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A squeezed state approach for the large polarons

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Abstract. The ground state energy of large polarons is investigated by means of squeezed states. First we introduced single-mode squeezed states and used the variational method to calculate this energy. This gives a result that is valid in the weak-coupling regime and only for very small values of the coupling constant. In order to improve the result we have considered two-mode squeezed states in which the correlation between phonons is involved. In this way the ground state energy is found to be lower than the Feynman result in the intermediate-coupling regime for $\alpha < 3.7$.

1. Introduction

The polaron concept was proposed by Landau [1] to examine the self-trapping phenomena of an electron in crystal lattices. However, it is usually considered today that the subject of the polaron was developed, by the pioneering work of Fröhlich [2], whose formulation was based on quantum field theory arguments. An electron interacting with LO phonons is described by the Fröhlich Hamiltonian (FH)

$$H = \frac{p^2}{2m} + \sum_{q} \hbar \omega_q b_q^{\dagger} b_q + \sum_{q} V_q (b_q^{\dagger} \exp(-iq \cdot r) + HC)$$
(1)

where $p = \hbar k$ is the electron momentum with band mass *m* and the $b_q^{\dagger}(b_q)$ are the creation (annihilation) operators for an LO phonon with a wave vector *q* and energy $\hbar \omega_q$. The interaction of the electron with phonons is represented by the last term, where

$$V_{q} = -i(\hbar\omega_{0}/qu^{1/2})(4\pi\alpha/V)^{1/2}.$$
(2)

Here V is the volume of the system, α is the coupling strength, and $u = (2m\omega_0/\hbar)^{1/2}$. In (2), the LO phonons are assumed to be dispersionless, i.e. $\omega_a = \omega_0$.

Although the FH has not been exactly solved so far, depending on the values of α , it is possible to obtain solutions by various approaches. For $\alpha < 1$, the weak-coupling region, perturbation theories give satisfactory results. For $\alpha > 6$, which is the strong-coupling region, the best available result is due to Miyake [3]. In the intermediate-coupling region between these two, the unitary transformation and variational methods developed by Lee, Low and Pines (LLP) [4] is a widely used approximation in the polaron theory. Feynman [5] has successfully applied his path integral formulation of quantum mechanics to solve the FH for all coupling strengths, and his method is now used as the standard to which other theories are compared.

In recent years squeezed states of the electromagnetic field have become common knowledge to those who are interested in quantum optics. These states are non-classical in the sense that uncertainty in one variance is compressed at the expense of the complementary variance of two non-commuting operators, while keeping their product at a minimum value as predicted for coherent states [6]. Similar arguments should be valid for lattice waves in solids. In this connection, such treatments as squeezed states of phonons are succesfully applied to small polarons in one dimension [7], to the ground state of a tunnelling particle coupled to boson excitation [8] and to acoustic polarons in three dimensions [9].

In the present work, our aim is to choose a single LO phonon from the phonon cloud accompanying the electron, and to form single-mode squeezed states. In order to observe the effect of such states on the polaron, in section 2 we calculate within the LLP model the ground state energy. In section 3 we consider two-mode squeezed states by which the correlation between phonons is included in the energy calculation. In the last section we compare the approach introduced in the previous sections with different theories and discuss the validity of our results.

2. Single-mode squeezed states

2.1. The Lee-Low-Pines transformations

The conservation of the total momentum P allows us to eliminate the electron coordinate r, through the first canon-ical transformation introduced by LLP [4]

$$U_1 = \exp\left[i\left(P - \sum_{q} \hbar q b_q^{\dagger} b_q\right) \cdot r\right].$$
(3)

The second transformation used by LLP is

$$U_2 = \exp\left[\sum_{q} \left(f_q b_q^{\dagger} - f_q^* b_q\right)\right] \tag{4}$$

where f_q is used as a variational function to be determined by minimizing the energy functional. The last transformation generates coherent states for phonon fields.

In the present work we are interested in the ground state energy; owing to this fact and to make later calculations more manageable we will in what follows take P = 0.

