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Some of Bipolaron Problems

Masao Hirokawa*
Department of Mathematics, Okayama University

a piece of "condensed matter" consists of an enormous swarm of electrons moving nonrelativistically
— A. Zee, "Quantum Field Theory in a Nutshell"

Abstract

This is a brief report of the author's talk on some of bipolaron problems in the light of mathematical physics.

1 Introduction

Over the past few decades a considerable number of studies have been made on bipolaron by physicists from the point of view of physics on high-temperature superconductor [5, 3], and also by chemists from the point of view of chemistry on conducting polymers [20]. In this paper we will focus our mind on some of bipolaron problems in the light of mathematical physics. The details of physical aspects written in this report will appear in [11].

When the energy of a lattice vibration of an ionic crystal (or metal) is quantized, the energy is called a *phonon*. This vibration makes a transverse (T) wave or longitudinal (L) one in 3-dimensional space $\mathbb{R}^3$. Moreover, phonons are classified into two branches of dispersion relation, i.e., acoustic (A) phonon or optical (O) one. We treat two electrons coupled with LO phonons in this paper. By electron-phonon interaction, an electron in a crystal (or metal) dresses itself in the *phonon cloud*. This dressed electron is the so-called *polaron*. The electron-phonon interaction may be assumed to have the form of

$$r^{-1} \times \text{electron charge density} \times \text{ion charge density}, \tag{1.1}$$

where r is the distance of the electron and phonon. Moreover, we can expect electrons in the ionic crystal (or metal) to interact strongly with LO phonons through the electric field of the polarization wave. This electron dressed in LO-phonon cloud is the Fröhlich polaron.

We consider two electrons in the crystal now. Then, the Coulomb repulsion occurs between the two electrons. As written above, each electron makes a polaron.

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If the two electrons are far away from each other, each electron dresses itself in the individual phonon cloud. So, there is no exchange of phonons between the two electrons, and no force by the phonon exchange occurs between the two. Thus, there are two isolated *single polarons* in the crystal. On the other hand, if the distance between the two electrons is so short that the phonon exchange occurs, the attraction may appear between the two electrons and they are bound. This bound polarons is called *bipolaron.*

The author is interested in the following problems which have been considered by solid state physicists:

Problem 1. Find the critical point, namely, the border between existence and non-existence of ground state of bipolaron.

Problem 2. Estimate the size of a bipolaron.

Problem 3. Does the following hold?
Binding Energy $2E_{\mathrm{SP}} - E_{\mathrm{BP}} > 0 \Longleftrightarrow$ Bipolaron has a ground state, where E_{SP} and E_{BP} are the ground state energies of single polaron and bipolaron, respectively.

Problem 4. Calculate the effective mass of bipolaron.

Problem 5. Does H tend to the Hamiltonian of two single polarons in a sense, when $U \gg \lambda$? Here U is the strength of the Coulomb repulsion and λ the coupling strength with the phonon field.

Problem 6. We have to break translation invariance in the Hamiltonian of bipolaron we treat, when we obtain a ground state of bipolaron. Then, does the Nambu-Goldstone bosons appear to recover the translation invariance? If so, are such Goldstone bosons acoustic phonons?

etc.

Problem 1 proposes another enhanced-binding-problem than Hiroshima-Spohn's [13]:

Hiroshima-Spohn's Idea: Their physical image of enhanced binding is that the effective mass increases and $V(x)$ causes attraction. For the effective Hamiltonian with an effective mass m^*,

$$H_{\mathrm{eff}} = \frac{1}{2m^*}p^2 + V(x),$$

there is a critical mass m_c such that

$$\begin{cases} m^* > m_c & \Longrightarrow \quad H_{\mathrm{eff}} \text{ has a ground state,} \\ m^* < m_c & \Longrightarrow \quad H_{\mathrm{eff}} \text{ has no ground state.} \end{cases}$$

Namely, their $V(x)$ is attractive, but it is so shallow that H_{eff} has no ground state when $m^* < m_c$. Since $V(x)$ is attractive, once m^* puts on weight so that $m^* > m_c$, the attraction by $V(x)$ functions well and H_{eff} has a ground state. On the other hand, in our case $V(x)$ makes the Coulomb repulsion! So, their idea does not work well for the bipolaron problem. In this sense, bipolaron problems propose another enhanced-binding-problem.

