_\phi - \gamma_0 \phi_{\alpha'}(x=0)\hat{S}_{\alpha'} \tag{6}$$

Here, the first term is the Hamiltonian for the $O(N)$-symmetric scalar field theory in d spatial dimensions,

$$\mathcal{H}_\phi = \int d^d x \left\{ \frac{\pi_\alpha^2 + (\nabla\phi_\alpha)^2 + s_c\, \phi_\alpha^2}{2} + \frac{u_0}{4!}\left(\phi_\alpha^2\right)^2 \right\} \tag{7}$$

We use the notation where unprimed indices run from $\alpha = 1, 2, ..., N$, while primed indices only take the values $\alpha' = 1, 2$. Summation is implied over repeated indices, and it is understood that $\phi_\alpha^2 = \phi_\alpha \phi_\alpha$. The operators $\hat{S}_\alpha(t)$ satisfy the $SU(2)$ algebra,

$$\begin{aligned} [\hat{S}_\alpha, \hat{S}_\beta] &= i\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma \\ \mathrm{Tr}\left(\hat{S}_\alpha \hat{S}_\beta\right) &= \frac{1}{3}(2S+1)S(S+1)\delta_{\alpha\beta} \end{aligned} \tag{8}$$

where the spin operator only takes the values $\alpha = 1, 2, 3$. We continue to label the $1-2$ directions with primed indices, and refer to the third direction as the $z-$direction. We note that the total Hamiltonian in Eq. (6) has $O(2) \times O(N-2)$ symmetry. Here we will allow arbitrary values of spin, S, and give results for $S = 1/2$ at the end of the calculation. Although the operator $\hat{S}_z$ does not appear in this Hamiltonian, it has nontrivial correlations in the interacting theory due to the commutation relations. Its scaling dimensions will then determine the critical exponent associated with perturbing this theory by a term $h_z \hat{S}_z$.

We will study this system in the $\epsilon = 3-d$ expansion. We will use the minimal subtraction renormalization scheme of Ref. 16, where $s_c = 0$ and the bare fields and interaction strength

are replaced by

$$\begin{aligned} \phi_\alpha &= \sqrt{Z}\phi_{R\alpha} \\ u_0 &= \frac{\mu^\epsilon Z_4}{S_{d+1}Z^2}g \end{aligned} \tag{9}$$

Here, μ is an arbitrary energy scale, g is a dimensionless coupling constant, and

$$S_d = \frac{2}{\Gamma(d/2)(4\pi)^{d/2}} \tag{10}$$

is a convenient phase factor. To leading order in g, the renormalization constants are given by

$$\begin{aligned} Z &= 1 - \frac{(N+2)}{144\epsilon}g^2 \\ Z_4 &= 1 + \frac{(N+8)}{6\epsilon}g + \left(\frac{(N+8)^2}{36\epsilon^2} - \frac{(5N+22)}{36\epsilon}\right)g^2 \end{aligned} \tag{11}$$

The beta function follows immediately from Eqns. (9) and (11)

$$\beta_g \equiv \mu\frac{dg}{d\mu}\bigg|_{u_0} = -\epsilon g + \frac{(N+8)}{6}g^2 - \frac{(3N+14)}{12}g^3 \tag{12}$$

from which we determine the bulk fixed point by finding the value of g where the beta function vanishes:

$$g^* = \frac{6\epsilon}{(N+8)}\left[1 + \frac{3(3N+14)}{(N+8)^2}\epsilon\right] \tag{13}$$

The addition of a localized bulk-impurity interaction cannot significantly alter the bulk correlation functions, so the above results also hold for the full theory $\mathcal{H}$. However, we must now consider the renormalization of the impurity operators and their interaction with the bulk order parameter. We define the constants

$$\begin{aligned} \hat{S}_{\alpha'} &= \sqrt{Z'}\hat{S}_{R\alpha'} \\ \hat{S}_z &= \sqrt{Z_z}\ \hat{S}_{Rz} \\ \gamma_0 &= \frac{\mu^{\epsilon/2}Z_\gamma}{\sqrt{ZZ'\tilde{S}_{d+1}}}\gamma \end{aligned} \tag{14}$$

Here, γ is another dimensionless renormalized interaction, and we have introduced another convenient phase factor

$$\tilde{S}_d = \frac{\Gamma(d/2-1)}{4\pi^{d/2}} \tag{15}$$

In terms of the above constants, we find that the impurity beta function is given by

$$\beta_\gamma \equiv \mu \frac{d\gamma}{d\mu}\bigg|_{u_0,\gamma_0} = -\frac{\frac{\epsilon}{2}\gamma + \gamma\beta_g \frac{d}{dg}\log\left(Z_\gamma/\sqrt{ZZ'}\right)}{1+\gamma\frac{d}{d\gamma}\log\left(Z_\gamma/\sqrt{ZZ'}\right)} \tag{16}$$

One major result of this paper is the determination of the beta function to two-loop order, from which we find an infrared fixed point at a critical value of γ^* which is perturbative in ϵ. The major observables associated with this fixed point are the universal decay of the spin operators. We introduce the anomalous dimensions,

$$\begin{aligned} \left\langle \hat{S}_{\alpha'}(t)\hat{S}_{\alpha'}(0)\right\rangle &\sim \frac{1}{t^{\eta'}} \\ \left\langle \hat{S}_z(t)\hat{S}_z(0)\right\rangle &\sim \frac{1}{t^{\eta_z}} \end{aligned} \tag{17}$$

where algebraic decay is forced by scale invariance, and the exponents are given by

$$\begin{aligned} \eta' &= \beta_\gamma \frac{d}{d\gamma}\log Z' + \beta_g \frac{d}{dg}\log Z' \\ \eta_z &= \beta_\gamma \frac{d}{d\gamma}\log Z_z + \beta_g \frac{d}{dg}\log Z_z \end{aligned} \tag{18}$$

These anomalous dimensions, which are twice the scaling dimension of the spin operators, are new data associated with the universality class of this phase transition.

Once the anomalous dimension of $\hat{S}_z$ is determined, we can also determine the critical exponents associated with perturbing the critical theory. The leading relevant perturbations to Eq. (6) are given by

$$\begin{aligned} \Delta\mathcal{H}' &= h'\hat{S}_{\alpha'} \\ \Delta\mathcal{H}_z &= h_z\hat{S}_z \end{aligned} \tag{19}$$

for any of the three $\hat{S}_\alpha$. This perturbation will introduce a large timescale ξ characterizing an exponential decay of the spin correlation functions, and by scaling arguments, it is straightforward to show that

$$\begin{aligned} \xi' &= |h'|^{-\nu'} \\ \xi_z &= |h'|^{-\nu_z} \end{aligned} \tag{20}$$

where

$$\begin{aligned} \nu' &= \frac{1}{1-\eta'/2} \\ \nu_z &= \frac{1}{1-\eta_z/2} \end{aligned} \tag{21}$$

Here, exponent ν_z corresponds to the critical exponent defined in the microscopic model above.