Under these transformations the FH becomes

$$\mathcal{H} = U_2^{-1} U_1^{-1} H U_1 U_2 = \sum_{i=0}^{4} H_i$$
(5)

where

$$H_0 = \sum_{q} \hbar \Omega_q |f_q|^2 + \sum_{q} (V_q f_q + V_q^* f_q^*)$$
(6a)

$$H_1 = \sum_{q} \left[(\hbar \Omega_q f_q + V_q^*) b_q^{\dagger} + \text{HC} \right]$$
(6b)

$$H_{2} = \sum_{q} \hbar \Omega_{q} b_{q}^{\dagger} b_{q} + \frac{\hbar^{2}}{2m} \sum_{qq'} q \cdot q' (f_{q} f_{q'} b_{q}^{\dagger} b_{q'}^{\dagger} + 2f_{q} f_{q'}^{*} b_{q}^{\dagger} b_{q'} + f_{q}^{*} f_{q'}^{*} b_{q} b_{q'})$$
(6c)

$$H_{3} = \frac{\hbar^{2}}{m} \sum_{qq'} q \cdot q' (f_{q'} b_{q'}^{\dagger} b_{q}^{\dagger} b_{q} + \text{HC})$$
(6d)

$$H_4 = \frac{\hbar^2}{m} \sum_{qq'} q \cdot q' b_q^{\dagger} b_{q'}^{\dagger} b_q b_{q'}$$
(6e)

$$\Omega_q = \omega_0 + \hbar q^2 / 2m. \tag{6f}$$

The expectation value of the transformed Hamiltonian \mathcal{H} and its variation with respect to f_q is known as the intermediate-coupling theory. To further this approximation, we will introduce a third transformation, by which H_2 becomes diagonal. The third transformation in this work will be through squeezed states and differs from that of Barentzen [10].

2.2. Single-mode squeezed state transformation

Let us now introduce squeezed state transformation for a single LO phonon mode

$$U_3 = \exp\left(\sum_{\boldsymbol{q}} \frac{\varphi_{\boldsymbol{q}}}{2N} (b_{\boldsymbol{q}}^{\dagger 2} - b_{\boldsymbol{q}}^2)\right)$$
(7)

where N is the total number of LO phonon modes and a crucial factor in determining the squeezing angle φ_q . This angle is assumed to be real to preserve the unitarity of the transformation and will be used as an additional parameter to minimize the energy.

The transformed Hamiltonian under U_3

$$\tilde{H} = U_3^{-1} \mathcal{H} U_3 = \sum_{i=0}^4 \tilde{H}_i$$
(8)

where \tilde{H}_0 is the same as H_0 of (6a) and

$$\tilde{H}_{2} = N \sum_{q} \left(\hbar \Omega_{q} \sinh^{2} \varphi_{q} + \frac{\hbar^{2} q^{2}}{2m} \left[\left(f_{q}^{2} + f_{q}^{*^{2}} \right) \sinh \varphi_{q} \cosh \varphi_{q} + 2|f_{q}|^{2} \sinh^{2} \varphi_{q} \right] \right) + O(b_{q}^{\dagger}, b_{q})$$
(9)

where $O(b_q^{\dagger}, b_q)$ represents the terms containing all b_q^{\dagger} and b_q ordered in normal form, and they will vanish on taking the expectation value. The squeezed state vector for the ground state of the phonon subsystem is formed as follows:

$$|\Psi_{\rm ph}\rangle_{\rm s} = U_3 |\rm vac\rangle \tag{10}$$

where the ket on the right is the zero phonon state. To calculate the ground state energy functional by these state vectors is equivalent to first transforming \mathcal{H} by U_3 and then forming the expectation value of this transformed Hamiltonian in the zero phonon state.

In each case we obtain an effective Hamiltonian for the electron

$$H_{\rm eff} = H_0 + {}_{\rm s} \langle \Psi_{\rm ph} | H_2 | \Psi_{\rm ph} \rangle_{\rm s} \tag{11}$$

and then the ground state energy becomes

$$\bar{E}(f_q, \varphi_q) = \sum_q \left(\bar{V}_q f_q + \bar{V}_q^* f_q^* + \bar{\Omega}_q |f_q|^2 \right) + N \sum_q \bar{\Omega}_q \sinh^2\left(\frac{\varphi_q}{N}\right) + N \sum_q \left(\frac{q}{u}\right)^2 |f_q|^2 \left[2 \sinh^2\left(\frac{\varphi_q}{N}\right) - \sinh\left(\frac{2\varphi_q}{N}\right) \right]$$
(12)

where for convenience we take $\bar{E} = E/\hbar\omega_0$, $\bar{V}_q = V_q/\hbar\omega_0$, $\bar{\Omega}_q = \Omega_q/\omega_0$. The minimization procedure with respect to f_q and φ_q gives two coupled equations:

$$\{1 + (q/u)^2 + (q/u)^2 N \Big[2\sinh^2(\varphi_q/N) - \sinh(2\varphi_q/N) \Big]\} f_q + \bar{V}_q^* = 0$$
(13a)

$$\exp(4\varphi_q/N) = 1 + 4(q/u)^2 |f_q|^2 / [1 + (q/u)^2].$$
(13b)

