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Ground State of a Spin-Phonon System. II. Adiabatic Limit

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The phase transition for a spin in a magnetic field B coupled to acoustic phonons by a coupling constant α is studied. The case $B \gg 1$ with an upper cutoff of unity for the phonons is studied systematically by using an adiabatic canonical transformation. In leading order the transition line is at $\gamma = 2\alpha/B = 1$. In the normal phase ($\gamma < 1$) the ground-state energy is $-B/2$ plus a function of γ that is given explicitly as the solution of a pair theory. In the broken symmetry phase ($\gamma > 1$) the energy is the classical energy plus the same function of $\sigma = 1/\gamma^2$. It is found that the first derivatives of the energy with respect to α and with respect to B have finite jumps across the transition line. Quantum fluctuations in both phases are treated. Higher-order terms are a series of powers of $1/B$ times functions of γ. The case of a small transverse field B is also studied. The sharp transition disappears and is replaced by rapid variation in a region of order $(B_1/B)^{2/3}$ about $\gamma = 1$.

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

1. INTRODUCTION

I continue[1] the study of the phase transition in the ground-state energy $E_G(\alpha, B)$ for the Hamiltonian

$$H = -\frac{B}{2}\sigma_z - \frac{B_1}{2}\sigma_x - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \int \frac{Dq}{\sqrt{k}}\, d\mathbf{k}\, \sigma_x + \frac{1}{2}\int |k| \left[p(k)\, p(-k) + q(k)\, q(-k)\right] d\mathbf{k} \tag{1}$$

I have included a transverse field B_1 which leads to states that are not eigenfunctions of parity. When $B_1 \ll 1$ one can get insight into the development of the broken symmetry.

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Here I am interested in developing a systematic theory for the case $B \gg 1$.

The frequency associated with a spin flip is larger than all phonon frequencies, since the upper cutoff in $D(k)$ is unity. Direct emission of a single phonon is forbidden by energy conservation. The transition line lies near $\alpha = B/2$, which is the value given by the classical theory. The energy in the classical theory is given by $(B_1 = 0)$

$$
\begin{aligned}
E_G &= -\frac{\alpha}{2} - \frac{B^2}{8\alpha} \qquad \alpha > \frac{B}{2} \\
&= -\frac{B}{2} \qquad\qquad\quad \alpha < \frac{B}{2}
\end{aligned}
\tag{2}
$$

The first derivatives are $(\partial E_G/\partial\alpha)_B = 0$, $(\partial E_G/\partial B)_\alpha = -1/2$ and are continuous across the transition line. The second derivatives exhibit jumps $(\partial^2 E_G/\partial B^2)_\alpha = -1/2B$ and $(\partial^2 E_G/\partial^2\alpha)_B = -2/B$. However, the classical theory neglects quantum fluctuations and is trivial in the normal phase.

I will develop a systematic theory for $B \gg 1$ based on a canonical transform that corresponds to the adiabatic approximation. The non-adiabatic terms can be explicitly calculated. However, the canonical transform must be adapted to account for the broken symmetry phase that is a consequence of the infinite number of phonon degrees of freedom together with the large number of long-wave acoustic phonons. The nonclassical energy is a series in $1/B$ of the form $L_0(\alpha/B) + (1/B)\, L_1(\alpha/B) + \cdots$. In both normal and broken symmetry phases we take account of quantum fluctuations. The transition line still lies near $\alpha \sim B/2$ but the nature of the phase transition is altered. There is now a small jump in the first derivatives of the energy across the line.

I introduce the broken symmetry with

$$
U_c = \exp\left(i \int ph\, d\mathbf{k}\right), \qquad U_c q(k)\, U_c^{-1} = q + h(k) \tag{3}
$$

$$
U_c H U_c^{-1} = H + \frac{1}{2}\int kh^2\, d\mathbf{k} - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \int \frac{Dh}{\sqrt{k}}\, d\mathbf{k}\, \sigma_x + \int khq\, d\mathbf{k} \tag{4}
$$

Next introduce the spin rotation with

$$
W_A = e^{i\sigma_y \theta_A/2}, \qquad \tan\theta_A = \int Y(k)\, q(k)\, d\mathbf{k} \tag{5}
$$

