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Ground State of a Spin-Phonon System. III. Small-B Limit

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The ground state of the spin-one-half acoustic phonon system is studied in the limit $B \ll 1$. The technique is to combine the Brillouin–Wigner variational perturbation theory with a source canonical transformation. With the $B=0$ source transform the energy is calculated as a function of coupling constant through terms of order B^2. To this order there is no phase transition. The theory gives the crossover from perturbation theory to an improved classical theory with quantum fluctuations. With a source transform with a nonzero inverse length β the energy estimate is further improved to next order in the coupling constant and for larger values of B. The soft, infinite-order transition of the modified source theory is removed in the limit $B \ll 1$.

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

1. INTRODUCTION

I continue[1] the study of the spin phonon system with unperturbed splitting B, coupling constant α, and upper phonon cutoff unity. My goal is the systematic study of the $B \ll 1$ limit. The variational calculations of part I showed that there are two regions of α where there are changes in behavior. The variational extension of the modified source theory gave a continuous crossover to a classical energy near $\alpha = 1/2$. This occurs with a parity eigenfunction, nonzero overlap Z, and a finite inverse length β for the correlation functions. However, in the region $1/2 < \alpha < 1$, when $B \ll 1$, we have $Z = (\beta e)^{\alpha/1-\alpha}$ and both Z and β are very small. Still at $\alpha \sim 1$ there is a weak, infinite-order transition superposed on the smooth classical behavior. Another, symmetry-breaking, theory also locates the crossover to classical behavior at $\alpha \sim 1/2$. But it gives a second-order phase transition

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with long-range correlation functions for all $\alpha > 1/2$ and classical behavior with quantum fluctuations. Nothing unusual happens near $\alpha \sim 1$. If one puts an infrared cutoff $k_0 \ll 1$, both theories give the crossover to classical behavior at $\alpha \sim 1/2$, and have everywhere continuous energies and finite range (which, however, depends on k_0).

These calculations illuminate the deficiencies of the simple modified source and classical theories. Here I try a different approach that focuses specifically on $B \ll 1$.

I examine the simplest approach in Sections 2–4. It features a source transformation with $f_0(k) = \frac{1}{2}(\alpha/\pi)^{1/2} D/k^{3/2}$. The transformed Hamiltonian has the constant $-\alpha/2$ and a spin-dependent term that is proportional to B. The diagonal part, proportional to B, is zero because the overlap is zero. The Hamiltonian is adapted to a perturbation treatment for $B \ll 1$. However, simple Rayleigh–Schrödinger perturbation theory is not appropriate. Instead, Brillouin–Wigner theory, which incidentally yields an upper bound, provides an effective control of the infrared behavior. The analysis can be carried out through terms of order B^2. In fact, for $\alpha \ll 1$ one finds the additional term $-B/2$, which is present in ordinary perturbation theory as applied to the original Hamiltonian. At $\alpha = 1/2$ there is a smooth crossover to the classical theory with additional quantum fluctuations. The width of the crossover depends logarithmically on B. The analysis uses explicit parity eigenfunctions and indicates that there is no transition at all near $\alpha = 1$, to order B^2.

In Section 5, I prepare the Hamiltonian with a modified source transformation

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

and then apply the Brillouin–Wigner (BW) analysis. If one uses the $\beta = BZ$ of the standard modified source theory, one starts with a diagonal part that has the phase diagram of that theory and with an off-diagonal part that is again proportional to B. The BW improvement now supplies the smooth crossover to classical behavior near $\alpha = 1/2$ that is missing in the modified source theory. It also yields quantum fluctuation corrections to the classical theory. On the other hand, the weak, infinite-order transition near $\alpha = 1$ remains. This theory is also valid for larger values of B in the region $\alpha \ll B/2$.

The analysis can be extended by leaving β free for variation at the end of the BW procedure. If $B \ll 1$, one finds that $\beta \ll 1$ can be chosen to be nonzero and to lower the energy. This wipes out the infinite-order transition of the modified source theory. The extra terms in the energy are very small $[\sim(B^2/\alpha)\exp(-2\alpha^2/B^2)]$, so that there is no conflict with the results of Section 2, which holds to order B^2.

Together with the results of part II which yield a first-order transition in $B \gg 1$ we have a partial understanding of the phase diagram. The region $B \sim 1$ is at present only treated by the variational approximations of I. There is still no convincing theory of this region.