Making use of the smallness of φ_q/N one can easily obtain

$$f_q = -\bar{V}_q^* / \left[1 + (q/u)^2 - 2\varphi_q (q/u)^2 \right]$$
(14*a*)

$$\varphi_q = \left\{ (q/u)^2 / [1 + (q/u)^2] \right\} a / [1 + (q/u)^2 - 2\varphi_q (q/u)^2]^2$$
(14b)

where $a = 3\alpha v_0/v$. Here v is the volume of the unit cell, and $v_0 = \frac{4}{3}\pi (1/u)^3$. In the terminology of polarons the mean extension in space of the phonon cloud is called the polaron radius. It is also possible to define this quantity as the meansquare deviation of the electron from the polaron centre [11]. In both cases, a thorough calculation reveals

that 1/u is approximately equal to the polaron radius. Therefore, v_0 represents the volume corresponding to the polaron radius.

With (14a,b) the energy expression becomes

$$\bar{E} = -\sum_{q} \frac{|\bar{V}_{q}|^{2}}{[1 + (q/u)^{2} - 2\varphi_{q}(q/u)^{2}]} + \sum_{q} \tilde{\Omega}_{q} \left(\frac{\varphi_{q}}{N}\right)^{2}$$
(15)

where the second term is the energy due to phonons created in the squeezed vacuum.

It appears from (14b) that φ_q is proportional to the coupling constant α ; but this does not mean that the degree of squeezing increases with that of the coupling strength. φ_q lies in a certain range of values because of the restriction imposed by the q dependence and accordingly this sets a limit to the value of α , which results in the validity of the approximation.

It is possible to draw numerically the curve of φ_q against q as shown in figure 1. It is a continuous function of q for values of a smaller than unity. As it increases towards unity, a gap appears, in which φ_q takes imaginary values, in contradiction with our previous assumption. When the value of a increases further, this gap enlarges in q with the consequence that φ_q finally takes a single value at q = 0, and vanishes at the other end, i.e. as q goes to infinity.



Figure 1. φ_q plotted against q/u for various values of a. Note that φ_q is equal to a at q/u = 0.

Figure 2. φ_q plotted against q/u for a = 0.5. The fine curve is the result from the continued fraction after first iteration. The bold curve is the result of the numerical calculation. After three iterations the two curves coincide.

1.2 1.4 1.6 1.8

In view of the above argument we conclude that the single-mode squeezed state approach is meaningful only for values of a smaller than unity. As a matter of fact, φ_q of (14b) is a continued fraction, and can be calculated by iterative methods to a certain accuracy in case of small values of a. Figure 2 shows the result of such a calculation. Once φ_q is known, the sums of (15) can be easily calculated and the resulting ground state energy is

$$\bar{E} = -\alpha (1 + 0.0391a + 0.0121a^2 + \cdots)).$$
⁽¹⁶⁾

Here the first term is the well known LLP result; the second and third terms are the corrections of the present work. Although this result shows a certain amount of lowering in the ground state energy, unfortunately it is valid only for very small values of α . This restriction arises because the size of weak-coupling polarons is very large in comparison with the dimensions of the unit cell and α is the product of v_0/v and α . The reason for this poor result can be attributed to the correlation between the modes, which is absent in the single-mode case. Therefore to improve this approach, we next consider two-mode squeezed states in which the phonon subsystem is in a correlated state. This has been recently applied to a model system with strong electron-phonon coupling [12].

3. Two-mode squeezed states

Let us consider two LO phonon modes specified by the wave vectors q and q', which of course have the same range of allowed values. In order to take into account the correlation between these two relevant modes we propose two-mode squeezing by the following transformation:

$$U_3 = \exp\left(\sum_{q \neq q'} \frac{\varphi_{qq'}}{N} \left(b_q^{\dagger} b_{q'}^{\dagger} - b_q b_{q'} \right) \right)$$
(17)

where now the squeezing angle $\varphi_{qq'}$ depends on q and q', and is defined as an element of a symmetrical 2×2 matrix with zero diagonal elements [13].

