

Schwinger-boson theory of the quantum XXZ model

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The quantum XXZ model is studied with the help of the Schwinger-boson formalism. The technique is particularly suited to describe the disordered state of low-dimensional quantum magnets. The Hubbard-Stratonovich transformation is employed to construct the saddle-point equations of the theory. The solution of these equations in one dimension yields the dependence of the Haldane gap as a function of the XY anisotropy.

I. INTRODUCTION

A paradigmatic model of quantum magnetism is the Heisenberg spin chain and its study has always been a prime testing ground for new concepts and for sharpening accepted understanding. Its study goes back at least to the remarkable exact solution of the spin one-half case by Bethe in 1931.¹ In the 1950's the spin-wave theory, developed primarily by Anderson² and Kubo,³ predicted for higher dimensional magnets the existence of an ordered ground state and gapless spin-wave excitations above it, the Goldstone modes. However, straightforward calculations revealed that in low dimensions the ordered ground state is destroyed by the spin waves, and genuinely new concepts are needed. The picture has been molded after the Bethe ansatz solution, assuming "quasi-long-range order," when there are gapless excitations in the system, even though the ground state does not support a true order parameter. Many analogous systems were identified, such as the one-dimensional quantum and two dimensional classical XY model with the Kosterlitz-Thouless phase and its countless realizations in different physical systems with the same $O(2)$ symmetry.

This widely accepted picture was shattered, when, in 1983, Haldane proposed that the integer and half-integer spin chains differ in a radical way. The above reasonings still hold for the half-integer case, but the integer chains were suggested to have a gap in the excitation spectrum.⁴ The proposal was based on advanced topological arguments, and immediately became the focus of both analytic and numerical attention. It took several years of hard numerical work to investigate this gap, as the convergence often was not fast enough, as some of the low-lying levels behaved in quite an unusual way.⁵ Eventually, however, agreement has been reached and now the existence of the gap in integer spin systems is generally accepted.

On the theoretical front our understanding improved considerably as well. The original argument for the existence of the gap made use of a large S mapping to the nonlinear σ model. The study of the topological terms strangely inverted the problem: In fact it was more straightforward to see the compelling evidence *in favor of the existence of the gap*, and nontrivial argu-

ments were needed to show its absence for half-integer spin chains.⁴ Later it was shown that the celebrated Lieb-Shultz-Mattis theorem,⁶ which clearly established the nonexistence of a gap in $S = 1/2$ chains (for a non-degenerate ground state), fails for integer spins.⁷

Additional light was shed on the physics of the Haldane phase with the introduction of several exactly solvable models, such as the Affleck-Kennedy-Lieb-Tasaki (AKLT) model, which is the Heisenberg Hamiltonian with an additional biquadratic term.⁸ In these models it was possible to write down the ground state wave functions exactly.⁹ These are typically different valence bond states with the spin rotational symmetry preserved. The Haldane gap was shown to persist in a finite region around the Heisenberg point.⁸ Hence it has been argued that these valence bond states can be smoothly deformed by adiabatic continuation into the Heisenberg ground state; thus they grasp the physics of the Heisenberg chain correctly.^{8,10} Considerable work went into studying the states at the ends of the finite length chains. These states held new surprises, as their quantum numbers were identified to be $S = 1/2$.¹¹ The recent development in the field has been the construction of a stringlike order parameter for the Haldane phase.^{12,13} Its existence has now been numerically confirmed as well.^{14,25}

Finally all these exotic studies have been put to the experimental test in the quasi-one-dimensional systems of CsNiCl_3 , $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4$, and most recently Y_2NiBaO_5 . The detailed analysis of the neutron scattering data yielded a quantitative agreement with predictions of the theory. In particular the existence of the gap,¹⁵ the shape of the excitation spectrum, and the exotic quantum numbers of the end states have been confirmed.¹⁶

Given the complexity of the problem it is not surprising that it proved to be relatively hard to develop a simple formalism which would grasp the essentials of the physics and yet would be transparent enough for wider applications. An important step towards such a description of the Haldane phase came with realization by Arovas, Auerbach, and Haldane that the exact ground state of the AKLT model⁸ could be expressed simply in terms of the Schwinger bosons.¹⁰ Subsequently Arovas and Auerbach developed a powerful mean field theory based on the