2. BRILLOUIN–WIGNER TREATMENT

Let us start by transforming the Hamiltonian with

$$U = \exp\left(i\sigma_x \int f_0\, p\, d\mathbf{k}\right) \tag{1}$$

$$f_0(k) = \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D}{k^{3/2}} \tag{2}$$

Then

$$\begin{aligned} H_T &= UHU^{-1} = H_0 + V - \frac{\alpha}{2}(1 - k_0) \\ V &= -\frac{B}{2}\left(\sigma_z \cos 2\int f_0\, p\, d\mathbf{k} + \sigma_y \sin 2\int f_0\, p\, d\mathbf{k}\right) \end{aligned} \tag{3}$$

When there is an infrared cutoff the overlap is

$$Z \equiv \int \phi_0^2 \cos\left(2\int f_0\, p\, d\mathbf{k}\right) d\mathbf{p} = \exp\left(-\int f_0^2\, d\mathbf{k}\right) = k_0^{\alpha} \tag{4}$$

This form of the Hamiltonian has the perturbation V strictly proportional to B and is the natural starting point when $B \ll 1$. The unitary operator commutes with the parity operator. We will use wave functions that involve operators that commute with parity operating on a noninteracting ground state $\phi_0\binom{1}{0}$. Thus, we will have a ground state that is always an eigenfunction of parity. It turns out that we do not need the infrared cutoff and can set $k_0 = 0$ from the start.

I will show that as α starts out from zero, the energy starts as $-\alpha/2 - B^{(1+\alpha)}/2$ as in the source theory. But the transition region is near $\alpha = 1/2$ (rather than $\alpha = 1$) as for the variational calculation of part I. For $\alpha > 1/2$ one approaches the result of the classical theory $-\alpha/2 - B^2/8\alpha$. The theory includes quantum fluctuations and is everywhere superior to both. The energy and all its derivatives with respect to α are continuous functions of α.

My aim is to calculate the energy accurately through terms of order B^2. (From this point on I leave off the constant $-\alpha/2$, which can be restored at the end.) The energy will be calculated by the lowest order Brillouin–Wigner perturbation theory. If $H_T = H_0 + V$, the energy is

$$E \leqslant -W(E) \tag{5}$$

where

$$W(E) = \langle \Phi_0 | \, V \frac{1}{H_0 - E} V \, | \Phi_0 \rangle \tag{6}$$

Here Φ_0 is the noninteracting ground state, and it is assumed that $\langle \Phi_0 | \, V \, | \Phi_0 \rangle = 0$ as in the present situation. The presence of E in the propagator $1/(H_0 - E)$ is essential, and one would lose everything with the Rayleigh–Schrödinger form.

The variational basis of the BW theory is that the true energy

$$E \leqslant \frac{\langle \Phi | \, H_0 + V \, | \Phi \rangle}{\langle \Phi \mid \Phi \rangle} \tag{7}$$

for any trial function Φ. Choose the unnormalized

$$\Phi = \left(1 - \lambda \frac{1}{H_0 - E} V \right) \Phi_0 \tag{8}$$

where λ and E are variational parameters. There is no problem in taking E to be the true energy. Then for $\lambda = 1$ a short calculation gives the above result. For $\lambda \neq 1$ we have

$$E \leqslant (\lambda^2 - 2\lambda) \, W(E) \tag{9}$$

where the minimization with respect to λ gives

$$\lambda^2 W \frac{\partial W}{\partial E} + \lambda \left(W + E \frac{\partial W}{\partial E} \right) - W = 0 \tag{10}$$

However, we do not need this improvement in the calculation through terms of order B^2. In all of these arguments one notes that expressions with an odd number V operators also do not contribute.

To have an explicit form, use the parametrization

$$\frac{1}{H_0 + |E|} = \int_0^\infty dy \, e^{yE} e^{-yH_0}, \qquad \varepsilon = |E| \tag{11}$$

We have the integrals

$$\left\langle\left[\exp\left(i2\int fp\,d\mathbf{k}\right)\right]\phi_0\,|\exp(-yH_0)|\left[\exp\left(i2\int fp\,d\mathbf{k}\right)\right]\phi_0\right\rangle$$
$$= \exp\left\{-2\int f^2[1-\exp(-yk)]\,d\mathbf{k}\right\}$$
$$\left\langle\left[\exp\left(i2\int fp\,d\mathbf{k}\right]\phi_0\,|\exp(-yH_0)|\left[\exp\left(-i2\int fp\,d\mathbf{k}\right)\right]\phi_0\right\rangle \tag{12}$$
$$= \exp\left\{-2\int f^2[1+\exp(-yk)\,d\mathbf{k}\right\}$$

The second integral vanishes as the infrared cutoff goes to zero. This is the usual zero overlap with our $f(k)=f_0(k)$.