Now the squeezed vacuum is formed by means of the vacuum state for the phonon subsystem,

$$|\Psi_{\rm ph}\rangle_{\rm s} = U_3 |\rm vac\rangle. \tag{18}$$

Since two LO phonons are involved in the trial wave function it is essential to rewrite the Hamiltonian consistently in a way to reflect these features of the phonon cloud. As before, we try to diagonalize H_2 of (6), and therefore the relevant Hamiltonian is written

$$H_{0} = \frac{1}{2}H_{0}(q) + \frac{1}{2}H_{0}(q')$$

$$H_{2} = \frac{1}{2}\sum_{q} \Omega_{q}b_{q}^{\dagger}b_{q} + \frac{1}{2}\sum_{q'} \Omega_{q'}b_{q'}^{\dagger}b_{q'}$$

$$+ \frac{\hbar^{2}}{2m}\sum_{qq'} q \cdot q'(f_{q}f_{q'}b_{q}^{\dagger}b_{q'}^{\dagger} + 2f_{q}f_{q'}^{*}b_{q}^{\dagger}b_{q'} + f_{q}^{*}f_{q'}^{*}b_{q}b_{q'}).$$
(19)

Now the expectation value of the energy, within a certain approximation (see the appendix) is

$$\begin{split} \bar{E}(f_{q},\varphi_{qq'}) &= \frac{1}{2} \sum_{q} \tilde{\Omega}_{q} |f_{q}|^{2} + \frac{1}{2} \sum_{q'} \tilde{\Omega}_{q'} |f_{q'}|^{2} + \frac{1}{2} \sum_{q} (\bar{V}_{q} f_{q} + \text{HC}) + \frac{1}{2} \sum_{q'} (\bar{V}_{q'} f_{q'} + \text{HC}) \\ &+ \frac{1}{2} \sum_{q,q'} \tilde{\Omega}_{q} \sinh^{2} \left(\frac{\varphi_{qq'}}{N} \right) + \frac{1}{2} \sum_{q,q'} \tilde{\Omega}_{q'} \sinh^{2} \left(\frac{\varphi_{qq'}}{N} \right) \\ &+ \sum_{q,q'} \frac{q}{u} \cdot \frac{q'}{u} (f_{q} f_{q'} + f_{q}^{*} f_{q'}^{*}) \sinh \left(\frac{\varphi_{qq'}}{N} \right) \cosh \left(\frac{\varphi_{qq'}}{N} \right). \end{split}$$
(20)

It should be noted that the last three terms do not contain a factor N in contrast to the last term of (12). This is because of the second sum over q' that will provide this factor. The minimization of this energy with respect to f_q and $\varphi_{qq'}$ gives

$$\bar{\Omega}_q f_q + \bar{V}_q^* + \sum_{q'} \frac{q}{u} \cdot \frac{q'}{u} f_{q'}^* \sinh\left(\frac{2\varphi_{qq'}}{N}\right) = 0$$
(21*a*)

$$(\bar{\Omega}_{\boldsymbol{q}} + \bar{\Omega}_{\boldsymbol{q}'}) \sinh\left(\frac{2\varphi_{\boldsymbol{q}\boldsymbol{q}'}}{N}\right) + 4\frac{\boldsymbol{q}}{\boldsymbol{u}} \cdot \frac{\boldsymbol{q}'}{\boldsymbol{u}} f_{\boldsymbol{q}} f_{\boldsymbol{q}'} \cosh\left(\frac{2\varphi_{\boldsymbol{q}\boldsymbol{q}'}}{N}\right) = 0.$$
(21b)

It is easy to show that inserting (21a,b) into (20) one can obtain the energy as follows:

$$\bar{E} = \frac{1}{2} \sum_{qq'} (\bar{\Omega}_q + \bar{\Omega}_{q'}) \sinh^2 \left(\frac{\varphi_{qq'}}{N}\right) + \frac{1}{4} \sum_q (\bar{V}_q f_q + \bar{V}_q^* f_q^*) + \frac{1}{4} \sum_{q'} (\bar{V}_{q'} f_{q'} + \bar{V}_{q'}^* f_{q'}^*)$$
(22)

Calculation of this energy requires the solution of two coupled equations (21a,b) for f_q and $\varphi_{qq'}$. In view of the difficulty of solving them exactly, we try to get results to a first approximation. In the first instance we put (21a, b) in the following form:

$$f_{q} = -\frac{V_{q}^{*}}{\bar{\Omega}_{q}} - \frac{1}{\bar{\Omega}_{q}} \sum_{q'} \frac{q}{u} \frac{q'}{u} \cos \gamma f_{q'}^{*} \frac{2\varphi_{qq'}}{N}$$
(23*a*)

$$\varphi_{qq'}/N = -\left[2(q/u)(q'/u)\cos\gamma/(\bar{\Omega}_q + \bar{\Omega}_{q'})\right]f_qf_{q'}$$
(23b)

where $\cos \gamma = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\phi - \phi')$. Again, to obtaim the above results, we used the first terms in the expansion of the hyperbolic function in powers of $\varphi_{qq'}/N$ that are very small. Now, let f_q be choosen as $-\bar{V}^*/\bar{\Omega}_q$, corresponding to the unsqueezed case, then it can be used in (23*a*,*b*) to obtain new f_q and $\varphi_{qq'}$.