In contrast to the rotation in the classical theory, here $\tan\theta_A$ is linear in the phonon coordinates. As a consequence, there are "recoil" terms. The transform is completed with

$$\begin{aligned} W_A p(k) W_A^{-1} &= p(k) - \frac{\sigma_y}{2} Y(k) \frac{1}{[1+\int Y(k)\, q(k)\, d\mathbf{k}]^2} \\ W_A \sigma_x W_A^{-1} &= \sigma_x \cos\theta_A - \sigma_z \sin\theta_A \\ W_A \sigma_z W_A^{-1} &= \sigma_z \cos\theta_A + \sigma_x \sin\theta_A \end{aligned} \tag{6}$$

2. NORMAL PHASE

Let us concentrate first on the normal phase, where $h(k)=0$. The simplest choice is (for $B_1 = 0$)

$$Y(k) = \left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D}{\sqrt{k}} \frac{1}{B} \tag{7}$$

The transformed Hamiltonian is

$$W_A H W_A^{-1} = H_0 - \sigma_z T \frac{B}{2} + \frac{\alpha}{6B^2} T^{-4} - \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{\sigma_y}{2B} \left\{ \int Dp\, k^{1/2}\, d\mathbf{k},\, T^{-2} \right\}_+ \tag{8}$$

where

$$T^2 = 1 + \frac{\alpha}{\pi B^2} \left(\int \frac{Dq}{\sqrt{k}}\, d\mathbf{k} \right)^2 \tag{9}$$

This is of course exactly equivalent to the original Hamiltonian. The last term, representing a spin flip, contributes in perturbation theory an amount α/B^3. It can be ignored if we calculate to order $1/B$. The third term is $(\alpha/B)(1/6B)$ accurate to $1/B$.

The ground state in the transformed system is $\binom{1}{0}\phi$, where ϕ is the lowest eigenfunction of

$$\mathscr{H} = H_0 - \frac{B}{2} T + \frac{\alpha}{6B^2} \tag{10}$$

Expanding the square root, we obtain

$$\begin{aligned} \mathscr{H} = &-\frac{B}{2} + \frac{\alpha}{6B^2} + H_0 - \frac{\alpha}{4\pi B} \left(\int \frac{Dq}{\sqrt{k}}\, d\mathbf{k} \right)^2 \\ &+ \left(\frac{\alpha}{4\pi B}\right)^2 \frac{1}{B} \left(\int \frac{Dq}{\sqrt{k}},\, d\mathbf{k} \right)^4 \end{aligned} \tag{11}$$

The quartic term is of order $1/B$. In the normal phase the Hamiltonian is (as $B \to \infty$)

$$\mathscr{H} = -\frac{B}{2} + H_0 - \frac{\gamma}{8\pi}\left(\int \frac{Dq}{\sqrt{k}}\, d\mathbf{k}\right)^2, \qquad \gamma = \frac{2\alpha}{B} \tag{12}$$

The eigenvalues are functions of γ. There is no lower bound for $\gamma > 1$ since the equation determining the eigenvalues Ω gives as the condition for a bound state

$$1 = \gamma \int_0^1 \frac{k^2\, dk}{k^2 + |\Omega|^2}, \qquad \Omega^2 = -|\Omega|^2 \tag{13}$$

which has a solution when $\gamma > 1$. This represents a runaway mode. However, the energy is finite when $\gamma < 1$ and as $\gamma \to 1$. The ground-state energy of this pair theory is given by[2]

$$E = -\frac{B}{2} + E_2 \tag{14}$$

$$E_2 = \frac{1}{2\pi} \int_0^\infty dk\, \delta(k)$$

$$\tan \delta(k) = \gamma^2 \frac{\pi}{2} \frac{k D^2(k)}{\rho} \tag{15}$$

$$\rho = 1 - \gamma^2 f \frac{D^2(k_1)\, k_1^2\, dk_1}{k_1^2 - k^2}$$

For our case of a sharp cutoff $D(k) = \theta(1-k)$

$$\rho(k) = 1 - \gamma^2 + \gamma^2 \frac{k}{2} \ln \frac{1+k}{1-k} \tag{16}$$

At $\gamma = 1$ the energy has the finite value

$$E_2(\gamma = 1) = -\frac{1}{2} \int_0^\infty \frac{dy}{\pi^2 + y^2} \tanh \frac{y}{2} \tag{17}$$

The expression for E_2 is complicated in the rest of the region $\gamma < 1$. However, for $\gamma \ll 1$ we obtain the perturbation result

$$E_2 \to -\frac{\gamma}{8} = -\frac{\alpha}{4B} \tag{18}$$

(valid, of course, for $B \gg 1$).