Schwinger-boson formulation to describe broad classes of low-dimensional quantum magnets.¹⁷ This technique provides a useful starting point to characterize spin-liquid and valence bond states as the nonvanishing expectation value of the mean field is attributed to a *bond variable*, representing the short-range correlations of the system without assuming long-range order. As these bond correlations were argued to be essential for the understanding of the Haldane phase,^{10,9} and by virtue of the above adiabatic connection between the AKLT model and the Heisenberg chain, this simple formalism is indeed suited to capture the essential physics of the Haldane phase, in particular the existence of the gap. However, while several generalizations of the Heisenberg model have been studied by other means, the Schwinger-boson technique has not yet been applied away from the spin-isotropic point. This is what we set out to do in the present paper.

In Sec. II we develop the formalism for arbitrary dimensions, Sec. III then gives the specific results for the case of one dimension, and in Sec. IV we summarize our results. The Appendix provides the calculational details.

II. FORMALISM

The generalized XXZ model is given by the Hamiltonian:

$$H = \sum_{\langle i,j \rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z, \quad (1)$$

where $\Delta = -1$ represents the case of the ferromagnet and $\Delta = 1$ characterizes that of the antiferromagnet. As stated in the Introduction one of our chief goals is to capture the Haldane gap of the XXZ model in one dimension. The Schwinger-boson (SB) approach allows for a large N generalization and a consequent, well-controlled $1/N$ expansion at the spin-isotropic point.¹⁷ Away from this point the symmetry reduces to $U(1) \times Z(2)$. Unfortunately the Schwinger bosons are not a useful tool in representing the $U(1)$ symmetry, as can be seen by direct inspection. Thus no attempt was made to develop a $U(N) \times Z(2)$ type generalization of the model. On the other hand the SB's provide a very natural representation of the spin operators, which remains useful away from isotropy. For these two reasons we choose to retain

the original Schwinger representation of the spin operators, and we work explicitly on the $SU(2)$ level.

In the Schwinger-boson approach one introduces two boson fields, a and b , which obey the typical Bose commutation rules $[a_i, a_j^\dagger] = \delta_{ij}$ and $[a_i, b_j^\dagger] = 0$ with the constraint that only $2S$ bosons can occupy each site, $a_i^\dagger a_i + b_i^\dagger b_i = 2S$. Here S is the representation label of the spin algebra. The spin operators are given in terms of the SB's as $S_i^+ = a_i^\dagger b_i$ and $S_i^z = 1/2(a_i^\dagger a_i - b_i^\dagger b_i)$. The generalized XXZ Hamiltonian in terms of these operators then takes the form

$$H = -1/2 \sum_{\langle i,j \rangle} \left[(a_i^\dagger b_j^\dagger a_j b_i + \text{H.c.}) - \Delta (a_i^\dagger a_j^\dagger a_i a_j + b_i^\dagger b_j^\dagger b_i b_j) \right], \quad (2)$$

where we performed a rotation about the z axis on one of the sublattices, assuming a bipartite lattice. Next, in order to introduce a Hubbard-Stratonovich transformation one rewrites the Hamiltonian in terms of two bond variables:

$$H = -\frac{1}{4} \sum_{\langle i,j \rangle} (1 - \Delta) : \mathbf{A}_{ij}^\dagger \mathbf{A}_{ij} : + (1 + \Delta) : \mathbf{B}_{ij}^\dagger \mathbf{B}_{ij} : , \quad (3)$$

where

$$\mathbf{A}_{ij} = (a_i^\dagger a_j + b_i^\dagger b_j), \quad \mathbf{B}_{ij} = (a_i b_j + b_i a_j), \quad (4)$$

and the colons represent normal ordering. One more bond decoupling is conceivable besides the two shown above; however, it generates additional terms, which are not present in the original Hamiltonian. Site decouplings were not considered, as they describe a state with long-range order, clearly an unwanted proposition in low dimensions. The two fields chosen are also the ones which arise naturally in the case of the isotropic ferromagnet and antiferromagnet;¹⁷ thus one expects our formulation to interpolate smoothly between these two known limits.