Concerning Problems 1-3, we will mainly study formation and deformation in this paper.

2 Hamiltonians

Let m be the mass of electron. The LO phonons are scalar bosons and can be assumed to be dispersionless, $\omega_k = \omega_{\rm LO}$. The free polaron radius is defined by $r_{\rm fp} \equiv (\hbar/2m\omega_{\rm LO})^{1/2}$. Let ϵ_∞ be the optic (high-frequency) dielectric constant and ϵ_0 the static dielectric constant. We set $V_k \equiv -\hbar\omega_{\rm LO}\left(4\pi\alpha r_{\rm fp}/k^2V\right)^{1/2}$ for the crystal volume V. For the electric charge e, the dimensionless electron-phonon coupling constant is defined by

$$\alpha \equiv \frac{1}{\hbar\omega_{\rm LO}}\frac{e^2}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\frac{1}{r_{\rm fp}}.$$

The ionicity of the crystal is defined by $\eta \equiv \epsilon_\infty/\epsilon_0$, which satisfies $0 < \eta < 1$. The strength of the Coulomb repulsion is denoted by $U \equiv e^2/\epsilon_\infty$.

The total Hamiltonian of bipolaron is given by

$$H = \sum_{j=1,2}\left[\frac{1}{2m}p_j^2 + \sum_k\left\{V_k e^{ikx_j}a_k + V_k^* e^{-ikx_j}a_k^\dagger\right\}\right] + \frac{U}{|x_1-x_2|} + \sum_k \hbar\omega_k\, a_k^\dagger a_k,$$

where a_k and $a_k^\dagger$ are annihilation and creation operators of LO phonon with the momentum $\hbar k$, respectively. Each position of the two electrons are denoted by $x_j \in \mathbb{R}^3$, $j = 1, 2$.

Kornilovitch studied bipolaron problems introducing the attraction radius $R > 0$ [15]. We take this R into H.

Let $\gamma_j \in C^\infty(\mathbb{R}^3)$, $j = 1, 2$, satisfying $|\gamma_j(y)| \le 1$ for every $y \in \mathbb{R}^3$, $\operatorname{supp}\gamma_2 \subset \{y \in \mathbb{R}^3 \,|\, |y| \le R\}$, and $\gamma_1(0) = 1$. Then, the Hamiltonian with R is

$$\begin{aligned} H(R) &= \sum_{j=1,2}\frac{1}{2m}p_j^2 + +\frac{U}{|x_1-x_2|} + \sum_k \hbar\omega_k\, a_k^\dagger a_k \\ &\quad +\gamma_1(x_1+x_2)\gamma_2(x_1-x_2)\sum_{j=1,2}\sum_k\left\{V_k e^{ikx_j}a_k + V_k^* e^{-ikx_j}a_k^\dagger\right\}. \end{aligned}$$

Namely, the attraction caused by phonon exchange occurs in the region $|x_1 - x_2| \le R$. Here γ_1 may play a role to break the translation invariance in $H(R)$. If we want to keep the translation invariance, we have only to use 1 as γ_1, i.e., $\gamma_1(x_1 + x_2) = 1$. And, if we want to break the translation invariance, we may take γ_1, for example, satisfying $\operatorname{supp}\gamma_1 \subset B_L$ in the case where the crystal is a ball $B_L = \{x \in \mathbb{R}^3 \,|\, |x| \le L\}$, or $\operatorname{supp}\gamma_1 \subset C_L$ in the case where the crystal is a cube $C_L = [-L/2.L/2]^3$.

