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Ground State of a Spin-Phonon System. I. Variational Estimates

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A study is made of the ground-state energy of a spin-one-half particle in a field B and interacting with a phonon bath. The infrared-sensitive case of acoustic phonons with point coupling in three dimensions is characterized by two parameters, a coupling constant α and B. Units are used where the high-momentum phonon cutoff is unity. There is a curve $\alpha(B)$ separating a symmetry-breaking region with a long-range phonon field from a normal region. Two simple, well-known, approximations are compared. The source theory yields discontinuities in the first derivatives of the energy with respect to B and α when $B > e^{-1}$ and an infinite-order transition when $B < e^{-1}$, but is trivial in the large-α region. The classical theory yields discontinuities in the second derivatives but is trivial in the small-α region. An improved variationally fixed ground-state wave function is analyzed. It gives a new $\alpha(B)$ curve with an infinite-order transition with continuous energy derivatives when $B < e/(e^2 - 1/4)$ and with discontinuous derivatives when B is larger than this value. It is nontrivial in the entire $\alpha(B)$ plane. The crossover to classical behavior occurs near $\alpha = 1/2$ for $B \ll 1$. But the wave function does not describe quantum fluctuations in the large-α phase. A second way of combining source and classical effects is described. It yields a second-order transition (near $\alpha = 1/2$ for $B \ll 1$) everywhere. These theories are special cases of a symmetry-breaking transformation together with a one-mode treatment of quantum fluctuations. The transition is viewed in terms of a single mode with a variable length, coupled dynamically to the spin.

KEY WORDS: Spin phonon transition; Spin phonon ground state.

1. INTODUCTION

A two-level system coupled to a boson field can be used to describe processes in quantum optics, condensed matter physics, chemical physics, meson theory, etc. A spin-1/2 description may be used for the two-level

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system and the unperturbed spin Hamiltonian is $-\frac{1}{2}B\sigma_z$. The boson field $\phi(x)$ is characterized by a spectrum $\omega(k)$. The coupling to the spin is proportional to σ_x and to the field $\phi(x)$ with a form factor $D(x)$. The interaction consists of a spin flip together with emission or absorption of a boson.

In the case of optical modes where $\omega(k)$ is a constant, independent of k, the problem is soluble. The boson field can be described in terms of modes, chosen so that the spin is coupled to a single mode. The exact eigenfunctions and eigenvalues may be determined by solving a three-term recurrence relation numerically to any desired accuracy. As a consequence, one can determine the thermodynamics and response functions. However, energy conservation forbids irreversible decay of the spin from the excited state.

With a more general $\omega(k)$, irreversible decay is permitted, and one is interested in the properties as a function of B and a coupling constant α. The response functions have been studied intensively in the past decade by a large number of analytic approaches. Path integral techniques have been particularly successful. The subject is extensively reviewed in the article by Leggett *et al.*[1] The case of an acoustic spectrum $\omega(k) = c|k|$ is especially subtle and challenging. In three dimensions with a point coupling $D(\mathbf{x}) - \delta(\mathbf{x})$, the field $\phi(\mathbf{x})$ has a $1/|x|$ behavior when couplied to a fixed source. The energy is finite, but there is an infinite number of quanta, i.e., an infrared divergence connected with the $1/|x|$ dependence. On the other hand, if recoil of the source is included and the problem is treated by perturbation theory, the divergence disappears. The present paper focuses on this case and examines the behavior of the grund-state energy E as a function of the coupling constant α and of the magnetic field B.

The crudest approximations indicate that there is a curve $\alpha(B)$ such that on one side ϕ has the $1/|x|$ behavior and on the other a shorter range behavior. Two such approximations are reviewed in Section 3. One is a variational extension of the source-type solution. It has the property that $\partial E/\partial B$ at fixed α and $\partial E/\partial \alpha$ at fixed B have discontinuities across the $\alpha(B)$ line when $B > e^{-1}$. For $B < e^{-1}$ there is a very soft infinite-order transition. The second is a semiclassical theory based on introducing a symmetry-breaking mean value for the boson field. The $\alpha(B)$ curve is very different, but $(\partial^2 E/\partial B^2)_\alpha$ and $(\partial^2 E/\partial \alpha^2)_B$ exhibit discontinuities. The magnitude of the long-range symmetry-breaking field tends to zero as one approaches the line. The two approximations are compared in Section 4 by matching energies. This leads to a new $\alpha(B)$ line, which now has a first-order transition. I define a first-order transition as one where the first derivatives of energy jump. The theories are nontrivial in the entire $\alpha(B)$ plane.

The existence of the $\alpha(B)$ line has been discussed from a more rigorous point of view by Spohn and Dumcke.[2] They use a functional integral formulation and relate the problem to the one-dimensional Ising model with long-range interactions.

The problem has been discussed by many people using different approaches. The $B \ll 1$ region has been treated by Emery and Luther,[3] Chakravarty,[4] Silbey and Harris,[5] Tanaka and Sakurai,[6] and Prelovsek.[7] The $B \gg 1$ region has been studied by an equation of motion technique by Beck *et al.*[8] and Prelovsek.[7] However, it appears to us that neither the position of the $\alpha(B)$ line nor the behavior of the derivatives of the energy at the line have been definitively established. There is disagreement about whether the transition occurs near $\alpha = 1/2$ or $\alpha = 1$ for $B \ll 1$ and there is disagreement as to whether the transition is first order or second order for $B \gg 1$.

It is not easy to compare the theories, since they are based on different formalisms. The present approach is to start with simple ground-state wave functions which correspond to some of the theories. I then enrich the functions so as to incorporate physical effects that are neglected or treated inadequately. In particular, one must pay attention to multiquanta effects in the transition to classical behavior and must treat quantum fluctuation effects equally accurately in both normal and broken symmetry phases. What emerges is that the crossover to classical behavior is near $\alpha = 1/2$ when $B \ll 1$. If there is a phase transition, it is very soft, with all finite derivatives continuous and occurring near $\alpha = 1$. In fact, in a separate paper I treat the $B \ll 1$ limit rigorously by another method. I show that there is no transition to order B^2 in the energy. I will also treat the $B \gg 1$ limit rigorously and show that the transition is first order.

My concern in this paper is with theories which give $E(\alpha, B)$ over the entire (α, B) plane, and to make clear the physical effects that play a role.

In Section 5 I examine one wave function with parameters that can be chosen to reduce to the classical and modified source parameters. It is superior to both and shows a continuous crossover to classical behavior near $\alpha = 1/2$ $(B \ll 1)$. There is a transition near $\alpha = 1$ similar to that of the source theory. For $B < B_{cr} = e/(e^2 - 1/4) = 0.38076$ the energy derivatives are continuous. There is a quantity β which is the inverse of a length, which tends to zero as one approaches the $\alpha(B)$ line. This line is $\alpha = [1 + (1 + B^2)^{1/2}]/2$. The numbers refer to units where the sound speed and phonon upper cutoff are taken to be 1. For $B > B_{cr}$ the transition is first order. In contrast to the source theory, the high-α phase is not trivial, and in fact agrees with the classical theory. However, quantum fluctuation effects in the high-α phase are not treated.