III. RENORMALIZATION

We determine the renormalization parameters above using bare perturbation theory. In particular, we will work in imaginary time τ, and compute the following correlation functions to two-loop order:

$$\mathcal{G}'(\tau)\delta_{\alpha'\beta'} = \left\langle \hat{S}_{\alpha'}(\tau)\hat{S}_{\beta'}(0)\right\rangle$$

$$\mathcal{G}^z(\tau) = \left\langle \hat{S}_z(\tau)\hat{S}_z(0)\right\rangle$$

$$\mathcal{V}(x,\tau)\delta_{\alpha'\beta'} = \left\langle \phi_{\alpha'}(x,\tau)\hat{S}_{\beta'}(0)\right\rangle \tag{22}$$

All correlation functions are understood to be imaginary time-ordered, we take $\tau > 0$, and a trace is taken over the spin indices. This calculation will result in divergences in the form of poles in ϵ, but we choose the constants Z', Z_3, and Z_4 such that these poles cancel when the correlation functions are expressed in terms of renormalized operators and couplings.

Due to the nontrivial commutator in Eq. (8), the perturbative expansion for these correlation functions does not obey Wick's theorem, nor do disconnected diagrams cancel. We must expand the numerator and denominator of the correlation functions separately as a series in u_0 and γ_0, and by carefully keeping track of the time-ordering of the spin operators we can obtain the desired correlation functions. This procedure can be represented by a form of diagrammatic perturbation theory developed in Ref. 10.

We first write the correlation function of the interacting theory in terms of free correlators, where the free part of our theory is the quadratic part of $\mathcal{H}_\phi$.

$$\langle \mathcal{O}\rangle = \frac{\left\langle \mathcal{O}e^{-\beta\mathcal{H}_I}\right\rangle_0}{\left\langle e^{-\beta\mathcal{H}_I}\right\rangle_0} \tag{23}$$

We introduce a finite inverse temperature β as an intermediate step. The Hamiltonian which appears on the right-hand side is the interaction Hamiltonian,

$$\mathcal{H}_I = \frac{u_0}{4!}\int d^dx \left(\phi_{I\alpha}(x)^2\right)^2 - \gamma_0\phi_{I\alpha'}(x=0)\hat{S}_{\alpha'} \tag{24}$$

The operators $\phi_{I\alpha}$ are the familiar interaction representation of our original bosonic fields (the interaction and Schrödinger representations of $\hat{S}_\alpha$ are equivalent in our model). Then

we expand the exponentials in the numerator and denominator, and the expectation values break into simple products of bosonic correlators and spin correlators. The bosonic operators obey Wick's theorem, so we obtain integrals over products of the free finite-temperature bosonic Green's function:

$$D_T(x,\tau) = \langle \phi_\alpha(x,\tau)\phi_\beta(0,0)\rangle_0 \tag{25}$$

However, the time-ordering over spin expectation values will result in a corresponding time-ordering over dummy integration variables.

We represent the imaginary time-ordered expectation value of an arbitrary operator $\langle A\rangle_0$ with the following diagrammatic rules:

- Every diagram contains a single directed loop along which imaginary time runs periodically from 0 to β, represented by a full line.
- External factors of $\hat{S}_\alpha(\tau)$ contained in A are represented by open circles placed on the directed loop at the appropriate external value of τ.
- External factors of $\phi_\alpha(\tau, x)$ contained in A are represented by open boxes which are placed outside of the directed loop.
- Factors of the interaction γ_0 are represented by closed circles placed on the directed loop, and a bosonic propagator always emerges from this vertex.
- Factors of the interaction u_0 are represented by a filled square, which connects to four bosonic propagators.
- Internal bosonic propagators connecting vertices placed at (x_i, τ_i) and (x_j, τ_j) give a factor of $D_T(x_i - x_j, \tau_i - \tau_j)$, and we integrate over all internal x_i and τ_i. However, the ordering of all the τ_i's appearing on the directed loop must be kept in determining the integration region.
- We trace over the spins along the directed line. If there are no spin operators inserted, this is interpreted at $\mathrm{Tr}\,\mathbb{I} = (2S+1)$.

We obtain the correction to $\langle A\rangle$ at a given order of u_0 and γ_0 by writing down all possible diagrams which obey the above rules and have the correct number of interaction vertices, and then sum them. We will demonstrate how to apply these rules in detail for the relatively simple one-loop case, before giving the full two-loop results.

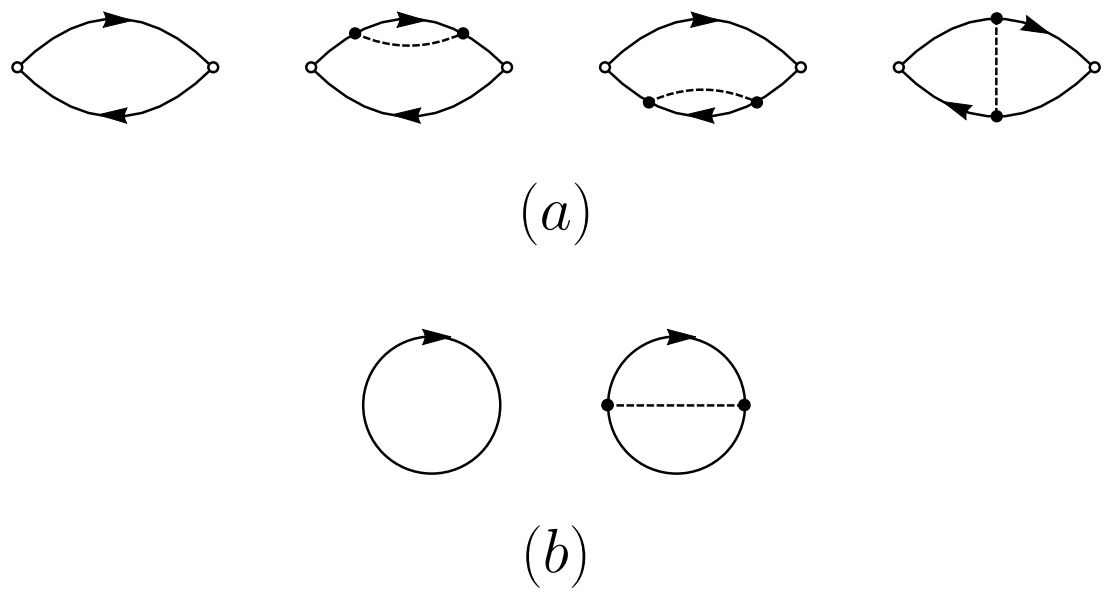

FIG. 1. The diagrammatic expansion for the spin-spin correlation function at one-loop, using the Feynman rules specified in the Section III. The diagrams contributing to the numerator and denominator of the correlation function are pictured in (a) and (b) respectively. As described in the main text, the integrals contributing to the numerator and denominator can be combined, so that we only need to keep track of differing spin traces.