Inserting these new values of f_q and $\varphi_{qq'}$ into (22) one can obtain the ground state energy

$$\bar{E} = -\alpha - \frac{\alpha^2}{2\pi^4} \int \int d\Omega \, d\Omega' \cos^2 \gamma \int \int dx \, dx' \frac{x^2 x''}{(1+x^2)^2 (1+x'^2)^2 (2+x^2+x'')}$$
(24)

where x and x' are equal to q/u and q'/u respectively. After taking integrals we finally obtain

$$\tilde{E} = -\alpha - 0.0135\alpha^2 + O(\alpha^3).$$
 (25)

Here the first term is the well known result of the intermediate coupling theory; the second term is the correction due to the two-mode squeezing process.

This result agrees formally with the existing works where the differences of the approximation appear in the coefficient of α^2 , which is 0.0123 in the Feynman result, 0.0126 in that of Barentzen.

4. Discussion of results

In the present paper we have studied the ground state energy of large polarons by making use of squeezed phonon states. First we formed single-mode squeezed states by which the energy turned out to be valid for a < 1, where $a = 3\alpha v_0/v$. When the electron-phonon interaction is weak, the ratio of v_0/v is large; consequently the resulting ground state energy is limited to a narrow region of α , contingent upon v_0/v . If we take this ratio arbitrarily to be about, for example, 10, then this energy can be used for the region $\alpha < \frac{1}{30}$. The result (16) is to be compared with the exact result as obtained from fourth-order perturbation theory [14]:

$$\tilde{E} = -\alpha - 0.01592\alpha^2 + O(\alpha^3)$$
(26)

where $\alpha < 1$. The present result is lower than (26), but it is valid for very small values of α as discussed above.

In section 3 we have therefore generalized this method to the case of two-mode squeezing. In this way it has become possible to take into account the correlation between the phonons. The energy of (25) is lower than the result of Feynman and those of other works with the exception of that by Larsen [15], where the correlation between phonons

is more carefully handled. The last approach gives the same result as (26) in the weakcoupling limit, and the numerical results for the ground state energy in the intermediate regime are slightly lower than those given by (25) and valid for $\alpha < 2.5$.

In order to judge the validity of the approximation in the present work, let us combine f_q and $\varphi_{qq'}$ of (23*a*,*b*) to obtain a relation for f_q ,

$$f_q = -\frac{\bar{V}_q^*}{\bar{\Omega}_q} \bigg/ \bigg[1 - \frac{4}{\bar{\Omega}_q} \left(\frac{q}{u}\right)^2 \sum_{q'} \left(\frac{q'}{u}\right)^2 \cos^2 \gamma \frac{|f_{q'}|^2}{(\bar{\Omega}_q + \bar{\Omega}_{q'})} \bigg].$$
(27)

This is still an exact result. Variational techniques of various types used in the intermediatecoupling regime exhibit a critical behaviour in which a free polaron undergoes a formal phase transition from an itinerant state to a localized one at a critical value α_c . This feature is observed as discontinuous changes of the polaron ground state energy and its first and second derivatives with respect to α . However, as first pointed out by Peeters and Devreese [16], the existence of the phase transition is an artifact of the approximation used and not a pertinent property of the FH. In fact, recently the absence of such phase transitions in polaron systems was rigorously proved [17]. In our case, the zero of the denominator of (27) causes a discontinuity in f_q and consequently in the energy and its derivatives, and will give a critical value α_c , but it seems unlikely that this can be considered as a phase transition, and furthermore our result is free from this effect due to the approximation made on f_q .