In Section 6 I examine a different function with broken symmetry, which also reduces to both source and classical theories. This function treats quantum fluctuations in the high-α phase, and the energy is continuous in the vicinity of $\alpha = 1$ ($B \ll 1$). The transition to classical behavior again occurs near $\alpha = 1/2$, but now there is a second-order transition. This persists over the entire plane, and for $B \gg 1$ is near $\alpha = B/2$. This theory reduces to the source theory in the low-α region.

In Section 7 I outline an approach that involves a symmetry-breaking field together with a one-mode reduction of the Hamiltonian. The spin is coupled dynamically to the mode. All earlier approximations are special cases of this formulation. The mode has a parameter β characterizing the spatial extent of the mode. The transition is determined by the behavior of this parameter. The one-mode problem can be solved exactly numerically, but this is not done here.

2. NOTATION

Let us study the Hamiltonian

$$H = -\frac{B}{2}\sigma_z - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \sigma_x \int \frac{D(\mathbf{k})}{(2k)^{1/2}} [a(\mathbf{k}) + a^+(\mathbf{k})]\, d\mathbf{k} + \int |k|\, a^+(k)\, a(\mathbf{k})\, d\mathbf{k} \tag{1}$$

A spin-1/2 (units $\hbar = 1$) particle interacts with a boson field

$$[a(\mathbf{k}), a^+(\mathbf{l})] = \delta(\mathbf{k} - \mathbf{l}) \tag{2}$$

Introducing

$$q(\mathbf{k}) = \frac{a(\mathbf{k}) + a^+(-\mathbf{k})}{\sqrt{2}}, \qquad p(\mathbf{k}) = i\frac{a^+(\mathbf{k}) - a(-\mathbf{k})}{\sqrt{2}} \tag{3}$$

$$[q(\mathbf{k}), p(\mathbf{l})) = i\delta(\mathbf{k} - \mathbf{l}), \qquad q^+(\mathbf{k}) = q(-\mathbf{k}) \tag{4}$$

the Hamiltonian is

$$H = -\frac{B}{2}\sigma_z - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \int \frac{D(\mathbf{k})}{\sqrt{\omega}} q(\mathbf{k})\, dk + H_{\text{ph}} \tag{5}$$

$$H_{\text{ph}} = \frac{1}{2}\int \omega\{p(\mathbf{k})\, p(-\mathbf{k}) + q(\mathbf{k})\, q(-\mathbf{k}) - 1\}\, d\mathbf{k} \tag{6}$$

This allows us to have a collection of unit-frequency oscillators in the absence of interaction. The unperturbed ground state of the boson field is

$$\phi_0 = Q \exp\left\{-\frac{1}{2}\int q(\mathbf{k})\, q(-\mathbf{k})\, d\mathbf{k}\right\} \tag{7}$$

The prefactor Q stands for normalization in the continuum limit.

Note that these coordinates are different from the Fourier components of the field, and that

$$\phi(\mathbf{x}) = \frac{1}{(2\pi)^3} \int \frac{q(\mathbf{k})}{\sqrt{\omega}} \exp(i\mathbf{k}\cdot\mathbf{x})\, d\mathbf{k} \tag{8}$$

We are particularly interested in the acoustic case where $\omega(\mathbf{k}) = c|\mathbf{k}|$. The sound speed c will be taken to be unity. $D(k)$ is a constant up to a cutoff k_0,

$$\begin{aligned} D(k) &= 1 \qquad \text{for} \quad k < k_0 \\ &= 0 \qquad \text{for} \quad k > k_0 \end{aligned} \tag{9}$$

This case has subtle behavior in the infrared. Complete the specification of units by taking $k_0 = 1$.

The parity operator

$$P = \exp\left[i \left(\frac{\sigma_z}{2} + \int a^+ a\, d\mathbf{k} \right) \pi \right] \tag{10}$$

commutes with H,

$$Pa(\mathbf{k})P^{-1} = -a(\mathbf{k}), \qquad P\sigma_x P^{-1} = -\sigma_x \tag{11}$$

The exact eigenstates of H can be classified as even or odd parity states. By performing a rotation about the y axis, one can transform the Hamiltonian so that $\sigma_x \to -\sigma_z$, $\sigma_z \to \sigma_x$. This is a formulation as a tunneling problem.

We are particularly interested in the ground-state energy of the system as a function of α and B. Note that the magnetization is

$$\langle \Psi_G | \sigma_z | \Psi_G \rangle = -2\, \partial E_G / \partial B \tag{12}$$

3. SOURCE AND CLASSICAL APPROXIMATIONS

Two limiting situations serve as reference points.

3.1. Source Approximation

When $\alpha = 0$ the ground state is nondegenerate with energy $-B/2$, and is

$$\Psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Psi_0 \qquad \text{with} \quad a(\mathbf{k})\Phi_0 = 0 \tag{13}$$

or

$$\Psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \phi_0 \qquad \text{in the } q(\mathbf{k}) \text{ representation}$$

This is an eigenstate of parity.

When $B = 0$ the eigenstates are given by the unitary transform U_s

$$U_s = \exp\left[i \int p(\mathbf{k}) f_0(\mathbf{k}) \sigma_x \, d\mathbf{k} \right], \qquad U_s H U_s^{-1} = H_0 - \alpha/2 \tag{14}$$

Here

$$f_0(k) = \frac{1}{2} \left(\frac{\alpha}{\pi} \right)^{1/2} \frac{D(k)}{\sqrt{k}} \frac{1}{k} \tag{15}$$

U_s commutes with the parity operator. The ground state is degenerate with energy $-\alpha/2$. The even-parity ground state is

$$\Psi = U_s^{-1} \phi_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{16}$$

or

$$\Psi = \left(\frac{\phi_+ + \phi_-}{2} \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \left(\frac{\phi_- - \phi_+}{2} \right) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{17}$$

Here

$$\phi_\pm = Q \exp\left\{ - \int [q(\mathbf{k}) \pm f_0(\mathbf{k})][q(-\mathbf{k}) \pm f_0(-\mathbf{k})] \, d\mathbf{k} \right\} \tag{18}$$

The expectation of the number operator with either of these states is

$$\langle \Psi | \int a^+ a \, d\mathbf{k} \, | \Psi \rangle = \int f_0^2 \, d\mathbf{k} = \frac{\alpha}{2} \int \frac{dk}{k} = \frac{\alpha}{2} \ln \frac{1}{k_0} \tag{19}$$

In the acoustic case this tends to infinity as the cutoff $k_0 \to 0$. This is an infrared divergence arising from contributions from long wavelengths. The overlap integral for the phonon parts of the degenerate states is $\langle \phi_- | \phi_+ \rangle = \exp(-\int f_0^2 \, d\mathbf{k})$ and tends to zero for the acoustic case. The expectation value of σ_z is zero; the overlap integral is zero.