2.1 Continuum Approximation

For the sake of simplicity in a mathematical treatment, we employ the units, $\hbar = m = \omega_{\rm LO} = 1$, and the following continuum approximation:

$$\left(\frac{V}{(2\pi)^3}\right)^{1/2} a_k \approx a(k) \qquad \text{and} \qquad \frac{1}{V}\sum_k \approx \int \frac{d^3k}{(2\pi)^3}.$$

For an ultraviolet cutoff Λ with the dimension of wave number, we define

$$\chi_{R,L,\Lambda}(x,y,k) := \gamma_1(x)\gamma_2(y)\chi_{|k|\le\Lambda}(|k|), \qquad x,k\in\mathbb{R}^3,$$

where $\chi_S(r)$ is the characteristic function on a set S, i.e.,

$$\chi_S(r) = \begin{cases} 1 & \text{if } r\in S, \\ 0 & \text{if } r\notin S. \end{cases}$$

The continuum-approximated Hamiltonian is

$$\begin{aligned} H_{\rm BP}(R) &= \sum_{j=1,2}\Bigg[\frac{1}{2}p_j^2 + \lambda\int\frac{d^3k}{\sqrt{(2\pi)^3}}\chi_{R,\Lambda}(x_1+x_2, x_1-x_2, k) \\ &\qquad\qquad \times\Big\{g(k)e^{ikx_j}a(k) + g(k)^* e^{-ikx_j}a^\dagger(k)\Big\}\Bigg] \\ &\quad + \frac{U}{|x_1-x_2|} + \int d^3k\, a^\dagger(k)a(k), \end{aligned}$$

where $\lambda \equiv (4\pi\alpha r_{\rm fp})^{1/2}$, $g(k)\equiv -i|k|^{-1}$.

We have to note that the continuum approximation may be unacceptable for the intermediate-coupling large bipolaron as in Alexandrov-Mott's textbook [3].

3 Deformation of Bipolaron

Let $E_{\rm BP}(R)$ be the ground state energy of $H_{\rm BP}(R)$. Let $E_{\rm SP}(R)$ be the ground state energy of the Hamiltonian of single polaron:

$$\begin{aligned} H_{\rm SP}(R) &= \frac{1}{2}p^2 + \lambda\int\frac{d^3k}{\sqrt{(2\pi)^3}}\chi_{R,\Lambda}(x,k)\Big\{g(k)e^{ikx}a(k) + g(k)^* e^{-ikx}a^\dagger(k)\Big\} \\ &\quad + \int d^3k\, a^\dagger(k)a(k), \end{aligned}$$

where p and x are the momentum and position operators of electron and $\chi_{R,\Lambda}(x,k) := \gamma_1(0)\gamma_2(x)\chi_{|k|\le\Lambda}(|k|)$.

Taking account of Emin's work [6], there may be an energy $E(R)>0$ such that

$$E_{\rm BP}(R) = 2E_{\rm SP}(R) - E(R) + \frac{U}{R}.$$

Therefore, we have

$$\text{Binding Energy } 2E_{\rm SP}(R) - E_{\rm BP}(R) < 0 \Longleftrightarrow E(R) < \frac{U}{R}.$$

Thus, if $E(R) < U/R$, we cannot expect that bipolaron has a ground state, because it is more stable that each of the two electrons is in the individual ground state of two isolated single polarons than it is that they are in the ground state of bipolaron. We now regard $E(R)$ as coming from the phonon field and estimate it at a constant E independent of R.

We set

$$E = \frac{2\lambda^2\Lambda}{\pi^2}. \tag{3.1}$$

Then, by developing Lieb's idea in [19], we obtain that even if γ_1 breaks the translation invariance, $H_{\mathrm{BP}}(R)$ *has no ground state so long as* $E < U/R$.

4 Formation of Bipolaron

In this section we consider formation of bipolaron following the method which is similar to Adamowski's in [1] and ours in [12],

4.1 Strategy for Existence of Ground State

Step 1: Our Hamiltonian $H_{\mathrm{BP}}(R)$ has the form of

$$H_{\mathrm{BP}}(R) = H_{\text{el-el}} + H_{\mathrm{ph}} + H_{\text{el-ph}}(R, \Lambda).$$

So, we find a canonical transformation $U(\theta)$ with a parameter $\theta \geq 0$ such that

$$\begin{aligned} U(\theta)^* H_{\mathrm{BP}}(R) U(\theta) &= H_{\mathrm{eff}}(\theta, R) + H_{\mathrm{ph}} + H_{\text{el-ph}}(\theta, R, \Lambda) \\ &\quad + \mathrm{Error}_\theta(R, \Lambda) + \Sigma_\theta(R, \Lambda), \end{aligned} \tag{4.1}$$

where $\Sigma_\theta(R,\Lambda)$ is an UV divergent energy in $U(\theta)^* H_{\mathrm{BP}}(R) U(\theta)$, $\mathrm{Error}_\theta(R,\Lambda)$ an error term (bounded operator) such that $\lim_{\Lambda\to\infty} \mathrm{Error}_\theta(R,\Lambda) = 0$ for every $R > 0$.