The first-order approximation in the present work corresponds to taking $f_{q'} = -\bar{V}_{q'}^*/\bar{\Omega}_{q'}$ in the right hand side of (27) and then expanding it in powers of α , on the assumption that

$$\frac{4}{\bar{\Omega}_{q}} \left(\frac{q}{u}\right)^{2} \sum_{q'} \left(\frac{q'}{u}\right)^{2} \cos^{2} \gamma \frac{|\bar{V}_{q'}|^{2}}{\bar{\Omega}_{q'}^{2}(\bar{\Omega}_{q} + \bar{\Omega}_{q'})} < 1.$$
(28)

This defines a range for α where the approximation is valid. However, in this form it is impossible to obtain a meaningful result; we therefore arrange (28) in a convenient form and take the sum over q of both sides. The right hand side diverges at the upper limit; corresponding to an approximation that is valid for all values of α , which is obviously not correct. We therefore introduce a weight function g(q) into both sides to obtain a convergent result. With this auxiliary function, (28) becomes

$$4\sum_{q,q'} g(q) \left(\frac{q'}{u}\right)^2 \frac{\cos^2 \gamma |\bar{V}_{q'}|^2}{\bar{\Omega}_{q'}^2(\bar{\Omega}_q + \bar{\Omega}_{q'})} < \sum_q g(q) \frac{\bar{\Omega}_q}{(q/u)^2}.$$
(29)

If we choose $g(q) = 1/\overline{\Omega}_q^{\beta}$, we obtain a finite result depending on the value of β . For $\beta = 2$, (29) gives the lowest value for α : $\alpha < 3\pi^2/8 = 3.7$. If β is increased, this value increases and hence we can take $\alpha < 3.7$ as the lowest upper bound of the coupling constant below which our approximation can be safely used.

We conclude from our investigation that squeezed states which provide innovations in quantum optics can play a major role in condensed matter physics. In the present paper we have considered a squeezed state approach for the large polarons. In that connection the self-energy of the polarons has been calculated accurately by means of squeezed states; in particular two-mode squeezed states in which the correlation between phonons is involved in a natural way are successful, comparing with other sophisticated works.

Appendix

The two-mode squeezing angle $\varphi_{qq'}$ introduced in (17) is defined as the elements of the symmetrical matrix Φ

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$$\Phi = \begin{pmatrix} 0 & \varphi_{qq'} \\ \varphi_{q'q} & 0 \end{pmatrix}$$
(A1)

with the properties $\varphi_{qq'} = \varphi_{q'q}$, $\varphi_{qq} = \varphi_{q'q'} = 0$ [13], as well as $\varphi_{qk} = \varphi_{q'k'} = 0$ in the present case.

In consequence of the properties of the matrix Φ , the transformed operators take on the following forms:

$$U_3^{-1}b_q U_3 = \sum_{q'} \left[b_q \cosh\left(\frac{\varphi_{qq'}}{N}\right) + b_{q'}^{\dagger} \sinh\left(\frac{\varphi_{qq'}}{N}\right) \right]$$
(A2)

$$U_3^{-1}b_{q'}U_3 = \sum_{q} \left[b_{q'} \cosh\left(\frac{\varphi_{qq'}}{N}\right) + b_q^{\dagger} \sinh\left(\frac{\varphi_{qq'}}{N}\right) \right]$$
(A3)

$$U_{3}^{-1}b_{q}^{\dagger}b_{q}U_{3} = \sum_{q'} \sinh^{2}\left(\frac{\varphi_{qq'}}{N}\right) + O_{1}(b_{q}^{\dagger}, b_{q})$$
(A4)

$$U_3^{-1}b_q^{\dagger}b_{q'}^{\dagger}U_3 = \sum_k \sinh\left(\frac{\varphi_{qq'}}{N}\right)\cosh\left(\frac{\varphi_{kq'}}{N}\right) + O_2(b_q^{\dagger}, b_q) \tag{A5}$$

$$U_3^{-1}b_q b_{q'} U_3 = \sum_{k'} \sinh\left(\frac{\varphi_{qq'}}{N}\right) \cosh\left(\frac{\varphi_{qk'}}{N}\right) + O_3(b_q^{\dagger}, b_q) \tag{A6}$$

$$U_3^{-1}b_q^{\dagger}b_{q'}U_3 = \sum_{kk'}\delta_{kk'}\sinh\left(\frac{\varphi_{qk'}}{N}\right)\sinh\left(\frac{\varphi_{kq'}}{N}\right) + O_4(b_q^{\dagger}, b_q)$$
(A7)

where all the O functions of operators in normal order vanish when we take the expectation value of H_2 with the vacuum state. For the sake of simplicity we take k = q in the sum of (A5) and k' = q' in (A6), and the ground state energy has been calculated in this approximation. Because of the properties of Φ the term arising from (A7) vanishes and gives no contribution to the energy.

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