This transformation introduces a displacement of the $q(k)$ variables relative to the instantaneous value of the spin variable σ_x. I will refer to it as the source transformation.

The analysis refers to the case $B=0$. The $B \to 0$ limit is subtle. If $B \neq 0$, ordinary nondegenerate perturbation theory, starting from the states for $\alpha=0$, given an energy

$$E= -\frac{B}{2}-\frac{\alpha}{2}\left(1-B\ln\frac{1+B}{B}\right) \tag{20}$$

The wave function is

$$\Psi = N^{-1}\left\{\Phi_0\begin{pmatrix}1\\0\end{pmatrix}-\frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2}\int\frac{D(k)}{(2k)^{1/2}}\frac{a^+(\mathbf{k})}{k+B}\,d\mathbf{k}\;\Phi_0\begin{pmatrix}0\\1\end{pmatrix}\right\} \tag{21}$$

The norm is finite because $B \neq 0$,

$$N^2 = 1+\frac{\alpha}{2}\,\xi(B), \qquad \xi(B)=\ln\left(\frac{1+B}{B}\right)-\frac{1}{1+B} \tag{22}$$

The expectation value of the number operator is, to order α,

$$\langle\Psi|\int a^+a\,d\mathbf{k}\,|\Psi\rangle=\tfrac{1}{2}\alpha\xi(B) \tag{23}$$

and becomes vanishingly small if B is fixed and $\alpha \to 0$.

The distinction between the two cases $\alpha \ll B$ and $B \ll \alpha$ (with both B and α less than unity) is clear when one uses the source transformation, leaving $f(k)$ free to be determined by the variational principle. This was done by Emery and Luther[3] and Silbey and Harris.[5] The source transform rotates the spin about the x axis and induces a displacement of $q(\mathbf{k})$. Taking the expectation value with a state vector $\Phi_0\binom{1}{0}$, one finds

$$E_s= -\frac{B}{2}\exp\left(-\int f^2\,d\mathbf{k}\right)-\frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2}\int\frac{D}{\sqrt{k}}f\,d\mathbf{k}+\frac{1}{2}\int kf^2\,d\mathbf{k} \tag{24}$$

The state vector of the original Hamiltonian is the parity eigenfunction, Eq. (17). Now we have the possibility of a nonzero overlap $Z=\exp(-\int f^2\,d\mathbf{k})$.

Varying $f(k)$, we find

$$f(k)\{k+Bz\}=\frac{D(k)}{\sqrt{k}}\frac{\sqrt{\alpha}}{2\sqrt{\pi}} \tag{25}$$

$$-\ln Z=\frac{\alpha}{1-\alpha}\left[\ln\left(\frac{1+BZ}{B}\right)-\frac{1}{1+BZ}\right] \tag{26}$$

$$E=\frac{-BZ}{2}-\frac{\alpha}{2}\frac{1}{1+BZ} \tag{27}$$

These equations have been studied by Tanaka and Sakurai.[6] One first analyzes the equation for Z.

When $\alpha < 1$, $Z(B)$ goes smoothly from 0 to 1 as B goes from zero to infinity. There is a unique Z for any B. For fixed B as $\alpha \to 0$, Z is near to 1. But for fixed $\alpha < 1$, as $B \to 0$, $Z \to 0$.

For $\alpha = 1$, Z is zero at $B = 1/e$ and there is a solution for $B > 1/e$. But for $B > 1/e$ there is no solution. With the trial function generated by the source transform, for $B < 1/e$, one must switch to a solution with $Z = 0$ and energy equal to $-\alpha/2$ and independent of B. The theory is trivial in this region. The switch at $B = 1/e$ involves a jump to finite Z. In the $B < 1/e$, $\alpha > 1$ region the boson field is long range, as it is for $B = 0$. When $Z \neq 0$ the field is of shorter range. More precisely, with parity, eigenfunctions $\overline{\sigma_x \phi} \equiv \langle \psi | \sigma_x \phi | \psi \rangle$ must be considered, since $\langle \psi | \phi(x) | \psi \rangle = 0$. For $Z \neq 0$,

$$\overline{\sigma_x \phi(x)} = \left(\frac{\alpha}{\pi}\right)^{1/2} \frac{1}{(2\pi)^2} \frac{1}{|x|} \int_0^1 \frac{\sin k\,|x|}{k + BZ}\, dk \tag{28}$$

Thus

$$\overline{\sigma_x \phi(x)} = \left(\frac{\alpha}{\pi}\right)^{1/2} \frac{1}{(2\pi)^2} \frac{1}{|x|^2} \left(\frac{1}{BZ} - \frac{\cos |x|}{1 + BZ}\right) + \cdots \qquad \text{as} \quad |x| \to \infty \tag{29}$$

When $\alpha > 1$, there are two solutions when B is greater than a critical value (depending on α). The lowest energy as obtained for the larger Z solution. There is no solution for B less than this value and one switches to the B-independent $f_0(k)$ and energy $-\alpha/2$.

The behavior on the transition line is interesting. Assuming that $Z \ll 1$, the equations become

$$E = \frac{-\alpha}{2} \frac{-B}{2} (1 - \alpha) Z \tag{30}$$

with

$$Z \to (Be)^{\gamma}, \qquad \gamma \equiv \frac{\alpha}{1 - \alpha} \tag{31}$$

Thus, for $Be < 1$, Z does tend to zero as $\alpha \to 1$ from below. The transition occurs at $\alpha = 1$. The γ term dominates so that any finite derivative with respect to B approaches zero. On the other hand, for $Be > 1$ the transition occurs on an $\alpha(B)$ line with a finite jump in the magnetization, i.e., it is first order. For $B \ll 1$, Eq. (33) shows that for $1/2 < \alpha < 1$, the B-dependent energy is smaller than B^2.

3.2. Classical Theory

The preceding calculation must compete with the variational estimate from a semiclassical, Hartree-type theory. Here one uses the unitary transform

$$U_c = \exp\left\{i\int p(\mathbf{k})\, h(\mathbf{k})\, d\mathbf{k}\right\}$$
$$U_c q(\mathbf{k}) U_c^{-1} = q(\mathbf{k}) + h(\mathbf{k}) \tag{32}$$

This is independent of the instantaneous values of the spin variable. $h(\mathbf{k})$ is the classical value of the boson field. It depends on a mean value of the spin

$$\langle \psi_0 | U_c H U_c^{-1} | \psi_0 \rangle = \frac{-B}{2}\sigma_z + \frac{1}{2}\int k h^2\, d\mathbf{k} - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \int \frac{Dh}{\sqrt{k}}\, d\mathbf{k}\, \sigma_x \tag{33}$$

after averaging with a phonon state ϕ_0. The spin is treated quantum mechanically. So this is really a semiclassical theory. It is a well-known approximation in quantum optics.