Switching to a path integral representation, we perform Hubbard-Stratonovich transformations using the complex bond variables A_{ij} and B_{ij} to express the partition function Z as

$$Z = \int \mathbf{D}[a, b, A, B; \lambda] \exp^{-S[a, b, A, B; \lambda]}, \quad (5)$$

where S is given as

$$\begin{aligned} S = & \int_0^\beta d\tau \frac{1}{2} [a(\tau)_i^\dagger \partial_\tau a(\tau)_i - \partial_\tau a(\tau)_i^\dagger a(\tau) + b(\tau)_i^\dagger \partial_\tau b(\tau) - \partial_\tau b(\tau)_i^\dagger b(\tau)] \\ & + \frac{4}{(1 - \Delta)} \sum_{\langle i,j \rangle} A_{ij}^\dagger A_{ij} + \frac{4}{(1 + \Delta)} \sum_{\langle i,j \rangle} B_{ij}^\dagger B_{ij} + \sum_{\langle i,j \rangle} (A_{ij}^\dagger \mathbf{A}_{ij} + \mathbf{A}_{ij}^\dagger A_{ij} + B_{ij}^\dagger \mathbf{B}_{ij} + \mathbf{B}_{ij}^\dagger B_{ij}) \\ & + \sum_i \lambda_i (a_i^\dagger a_i + b_i^\dagger b_i - 2S). \end{aligned} \quad (6)$$

The constraint on the number of bosons is enforced by the field λ_i separately at each site, with the corresponding integral running along the imaginary axis, from $-i\infty$ to $+i\infty$. We proceed by developing a mean field approximation for this so far exact equation by choosing A_{ij} ,

B_{ij} , and λ_i to be static and assume the spatially uniform values A , B , and λ , respectively. These values are subsequently determined self-consistently in the steepest descent approximation. Converting to Fourier space the mean field (MF) Hamiltonian takes the form

$$H_{\text{MF}} = \frac{2}{(1-\Delta)} A^2 z + \frac{2}{(1+\Delta)} B^2 z - N 2 S \lambda + \frac{1}{2} \sum_{\mathbf{k}} \left[(\gamma_{\mathbf{k}} A z + \lambda) (a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}) + \gamma_{\mathbf{k}} B z (a_{\mathbf{k}} b_{-\mathbf{k}} + a_{-\mathbf{k}} b_{\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger) \right], \quad (7)$$

where z is the coordination number, and $\gamma_{\mathbf{k}} g = \frac{1}{z} \sum_{\delta} e^{i\mathbf{k} \cdot \delta}$, with δ indexing the nearest neighbors. We explicitly verified that the mean field Hamiltonian retains the original $U(1)$ symmetry [$a \rightarrow \exp(i\phi/2) a$; $b \rightarrow \exp(-i\phi/2) b$, sending $S^+ \rightarrow \exp(i\phi) S^+$; $S^- \rightarrow \exp(-i\phi) S^-$] by calculating the commutator of the Hamiltonian with the generator of global rotations about the z axis. This is the main advantage of the present formulation over spin-wave-based approaches, as those break this XY rotational symmetry, leading to the appearance of a spurious Goldstone mode. This of course obliterates any trace of the Haldane gap. To capture the gap one typically employs a mapping to the nonlinear σ model and performs a renormalization group analysis.^{4,9}

We now proceed to determine the spectrum of the Hamiltonian by using the Bogoliubov transformation. One introduces the mutually independent quasiparticle operators

$$\alpha_{\mathbf{k}} g = (u_{\mathbf{k}} a_{\mathbf{k}}^\dagger + v_{\mathbf{k}} b_{-\mathbf{k}}), \quad \beta_{\mathbf{k}} g = (v_{\mathbf{k}} a_{\mathbf{k}}^\dagger + u_{\mathbf{k}} b_{-\mathbf{k}}), \quad (8)$$