A. Spin-spin correlation function

We show the lowest-order diagrams contributing to the spin-spin correlation functions in Fig. 1.(b). Below we will evaluate spin traces using the identities enumerated in Appendix A. We first write out the diagrams in the denominator, obtaining from the above rules

$$\mathcal{Z} = (2S+1) + \mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\alpha'}\right)\gamma_0^2 \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 D_T(\tau_1-\tau_2) + \cdots \tag{26}$$

We then rewrite this expression for reasons which will become clear shortly:

$$\begin{aligned}\mathcal{Z} = (2S+1) + \ (2S+1)\frac{2S(S+1)}{3}\gamma_0^2\Bigg[\int_0^\tau d\tau_1 \int_{\tau_1}^\tau d\tau_2 + \int_\tau^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \\ + \int_0^\tau d\tau_1 \int_\tau^\beta d\tau_2\Bigg] D_T(\tau_1-\tau_2) + \cdots\end{aligned} \tag{27}$$

We now consider the numerator of the spin-spin correlator in Eq. (22), given by the

diagrams in Fig. 1.(a).

$$\mathcal{Z}\mathcal{G}(\tau) = \mathrm{Tr}\left(\hat{S}_\alpha \hat{S}_\beta\right) + \mathrm{Tr}\left(\hat{S}_\alpha \hat{S}_{\sigma'} \hat{S}_{\sigma'} \hat{S}_\beta\right) \gamma_0^2 \int_0^\tau d\tau_1 \int_{\tau_1}^\tau d\tau_2 D_T(\tau_1 - \tau_2)$$
$$+ \ \mathrm{Tr}\left(\hat{S}_\alpha \hat{S}_\beta \hat{S}_{\sigma'} \hat{S}_{\sigma'}\right) \gamma_0^2 \int_\tau^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 D_T(\tau_1 - \tau_2)$$
$$+ \ \mathrm{Tr}\left(\hat{S}_\alpha \hat{S}_{\sigma'} \hat{S}_\beta \hat{S}_{\sigma'}\right) \gamma_0^2 \int_0^\tau d\tau_1 \int_\tau^\beta d\tau_2 D_T(\tau_1 - \tau_2) + \cdots \tag{28}$$

Here, we take the external indices to either be α', β' to define $\mathcal{G}'(\tau)$, or 3 to denote $\mathcal{G}_3(\tau)$. We notice that the three integrals contributing to the numerator are identical to the three we used to split up the denominator. Thus, to calculate the full correlation function, we only need to compute these three integrals and keep track of the difference in spin traces which appear in the numerator and denominator. This simplification is minor for the one-loop case, but it simplifies the two-loop calculation enormously.

We now write the one-loop correlation function in terms of the spin traces given in Appendix A. Here, the traces on the right-hand side correspond to either the $\mathcal{S}_i'$ or $\mathcal{S}_i^z$ in the appendix depending on whether the left-hand side represents the correlator $\mathcal{G}'(\tau)$ or $\mathcal{G}^z(\tau)$ respectively.

$$\mathcal{G}(\tau) = \frac{S(S+1)}{3}\Bigg\{1 + \left[\mathcal{S}_1 - \frac{2S(S+1)}{3}\right] \gamma_0^2 \int_0^\tau d\tau_1 \int_{\tau_1}^\tau d\tau_2 D_T(\tau_1 - \tau_2)$$
$$+ \left[\mathcal{S}_1 - \frac{2S(S+1)}{3}\right] \gamma_0^2 \int_\tau^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 D_T(\tau_1 - \tau_2)$$
$$+ \left[\mathcal{S}_2 - \frac{2S(S+1)}{3}\right] \gamma_0^2 \int_0^\tau d\tau_1 \int_\tau^\beta d\tau_2 D_T(\tau_1 - \tau_2) + \cdots\Bigg\} \tag{29}$$

We now consider the evaluation of these integrals. For the purpose of renormalizing our theory, we can work in the $T = 0$ limit, where the bosonic propagator takes the form

$$D_0(\tau) = \int \frac{d^d k}{(2\pi)^d} \frac{d\omega}{2\pi} \frac{e^{-i\omega\tau}}{k^2 + \omega^2} = \frac{\tilde{S}_{d+1}}{|\tau|^{d-1}} \tag{30}$$

Finally, the integrations over imaginary time must be extended with care, since imaginary time is really compact: $\beta \sim 0$. Therefore, we need to extend the integration domain as

$$\int_0^\beta \longrightarrow \int_0^\infty + \int_{-\infty}^0 \tag{31}$$

so that the integration still forms a loop in imaginary time. So the three integrals appearing in Eq. (29) respectively become

$$\int_0^\tau d\tau_1 \int_{\tau_1}^\tau d\tau_2 D_0(\tau_1 - \tau_2) = -\frac{\tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} \tag{32}$$

$$\left[\int_\tau^\infty d\tau_1 \int_{\tau_1}^\infty d\tau_2 + \int_\tau^\infty d\tau_1 \int_{-\infty}^0 d\tau_2 + \int_{-\infty}^0 d\tau_1 \int_{\tau_1}^0 d\tau_2\right] D_0(\tau_1 - \tau_2) = -\frac{\tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} \tag{33}$$

$$\left[\int_0^\tau d\tau_1 \int_\tau^\infty d\tau_2 + \int_0^\tau d\tau_1 \int_{-\infty}^0 d\tau_2\right] D_0(\tau_1 - \tau_2) = \frac{2\tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} \tag{34}$$

where we have used the dimensional regularization "identity" $\int_0^\infty d\tau \tau^\alpha = 0$.

Collecting all of the above results, we find that the leading-order spin-spin correlation functions are given by

$$\mathcal{G}'(\tau) = \frac{S(S+1)}{3}\left[1 - \frac{\gamma_0^2 \tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} + \cdots\right] \tag{35}$$

$$\mathcal{G}^z(\tau) = \frac{S(S+1)}{3}\left[1 - \frac{2\gamma_0^2 \tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} + \cdots\right] \tag{36}$$

The procedure at two-loop is done using the same procedure; we fill in the intermediate steps in Appendix B. Our final result is

$$\begin{aligned}\left\langle \hat{S}_{\alpha'}(\tau)\hat{S}_{\beta'}(0)\right\rangle = \delta_{\alpha'\beta'}\frac{S(S+1)}{3}\Bigg[1 - \frac{\gamma_0^2 \tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} \\ + \left(\gamma_0^2 \tilde{S}_{d+1}\tau^\epsilon\right)^2\left(\frac{1}{\epsilon^2} + \frac{5}{2\epsilon} + \cdots\right)\Bigg]\end{aligned} \tag{37}$$

$$\begin{aligned}\left\langle \hat{S}_z(\tau)\hat{S}_z(0)\right\rangle = \frac{S(S+1)}{3}\Bigg[1 - \frac{2\gamma_0^2 \tilde{S}_{d+1}\tau^\epsilon}{\epsilon(1-\epsilon)} \\ + \left(\gamma_0^2 \tilde{S}_{d+1}\tau^\epsilon\right)^2\left(\frac{3}{\epsilon^2} + \frac{6}{\epsilon} + \cdots\right)\Bigg]\end{aligned} \tag{38}$$

where we only keep the divergent part of the γ_0^4 term.