Perform a rotation

$$W = \exp\left(i\sigma_y \frac{\theta}{2}\right), \qquad \tan\theta = B\int \frac{Dh}{\sqrt{k}}\, d\mathbf{k}\left(\frac{\alpha}{\pi}\right)^{1/2} \tag{34}$$

and take the expectation value with $\binom{1}{0}$. The wave function for the original Hamiltonian is a product function of spin and boson variables, with θ and $h(k)$ determined self-consistently. This gives

$$E_c = -\left[\left(\frac{B}{2}\right)^2 + \frac{\alpha}{4\pi}\left(\int \frac{Dh}{\sqrt{k}}\, d\mathbf{k}\right)^2\right]^{1/2} + \frac{1}{2}\int k h^2\, d\mathbf{k} \tag{35}$$

Minimization of the energy with respect to $h(\mathbf{k})$ gives

$$h(k) = \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D}{\sqrt{k}}\frac{1}{k}\sin\theta \tag{36}$$

$$\cos\theta = B/2\alpha$$

$$E_c = \frac{-\alpha}{2} - \frac{B^2}{8\alpha}, \qquad \alpha > \frac{B}{2} \tag{37}$$

The expectation value of σ_z is $\cos\theta$.

The solution only exists when $2\alpha > B$. When the condition is violated (i.e., for small α) we must take $h(k)=0$, and the energy is $-B/2$, i.e., independent of α. So the theory is trivial, and there is no coupling to phonons. The state vector is

$$\Psi_c = \cos\left(\frac{\theta}{2}\right)\phi_-\begin{pmatrix}1\\0\end{pmatrix} + \sin\left(\frac{\theta}{2}\right)\begin{pmatrix}0\\1\end{pmatrix}\phi_- \tag{38}$$

The displacement in ϕ_- is $h(k)$. This state vector is not an eigenfunction of parity. We can apply $(-i)P$ to Ψ_c and construct the symmetric combination

$$\Psi = \cos\left(\frac{\theta}{2}\right)[\phi_- + \phi_+]\begin{pmatrix}1\\0\end{pmatrix} + \sin\left(\frac{\theta}{2}\right)[\phi_- - \phi_+]\begin{pmatrix}0\\1\end{pmatrix} \tag{39}$$

This is an eigenfunction of the parity operator. However, ϕ_- and ϕ_+ involve the displacement $h(k)$ and the overlap $\langle\phi_-|\phi_+\rangle = 0$. Thus, forming the combination does not lower the energy. The antisymmetric combination has the same energy. The classical theory has $Z \equiv 0$ and the spatial phonon field associated with $h(k)$ has the long-range $1/|x|$ behavior. With the parity eigenfunction constructed from the classical function it is $\overline{\sigma_x \phi(x)}$ that has this behavior.

4. COMPARISON OF SOURCE AND CLASSICAL THEORIES

The next step is to compare the energies of the source and classical approximations.

The result of the numerical analysis of $E(\alpha)$ for different values of B is summarized in Table I. The α_D are critical coupling constants. For any B, $\alpha < \alpha_D$ corresponds to the superiority (lower energy) of the source theory. The situation $\alpha > \alpha_D$ corresponds to a lower energy for the classical theory. Z_D is the value of the overlap at the intersection of energy curves. α_D and Z_D are obtained by equating $E_s = E_c$. One has

$$\frac{\alpha}{2} + \frac{B^2}{8\alpha} = \frac{BZ}{2} + \frac{\alpha}{2}\frac{1}{1+BZ} \tag{40}$$

Table I. Source versus Classical Theories

B	0.0012	0.0101	0.05	0.1	0.1405	0.20	0.24	0.30	0.368	0.50	0.70	1.00	2.00	4.00
α_D	0.540	0.540	0.60	0.635	0.653	0.69	0.712	0.778	0.800	0.875	1.02	1.20	1.6	3.0
Z_D	0.0012	0.011	0.05	0.10	0.15	0.215	0.26	0.32	0.37	0.482	0.60	0.70	0.88	0.92
$\sin\psi_c$	0.0011	0.009	0.042	0.079	0.108	0.145	0.169	0.200	0.230	0.313	0.343	0.417	0.625	0.667

We see that for $B \ll 1$ the jump in Z_D (since $Z \equiv 0$ in classical theory) is small. The transition to the classical theory is at α near 1/2. When $B > 1$ the jump tends to unity. There is also a jump in angle. The source theory corresponds to $\sin \psi = 0$ and for the classical theory $\sin \psi_c = B/2\alpha$ $(\psi = \pi/2 - \theta)$.

Let us consider $E(B)$ for different regions of α.

(i) $\alpha < 1/2$. The source theory is superior for all B. When $BZ < 1$, we have $Z \to (Be)^\gamma$, $\gamma = \alpha/(1-\alpha)$, and

$$E \to -\frac{\alpha}{2} - \frac{\alpha - 1}{2} B(Be)^\gamma \tag{41}$$

When $B \gg 1$,

$$Z \sim 1 - \frac{\alpha}{2B^2}, \qquad E \to -\frac{B}{2} - \frac{\alpha}{4B} \tag{42}$$

There is no transition as B varies.

(ii) $1/2 < \alpha < 1$. For given α the classical theory is valid for small B, the source theory for larger B. From the table, at $\alpha = 0.60$ the divide is at $B = 0.05$. For $\alpha = 0.875$ it is at $B = 0.50$.

(iii) $\alpha = 1$. Here the source approximation fails for $B < 1/e = 0.3679$. But the classical approximation is in fact better for $B < 0.67$ when $Z \sim 0.57$.

(iv) $\alpha > 1$. As α increases, the source theory fails in the region $B < 1$. At $\alpha = 1.02$ the classical theory is superior for $B < 0.70$, the source theory is superior for $B > 0.70$.

(v) $\alpha \gg 1$. The intersection occurs at $\alpha \sim \frac{1}{2}B[1 + (2B)^{-1/2}]$ when $Z \sim 1 - \alpha/2B^2$.

In sum, comparison of the crude source and classical theories yields a picture of crossing of energies. With increasing α there is a jump in the overlap factor and a transition to the symmetry-breaking long-range boson field with $Z \equiv 0$. Thus, the transition is first order across the $\alpha(B)$ line. This is not surprising, since direct comparison of energies for different approximations would be expected to give a first-order transition. The description at the intersection is defective. In the next section I use an improved wave function to give a better account of the intersection. The result is that the transition is very similar to that of the source theory, but is nontrivial in the large-α region. In addition, the crossover to classical behavior occurs ner $\alpha = 1/2$, but continuously, rather than with a jump in the first derivatives.