Hence the expression for the energy is

$$|E|\geqslant\left(\frac{B}{2}\right)^2\int_0^\infty dy\,e^{-y\varepsilon}e^{-2\alpha J(y)} \tag{13}$$

Here

$$J(y)=\int_0^y dk\,\frac{1-e^{-k}}{k}=\int_0^1\frac{dk}{k}(1-e^{-yk}) \tag{14}$$

$J(y)$ can be expressed in terms of the exponential integral

$$J(y)=\ln y+\gamma+E_1(y), \qquad \gamma=0.5772... \tag{15}$$

It has the limiting behavior

$$J(y)\to y-\frac{y^2}{4} \qquad \text{as} \quad y\to 0$$
$$\to \ln y+\gamma+\frac{e^{-y}}{y} \qquad \text{as} \quad y\to\infty \tag{16}$$

3. ANALYSIS OF $I(b|\epsilon)$

Let

$$b=2\alpha-1$$
$$I(b\,|\,\varepsilon)=\int_0^\infty dy\,e^{-y\varepsilon}e^{-(1+b)J(y)} \tag{17}$$

We are particularly interested in the behavior as $\varepsilon \to 0$. There is an upper bound that arises because

$$J(y) \geqslant \ln(1+y) \tag{18}$$

The leading terms are the same for $y \to 0$ and $y \to \infty$ but differ by the Euler constant γ as $y < \infty$. The bound is

$$I(b \mid \varepsilon) \leqslant I_0(b \mid \varepsilon) \tag{19}$$

$$\begin{aligned} I_0(b \mid \varepsilon) &= \int_0^\infty dy\, e^{-y\varepsilon}(1+y)^{-(1+b)} \\ &= e^{\varepsilon}\varepsilon^b \Gamma(-b \mid \varepsilon) \end{aligned} \tag{20}$$

Here Γ is the incomplete gamma function.[2] The expansion in ε for all noninteger b is

$$I_0(b \mid \varepsilon) = e^{\varepsilon}\left\{\varepsilon^b \Gamma(-b) + \frac{1}{b} + \frac{\varepsilon}{1-b} - \frac{\varepsilon^2}{2(2-b)} + \cdots\right\} \tag{21}$$

If $b > 1$ $(\alpha > 1)$, the leading terms are

$$I_0(b \mid \varepsilon) \to \frac{1}{b} + \frac{\varepsilon}{b(1-b)} \tag{22}$$

If $b < 1$ $(\alpha < 1)$, the noninteger power of ε is important

$$I_0(b \mid \varepsilon) \to \frac{1}{b} + \varepsilon^b \Gamma(-b) + \cdots \tag{23}$$

In addition, for $b < 0$ $(\alpha < 1/2)$, the ε^b term dominates the constant $1/b$. The Γ function is analytic in b in the vicinity of $b = 0$, but there is a confluence of ε^b and the constant term, leading to logarithmic terms in ε. We have

$$\Gamma(b \mid \varepsilon) = -\gamma - \ln \varepsilon + \varepsilon - b\left(\frac{\ln^2 \varepsilon}{2} + \gamma \ln \varepsilon + c_2\right) \tag{24}$$

Here I have used

$$\begin{aligned} \Gamma(-b) &= -\frac{1}{b} - \gamma - bc_2 \\ c_2 &= \frac{\pi^2}{12} + \frac{\gamma^2}{2} \end{aligned} \tag{25}$$

There is the same type of behavior at all integer b. At $b=1$

$$I_0(1\,|\,\varepsilon)=e^{\varepsilon}\{1+\varepsilon\ln\varepsilon+(\gamma-1)\,\varepsilon+\cdots\} \tag{26}$$

I now turn to the analysis of $I(b\,|\,\varepsilon)$. The results are similar to those for $I_0(b\,|\,\varepsilon)$. When $b>1$ we only need

$$I(b\,|\,\varepsilon)\to K_0(b)-\varepsilon K_1(b)+\cdots \tag{27}$$

We have two sets of moments

$$\begin{aligned} K_n(b)&=\int_0^\infty dy\; y^n e^{-(1+b)J(y)} \\ L_n(b)&=\int_0^\infty dy\; y^n e^{-y} e^{-(1+b)J(y)} \end{aligned} \tag{28}$$

The K_n only exist for $n<b$. Integrating by parts, we have the relation

$$K_n(b)=\frac{b+1}{b-n}\,L_n(b) \tag{29}$$

For any given $b>1$, terms in $\ln\varepsilon$ appear for $n>b$, but will not be needed in this analysis.