B. Vertex renormalization

We now consider the renormalization of the vertex function $\mathcal{V}(x,\tau)$, defined in Eq. (22). In writing down all possible diagrams up to two-loop order, it becomes apparent that every diagram which does not depend on u_0 is identical to a diagram appearing in Fig. 1, but with the insertion of an external boson. Therefore, the only loop diagrams which contribute to renormalizing the bare interaction γ_0 are those which involve the bulk interaction; these are shown in Fig. 2. This implies the *exact* relation

$$Z_\gamma = 1 \quad \text{at} \quad g = 0 \tag{39}$$

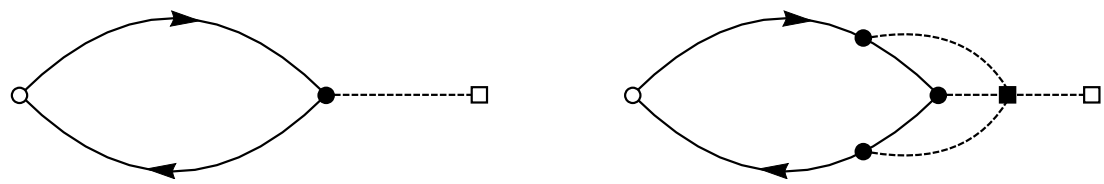

FIG. 2. The diagrams which renormalize the impurity interaction γ.

We now evaluate the diagrams in Fig. 2 using the Feynman rules specified above. There is only one loop diagram which corrects the tree-level interaction, but there are three distinct ways to evaluate the spin traces. We find

$$\begin{aligned}\mathcal{V}(x,\tau) = &\frac{S(S+1)}{3}\gamma_0 \int \frac{d^dk}{(2\pi)^d}\frac{e^{ikx}}{k^2} \\ &- \frac{S(S+1)}{3}\frac{\gamma_0^3 u_0}{18}\int \frac{d^dk}{(2\pi)^d}\frac{e^{ikx}}{k^2}\int \frac{d^dk_1}{(2\pi)^d}\int \frac{d^dk_2}{(2\pi)^d}\frac{2\mathcal{S}_1' + \mathcal{S}_2'}{k_1^2 k_2^2 (k+k_1+k_2)^2}\end{aligned} \tag{40}$$

where the spin traces $\mathcal{S}_i'$ are specified in Appendix A. Evaluating the divergent part of the integral,

$$\begin{aligned}\mathcal{V}(x,\tau) = &\frac{S(S+1)}{3}\int \frac{d^dk}{(2\pi)^d}\frac{e^{ikx}}{k^2}\Bigg[\gamma_0 \\ &- \gamma_0^3 u_0 \left(S(S+1) - \frac{1}{3}\right)\left(k^2\right)^{-\epsilon}\tilde{S}_{d+1}^2\left(\frac{2\pi^2}{15\epsilon} + \cdots\right)\Bigg]\end{aligned} \tag{41}$$

IV. RENORMALIZATION GROUP SUMMARY

The RG equations can be obtained directly from the Eqns. (37), (38), (41), along with the definitions of the renormalization constants in Section II. After some algebra, we obtain

$$\begin{aligned}Z' &= 1 - \frac{\gamma^2}{\epsilon} + \frac{1}{2\epsilon}\gamma^4 \\ Z_z &= 1 - \frac{2\gamma^2}{\epsilon} + \frac{1}{\epsilon^2}\gamma^4 \\ Z_\gamma &= 1 + \frac{2\pi^2\left[S(S+1) - \frac{1}{3}\right]}{15\epsilon} g\gamma^2\end{aligned} \tag{42}$$

The beta function now follows from Eq. (16):

$$\beta_\gamma = -\frac{\epsilon}{2}\gamma + \frac{1}{2}\gamma^3 - \frac{1}{2}\gamma^5 + \frac{(N+2)}{144}g^2\gamma + \frac{4\pi^2}{15}\left[S(S+1) - \frac{1}{3}\right]g\gamma^3 \tag{43}$$

Tuning the bulk interactions to their fixed point, $g = g^*$, we find a fixed point for the impurity interactions which is also perturbative in ϵ. To leading order,

$$\gamma^{*2} = \epsilon + \left[1 - \frac{N+2}{2(N+8)^2} - \frac{16\pi^2}{5(N+8)}\left(S(S+1) - \frac{1}{3}\right)\right]\epsilon^2 \tag{44}$$

Since our model is symmetric under $\gamma \to -\gamma$, all physical quantities only depend on γ^2. The initial flow depends on the sign of the bare value of γ_0, after which the theory will flow to either γ^* or $-\gamma^*$.

The anomalous dimensions of the spin operators follow from Eq. (18):

$$\eta' = \gamma^2 - \gamma^4 \tag{45}$$

$$\eta_z = 2\gamma^2 \tag{46}$$

where the $\mathcal{O}(\gamma^4)$ contribution to η_z vanishes. Evaluating these at $\gamma = \gamma^*$:

$$\eta' = \epsilon - \left(\frac{N+2}{2(N+8)^2} + \frac{16\pi^2}{5(N+8)}\left[S(S+1) - \frac{1}{3}\right]\right)\epsilon^2 \tag{47}$$

$$\eta_z = 2\epsilon + \left(2 - \frac{N+2}{(N+8)^2} - \frac{32\pi^2}{5(N+8)}\left[S(S+1) - \frac{1}{3}\right]\right)\epsilon^2 \tag{48}$$

As an aside, we mention the model with a Gaussian bulk, $g = 0$. This theory is infrared unstable to interactions, but the simple relation $Z_\gamma = 1$ allows us to derive an exact result for the anomalous dimension of the spin operators. Since the beta function for γ only depends on Z' in this theory, and $\beta_\gamma = 0$ at the interacting fixed point, Eqns. (16)-(18) imply

$$\eta' = \epsilon \quad \text{at} \quad g = 0 \tag{49}$$

to all orders in ϵ. In contrast, η_z will generically receive corrections at every order in ϵ at the Gaussian fixed point.