5. A VARIATIONAL EXTENSION

Consider the problem in the $q(\mathbf{k})$ representation. Denote $\phi_\pm$ as ϕ_0 with $q(\mathbf{k}) \to q(\mathbf{k}) \pm f(k)$. The overlap between the two functions is

$$Z \equiv \langle \phi_+ | \phi_- \rangle = \exp(-\xi), \qquad \xi = \int f^2 \, d\mathbf{k} \tag{43}$$

Take as the trial function Eq. (39). The normalization is

$$\langle \Psi | \Psi \rangle = 2(1 + Z \cos \theta) \tag{44}$$

We also have ($\psi = \pi/2 - \theta$)

$$\begin{aligned} \langle \Psi | \sigma_z | \Psi \rangle / \langle \Psi | \Psi \rangle &= (\sin \psi + Z)/(1 + Z \sin \psi) \\ \langle \Psi | \sigma_x | \Psi \rangle / \langle \Psi | \Psi \rangle &= 0 \end{aligned} \tag{45}$$

This function involves an angle θ and a function $f(k)$, and is an eigenfunction of the parity operator. For $\theta = \pi/2$ it is

$$\left\{ \phi_- \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \phi_+ \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\} \frac{1}{\sqrt{2}}$$

and is a linear combination of the degenerate source functions. In that case the overlap Z is not zero.

For general θ but $f(k) \sim D/k^{3/2}$ we have a classical function with overlap zero, i.e., the long-range spatial behavior. The projection to an eigenfunction of parity gains nothing in energy in the large-α region.

Our wave function uses the angle θ when $Z \neq 0$ to give a better fit of the source and classical theories. θ and $f(\mathbf{k})$ are to be freely varied.

It is convenient to use the angle $\psi = \pi/2 - \theta$ so that $\sin \psi = \cos \theta$, $\cos \psi = \sin \theta$. We have

$$E\{1 + Z \sin \psi\} = -\frac{B}{2} [\sin \psi + Z] - \left(\frac{\alpha}{\pi} \right)^{1/2} \cos \psi \, D_1 + \frac{J}{2} (1 - Z \sin \psi) \tag{46}$$

where

$$D_1 \equiv \int \frac{Df}{\sqrt{k}} \, d\mathbf{k}, \qquad J = \int k f^2 \, d\mathbf{k} \tag{47}$$

Variation of E with respect to ψ gives

$$\left(\frac{\alpha}{4\pi} \right)^{1/2} D_1 (\sin \psi + Z) = \cos \psi \left\{ \frac{B}{2} (1 - Z^2) + ZJ \right\} \tag{48}$$

Variation of E with respect to $f(k)$ shows that $f(k)$ has the form

$$f(k)=\frac{\sqrt{\alpha}}{2\sqrt{\pi}}\frac{\cos\psi}{1-Z\sin\psi}\frac{D(k)}{(k+\beta)\sqrt{k}} \tag{49}$$

$$\beta(1-Z^2\sin^2\psi)=Z\left[B\cos^2\psi-\frac{\alpha}{2\sqrt{\pi}}\sin(2\psi)\int\frac{Df}{\sqrt{k}}+2J\sin\psi\right] \tag{50}$$

We have the basic integrals

$$\begin{aligned}\xi&=\frac{1}{4\pi}\int\frac{D^2\,d\mathbf{k}}{k(k+\beta)^2}=\ln\left(\frac{1+\beta}{\beta}\right)-\frac{1}{1+\beta}\\ D_0&=\frac{1}{4\pi}\int\frac{D^2\,d\mathbf{k}}{k(k+\beta)}=1-\beta\ln\frac{1+\beta}{\beta}\\ J_0&=\frac{1}{4\pi}\int\frac{D^2\,d\mathbf{k}}{(k+\beta)^2}=\left(1+\frac{\beta}{1+\beta}-2\beta\ln\frac{1+\beta}{\beta}\right)\end{aligned} \tag{51}$$

We can now write the equations of the theory in a more convenient form. The energy functional can be written as

$$E(1-Z^2\sin^2\psi)=-\frac{B}{2}\sin\psi(1-Z^2)-\frac{BZ}{2}\cos^2\psi-\frac{\alpha}{2}\frac{\cos^2\psi}{1+\beta} \tag{52}$$

We also have

$$\ln\frac{1}{Z}=\frac{\alpha\cos^2\psi\xi}{(1-Z\sin\psi)^2} \tag{53}$$

There are two equations representing variation with respect to f and ψ. The β equation, after some manipulation, is

$$\begin{aligned}&\beta\left[1-Z^2\sin^2\psi+2Z\ln\frac{1}{Z}(1-Z\sin\psi)\sin\psi\right]\\ &\quad=Z\cos^2\psi\left[B+\frac{2\alpha Z\sin^2\psi}{1-Z\sin\psi)^2}J_0(\beta)\right]\end{aligned} \tag{54}$$

The angle equation may be put in the form [using the form of $f(k)$]

$$\sin\psi=\frac{R}{2}-\left[\left(\frac{R}{2}\right)^2+s\right]^{1/2} \tag{55}$$

$$S=\frac{\alpha Z\beta\xi-(B/2)(1-Z^2)}{\Delta},\qquad R=\frac{1-Z^2}{\Delta}(BZ+\alpha D^0)$$

with

$$\Delta = Z\left[\frac{BZ}{2}(1-Z^2)+\alpha\beta\xi\right] \tag{56}$$

The theory is characterized by three intricately connected equations for Z, β, ψ. The preceding forms are efficient for computation in the region $\beta < 1$. One may start with a $\sin\psi$ equal to the classical $B/2\alpha$ and find Z and β from the $\ln(1/Z)$ and β equations. Then one recomputes $\sin\psi$ and iterates to self-consistency.

One can study the $\beta \ll 1$, $Z \ll 1$ limit analytically. The energy functional has the limiting form

$$E \rightarrow -\frac{B}{2}\sin\psi - \frac{\alpha}{2}\cos^2\psi \tag{57}$$

$$-\frac{\beta}{2}Z\,\mathrm{co}^2\,\psi + \frac{\alpha}{2}\cos^2\psi\beta \tag{58}$$

Let $\alpha^* = \alpha\cos^2\psi$ and $B^* = B\cos^2\psi$. We vary with respct to β after inserting

$$Z \rightarrow (e)^{\alpha^*} \tag{59}$$

which is the limiting value of

$$\ln\left(\frac{1}{Z}\right) = \alpha^*\xi(\beta) \rightarrow \alpha^*\ln\left(\frac{1}{\beta e}\right)$$

Then

$$Z \rightarrow (B^*e)^{\gamma^*} \qquad \gamma^* = \alpha^*/(1-\alpha^*)$$

$$\beta \rightarrow B^*Z$$

$$E = \frac{-B}{2}\sin\psi - \frac{\alpha}{2}\cos^2\psi + \frac{B^*}{2}(\alpha^*-1)(B^*e)^{\gamma^*} \tag{61}$$

The energy shift is positive for $\alpha^* > 1$. This form can be used to establish that there is an infinite-order transition, by an argument like that used for for the source theory.