In (4.1) $H_{\mathrm{eff}}(\theta, R) = H_{\text{el-el}} + V(\theta, R)$ becomes an effective Hamiltonian in quantum mechanics. The potential $V(\theta, R)$ in $H_{\mathrm{eff}}(\theta, R)$ should be derived from the electron-phonon interaction, and we expect that there exists a critical θ_c such that for the Hamiltonian $H_{\mathrm{eff}}^{\mathrm{rel}}(\theta, R)$ of the relativistic motion of $H_{\mathrm{eff}}(\theta, R)$,

$$\begin{cases} \theta > \theta_c \implies H_{\mathrm{eff}}^{\mathrm{rel}}(\theta, R) \text{ has a ground state,} \\ \theta < \theta_c \implies H_{\mathrm{eff}}^{rel}(\theta, R) \text{ has no ground state.} \end{cases}$$

Here the Hamiltonian of the relativistic motion of $H_{\mathrm{eff}}(\theta, R)$ means the Hamiltonian after separating the part of the center-of-mass motion from $H_{\mathrm{eff}}(\theta, R)$. Based on (1.1), we can expect $V(\theta, R)$ include a Coulomb attractive potential. We derive $H_{\mathrm{eff}}(\theta, R)$ in the following. In the physicists' context, for the phonon vacuum Ω_{ph},

$$H_{\mathrm{eff}}(\theta, R) = \lim_{\Lambda\to\infty} \langle \Omega_{\mathrm{ph}} \,|\, U(\theta)^* H_{\mathrm{BP}}(R) U(\theta) - \Sigma_\theta(R, \Lambda) \,|\, \Omega_{\mathrm{ph}} \rangle,$$

which means

$$H_{\mathrm{eff}}(\theta, R) P_{\Omega_{\mathrm{ph}}} \equiv \lim_{\Lambda\to\infty} P_{\Omega_{\mathrm{ph}}} \left(U(\theta)^* H_{\mathrm{BP}}(R) U(\theta) - \Sigma_\theta(R, \Lambda) \right) P_{\Omega_{\mathrm{ph}}},$$

where $P_{\Omega_{\mathrm{ph}}}$ is the projection onto the space spanned by the phonon vacuum Ω_{ph}.

Step 2: We consider whether the Hamiltonian $\widetilde{H}_{\mathrm{BP}}^{\mathrm{rel}}(\theta, R)$ of the relativistic motion of

$$\widetilde{H}_{\mathrm{BP}}(\theta, R) = H_{\mathrm{eff}}(\theta, R) + H_{\mathrm{ph}} + H_{\text{el-ph}}(\theta, R, \Lambda)$$

has a ground state or not.

4.2 Effective Hamiltonians in Quantum Mechanics

As we succeeded in deriving the Coulomb attractive potential from the electron-phonon interaction in [12], we use the canonical transformation with test functions. This canonical transformation appears before we determine the test functions for a self-energy in the procedure for Tomonaga's intermediate coupling approximation [26] by Lee, Low, and Pines [17, 16, 18]. From now on, we take $\gamma_1(y) = 1$ for every $y \in \mathbb{R}^3$.