To handle the case of $b<1$, note the functional equation (obtained by integration by parts

$$\left(\varepsilon\frac{\partial}{\partial\varepsilon}-b\right)I(b\,|\,\varepsilon)=-(b+1)\,I(b\,|\,\varepsilon+1) \tag{30}$$

Near $\varepsilon=0$

$$I(b\,|\,\varepsilon+1)=\sum\frac{(-1)^n}{n!}\,L_n \tag{31}$$

For noninteger b we have the solution

$$I(b\,|\,\varepsilon)=C(b)\,\varepsilon^b-\sum_n\frac{b+1}{n-b}\frac{(-1)^n}{n!}\,\varepsilon^n L_n \tag{32}$$

The constant $C(b)$ is obtained by equating the two different expressions for $I(b\,|\,1)$,

$$C(b)=-\frac{1}{b}\,L_0+\sum_{n\neq 0}\frac{1+b}{1-b}\frac{(-1)^n}{n!}\,L_n(b) \tag{33}$$

At $b=0$ ($\alpha=1/2$), dropping terms that vanish as $\varepsilon \to 0$,

$$I(0 \mid \varepsilon) = -e^{-\gamma} \ln \varepsilon - \sum_{n \neq 0} \frac{1}{n} \frac{(-1)^n}{n!} L_n(0) \tag{34}$$

Near $b=0$, keeping only terms that become infinite as $\varepsilon \to 0$,

$$I(b \mid \varepsilon) = -e^{-\gamma} \ln \varepsilon - b \left\{ e^{-\gamma} + L_0^1(0) - \sum_{n \neq 0} \left[\frac{(-1)^n}{n!} \frac{L_n(0)}{n} \right] \ln \varepsilon + e^{-\gamma} \ln^2 \varepsilon \right\} \tag{35}$$

At $b=1$ ($\alpha=1$) the solution is

$$I(1 \mid \varepsilon) = 2e^{-\gamma} + e^{-2\gamma} \varepsilon \ln \varepsilon + O(\varepsilon) \tag{36}$$

The expressions involve the quantities $L_n(b)$. Certain special values can be obtained exactly. Using the expression for $J(y)$ in terms of the exponential integral $E_1(y)$ and integrating by parts, we find

$$L_n(n) = \frac{e^{-(1+n)\gamma}}{1+n} \tag{37}$$

Since $dJ/dy \geqslant 0$, we have $(dL_n/db)(b) < 0$ with $L_n(-1) = n!$.

In particular, $L_0(b)$ dominates for $b > 1$ as $\varepsilon \to 0$ and is important for all b. It is a smooth decreasing function starting at $L_0(-1) = 1$ with $L_0(0) = e^{-\gamma} = 0.5614$. For large b there is the asymptotic expansion

$$L_0(b) \to \frac{1}{1+b} \left[1 - \frac{1}{2(1+b)} + \cdots \right] \tag{38}$$

There is an elementary lower bound that follows from $J(y) \leqslant y$. It is

$$L_0 \leqslant 1/(b+2) \tag{39}$$

There is a stronger lower bound that follows from Jensen's inequality with a weight function $w(t) = te^{-yt}$. The optimum t is

$$t = \alpha + (1+\alpha^2)^{1/2} \tag{40}$$

$$L_0 \geqslant \exp\left[(2\alpha - 1) \ln t + 1 - \frac{1}{t} - 2\alpha \ln(1+t) \right] \tag{41}$$

The value at $\alpha = 1/2$ ($b=0$) is 0.560, close to the exact 0.5614.

There is an upper bound that follows from $J(y) \geqslant \ln(1+y)$,

$$L_0 \leqslant e^1 \Gamma(-b \mid 1) \tag{42}$$

and may be computed from tables of the incomplete gamma function.