From Eqn. (21), we find the critical exponents

$$\nu' = 1 + \frac{\epsilon}{2} + \left(\frac{1}{4} - \frac{N+2}{4(N+8)^2} - \frac{8\pi^2}{5(N+8)}\left[S(S+1) - \frac{1}{3}\right]\right)\epsilon^2 \tag{50}$$

$$\nu_z = 1 + \epsilon + \left(2 - \frac{N+2}{2(N+8)^2} - \frac{16\pi^2}{5(N+8)}\left[S(S+1) - \frac{1}{3}\right]\right)\epsilon^2 \tag{51}$$

We now compare these to numerical results. For $N = 2$ and $S = 1/2$, we predict the critical exponents

$$\nu' \approx 1.08$$
$$\nu_z \approx 2.66 \tag{52}$$

In Refs 6 and 12, both the microscopic model of Eqn. (1) and the field theory model of Eqn. (refspincoup) were studied in numerical simulations. These authors claculated the above critical exponents to be

$$\nu' \approx 1.13(2)$$
$$\nu_z \approx 2.33(5) \tag{53}$$

The numerics show impressive agreement with the ϵ expansion.

V. COMPRESSIBILITY

In this section, we consider the finite-temperature response of the critical theory to an external probe coupled to the conserved $O(2)$ charge associated with particle number in the superfluid. Physically, this corresponds to the compressibility of the superfluid. We compute this by altering our Lagrangian,

$$\frac{1}{2}\int d^dx\left[(\partial_\tau\phi_1)^2+(\partial_\tau\phi_2)^2\right]\longrightarrow\frac{1}{2}\int d^dx\left[(\partial_\tau\phi_1+iH\phi_2)^2+(\partial_\tau\phi_2-iH\phi_1)^2\right]-H\hat{S}_z \tag{54}$$

and then taking variational derivatives of the free energy

$$\chi=\left.\frac{\delta^2\left(T\log Z\right)}{\delta H^2}\right|_{H=0} \tag{55}$$

Here, we will continue working with our generalized theory, Eq. (6), with $O(2)\times O(N-2)$ symmetry, where the probe field H couples to the $O(2)$ charge. The contribution of the bulk degrees of freedom to this quantity were computed in Ref. 17, so here we focus only on terms which depend on γ, and we denote this part of the compressibility by χ_{imp}. Because this is a correlation function of a conserved current, its scaling dimension cannot renormalize, so at finite temperature it must take the form

$$\chi_{\text{imp}}=\frac{\mathcal{C}_1}{T} \tag{56}$$

where $\mathcal{C}_1$ is a *universal* number. We can also interpret $\mathcal{C}_1 = S_{\text{eff}}(S_{\text{eff}}+1)/3$ as the "effective spin" in the presence of interactions with the bulk, since for $\gamma = 0$,

$$\chi_{\text{imp}}\Big|_{\gamma=0} = \frac{S(S+1)}{3T} \tag{57}$$

In our calculations at $T = 0$, we found that bulk interactions did not contribute to the impurity critical exponents until two-loop order. However, the structure of the ϵ-expansion for the bulk theory is rather different at finite temperature. In the critical regime, physical quantities become an expansion in $\sqrt{\epsilon}$ (with possible extra factors of $\ln\epsilon$) [17]. This dependence enters through the finite-temperature bosonic propagator, which is now given by

$$D_T(x,\tau) = T\sum_{i\omega_n}\int \frac{d^dk}{(2\pi)^d}\frac{e^{ikx}e^{-i\omega_n\tau}}{\omega_n^2+k^2+m^2} \tag{58}$$

with

$$m^2 = \left(\frac{N+2}{N+8}\right)\frac{2\pi^2T}{3}\epsilon \tag{59}$$

We will see that this leads to a $\sqrt{\epsilon}$-expansion for χ_{imp} as well.

Performing the functional derivative in Eq. (55), the compressibility is given by

$$\begin{aligned}\chi_{\text{imp}} = &\frac{1}{\beta}\int_0^\beta d\tau\int_0^\beta d\tau'\left\langle \hat{S}_z(\tau)\hat{S}_z(\tau')\right\rangle + \frac{1}{\beta}\int_0^\beta d\tau\int d^dx\ \left\langle\phi_{\alpha'}^2(\tau,x)\right\rangle\\ &-\frac{1}{\beta}\int_0^\beta d\tau\int_0^\beta d\tau'\int d^dx\int d^dx'\left\langle\left[\phi_2\partial_\tau\phi_1-\phi_1\partial_\tau\phi_2\right](\tau,x)\left[\phi_2\partial_{\tau'}\phi_1-\phi_1\partial_{\tau'}\phi_2\right](\tau',x')\right\rangle\\ &-\frac{2i}{\beta}\int_0^\beta d\tau\int_0^\beta d\tau'\int d^dx\left\langle\hat{S}_z(\tau)\left[\phi_2\partial_{\tau'}\phi_1-\phi_1\partial_{\tau'}\phi_2\right](\tau',x)\right\rangle\end{aligned} \tag{60}$$

These correlation functions can be computed using the same diagrammatic technique used in Section III, we simply do not take the zero temperature limit. A straight-forward computation leads to the expression

$$\chi_{\text{imp}} = \frac{S(S+1)}{3T}\left[1+\frac{\gamma_0^2}{2T}\int\frac{d^dk}{(2\pi)^d}\frac{\operatorname{csch}^2\left(\beta\sqrt{k^2+m^2}/2\right)}{k^2+m^2}\right] \tag{61}$$

Here we see why keeping the temperature-dependent mass in the bosonic propagator was crucial: for $m\to 0$ this expression in infrared singular, and an evaluation at finite m gives (at leading order)

$$\chi_{\text{imp}} = \frac{S(S+1)}{3T}\left[1+\gamma^2\frac{\pi}{\beta m}\right] \tag{62}$$

which lowers the order of the leading correction to

$$\chi_{\rm imp} = \frac{S(S+1)}{3T}\left[1 + \left(\frac{3(N+8)}{2(N+2)}\right)^{1/2}\sqrt{\epsilon}\right] \tag{63}$$

As has been seen in previous work on the finite temperature ϵ-expansion, the leading correction is not particularly small, so this may not give a good numerical estimate. For $S = 1/2$ and $N = 2$, we find

$$\mathcal{C}_1 \approx .734 \tag{64}$$

In Reference 12, the constant $\mathcal{C}_1$ is computed numerically in a finite volume geometry, with a result close to the free value. Due to finite size effects, their result cannot be directly compared to ours.

VI. CONCLUSIONS

Huang *et al.* [6] recently found a novel impurity quantum critical point in their study of the Bose-Hubbard model on the square lattice. They held the bulk square lattice at the superfluid-insulator quantum critical point, and then varied the strength of the trapping potential at a single site. They found a quantum phase transition, with a diverging length scale, at a critical value of the trapping potential where the impurity site occupation number jumped by unity.