We denote by $U(\beta_1, \beta_2)$ the unitary operator with test functions β_j, $j = 1, 2$, which makes our canonical transformation with test functions. We assume

$$\beta_j(k)^* = \beta_j(-k), \qquad j = 1, 2. \tag{4.2}$$

Now we choose β_j as $\beta_j(k) = \theta(1 + k^2/2)^{-1}$ for a parameter $\theta \geq 0$. In the case $\theta = 1$, $U(\beta_1, \beta_2)$ is the unitary operator in Tomonaga's intermediate coupling approximation, and it was named *canonical transformation of Gross* by Nelson [9, 10, 23]. Then, we have $U(\beta_1, \beta_2)^* H_{\mathrm{BP}}(R) U(\beta_1, \beta_2)$ in the same way as in [12]. Thus, we obtain

$$H_{\mathrm{eff}}(\theta, R) = H_{\mathrm{QM}} + \mathrm{error}_R(\theta), \tag{4.3}$$

where

$$\begin{aligned} H_{\mathrm{QM}} = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \sqrt{2}\alpha\left(\frac{1}{1-\eta} - \theta(2-\theta)\right)\frac{1}{|x_1 - x_2|} \\ +\sqrt{2}\alpha\theta(2-\theta)\frac{e^{-\sqrt{2}|x_1-x_2|}}{|x_1-x_2|} - \sqrt{2}\alpha\theta^2 e^{-\sqrt{2}|x_1-x_2|}, \\ \mathrm{error}_R(\theta) = \chi_{|x_1-x_2|\geq R}(|x_1 - x_2|)\Bigg(- \frac{\theta(2-\theta)}{|x_1-x_2|} + \sqrt{2}\alpha\theta(2-\theta)\frac{e^{-\sqrt{2}|x_1-x_2|}}{|x_1-x_2|} \\ -\sqrt{2}\alpha\theta^2 e^{-\sqrt{2}|x_1-x_2|}\Bigg). \end{aligned}$$

So, since $0 < \eta < 1$ and $0 \leq \theta(2-\theta) \leq 1$ for $0 \leq \theta \leq 2$, we cannot derive enough attraction from the electron-phonon interaction.

In order to derive a more effective attraction from the electron-phonon interaction, we use the notion of a virtual phonon as Feynman introduced in [7] (also see [22]). We regard the virtual phonon as a classical particle and assume it sits on the center $(x_1 + x_2)/2$ of the segment made by the two electrons. In this case, the two electrons can feel an attraction between themselves besides the Coulomb repulsion. Then, the two electrons do not have to become aware of the existence of the virtual phonon, though the attraction is actually made by the virtual phonon. Under this picture, we must be able to gain the Coulomb attraction between the two electrons as an effective potential $V(\theta, R)$. To derive such the Coulomb attraction, we employ β_j satisfying

$$\beta_1(k)^* + \beta_2(k) - \beta_1(k)^*\beta_2(k) = \theta/2, \qquad k \in \mathbb{R}^3 \tag{4.4}$$

from now on. For example, if we take $\beta_1(k) = -\beta_2(k) = \sqrt{\theta/2}$ or $\beta_1(k) = -(-1 + \sqrt{1+4\theta})/4$ and $\beta_2(k) = (-1 + \sqrt{1+4\theta})/2$, then β_1 and β_2 satisfy (4.4). Then, we obtain

$$H_{\mathrm{eff}}(\theta, R) = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \frac{U(\theta)}{|x_1 - x_2|} + \mathrm{error}_R(\theta), \tag{4.5}$$

where

$$U(\theta) = U - \frac{\lambda^2\theta}{2\pi},$$

$$\mathrm{error}_R(\theta) = \chi_{|x_1-x_2|\geq R}(|x_1 - x_2|)\frac{\lambda^2\theta}{2\pi|x_1 - x_2|}.$$

Let us fix $\mu > 0$ arbitrarily. *If θ and R are sufficiently large such that*

$$\mu + 2\sqrt{2}\alpha\left[\frac{1}{1-\eta} - \theta\left\{1 - \mu^2\left(R + \frac{1}{2\mu}\right)e^{-2\mu R}\right\}\right] < 0, \tag{4.6}$$

then $H^{\mathrm{rel}}_{\mathrm{eff}}(\theta, R)$ has a ground state. Some values of α for formation of bipolaron were physically studied in [1, 28]. For the case of finite temperature, see [25, 27].