4. GROUND-STATE ENERGY

Let us now turn to the results for the ground-state energy, given as the solution of

$$\varepsilon = (B/2)^2\, I(b \mid \varepsilon) \tag{43}$$

If we calculate only to order B^2, we can set $\varepsilon = 0$ on the right-hand side in the entire region $\alpha > 1/2$. Then

$$\varepsilon = \left(\frac{B}{2}\right)^2 \frac{2\alpha}{2\alpha - 1} L_0(b) \tag{44}$$

This approaches

$$\varepsilon = \left(\frac{B}{2}\right)^2 \frac{1}{2\alpha}\left(1 + \frac{1}{4\alpha} + \cdots\right) \tag{45}$$

when $2\alpha \gg 1$. The last term arises from quantum fluctuation corrections to the classical theory. As α approaches 1/2 from above

$$\varepsilon \to \left(\frac{B}{2}\right)^2 \frac{e^{-\gamma}}{2\alpha - 1} \tag{46}$$

Of course this no longer holds near $\alpha = 1/2$ when ε is large. Fractional and logarithmic terms only enter in higher order and there is nothing special about the region $\alpha \sim 1$.

In the region $\alpha < 1/2$ we need to retain the fractional ε^b term and the constant term in $I(b \mid \varepsilon)$. Then

$$\varepsilon = \left(\frac{B}{2}\right)^2 \left[C(b)\, \varepsilon^b + \frac{b+1}{b} L_0(b)\right] \tag{47}$$

Since $b < 0$, the fractional term dominates and

$$\varepsilon \to \{(B/2)^2\, C\}^{1/2(1-\alpha)} \tag{48}$$

At $b = 0$ ($\alpha = 1/2$) we use Eq. (34). ε is obtained as the solution of

$$\varepsilon^* = (B/2)^2\, e^{-\gamma} \ln 1/\varepsilon^* \tag{49}$$

ε^* involves an infinite series of logarithms of B. Then one uses Eq. (35), linear in b, to find ε in the vicinity of $b = 0$. The width of the crossover region is of order $b \sim 1/\ln(1/\varepsilon^*)$ and goes slowly to zero as $b \to 0$.

In the present theory, accurate to order B^2, the transition from the weak coupling to classical theory is smooth. It occurs near $\alpha = 1/2$. All of this is compatible with the variational calculation of I. On the other hand, the present analysis is superior for $\alpha \gg 1$, since it includes quantum fluctuations. The variational calculation gives an infinite-order transition at $\alpha = \frac{1}{2}[1 + (1 + B^2)^{1/2}]$ for $B < e/(e^2 - 1/4)$. The modified source theory gives the same type of transition at $\alpha = 1$ for $B < 1/e$. The present analysis gives no transition at all. The two results are in agreement when one calculates energies to order B^2. The energies in the variational and source calculations are of order $(Be)^{1/(1-\alpha)}$, i.e., vanishingly small near $\alpha = 1$.

What really happens for $B \ll 1$ is not settled by this analysis. The variational calculation neglects quantum fluctuations in the higher α phase and is therefore suspect. In the next section I attack the $B < 1$ region starting from a Hamiltonian that has been prepared to include the modified source theory in the unperturbed Hamiltonian. I show that there is in fact no transition at all near $\alpha = 1$ when $B \ll 1$.

5. APPLICATION TO SOURCE THEORY

One can apply the Brillouin–Wigner variational treatment to a Hamiltonian that is first prepared by making a source-type canonical transformation. The value of this procedure as a starting point for a systematic analysis was emphasized by Emery and Luther,[3] who noted that the $-(BZ/2)\,\sigma_z$ term removes the degeneracy at $B = 0$.

Let us introduce

$$U_s = \exp\left(i \int pf\, d\mathbf{k}\, \sigma_x\right) \tag{50}$$

$$f(k) = \frac{1}{2}\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{D}{\sqrt{k}} \frac{1}{k+\beta}, \qquad \ln\frac{1}{Z} = \xi(\beta) \tag{51}$$

We leave β free and arrange the Hamiltonian as

$$U_S H U_S^{-1} = -\frac{\alpha}{2}\frac{1}{1+\beta} - \frac{BZ}{2}\sigma_z + V_1 + V_2 + H_0 \tag{52}$$

$$V_1 = -\frac{B}{2}\sigma_z\left(\cos 2\int p\, d\mathbf{k} - Z\right) - \sigma_y\left(\frac{B}{2}\sin 2\int fp\, d\mathbf{k} - \beta \int pf\, d\mathbf{k}\right)$$

$$V_2 = \beta \int f(\sigma_y p - \sigma_x q)\, d\mathbf{k} \tag{53}$$

Note the consequences of this arrangement. First, V_2 vanishes when applied to the new unperturbed state vector $\binom{1}{0}\phi_0$, so that it does not enter in the BW calculation. Second, in the normal phase ($\beta \neq 0$) the σ_z part of

V_1 starts as α^2. The contribution from the off-diagonal σ_y part is $\sim\alpha^3$. So we will obtain results that are valid to order α^2 for all B. Third, if β is chosen to have the modified source value $\beta = BZ$, V_1 has an overall factor B. The treatment is thus again suited to a study of the $B \ll 1$ limit.