Let us first study the region $B \ll 1$. Later we will develop a systematic theory in that region. The simple equations of source and classical energies gave intersection nearly $\alpha = 1/2$ with the classical theory superior for the larger α values. With the present variational theory the transition is continuous. When $1/2 < \alpha^* < 1$ or $\gamma^* > 1$ the last term is negligible for $B \ll 1$. We can use the classical angle $\sin\psi = B/2\alpha$ and $\alpha^* = \alpha[1-(B/2\alpha)^2] \to \alpha$. Thus, the energy takes on the classical value in the region $1/2 < \alpha < 1$ when $B \ll 1$.

On the other hand, if $\alpha < 1/2$, the last term contributes the leading term $-B/2$ in energy. Using the classical angle, the energy through terms of order B^2 is

$$E = -\frac{\alpha}{2} - \left(\frac{B}{2\alpha}\right)^2 \frac{1}{2} - \frac{B}{2}(1-\alpha)(Be)^{\alpha/1-\alpha} \tag{62}$$

This exhibits a continuous crossover to classical behavior near $\alpha = 1/2$.

Next we study the $\alpha(B)$ transition as predicted by the variational wave function.

There is a line in the (α, B) plane such that the classical theory applies for α above the line. Coming down to the line from larger values of α, the angle approaches $\sin\psi = B/2\alpha$ on the line. As we move across the line, there are two distinct regions. When $B < B_c = e/(e^2 - 1/4) = 0.38076...$, β and Z are arbitrarily close to zero. So β, Z, ψ are continuous. All derivatives with respect to B vanish. I call this an infinite-order transition. The range tends to infinity near the line.

In the second region $B > B_c$ there is no such behavior and one has finite jumps in β, Z, ψ as one crosses the line. This is a "first-order" transition.

To prove these results, assume $\beta \ll 1$, $Z \ll 1$ and use Eqs. (60), (61).

The condition $\alpha^* = 1$ together with $\sin\psi = B/2\alpha$ defines a critical line $\alpha_c(B)$ with

$$\alpha_c = \frac{1 + (1 + B^2)^{1/2}}{2} \tag{63}$$

If now $B^*z < 1$, $Z \ll 1$ provided $\alpha^* < 1$ as $\alpha^* \to 1$. Then $\alpha^*/(1-\alpha^*) \to +\infty$. So we have the infinite-order region. The two conditions $\alpha^* = 1$, $B^*e = 1$ give the end of the the region at $B = B_c = e/(e^2 - 1/4)$. Just as for the source theory, the exponent γ^* dominates and any finite derivative with respect to B vanishes as $\alpha^* \to 1$.

It follows that for $B < B_c$ the divide coupling constant σ_D is pushed up to $\alpha_c = [1 + (1 + B^2)^{1/2}]/2$ and Z_D is pushed to $Z = 0$. Thus, the domain of a α where the symmetry is unbroken is extended considerably. The angle behavior is such that $\sin\psi$ is very small for $\alpha \ll 1$, rises to a maximum as α increases, and then falls off according to the classical formula $\sin\psi_c = B/2\alpha$. When B is small the angle remains small throughout.

Table II. Angle, Overlap, and Energy[a]

Z	α	$\sin\psi$	$\lvert E\rvert$	$\lvert E_{cl}\rvert$
0	1.0025	0.0499	0.50125	0.5025
0.01	0.779	0.064	0.3896	0.3911
0.04	0.711	0.071	0.3561	0.3573
0.045	0.700	0.072	0.3507	0.3518
0.07	0.869	0.0746	0.3357	0.3364
0.10	→0.635	0.0775	0.3295	0.3196←
0.20	0.545	0.0842	0.2798	0.2748
0.30	0.469	0.0887	0.2460	0.2371
0.50	0.331	0.0953	0.1826	
0.60	0.265	0.0938	0.1550	
0.70	0.199	0.0873	0.1280	
0.80	0.133	0.0719	0.1016	
0.90	0.067	0.0438	0.0757	

[a] The results of a numerical solution based on the small-angle formula. $B = 0.10$.

As an example, I give numerical results for $B = 0.10$ in Table II. The maximum angle is near $\alpha = 0.33$ when $Z = 0.50$ and is $\sin\psi = 0.095$. The crude divide is at $\alpha = 0.635$, $Z = 0.10$ when $\sin\psi = 0.078$. The energy going with the trial function is lower than the symmetry-breaking classical energy up to $\alpha = 1.0025$.

On the critical line $B = B_{cr}$ the behavior is similar but the angle reaches larger values.

The transition is first order when $B > B_{cr}$. The results are particularly simple when $B \gg 1$. The dividing coupling α_D is near $B/2$. One has

$$Z = 1 - \delta Z, \qquad \delta Z = \alpha/2B^2 \tag{64}$$

Matching E_s and E_c, we have the correction

$$\begin{aligned} \alpha_D &= \frac{B}{2}\left(1 + \frac{1}{\sqrt{2}}\frac{1}{\sqrt{B}} + \cdots\right) \\ E_s &\to -\frac{B}{2} - \frac{1}{8} - \frac{1}{8\sqrt{2}}\frac{1}{\sqrt{B}} \qquad \text{at} \quad \alpha \equiv \frac{B}{2} \end{aligned} \tag{65}$$

$$\sin\psi = \frac{\alpha}{4B^2} \tag{66}$$

The angle increases linearly with α and reaches the very small value $\sin\psi = 1/8B$ at $\alpha = B/2$. The energy shift is $\Delta E = -(1/8B^2)(\alpha/2B)^3$. The jump in in Z is $1 - 1/4B$. In fact, there is little change from the crude source theory.

For smaller values of B but with $B > B_{cr}$ one must have recourse to a numerical analysis of the complete equations.

In summary, the variational calculation improves on the source calculation in a number of ways. It shows a smooth transition to classical behavior near the line where source and classical energies match. For values of α between this line and the $\alpha(B)$ transition line it is superior to both. On the other hand, above the $\alpha(B)$ line the range is infinite and the theory is no better than the classical theory. This indicates that important quantum fluctuation effects are not included in the wave function. For $B^*e < 1$ the transition is infinite order and the nonclassical contribution is very small. In fact, for $B \ll 1$, calculation to order B^2 gives no transition at all. This is what will be found in a more systematic treatment. This variational calculation can be used for larger values of B even though the physical motivation for the wave function is less clear. The theory gives a jump in first derivatives of energy across the line. We will be able to give a systematic treatment for $B \gg 1$ which gives the same result but with a more trustworthy basis.