Judging from the sufficient condition for deformation of bipolaron and the R-dependence in (4.6), we may expect formation of bipolaron when $R = \infty$. Namely, when the distance between the two electrons gets longer and longer, the Coulomb repulsion between the two weakens. On the other hand, if the phonon cloud still grasps the two electrons, then there is a possibility that the attraction caused by phonons wins over the Coulomb repulsion and the two electrons are bound. Actually, we obtain

$$2E_{\mathrm{SP}}(\infty) - E_{\mathrm{BP}}(\infty) > 0, \tag{4.7}$$

developing the technique in [8].

For one of establishment of the above conjecture, we introduce the center-of-mass coordinates, $X_1 = (x_1 + x_2)/2$, $P_1 = -i\nabla_{X_1} = M_1\dot{X}_1 = p_1 + p_2$, and the relativistic coordinates, $X_2 = x_1 - x_2$, $P_2 = -i\nabla_{X_2} = M_2\dot{X}_2 = (p_1 - p_2)/2$. We set masses $M_1 = 2$ and $M_2 = 1/2$. Then, our Hamiltonian $H_{\mathrm{BP}}(R)$ can be identified with

$$\begin{aligned}\sum_{j=1,2}\Bigg[\frac{1}{2M_j}P_j^2 + \lambda\int\frac{d^3k}{\sqrt{(2\pi)^3}}\chi_{R,\Lambda}(X_2,k)c(X_2,k)&\\ \times\left\{g(k)e^{ikX_1}a(k) + g(k)^*e^{-ikX_1}a^\dagger(k)\right\}\Bigg]&\\ +\frac{U}{|X_2|} + \int d^3k\, a^\dagger(k)a(k),&\end{aligned} \tag{4.8}$$

where

$$\begin{aligned} c(X_2,k) &= 2\cos\frac{kX_2}{2} = e^{ikX_2} + e^{-ikX_2},\\ s(X_2,k) &= 2\sin\frac{kX_2}{2} = e^{ikX_2} - e^{-ikX_2}.\end{aligned}$$

Because of the form of the electron-phonon interaction in (4.8), we cannot generally make the complete separation of the center-of-mass motion from $H_{\mathrm{BP}}(R)$.

In order to separate the center-of-mass motion from (4.8), we fix the center of mass of the two electrons as

$$Q = \frac{x_1 + x_2}{2}. \tag{4.9}$$

Then, the virtual phonon is also fixed at $X_1 = Q$ and it becomes the fixed source of the phonon field. Namely, the attraction which binds the two electrons for formation of bipolaron is similar to the nuclear force caused by the exchange of π-mesons in nucleon. Moreover, we nail down the virtual phonon at the origin, i.e., $Q = 0$. Because the virtual phonon attracts the two electrons, the center of mass of the two electron is also nailed down at the origin $Q = 0$ now. So, we have $x_1 = X_2/2$ and $x_2 = -X_2/2$. We have $p_1 = P_2$ and $p_2 = -P_2$ since $P_1 = p_1 + p_2 = \dot{x}_1 + \dot{x}_2 = 0$. Let $\beta_1(k) = -\beta_2(k) = \sqrt{\theta/2}$. Then, we are allowed to regard $\widetilde{H}_{\mathrm{BP}}(\theta, R)$ as the following.

$$\widetilde{H}_{\mathrm{BP}}(\theta, R) = \frac{1}{2M_1}P_1^2 + \widetilde{H}_{\mathrm{BP}}^{\mathrm{rel}}(\theta, R), \tag{4.10}$$