It is not hard to find the ground-state energy to order $1/B$. One needs the pair ground-state wave function $\Psi_p(q(k) \mid \gamma)$. The extra contributions are

$$\Delta E = \frac{\gamma}{12B} + \left\langle \Psi_p \left| \left(\int \frac{Dq}{\sqrt{k}} \, d\mathbf{k} \right)^4 \right| \Psi_p \right\rangle \frac{\gamma^2}{(8\pi)^2} \frac{1}{B} \tag{19}$$

or

$$\Delta E = \frac{\gamma}{12B} + \frac{3}{B} \left(\frac{\gamma}{8\pi} \right)^2 \iint \frac{D(k)\, D(l)}{(kl)^{1/2}} \underbrace{q(k)\, q(l)} \, d\mathbf{k}\, dl \tag{20}$$

The contraction

$$\underbrace{q(k)\, q(l)} = \langle \Psi_p \,| q(k)\, q(l) |\, \Psi_p \rangle$$

is a known function of γ, but we are not interested in the value here. Note that the first derivative $dE_2/d\gamma$ is finite as $\gamma \to 1$.

3. BROKEN SYMMETRY PHASE ($B_1 = 0$)

The corresponding expansion in the broken symmetry phase starts from

$$H = H_0 + \int hkq \, d\mathbf{k} + \frac{1}{2} \int kh^2 \, d\mathbf{k} - \frac{B}{2} \left\{ 1 + \frac{\alpha}{\pi B^2} \left[\int \frac{D}{\sqrt{k}} (h+q) \, d\mathbf{k} \right]^2 \right\}^{1/2} \tag{21}$$

Let

$$\sigma = 1 + \frac{\alpha}{\pi B^2} \left(\int \frac{Dh}{\sqrt{k}} \, d\mathbf{k} \right)^2 \tag{22}$$

and expand the square root. The condition, to order $1/B$, that the linear term in $q(k)$ vanishes is

$$h(k) = \frac{1}{2} \left(\frac{\alpha}{\pi} \right)^{1/2} \frac{D}{k^{3/2}} \sin \theta, \qquad \cos \theta = \frac{B}{2\alpha} \tag{23}$$

This is the same result as in the classical theory. One also finds that $\sigma = (B/2\alpha)^2 = \gamma^{-2}$. However, one now can compute quantum fluctuation effects in the broken symmetry phase. Neglecting the quartic term ($\sim 1/B$), one has the Hamiltonian

$$\mathscr{H} = -\frac{\alpha}{2} - \frac{\sigma}{8\pi} \left(\int \frac{Dq}{\sqrt{k}} \, d\mathbf{k} \right)^2 + H_0 \tag{24}$$

σ replaces γ in the energy E_2. Far above the transition line there is the fluctuation contribution $-\sigma/8$. The energies of normal and broken symmetry phases match at $\gamma=\sigma=1$, and the $1/B$ contributions are the same.

While the energy is continuous, the first derivatives are not. In the normal phase

$$\left(\frac{\partial E_2}{\partial \alpha}\right)_B = \frac{2}{B}\frac{dE_2}{d\gamma}, \qquad \left(\frac{\partial E_2}{\partial B}\right)_\alpha = -\frac{\gamma}{B}\frac{dE_2}{d\gamma} \tag{25}$$

In the broken symmetry phase

$$\left(\frac{\partial E_2}{\partial \alpha}\right)_B = -\frac{4}{B}\frac{1}{\gamma^3}\frac{dE_2}{d\sigma}, \qquad \left(\frac{\partial E_2}{\partial B}\right)_\alpha = \frac{2}{B}\frac{1}{\gamma^2}\left(\frac{dE_2}{d\sigma}\right) \tag{26}$$

At the transition line $\gamma=\sigma=1$ and $dE_2/d\gamma = dE_2/d\sigma$. So the first derivatives jump by an amount of order $1/B$.

4. WEAK TRANSVERSE FIELD

I now add a term $-(B_1/2)\,\sigma_x$ to the Hamiltonian. This term does not commute with the parity operator. When the coupling constant is zero the ground-state energy is $-[(B/2)^2+(B_1/2)^2]^{1/2}$. When $B=0$ the ground-state energy is no longer degenerate. It is $-B_1/2-\alpha/2$ with a state vector $\binom{1}{1}\phi_0$. We are interested here in the limit $B \gg 1$ with $B_1 \ll 1$. There is no longer any phase transition as a function of α. Instead there is a rapid transition from normal to ordered phase in the vicinity of $\alpha = B/2$. The width of the transition region is of order $(B_1/B)^{2/3}$.