6. SYMMETRY-BREAKING SOURCE THEORY

In the present section I examine a different way of combining the classical and modified source theories. It is a symmetry-breaking extension of the modified source theory. In the large-α phase it yields quantum fluctuation corrections to the classical theory. In this respect it is superior to the variational extension. On the other hand, in the small-α phase it reduces to the modified source theory and is therefore inferior to the variational extension. It will be clear that a better wave function should include both effects. This leads to a complicated theory that I have not analyzed.

The trial function of this section is

$$\psi_B = \exp\left(-i\int pf\,d\mathbf{k}\,\sigma_x\right)\left(-i\int ph\,d\mathbf{k}\right)\exp\left[-i\left(\frac{\theta}{2}\right)\sigma_y\right]\begin{pmatrix}1\\0\end{pmatrix}\phi_0 \qquad (67)$$

It leads to an $\alpha(B)$ line that starts at $\alpha = 1/2$ when $B \ll 1$ and tends to $\alpha = B/2$ when $B \gg 1$. The transition is everywhere second order, i.e., the first derivatives of the energy are continuous. The theory agrees with the variational extension in locating the crossover to classical behavior near $\alpha = 1/2$ (when $B \ll 1$), but describes it in terms of discontinuous second derivatives, rather than continuously. Of course ψ_B can be made into an even-parity eigenfunction so that we have a parity eigenfunction in the entire α, B plane. However, as was the case for the classical theory, this leads to no improvement in the energy in the broken symmetry phase.

ψ_B is a succession of unitary transforms involving two functions $f(k)$ and $h(k)$ and an angle θ. It includes the source and classical theories as special cases and given an account of quantum fluctuations in the broken symmetry phase. Let

$$Z_0 \equiv \exp\left(-\int f^2\, dk\right) \tag{68}$$

Then, carrying out the variation of the energy functional, we find

$$h(k) = L\left\{\frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D}{k^{3/2}} - f(k)\right\} \tag{69}$$

$$f(k) = \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D(k)}{\sqrt{k}\,(k+2\alpha-1)} \tag{70}$$

$$\tan\theta = \frac{2L}{B}\left(\alpha - \frac{1}{2}\right) \tag{71}$$

$$L^2 = 1 - \left(\frac{BZ_0}{2}\right)^2 \left(\frac{1}{\alpha - 1/2}\right)^2 \tag{72}$$

The order parameter L is nonzero when

$$BZ_0 < 2\alpha - 1 \tag{73}$$

The above equations lead to the explicit results in the broken symmetry phase

$$Z_0 = e^{1/2}\left(\frac{\alpha - 1/2}{\alpha}\right)^{\alpha} \tag{74}$$

$$E = -\frac{\alpha}{2} - \frac{1}{8}\frac{(BZ_0)^2}{\alpha - 1/2} \tag{75}$$

The inverse length $2\alpha - 1$ is continuous with the BZ inverse length of the source theory on the transition line. With the above simple function this length is independent of B in the broken symmetry phase. When $B \to 0$ the line starts at $\alpha = 1/2$ (as was the case with simple energy matching of classical and source theories).

The transition occurs along the line

$$B = \frac{2}{\sqrt{e}} \alpha^{\alpha} (\alpha - 1/2)^{1-\alpha} \tag{76}$$

$$\begin{aligned} \alpha &\to \frac{1}{2} + \frac{eB^2}{2} \qquad \text{small } B \\ \alpha &\to \frac{B}{2} + \frac{3}{8} \qquad \text{large } B \end{aligned} \tag{77}$$

Along the line the energy has the simple form

$$E = -\alpha + 1/4 \tag{78}$$

For every $\alpha > 1/2$ there is the appropriate B.

In the broken symmetry phase the first derivatives at the transition line are given by

$$\begin{aligned} \left(\frac{\partial E}{\partial \alpha}\right)_B &= -\frac{1}{2} - \left(\alpha - \frac{1}{2}\right) \ln \frac{\alpha - 1/2}{\alpha} \\ \left(\frac{\partial E}{\partial B}\right)_\alpha &= -\frac{\alpha - 1/2}{B} \end{aligned} \tag{79}$$

The second derivatives at the line are

$$\begin{aligned} \left(\frac{\partial^2 E}{\partial \alpha^2}\right)_B &= -\left[(2\alpha - 1) \ln^2 \frac{\alpha - 1/2}{\alpha} + \frac{1}{2\alpha}\right] \\ \left(\frac{\partial^2 E}{\partial \beta^2}\right)_\alpha &= -\frac{\alpha - 1/2}{B^2} \end{aligned} \tag{80}$$

In this phase at large α

$$Z_0 \to 1 - \frac{1}{8\alpha} \tag{81}$$

$$E \to -\frac{\alpha}{2} - \frac{B^2}{8\alpha}\left(1 + \frac{1}{4\alpha}\right) \tag{82}$$

$$L^2 \to 1 - \left(\frac{B}{2\alpha}\right)^2 \left(1 + \frac{3}{4\alpha}\right) \tag{83}$$

The last terms describe the effect of quantum fluctuations on the energy and order parameter.

The normal phase is described by the modified source approximation at the transition line $Z=Z_0$ and the first derivatives are the same as for the broken symmetry phase. The second derivatives at the line are

$$\begin{aligned}\left(\frac{\partial^2 E}{\partial\alpha^2}\right)_B &= \frac{-4\alpha(\alpha-1/2)}{4\alpha-1}\left[\ln\left(\frac{2\alpha}{2\alpha-1}\right)-\frac{1}{2\alpha}\right]^2\\ \left(\frac{\partial^2 E}{\partial B^2}\right)_\alpha &= \frac{1}{2}\frac{Z_0}{B}\frac{1}{4\alpha-1}\end{aligned}\tag{84}$$

The second derivatives are different for the two phases.