where

$$\begin{aligned}
&\widetilde{H}_{\mathrm{BP}}^{\mathrm{rel}}(\theta, R) \\
= \ & \frac{1}{2M_2}P_2^2 + \frac{U(\theta)}{|X_2|} + \int d^3k\, a^\dagger(k)a(k) \\
& +\lambda \int \frac{d^3k}{\sqrt{(2\pi)^3}} \chi_{R,\Lambda}(X_2, k) \\
& \times \left\{ g(k) \left(c(X_2, k) - i\sqrt{\frac{\theta}{2}}\left(1 + \frac{k^2}{2}\right) s(X_2, k) + i \sum_{j=1,2} \partial_j \gamma_2(X_2) \right) a(k) \right. \\
& \left. + g(k)^* \left(c(X_2, k) + i\sqrt{\frac{\theta}{2}}\left(1 + \frac{k^2}{2}\right) s(X_2, k) - i \sum_{j=1,2} \partial_j \gamma_2(X_2) \right) a^\dagger(k) \right\} \\
& + \frac{\lambda\sqrt{\theta}}{\sqrt{2}} \left\{ P_2 \int \frac{d^3k}{\sqrt{(2\pi)^3}} \chi_{R,\Lambda}(X_2, k) k g(k) c(X_2, k) a(k) \right. \\
& \qquad \left. + \int \frac{d^3k}{\sqrt{(2\pi)^3}} \chi_{R,\Lambda}(X_2, k) k g(k)^* c(X_2, k) a^\dagger(k) P_2 \right\} \\
& + \frac{\lambda^2\theta}{4} \sum_{j=1,2} \left\{ A_j^2 + 2A_j^\dagger A_j + A_j^{\dagger 2} \right\},
\end{aligned} \tag{4.11}$$

where

$$\begin{aligned}
A_1 &= \int \frac{d^3k}{\sqrt{(2\pi)^3}} \chi_{R,\Lambda}(X_2, k) k g(k) e^{ikX_2/2} a(k), \\
A_2 &= \int \frac{d^3k}{\sqrt{(2\pi)^3}} \chi_{R,\Lambda}(X_2, k) k g(k) e^{-ikX_2/2} a(k).
\end{aligned}$$

Namely, we can separate the center-of-mass motion from $\widetilde{H}_{\mathrm{BP}}(\theta, R)$ and the Hamiltonian of the relativistic motion is given by $\widetilde{H}_{\mathrm{BP}}^{\mathrm{rel}}(\theta, R)$. We note that the electron-phonon interaction in $\widetilde{H}_{\mathrm{BP}}^{\mathrm{rel}}(\theta, R)$ has the form obtained by combining the forms of the interaction of the Nelson model and that of Pauli-Fierz model. So, using the method in [8] and [24], we can say the following. Let us fix $\mu > 0$ arbitrarily. *If θ and R are sufficiently large such that (4.6) holds, then $H_{\mathrm{BP}}^{\mathrm{rel}}(R)$ has a ground state.*

5 Acoustic Phonons as Nambu-Goldstone Bosons

De Luca, Ricciardi, and Umezawa showed in [21] that acoustic phonons are the Nambu-Goldstone bosons recovering the translation invariance. We break the translation invariance in $H_{\text{BP}}(R)$ to obtain a ground state. Then, does the Nambu-Goldstone theorem work? If so, what are the Nambu-Goldstone bosons? Are there acoustic phonons as in [21]?

We remember the following. Let H_{S} be the Schrödinger operator with a delta potential:

$$H_{\text{S}} = -\frac{1}{2}\Delta + \delta(x), \qquad x \in \mathbb{R}^3.$$

We define a non-relativistic, classical field $\varphi(x,t)$ by

$$\varphi(x,t) := e^{-iH_{\text{S}}t}\varphi(x)$$

with an initial field $\varphi(x)$. Then, $\varphi(x,t)$ satisfies the wave equation,

$$i\frac{\partial}{\partial t}\psi(x,t) = H_{\text{S}}\psi(x,t).$$

Let $\widehat{\varphi}(x,t)$ be the second quantization of $\varphi(x,t)$ which satisfies the canonical commutation relation (CCR). We define the Hamiltonian $\widehat{H}$ by

$$\widehat{H} := \int \frac{1}{2}\nabla\widehat{\varphi}(x,t)^*\nabla\widehat{\varphi}(x,t)dx + \int\int \widehat{\varphi}(x,t)^*\widehat{\varphi}(y,t)^*\delta(x-y)\widehat{\varphi}(y,t)\widehat{\varphi}(x,t)dydx.$$

Inserting $\widehat{H}$ into the Heisenberg equation for $\widehat{\varphi}(x,t)$ and using CCR, we obtain the following non-linear Schrödinger equation,

$$i\frac{\partial}{\partial t}\widehat{\varphi}(x,t) = -\frac{1}{2}\Delta\widehat{\varphi}(x,t) + \widehat{\varphi}(x,t)^*\widehat{\varphi}(x,t)\widehat{\varphi}(x,t). \tag{5.1}$$

It is well known that the non-linear Schrödinger equation (5.1) causes the Nambu-Goldstone bosons. Therefore, the delta potential in the Schrödinger operator plays an important role to derive the Nambu-Goldstone bosons in a sense. In this point of view, we attempt to find a delta potential in $H_{\text{eff}}(\theta, R)$.