The results follow immediately when we use the angle

$$\tan\theta_A = \frac{B_1}{B} + \frac{1}{B}\left(\frac{\alpha}{\pi}\right)^{1/2} \int \frac{D}{\sqrt{k}}\,[h+q]\,d\mathbf{k} \tag{27}$$

To calculate to order $1/B$, we can again neglect the recoil terms, expand the leading square root term, and choose $h(k)$ to make the linear term in $q(k)$ vanish. This gives a Hamiltonian

$$\mathscr{H} = \xi_0 - \frac{\gamma}{8\pi B}\frac{1}{(1+u^2)^{3/2}}\left(\int \frac{Dq}{\sqrt{k}}\,d\mathbf{k}\right)^2 + H_0 \tag{28}$$

$$\xi_0 = -\frac{B}{2}(1+u^2)^{1/2} + \frac{\alpha}{2}\frac{u^2}{1+u^2} \tag{29}$$

The quantity u obeys the equation

$$\left(u - \frac{B_1}{B}\right)(1+u^2)^{1/2} = \left(\frac{2\gamma}{B}\right)u \tag{30}$$

One finds for the dispaced phonon field $h(k)$

$$h(k)=\frac{1}{2}(\alpha\pi)^{1/2}\frac{D}{k^{3/2}}\frac{u}{(1+u^2)^{1/2}} \tag{31}$$

Let us first analyze the equation for u. Note that at $\gamma=1$ the solution is $u^*=(2B_1/B)^{1/3}$, neglecting higher-order terms in (B_1/B). The coefficient of the pair term is $-(\gamma/8\pi h)[1-(3/2)(2B_1/B)^{2/3}]$. The energy ξ_0 becomes

$$\xi_0=-\frac{B}{2}-\frac{3}{16}\left(\frac{2B_1}{B}\right)^{2/3} \tag{32}$$

In the weak coupling region $\gamma<1$ we have

$$u\to\frac{B_1}{B}\frac{1}{1-\gamma} \tag{33}$$

provided we are outside of a B_1-dependent region near $\alpha=B/2$. Then

$$\xi_0=-\frac{B}{2}\left[1+\frac{1}{2}\left(\frac{B_1}{B}\right)^2\frac{1}{1-\gamma}\right] \tag{34}$$

To get the total ground-state energy, we must add the contribution from the pair term. In $\gamma\ll 1$ this is

$$-\frac{\gamma}{8}\left[1-\frac{3}{2}\left(\frac{B_1}{B}\right)^2\right] \tag{35}$$

We recover the perturbation result.

In the ordered or "broken symmetry" phase $\alpha/2B>1$

$$u\to(\gamma^2-1)^{1/2}-1+\frac{1}{1-(B/2\alpha)^2}\frac{B_1}{B} \tag{36}$$

$$\xi_0\to-\frac{\alpha}{2}-\frac{B^2}{8\alpha}-\frac{B_1}{2}\left[1-\left(\frac{B}{2\alpha}\right)^2\right]^{1/2} \tag{37}$$

When $\alpha\gg B/2$ the pair term gives the quantum fluctuation term $-1/32\, B^2/\alpha^2$.

In the limit $\alpha\to\infty$ we obtain the simple $\xi_0=-\alpha/2-B_1/2$ with the ground-state wave function $\binom{1}{1}\phi_0$.

5. CONCLUSIONS

The adiabatic canonical transformation prepares the Hamiltonian by referring the spin variable to the instantaneous phonon coordinates. It is in the spirit of the classical theory, which uses mean values of the phonon coordinates. However, the adiabatic approach gives a meaningful normal phase and a description of quantum fluctuations. It also changes the transition from second order to first order. It should be noted that many people have used this transformation before.[3] For spin-1/2 particles there is a clear-cut isolation of the nonadiabatic effects. This simplifies the systematic analysis as compared with the usual treatments of the adiabatic approximation, even though the physics is no different. What has been missing, and is supplied here, is the extension to the symmetry-breaking region and an analysis of the pair Hamiltonian.

The results for $B \gg 1$ can be obtained in other ways. For example, they can be found easily from the Green's function treatment, with symmetry breaking, of Prelovsek[4] and others. The adiabatic transformation has the advantage of making obvious the role of the parameter γ and the expansion in $1/B$. It should also be noted that the domain of validity of the adiabatic approach can be extended, as noted by Carmeli and Chandler.[5] A variational calculation can be made with a

$$Y(k) = \lambda \left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D}{\sqrt{k}} \frac{1}{k+\beta}$$

With $\gamma = 1$ and $\beta = B$ one obtains the lowest order result even if B is not large. However, my main concern has been with the behavior at the transition line.

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