In an earlier study of quantum antiferromagnets with SU(2) spin rotation symmetry, Ref. 9 examined impurities in dimerized, two-dimensional antiferromagnets at the bulk critical point point between a spin-gap state and Néel order described by the O(3) Wilson-Fisher conformal field theory. They found that impurities were universally characterized by a single spin quantum number, S, which specified a renormalization group fixed point with *no* relevant directions in the impurity field theory.

In this paper, we proposed that impurity criticality of the Bose-Hubbard model [6] is described by the $S = 1/2$ impurity fixed point found in Ref. 9, after the O(3) symmetry is reduced to O(2) in both the bulk and the impurity. We showed that with only O(2) symmetry, the impurity fixed point does allow for a *single* relevant perturbation in the impurity field theory: this relevant perturbation is associated with a longitudinal field acting on the $S = 1/2$ spin on the impurity site. We note that a model of $S = 1/2$ impurity has also been recently studied by Chen *et al.* [12]. With the presence of this relevant impurity

perturbation, we can understand the need for a critical trapping potential in the numerical study of Huang *et al.* [6].

We computed critical exponents and universal amplitudes associated with the O(2)-symmetric impurity fixed point in an expansion in $\epsilon = 3 - d$, where d is the bulk spatial dimensionality. Associated with two different relevant perturbations, we estimated from a computation to order ϵ^2 that the impurity length scale diverged with the exponents $\nu_z \approx 2.66$ and $\nu' \approx 1.08$; this compares well with the numerical results [6, 12] $\nu_z \approx 2.33$ and $\nu' \approx 1.13$. Additional tests of the ϵ-expansion results will be possible in further numerical studies.

Finally, we note that this novel impurity quantum criticality should be accessible in cold atom experiments, and we hope it will be studied in the near future.

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Appendix A: Spin traces

Here we tabulate spin traces. We give expressions in terms of the index $\mathcal{C}_S$ of the spin-S representation of $SU(2)$,

$$\mathcal{C}_S = \frac{1}{3}(2S+1)S(S+1) \tag{A1}$$

This is defined as the constant appearing in the bilinear trace

$$\mathrm{Tr}\left(\hat{S}_\alpha \hat{S}_\beta\right) = \mathcal{C}_S \delta_{\alpha\beta}, \tag{A2}$$

Below we give the relevant traces, where we distinguish $\sigma' = 1, 2$ from the $z = 3$ direction. These traces give zero if one replaces one of the two σ' indices with z.

At one-loop, we need the following traces:

$$
\begin{aligned}
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{\beta'}\right) &= \left[\frac{4}{5}S(S+1)-\frac{1}{10}\right]\mathcal{C}_S\delta_{\alpha'\beta'} = \mathcal{S}_1'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{z}\right) &= \left[\frac{2}{5}S(S+1)+\frac{1}{5}\right]\mathcal{C}_S = \mathcal{S}_1^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\beta'}\hat{S}_{\sigma'}\right) &= \left[\frac{4}{5}S(S+1)-\frac{3}{5}\right]\mathcal{C}_S\delta_{\alpha'\beta'} = \mathcal{S}_2'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{z}\hat{S}_{\sigma'}\right) &= \left[\frac{2}{5}S(S+1)-\frac{4}{5}\right]\mathcal{C}_S = \mathcal{S}_2^z\mathcal{C}_S
\end{aligned}
\tag{A3}
$$

At two-loop:

$$
\begin{aligned}
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\eta'}\hat{S}_{\beta'}\right) &= \frac{\mathcal{C}_S}{70}\left[48\ S^2(S+1)^2-6S(S+1)-5\right]\delta_{\alpha'\beta'} = \mathcal{S}_3'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\eta'}\hat{S}_{z}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2-S(S+1)+5\right] = \mathcal{S}_3^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\beta'}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{70}\left[48\ S^2(S+1)^2-48S(S+1)+9\right]\delta_{\alpha'\beta'} = \mathcal{S}_4'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{z}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2-15S(S+1)-2\right] = \mathcal{S}_4^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{\beta'}\hat{S}_{\eta'}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[24\ S^2(S+1)^2-17S(S+1)+8\right]\delta_{\alpha'\beta'} = \mathcal{S}_5'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\sigma'}\hat{S}_{z}\hat{S}_{\eta'}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2-S(S+1)+5\right] = \mathcal{S}_5^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\hat{S}_{\beta'}\right) &= \frac{\mathcal{C}_S}{35}\left[24\ S^2(S+1)^2-17S(S+1)+8\right]\delta_{\alpha'\beta'} = \mathcal{S}_6'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\hat{S}_{z}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2+27S(S+1)-16\right] = \mathcal{S}_6^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\beta'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\right) &= \frac{\mathcal{C}_S}{35}\left[24\ S^2(S+1)^2-38S(S+1)+15\right]\delta_{\alpha'\beta'} = \mathcal{S}_7'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{z}\hat{S}_{\eta'}\hat{S}_{\sigma'}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2-29S(S+1)+26\right] = \mathcal{S}_7^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\beta'}\right) &= \frac{\mathcal{C}_S}{70}\left[48\ S^2(S+1)^2-48S(S+1)+9\right]\delta_{\alpha'\beta'} = \mathcal{S}_8'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{z}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2+6S(S+1)-9\right] = \mathcal{S}_8^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\hat{S}_{\beta'}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[24\ S^2(S+1)^2-38S(S+1)+15\right]\delta_{\alpha'\beta'} = \mathcal{S}_9'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\sigma'}\hat{S}_{z}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2-22S(S+1)+12\right] = \mathcal{S}_9^z\mathcal{C}_S \\
\mathrm{Tr}\left(\hat{S}_{\alpha'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{\beta'}\hat{S}_{\sigma'}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[24\ S^2(S+1)^2-45S(S+1)+29\right]\delta_{\alpha'\beta'} = \mathcal{S}_{10}'\mathcal{C}_S\delta_{\alpha'\beta'} \\
\mathrm{Tr}\left(\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\eta'}\hat{S}_{z}\hat{S}_{\sigma'}\hat{S}_{\eta'}\right) &= \frac{\mathcal{C}_S}{35}\left[8\ S^2(S+1)^2-50S(S+1)+33\right] = \mathcal{S}_{10}^z\mathcal{C}_S
\end{aligned}
\tag{A4}
$$

Appendix B: Details of the two-loop calculation

In this appendix we detail some of the intermediate steps in the calculation of the two-loop contribution to the spin-spin correlation function quoted in Eqns. (37)-(38). The procedure proceeds in a very similar fashion to how the one-loop calculation is described in Section III A.