In this section we employ the approximation by Bassani, Iadonisi, *et al.* [14, 4]. We define the total momentum by

$$\Pi = P_1 + \int d^3k\, k a^\dagger(k)a(k).$$

Then, we have $[H_{\text{BP}}(R), \Pi] = 0$. We consider the case $\Pi = 0 \in \mathbb{R}^3$. We neglect a residual phonon-phonon interaction, i.e.,

$$\left(\int d^3k\; ka^\dagger(k)a(k)\right)^2 \approx \int d^3k\; k^2 a^\dagger(k)a(k),$$

and take the canonical transformation, $a(k) \longrightarrow e^{-ikX_1}a(k)$. Then, we reach

$$\begin{aligned} H_{\text{BP}}^{\Pi=0}(R) \;&=\; \frac{1}{2M_2}P_2^2 + \frac{U}{|X_2|} + \int d^3k\left(1 + \frac{k^2}{2M_1}\right)a^\dagger(k)a(k) \\ &\quad + \lambda\int \frac{d^3k}{(2\pi)^3}\chi_{R,\Lambda}(X_2,k)c(X_2,k)\left\{g(k)a(k) + g(k)^*a^\dagger(k)\right\}. \end{aligned} \tag{5.2}$$

We can show that for E given in (3.1) $H_{\mathrm{BP}}^{\Pi=0}(R)$ *has no ground state if* $E < U/R$. Moreover, *there is a unitary operator* $U(\theta)$ *such that*

$$\begin{aligned} H_{\mathrm{eff}}^{\Pi=0}(\theta,R) &= \lim_{\Lambda\to\infty}\langle\Omega_{\mathrm{ph}}\,|\,U(\theta)^*H_{\mathrm{BP}}^{\Pi=0}(R)U(\theta)-\Sigma_\theta^{\Pi=0}(R,\Lambda)\,|\,\Omega_{\mathrm{ph}}\rangle \\ &= \frac{1}{2M_2}P_2^2+\frac{U(\theta)}{|X_2|}+\gamma\delta(X_2)+\mathrm{error}_R(\theta), \end{aligned} \tag{5.3}$$

where $\Sigma_\theta^{\Pi=0}(R,\Lambda)$ is a divergent energy of $U(\theta)^*H_{\mathrm{BP}}^{\Pi=0}(R)U(\theta)$ and

$$\begin{aligned} U(\theta) &= U+\frac{\lambda^2}{2\pi}\left(\theta^2-\theta\right), \\ \gamma &= \lambda^2\theta^2\left(\frac{1}{M_1}+\frac{1}{4M_2}\right), \\ \mathrm{error}_R(\theta) &= \frac{\lambda^2}{2\pi}\left(\theta^2-\theta\right)\chi_{|X_2|\ge R}(|X_2|)\frac{1}{|X_2|}. \end{aligned}$$

Therefore, we can take $\theta=\theta_0\equiv\alpha/\sqrt{2}+\sqrt{\alpha^2/2-\sqrt{2}\alpha/(1-\eta)}$, provided that $(1-\eta)\alpha > 2\sqrt{2}$. Then, $U(\theta_0)=0$. Namely, $H_{\mathrm{eff}}^{\Pi=0}(\theta,R)$ becomes our desired Schrödinger operator. But we cannot say anything about whether acoustic phonons appear as the Nambu-Goldstone bosons in bipolaron yet.

We note the following. *Even if* $U(\theta) > 0$, $H_{\mathrm{eff}}^{\Pi=0}(\theta,R)$ *can have a bound state with negative energy under a certain boundary condition around* $X_2=0$ [2, Theorem 2.1.3].

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