I note the behavior for small and large B. The common first derivatives are

$$\begin{aligned}\left(\frac{\partial E}{\partial\alpha}\right)_B &\to -\frac{1}{2}+\frac{e}{2}B^2\ln(eB^2) \qquad \text{as} \quad B\to 0\\ &\to -\frac{1}{4B} \qquad \text{as} \quad B\to\infty\end{aligned}\tag{85}$$

$$\begin{aligned}\left(\frac{\partial E}{\partial B}\right)_\alpha &\to \frac{eB}{2} \qquad \text{as} \quad B\to 0\\ &\to -\frac{1}{2} \qquad \text{as} \quad B\to\infty\end{aligned}\tag{86}$$

In the broken symmetry phase

$$\begin{aligned}\left(\frac{\partial^2 E}{\partial\alpha^2}\right)_B &\to -[1+eB^2\ln^2(eB^2)] \qquad \text{as} \quad B\to 0\\ &\to -\frac{2}{B} \qquad \text{as} \quad B\to\infty\end{aligned}\tag{87}$$

$$\begin{aligned}\left(\frac{\partial^2 E}{\partial B^2}\right)_\alpha &\to -\frac{1}{16}e^2B^2 \qquad \text{as} \quad B\to 0\\ &\to -\frac{1}{2B} \qquad \text{as} \quad B\to\infty\end{aligned}\tag{88}$$

In the normal phase

$$\begin{aligned}\left(\frac{\partial^2 E}{\partial\alpha^2}\right)_B &\to -eB^2[1+\ln(eB^2)]^2 \qquad \text{as} \quad B\to 0\\ &-\frac{1}{2B} \qquad \text{as} \quad B\to\infty\end{aligned}\tag{89}$$

$$\left(\frac{\partial^2 E}{\partial B^2}\right)_\alpha \to -\frac{e}{2} \qquad \text{as} \quad B \to 0$$
$$-\frac{1}{4B^2} \qquad \text{as} \quad B \to \infty \tag{90}$$

7. FORMULATION AS A ONE-MODE PROBLEM

In this section I show that the approximations discussed so far are special cases of a one-mode Hamiltonian. This makes possible some improvements in the ground-states wave function. The transition is again relation to the behavior of an inverse length β entering in the privileged phonon mode. But we are not restricted to the variational treatment of the previous section. Let

$$q(\mathbf{k}) = q_0 X_0(\mathbf{k}) + \sum_{n \neq 0} q_n X_n(\mathbf{k}) \tag{91}$$

where X_0, X_n forms an orthonormal set. In the present paper I do not need to specify the X_n. I take the expectation value with a state vector that ϕ that has the property $A_n \Phi = 0$. Here

$$q_n = \frac{A_n + A_n^+}{\sqrt{2}} \tag{92}$$

Alternatively, the trial state vector has its q_n dependence in a factor $\exp\{-\sum_{n\neq 0}(q_n^2/2)\}$.

We have the one-mode Hamiltonian

$$H = -\frac{B}{2}\sigma_Z - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \int \frac{DX_0}{\sqrt{k}}\, d\mathbf{k}\, q_0 \sigma_x + \frac{T_{00}}{2}(p_0^2 + q_0^2 - 1)$$
$$T_{00} = \int k X_0^2\, dk \tag{93}$$

I now make a particular choice for the mode X_0

$$X_0(k) = \frac{1}{(4\pi\xi)^{1/2}} \frac{D(k)}{\sqrt{k}}\; k + \beta \tag{94}$$

For the acoustic case, this is the same ξ as was defined earlier. I note, in passing, that for the optical case, where $\omega(k)$ is constant, the full spin phonon Hamiltonian has only one phonon mode in interaction with the spin.

We have normalized $X_0(k)$. β is the only free parameter in this variational calculation.

The Hamiltonian takes the form

$$H = -\frac{B}{2}\sigma_z - \frac{D_0}{(\alpha\xi)^{1/2}} q_0\sigma_x + \frac{T_{00}}{2}(p_0^2 + q_0^2 - 1) \tag{95}$$

and

$$T_{00} + \beta = D_0/\xi \tag{96}$$

The above refers to the normal phase. When there is symmetry breaking we use U_c to transform the Hamiltonian first. We consider

$$V_c H V_c^{-1} = \frac{1}{2}\int kh^2\, d\mathbf{k} + \int khq\, d\mathbf{k} + H - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2}\int \frac{Dh}{\sqrt{k}}\, d\mathbf{k}\, \sigma_x \tag{97}$$

We need to find the ground state ξ_0 of the lst three terms as a functional of $h(k)$. Then $h(k)$ is determined from

$$kh(k) + \frac{\delta\xi_0}{\delta h(k)} = 0 \tag{98}$$

Our earlier theories involve $\int p(k) f(k)\, d\mathbf{k} = (\alpha\xi)^{1/2} p_0$ and thus can be viewed as particular approximations to the one-mode Hamiltonian. It is easy to think of better approximations. The problem is exactly soluble in the sense that there is a three-term recursion relation which may be studied numerically to any desired accuracy. There have been many papers devoted to the one-mode problem. Very important is the analysis of Shore and Sander.[9] They used the numerical solution to show the inadequacy of the source type of approximation, which predicts spurious discontinuities of the energy. They suggested an improved variational ansatz. The variational calculation of Section 4 is similar to theirs. For a discussion of analytic approaches to the one-mode Hamiltonian see Wagner[10] and Prelovsek.[7] The present involves the additional step of finding the optimum β, and in the symmetry-breaking phase of $h(k)$. I have not tried to do the extensive numerical work that is needed.

8. CONCLUSIONS

I have discussed the location of the $\alpha(B)$ line and the nature of the transition. The approach has been to start with two simple approximate ground-state wave functions. By contrasting them, one sees the deficiencies and strengths of each of them. I then construct better and more complicated functions that take account of multiple quantum excitations and quantum fluctuations in both normal and broken symmetry phases. The analysis is partly negative in that it shows why one should not believe the predictions of some simple theories. This line of thinking culminates in the formulation of Section 7 that involves a symmetry-breaking field $h(k)$ and a spin coupled dynamically to a single mode of the phonon field and characterized by an inverse length β. It is possible that a definite answer to the behavior for general B is contained in this Hamiltonian. However, I have not carried out the analysis to show this.

Definite conclusions can be obtained by other methods for the $B \ll 1$ case, where there is no transition to order B^2, and for $B \gg 1$, where there is a first-order transition. This is done in the accompanying papers.

Note that in the symmetry-breaking phase, one can always use parity eigenfunctions. We have ground-state wave functions that are eigenfunctions of parity for all α, B. It is just that the zero overlap means that there is no improvement in energy by using such functions. The broken symmetry coincides with the appearance of a $1/|x|$ behavior for the ground-state average $\overline{\sigma_x \phi(x)}$.

REFERENCES

1. A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. T. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys.* **59**:1 (1987).
2. H. Spohn and R. Dumcke, *J. Stat. Phys.* **41**:389 (1983).
3. V. J. Emery and A. Luther, *Phys. Rev.* B **9**:215 (1974).
4. S. Chekravarty, *Phys. Rev. Lett.* **49**:681 (1982).
5. R. Silbey and R. A. Harris, *J. Chem. Phys.* **80**:2615 (1984).
6. A. Tanaka and A. Sakurai, *Prog. Theor. Phys.* **76**:999 (1986).
7. P. Prelovsek, *J. Phys. C* **12**:1855 (1979).
8. R. Beck, N. Götze, and P. Prelovsek, *Phys. Rev. A* **20**:1140 (1979).
9. H. B. Shore and L. M. Sander, *Phys. Rev. B* **7**:4537 (1973).
10. M. Wagner, *Z. Physik B* **37**:225 (1979).