The relevant diagrams are pictured in Figures 3 and 4. Here, we have grouped the diagrams into three groups (a), (b), and (c). This is because, like the one-loop calculation in the main text, the three diagrams contributing to the denominator can be rewritten so that they are the sum of the diagrams in the numerator. Then we only need to compute the 15 diagrams which follow form the integrals pictured in Figure 3, while keeping track of the difference in spin traces between the numerator and denominator. In the $O(3)$ symmetric case considered in Reference 10, this resulted in large cancellations and only 7 diagrams need to be computed. In contrast, there are no cancellations here, and all 15 diagrams need to calculated.

We label the loop integrals which follow from Figure 3 as $\mathcal{I}_i$ for $i = 1, 2, ..., 15$, where we label the integrals from left-to-right and top-to-bottom according to the figure. In terms of these integrals, the two-loop contribution to $\mathcal{G}$ is

$$\begin{aligned}
\mathcal{G}^{(\text{two-loop})} = \frac{S(S+1)}{3}\gamma_0^4 \Bigg\{ & \left[\mathcal{S}_6 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_1 + \left[\mathcal{S}_4 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_2 \\
& + \left[\mathcal{S}_7 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_3 + \left[\mathcal{S}_4 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_4 \\
& + \left[\mathcal{S}_6 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_5 + \left[\mathcal{S}_3 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_6 \\
& + \left[\mathcal{S}_4 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_7 + \left[\mathcal{S}_5 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_8 \\
& + \left[\mathcal{S}_4 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_9 + \left[\mathcal{S}_3 - \frac{2S(S+1)}{3}\mathcal{S}_1'\right]\mathcal{I}_{10} \\
& + \left[\mathcal{S}_8 - \frac{2S(S+1)}{3}\mathcal{S}_2'\right]\mathcal{I}_{11} + \left[\mathcal{S}_8 - \frac{2S(S+1)}{3}\mathcal{S}_2'\right]\mathcal{I}_{12} \\
& + \left[\mathcal{S}_9 - \frac{2S(S+1)}{3}\mathcal{S}_2'\right]\mathcal{I}_{13} + \left[\mathcal{S}_9 - \frac{2S(S+1)}{3}\mathcal{S}_2'\right]\mathcal{I}_{14} \\
& + \left[\mathcal{S}_{10} - \frac{2S(S+1)}{3}\mathcal{S}_2'\right]\mathcal{I}_{15} \Bigg\}
\end{aligned} \tag{B1}$$

Within each bracket, the first spin sum is either $\mathcal{S}'$ or $\mathcal{S}^z$ depending on whether one wants

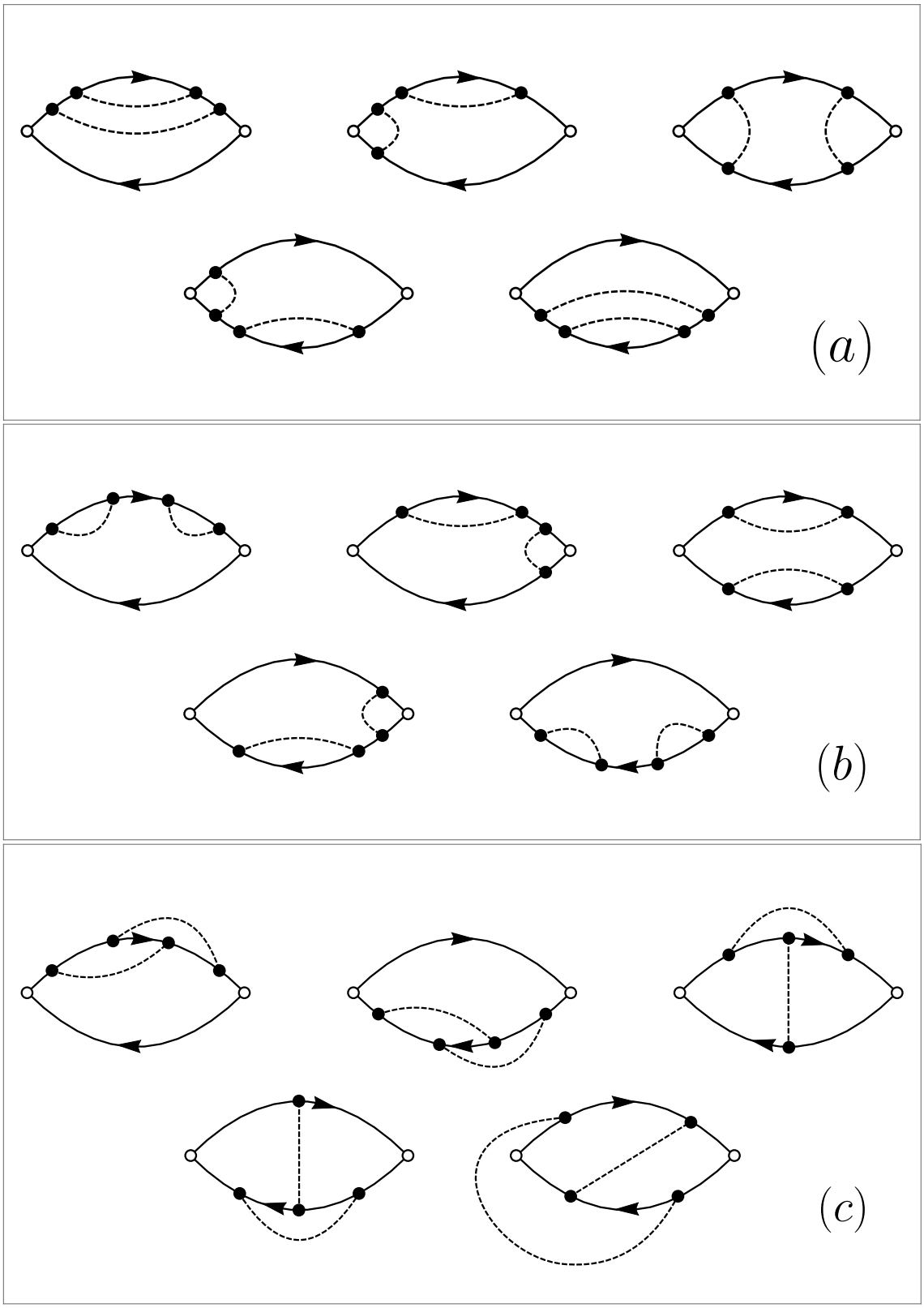

FIG. 3. The diagrams contributing to the numerator of the two-point function at two-loop.