such that

$$[\alpha_{\mathbf{k}'}, \alpha_{\mathbf{k}} g^\dagger] = \delta_{\mathbf{k}, \mathbf{k}'}, \quad [\beta_{\mathbf{k}'}, \beta_{\mathbf{k}} g^\dagger] = \delta_{\mathbf{k}, \mathbf{k}'}, \quad [\alpha_{\mathbf{k}'}, \beta_{\mathbf{k}} g^\dagger] = 0, \quad (9)$$

where

$$u_{\mathbf{k}} g = \frac{1}{2\omega_{\mathbf{k}}} (\lambda + \gamma_{\mathbf{k}} g A z + \omega_{\mathbf{k}})^{\frac{1}{2}}, \quad (10)$$

$$v_{\mathbf{k}} g = \frac{1}{2\omega_{\mathbf{k}}} (\lambda + \gamma_{\mathbf{k}} g A z - \omega_{\mathbf{k}})^{\frac{1}{2}}.$$

The Bogoliubov transformation determines the dispersion relation, and we find that $\omega_{\mathbf{k}} g$ is given by

$$\omega_{\mathbf{k}} g = [(\lambda + A z \gamma_{\mathbf{k}})^2 - (B z \gamma_{\mathbf{k}} g)^2]^{\frac{1}{2}}. \quad (11)$$

The frequency summation yields the mean field free energy, which can be expressed in terms of these variables as

$$f_{\text{MF}} = \frac{F_{\text{MF}}}{N} = \frac{1}{(1-\Delta)} A^2 z + \frac{1}{(1+\Delta)} B^2 z - (S + \frac{1}{2}) \lambda - \frac{A z}{2} \frac{1}{N} \sum_{\mathbf{k}} g \gamma_{\mathbf{k}} + \frac{1}{\beta} \frac{1}{N} \sum_{\mathbf{k}} g \ln(1 - e^{-\beta \omega_{\mathbf{k}}}) + \frac{1}{2} \frac{1}{N} \sum_{\mathbf{k}} g \omega_{\mathbf{k}}, \quad (12)$$

where N is the number of lattice sites.

The steepest descent equations are constructed from the extremum conditions of the mean field free energy f_{MF} with respect to the MF parameters, i.e., $\frac{\delta F}{\delta A} = \frac{\delta F}{\delta B} = \frac{\delta F}{\delta \lambda} = 0$:

$$A = \frac{(1-\Delta)}{2} \sum_{\mathbf{k}} g \left[1 - \frac{\lambda + A z \gamma_{\mathbf{k}} g}{\omega_{\mathbf{k}}} \coth \frac{1}{2} \beta \omega_{\mathbf{k}} \right] \frac{\gamma_{\mathbf{k}} g}{2},$$

$$\frac{2}{z} = \frac{(1+\Delta)}{2} \sum_{\mathbf{k}} g \frac{\gamma_{\mathbf{k}} g^2}{\omega_{\mathbf{k}}} \coth \frac{1}{2} \beta \omega_{\mathbf{k}},$$

$$\frac{(S+1)}{2} = \frac{1}{2} \sum_{\mathbf{k}} g \frac{\lambda + A z \gamma_{\mathbf{k}} g}{\omega_{\mathbf{k}}} \coth \frac{1}{2} \beta \omega_{\mathbf{k}}. \quad (13)$$

It is reassuring to note at this point that the mean field equations for the Heisenberg ferromagnet and antiferromagnet, derived by Arovass and Auerbach, can be attained from our formulas by setting A or B to zero, respectively.¹⁷ We now explore the solutions of these mean field equations in one dimension.

III. ONE DIMENSION

Here we solve the saddle-point equations for the $S = 1$ linear chain at $T = 0$ for values of the anisotropy parameter between $\Delta = -1$ and 1 . Changing our sums to integrals, the saddle-point equations and mean field free energy can be evaluated exactly. The mean field equations can then be expressed in terms of known elliptic functions. The details of these equations are given in the Appendix. At this point it is convenient to reexpress the formulas in terms of the reduced variables η_a and η_b , defined in terms of the original variables such that

$$\eta_a = \frac{(A+B)z}{\lambda}, \quad \eta_b = \frac{(A-B)z}{\lambda}. \quad (14)$$

The mean field equations can then be manipulated so that λ is expressed as an explicit function of η_a and η_b . Now Eqs. (13) are solved for the variable λ . Using this solution λ can then be replaced in $f_{\text{MF}}(\lambda, \eta_a, \eta_b)$, making the free energy a function of η_a and η_b only. In terms of these variables the solution of the mean field equations is no longer a saddle point of the free energy, but rather is the minima of $f_{\text{MF}}(\eta_a, \eta_b)$.