Finally, if $\beta = BZ$, the starting point is the full phase diagram of the modified source theory. The BW treatment allows us to incorporate quantum fluctuations and the crossover to classical theory for $1/2 < \alpha < 1$ when $B < 1$.

There is an advantage in leaving β free and determining it later by the variational principle. Introduce

$$\varepsilon_1 = -E - \frac{\alpha}{2}\frac{1}{1+\beta} - \frac{BZ}{2} \tag{54}$$

$$\eta(y) = \int f^2 e^{-yk}\, d\mathbf{k} \tag{55}$$

Using our earlier procedure

$$\varepsilon_1 \geqslant \left(\frac{B}{2}\right)^2 \int_0^\infty e^{-y\varepsilon_1}\, dy\, Z^2(\cosh 2\eta - 1) + \int_0^\infty e^{-y(e_1 - BZ)} \left\{\left(\frac{BZ}{2}\right)^2 \sinh 2\eta - \beta BZ\eta + \frac{\beta^2}{2}\eta\right\} \tag{56}$$

In the large-α region with $\beta = 0$ this is the theory of the previous section. However, we can now ask whether it is possible to improve the result by taking $\beta \neq 0$ in this region. This is indeed the case.

When $\beta \ll 1$ we expand $\eta(y)$. There is a term in $\beta \ln \beta$. Then the equation determining ε_1 simplifies to

$$\varepsilon_1 = (B/2)^2\, I(b \mid \varepsilon_2) \tag{57}$$

with

$$\varepsilon_2 = \varepsilon_1 - 4\beta \ln \frac{1}{\beta} \cdot \alpha \tag{58}$$

We determine β by examining the energy expression

$$|E| = \frac{\alpha}{2} - \frac{\alpha\beta}{2} + \frac{(\beta e)^\alpha}{2} + \varepsilon_1 \tag{59}$$

since $Z \to (\beta e)^\alpha$. In the region $\alpha > 1$

$$\varepsilon_1 \to \left(\frac{B}{2}\right)^2 \left\{K_0(b) + 4\alpha K_1(b)\, \beta \ln \frac{1}{\beta}\right\} \frac{1}{1 + (B/2)^2\, k_1} \tag{60}$$

It is now possible to choose $\beta \ll 1$ but $\neq 0$. The $\beta \ln \beta$ term dominates the β^α term of the source theory and we find $(B \ll 1)$

$$\beta e = \exp\left(-\frac{1}{2B^2}\frac{1}{K_1}\right) \to \exp\left(-\frac{2\alpha^2}{B^2}\right) \tag{61}$$

The energy of the $\beta = 0$ theory is lowered by the very small term

$$\frac{B^2}{4\alpha}\frac{1}{e}\exp\left(-\frac{2\alpha^2}{B^2}\right) \tag{62}$$

On the other hand, in the region $\alpha < 1$, ε_1 is again shifted by a term proportional to $\beta \ln(1/\beta)$. But this is small compared to the source term β^α. So β is determined for $\alpha < 1$ by the theory of Sections 2–4. In the close vicinity of $\alpha = 1$ there is a smooth change in β determined by the confluence of the two types of terms.

The result of this section is that the combination of the source transform with an inverse length β and the BW variational approach offers great advantages. Not only do we correct the source theory to cover the crossover to classical behavior plus quantum fluctuations near $\alpha = 1/2$, as was the case for the $\beta = 0$ theory. We also obtain a better calculation of the energy for larger values of B in the normal regime. This is already achieved with $\beta = BZ$.

By leaving β free for variation, we wipe out the soft transition of the source theory near $\alpha = 1$ and lower the energy further. Of course the full analysis of Eq. (56) is very complicated. We have no definite conclusions about the transition when $B \sim 1/e$. The results of Part II show that there is a first-order transition that develops at some point when B is increased.

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