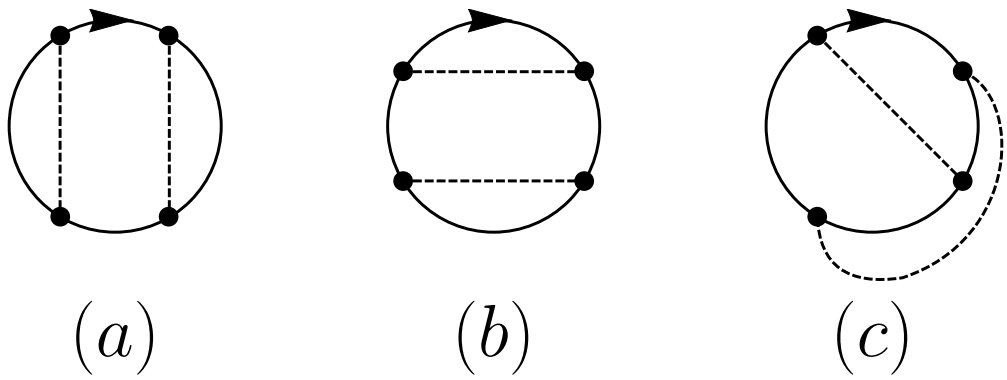

FIG. 4. The diagrams contributing to the denominator of the two-point function at two-loop.

the two point correlator $\mathcal{G}'$ or $\mathcal{G}^z$. We note that the denominator Z also contains an order γ_0^4 term from expanding the one-loop contribution to second order, but this contribution vanishes in dimensional regularization.

We now evaluate the 15 integrals above. Below, we will give the $T > 0$ integrals for each integral which follow from the diagrams in Fig. 3, and then state the evaluation of the divergent piece of the $T = 0$ limit. We take this limit according to the prescription described below Eq. 29 in the main text.

$$\begin{aligned}\mathcal{I}_1 &= \int_0^\tau d\tau_1 \int_{\tau_1}^\tau d\tau_2 \int_{\tau_1}^{\tau_2} d\tau_3 \int_{\tau_3}^{\tau_2} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4) \\ &\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{2\epsilon^2}+\frac{3}{2\epsilon}+\cdots\right) \end{aligned} \tag{B2}$$

$$\begin{aligned}\mathcal{I}_2 &= \int_0^\tau d\tau_1 \int_{\tau}^\beta d\tau_2 \int_{\tau_1}^{\tau} d\tau_3 \int_{\tau_3}^{\tau} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4) \\ &\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(-\frac{3}{2\epsilon^2}-\frac{3}{\epsilon}+\cdots\right) \end{aligned} \tag{B3}$$

$$\begin{aligned}\mathcal{I}_3 &= \int_0^\tau d\tau_1 \int_{\tau}^\beta d\tau_2 \int_{\tau_1}^{\tau} d\tau_3 \int_{\tau}^{\tau_2} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4) \\ &\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{2}{\epsilon^2}+\frac{3}{\epsilon}+\cdots\right) \end{aligned} \tag{B4}$$

$$\begin{aligned}\mathcal{I}_4 &= \int_0^\tau d\tau_1 \int_{\tau}^\beta d\tau_2 \int_{\tau}^{\tau_2} d\tau_3 \int_{\tau}^{\tau_3} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4) \\ &\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(-\frac{3}{2\epsilon^2}-\frac{3}{\epsilon}+\cdots\right) \end{aligned} \tag{B5}$$

$$\mathcal{I}_5 = \int_\tau^\beta d\tau_1 \int_\tau^{\tau_1} d\tau_2 \int_{\tau_2}^{\tau_1} d\tau_3 \int_{\tau_2}^{\tau_3} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{2\epsilon^2}+\frac{3}{2\epsilon}+\cdots\right) \tag{B6}$$

$$\mathcal{I}_6 = \int_0^\tau d\tau_1 \int_{\tau_1}^{\tau} d\tau_2 \int_{\tau_2}^{\tau} d\tau_3 \int_{\tau_3}^{\tau} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{\epsilon^2}+\frac{2}{\epsilon}+\cdots\right) \tag{B7}$$

$$\mathcal{I}_7 = \int_0^\tau d\tau_1 \int_{\tau_1}^{\tau} d\tau_2 \int_{\tau_2}^{\tau} d\tau_3 \int_{\tau}^{\beta} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(-\frac{3}{2\epsilon^2}-\frac{3}{\epsilon}+\cdots\right) \tag{B8}$$

$$\mathcal{I}_8 = \int_0^\tau d\tau_1 \int_{\tau_1}^{\tau} d\tau_2 \int_{\tau}^{\beta} d\tau_3 \int_{\tau_3}^{\beta} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{\epsilon^2}+\frac{2}{\epsilon}+\cdots\right) \tag{B9}$$

$$\mathcal{I}_9 = \int_0^\tau d\tau_1 \int_{\tau}^{\beta} d\tau_2 \int_{\tau_2}^{\beta} d\tau_3 \int_{\tau_3}^{\beta} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(-\frac{3}{2\epsilon^2}-\frac{3}{\epsilon}+\cdots\right) \tag{B10}$$

$$\mathcal{I}_{10} = \int_\tau^\beta d\tau_1 \int_{\tau_1}^{\beta} d\tau_2 \int_{\tau_2}^{\beta} d\tau_3 \int_{\tau_3}^{\beta} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{\epsilon^2}+\frac{2}{\epsilon}+\cdots\right) \tag{B11}$$

$$\mathcal{I}_{11} = \int_0^\tau d\tau_1 \int_{\tau_1}^{\tau} d\tau_2 \int_{\tau_1}^{\tau_2} d\tau_3 \int_{\tau_2}^{\tau} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(-\frac{1}{\epsilon^2}-\frac{5}{2\epsilon}\right) \tag{B12}$$

$$\mathcal{I}_{12} = \int_\tau^\beta d\tau_1 \int_{\tau}^{\tau_1} d\tau_2 \int_{\tau_2}^{\tau_1} d\tau_3 \int_{\tau}^{\tau_2} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(-\frac{1}{\epsilon^2}-\frac{5}{2\epsilon}\right) \tag{B13}$$

$$\mathcal{I}_{13} = \int_0^\tau d\tau_1 \int_\tau^\beta d\tau_2 \int_\tau^{\tau_2} d\tau_3 \int_{\tau_2}^\beta d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{\epsilon^2}+\frac{2}{\epsilon}+\cdots\right) \tag{B14}$$

$$\mathcal{I}_{14} = \int_0^\tau d\tau_1 \int_\tau^\beta d\tau_2 \int_0^{\tau_1} d\tau_3 \int_{\tau_1}^\tau d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{\epsilon^2}+\frac{2}{\epsilon}+\cdots\right) \tag{B15}$$

$$\mathcal{I}_{15} = \int_0^\tau d\tau_1 \int_\tau^\beta d\tau_2 \int_0^{\tau_1} d\tau_3 \int_\tau^{\tau_2} d\tau_4 D(\tau_1-\tau_2)D(\tau_3-\tau_4)$$
$$\overset{\beta\to\infty}{\Longrightarrow} \left(\tilde{S}_{d+1}\tau^\epsilon\right)^2 \left(\frac{1}{\epsilon}+\cdots\right) \tag{B16}$$

Plugging these values into Eq. (B1) and simplifying gives the full two-loop expression used in Eq. (38) in the main text.

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