This minimum of the free energy is determined by a numerical minima searching routine. The relevant regime is the square $(-1, 1; -1, 1)$ in the η_a, η_b space. The routine employed starts with three points in the (η_a, η_b) space, and moves towards the minima of the free energy surface, converging with accuracy depending on comparative values of f_{MF} . The minimum generated by this method was then double-checked against the original saddle-point equations, determining whether they were actual solutions. We chose this method over the iterative solution of the three coupled saddle-point equations, because it was far less time consuming and free of numerical instabilities. These instabilities come about because of the unusually flat bottom of the free energy surface in the

parameter space. In Fig. 1 we display the solutions to the mean field parameters A and B as functions of the anisotropy. Having determined the location of the saddle point, the gap is subsequently evaluated as a function of the anisotropy. The result is displayed in Fig. 2.

Here a remark is in order. The quantum number of the Schwinger bosons is $S = 1/2$, whereas the true low-lying excitations above the singlet ground state are expected to be triplets on simple physical grounds; i.e., the corresponding quantum number should be $S = 1$. The present technique is expected to capture this feature by binding together two of the $S=1/2$ excitations. As on the mean field level there is no interaction left among the quasi-particles, this binding will be driven by the fluctuations around the mean field, i.e., the $1/N$ type corrections, as has been shown by Read and Sachdev.¹⁸ Clearly then a gap in the true spectrum will be approximately twice the mean field gap of our model.

The value of the gap is obtained at the spin-isotropic antiferromagnetic (AFM) point as $E_{\text{gap}} \approx 0.17$. This is considerably off the best numerical estimate of $E_{\text{gap}} \approx 0.40$.⁵ This difference is not surprising, given that we are applying a mean field approximation in a low dimension. However, the large S asymptotics $E_{\text{gap}} \sim S \exp(-\pi S)$ of the gap is close to that predicted from the nonlinear σ model: $E_{\text{gap}} \sim S^2 \exp(-\pi S)$, a remarkable result.¹⁷ Instead of high numerical accuracy, the main advantage of using Schwinger bosons is in providing a simple and useful formulation of the Haldane problem for the XXZ model, which then can directly be generalized for more challenging problems, such as the case of the doped Haldane chain¹⁹ and the disordered spin chains.²⁰ This formulation is also expected to determine the tendencies of the physical quantities at least at the qualitative level. For instance, the precipitous drop of the gap for anisotropies just slightly less than 1 is rather unexpected. In the field theoretical formulation there is no compelling

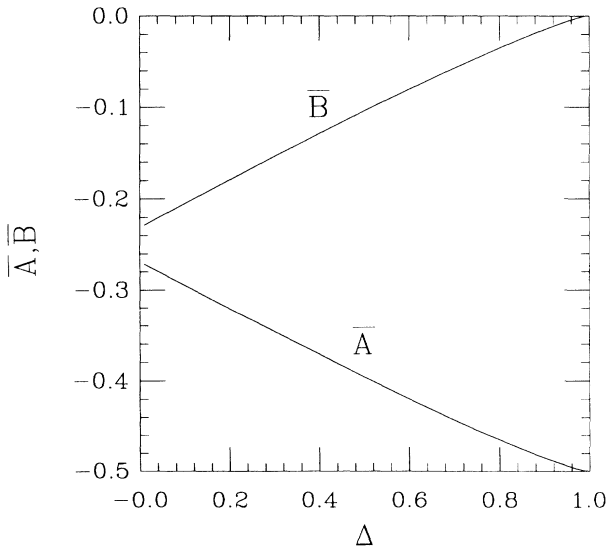


FIG. 1. The values of the normalized mean field parameters are plotted as a function of the anisotropy ($\bar{A} = A/\lambda$, $\bar{B} = B/\lambda$).

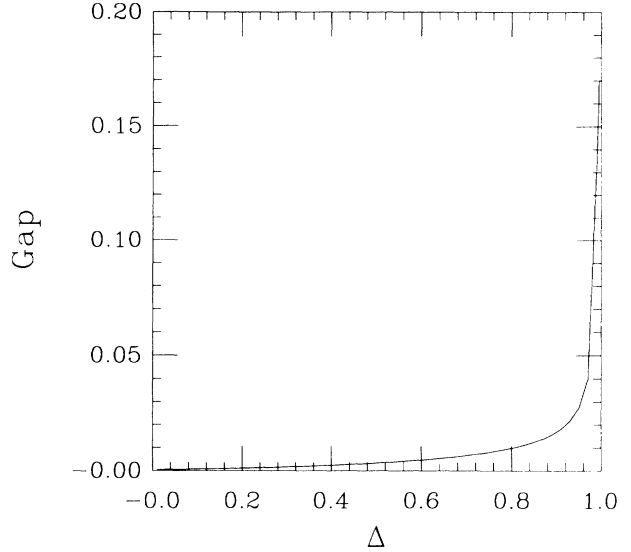


FIG. 2. The gap of the excitation spectrum is shown as a function of the spin anisotropy, Δ .

reason for such behavior; thus our result calls out for further physical understanding.

We are unaware of any published numerical work exploring the value of the gap in the XY region $|\Delta| < 1$. We find that the gap persists well into this regime. Analytic considerations expect the gap to disappear at the XY point ($\Delta = 0$). The structure of the saddle-point equations prevents the vanishing of the gap at the XY point. However, we find that the gap is indeed very small there: $E_{\text{gap}} \approx 0.0004$. Here we remark that the extreme small size of the gap in much of the anisotropic region might be the reason why it proved to be difficult to numerically determine its value and also the location of the boundary of the Haldane phase.

It should be noted that the Schwinger-boson mean field theory, as developed here, can be extended to higher dimensions. For the case of two dimensions at $T = 0$, the mean field equations are not analytically integrable. Furthermore, the mean field equations have no solution for low values of S . However, this can be remedied through the introduction of a condensate term when changing from sums to integrals, as was done at the ferro- and antiferromagnetic points.^{21,22} The introduction of such a condensate term in the free energy produces the expected spin-wave results for the excitation spectrum.

IV. DISCUSSION AND SUMMARY

In this paper we developed the Schwinger-boson description of the XXZ model. We constructed the most general, spin-rotationally invariant bond decoupling scheme and employed the Hubbard-Stratonovich transformation. The excitation spectrum has been determined in the mean field approximation. The gap is calculated by numerical study of the free energy minima in the whole range of the spin anisotropy. The spectrum clearly exhibits the Haldane gap in the antiferromagnetic regime.

At the Heisenberg point we obtain $E_{\text{gap}} \approx 0.17$, whereas the best numerical estimate is $E_{\text{gap}} \approx 0.40$. The difference is not unexpected, given that we are applying a mean field approximation in a low dimension. The analytic form of the gap in the large S limit is analogous to the form obtained from the nonlinear σ model. However, the precipitous drop of the gap for values of the anisotropy less than 1 is unexpected on field theoretical grounds; thus our result invites further physical understanding. Analytically the gap is expected to disappear at the XY point ($\Delta = 0$). For comparison we obtain $E_{\text{gap}} \approx 0.0004$.

We conclude that the Schwinger-boson-based mean field formalism offers a technically simple, easy-to-generalize, qualitatively satisfying approach to the one-dimensional XXZ model. It also provides a formal basis for the valence bond picture for the ground state, which has been suggested on more intuitive grounds before.

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APPENDIX

In this appendix we carry out the integrations explicitly for the mean field free energy and of the saddle-point equations for the linear chain at $T = 0$. We work in terms

of the reduced variables η_a and η_b and write

$$f_{\text{MF}} = \frac{1}{(1 - \Delta^2)} \frac{\lambda^2}{4} (\eta_a^2 + \eta_b^2) + \frac{\Delta}{(1 - \Delta^2)} \frac{\lambda^2}{2} \eta_a \eta_b - (S + \frac{1}{2})\lambda + \frac{\lambda}{2} \int \frac{dk}{(2\pi)} \frac{1}{\omega'_k} \quad (\text{A1})$$

and

$$\begin{aligned} \lambda &= -(1 - \Delta) \int \frac{dk}{(2\pi)} \frac{\left(\frac{1}{(\eta_a + \eta_b)} - \frac{\gamma_k}{2}\right) \gamma_k}{\omega'_k}, \\ \lambda &= \frac{(1 + \Delta)}{2} \int \frac{dk}{(2\pi)} \frac{\gamma_k^2}{\omega'_k}, \\ S + \frac{1}{2} &= \frac{1}{2} \int \frac{dk}{(2\pi)} \frac{1}{\omega'_k} + \frac{1}{4} (\eta_a + \eta_b) \int \frac{dk}{(2\pi)} \frac{\gamma_k}{\omega'_k}, \end{aligned} \quad (\text{A2})$$

where $\eta_a = \frac{(A+B)z}{\lambda}$, $\eta_b = \frac{(A-B)z}{\lambda}$, and $\omega'_k = \omega_k/\lambda = [(1 + \eta_a \gamma_k)(1 + \eta_b \gamma_k)]^{\frac{1}{2}}$. The integral that appears in the mean field equation is of the form

$$I = \int \frac{dk}{2\pi} \omega'_k, \quad (\text{A3})$$

while the integrals appearing in the saddle-point equations are all of the form

$$I_n = \int \frac{dk}{2\pi} \frac{\gamma_k^n}{\omega'_k}, \quad (\text{A4})$$

where $n = 0, 1$, or 2 .

These integrals are given in Ref. 23, and can be expressed with the help of the elliptic functions as

$$I = \frac{2}{\pi} [(1 + \eta_a)(1 - \eta_b)]^{-\frac{1}{2}} \left[E(k) + \frac{(1 - \eta_a)}{(1 - \eta_b)} \frac{\eta_b}{\eta_a} [\Pi(\alpha^2, k) - K(k)] + \frac{(1 - \eta_a)}{(1 + \eta_a)} \Pi(\alpha^2, k) \right] \quad (\text{A5})$$

and

$$I_0 = \frac{2}{\pi} [(1 + \eta_a)(1 - \eta_b)]^{-\frac{1}{2}} K(k), \quad (\text{A6})$$

$$I_1 = -\frac{2}{\pi} [(1 + \eta_a)(1 - \eta_b)]^{-\frac{1}{2}} \frac{1}{\alpha^2} [(\alpha^2 - \alpha_1^2) \Pi(\alpha^2, k) + \alpha_1^2 K(k)], \quad (\text{A7})$$

$$I_2 = \frac{2}{\pi} [(1 + \eta_a)(1 - \eta_b)]^{-\frac{1}{2}} \frac{1}{\alpha^4} [\alpha_1^4 K(k) + 2\alpha_1^2 (\alpha^2 - \alpha_1^2) \Pi(\alpha^2, k) + (\alpha^2 - \alpha_1^2)^2 V_1], \quad (\text{A8})$$

where

$$V_1 = \frac{1}{2(\alpha^2 - 1)(k^2 - \alpha^2)} [\alpha^2 E(k) + (k^2 - \alpha^2) K(k) + (2\alpha^2 k^2 + 2\alpha^2 - \alpha^4 - 3k^2 \alpha^2) \Pi(\alpha^2, k)] \quad (\text{A9})$$

and the variables α_1 and α are given by

$$\begin{aligned} \alpha^2 &= \frac{2\eta_a}{1 + \eta_a}, \quad \alpha_1^2 = \frac{2}{1 + \eta_a}, \\ k^2 &= \alpha^2 \left(\frac{\frac{1}{\eta_b} - \frac{1}{\eta_a}}{\frac{1}{\eta_b} - 1} \right), \end{aligned} \quad (\text{A10})$$

and K , E , and Π are the complete elliptic integrals of the first, second, and third kinds, respectively. The numerical routines used for determining the values of elliptical integrals were taken from Ref. 24. These functions, evaluated with these routines, are then used in the search for the minima of the free energy, as explained in the text.

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