Some of Bipolaron Problems

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

In my talk I would like to present some of bipolaron problems. The bipolaron problems considered here have been lively studied by many solid state physicists, especially, since the second half of the 1980s. I would like to consider some of them as the problems in mathematical physics.

When the energy of a lattice vibration of an ionic crystal is quantized, the energy is called a *phonon*. This vibration makes a wave in 3-dimensional space. In order to classify phonons, we have to remember the following facts: There are two sorts of wave of phonons, transverse (T) wave and longitudinal (L) one. The transverse wave makes up a vector field. On the other hand, the longitudinal wave makes up a scalar field. Also, there are two branches of dispersion relation of phonons, acoustic (A) branch and optical (O) one. By electron-phonon interaction, the electron in the crystal is dressed in the so-called *phonon cloud*. This dressed electron is the *polaron*. The electron-phonon interaction may be assumed to have the form r^{-1} × electron charge density × ion charge density. Moreover, we can expect electrons in the ionic crystal to interact strongly with *LO phonons* through the electric field of the polarization wave. Namely, *Fröhlich polaron*.

Now we consider two electrons. Between the two there is, of course, the Coulomb repulsion. We assume each electron is coupled with the phonon cloud (i.e., phonon field). Then, the bipolaron problems start. Should we consider the common phonon cloud or individual one for the two electrons? That is the entrance of our bipolaron problems. If the distance between the two electrons is very long, each electrons has to be dressed in the individual phonon cloud. So, there is no exchange of phonons. Thus, between the two electrons, there is the Coulomb repulsion only, no attraction. On the other hand, if the distance between the two electrons is short, the common phonon cloud grasps both the electrons. So, there is exchange of phonons. Namely, not only the Coulomb repulsion works, but also the attraction caused by phonon field works between the two electrons. Therefore, the tug of war by the Coulomb repulsion and the attraction caused by phonon cloud puzzles us.

We denote the momentum operator of the electrons by p_j, $j = 1, 2$. We denote the annihilation and creation operators of phonons by a_k and $a_k^\dagger$, respectively. Then, the Hamiltonian of the 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 $x_j \in \mathbb{R}^3$, $j = 1, 2$, and the LO phonons are assumed to be dispersionless, i.e., $\omega_k = \omega_{\mathrm{LO}}$. Each of the constants has the following physical meaning: m is the mass of electrons, $r_{\mathrm{fp}} \equiv$

$(\hbar/2m\omega_{\rm LO})^{1/2}$ the free polaron radius, $V_k \equiv -\hbar\omega_{\rm LO}\,(4\pi\alpha r_{\rm fp}/k^2 V)^{1/2}$, V the crystal volume, $\alpha \equiv (1/\hbar\omega_{\rm LO})(e^2/2)\,(\epsilon_\infty^{-1} - \epsilon_0^{-1})\,r_{\rm fp}^{-1}$ the dimensionless electron-phonon coupling constant, e the electric charge, ϵ_∞ the optic (high-frequency) dielectric constant, ϵ_0 the static dielectric constant, $U \equiv e^2/\epsilon_\infty$ the strength of the Coulomb repulsion, and $\eta \equiv \epsilon_\infty/\epsilon_0$ the ionicity of the crystal with $0 \le \eta < 1$.

Some of Bipolaron Problems:

I am interested in the following problems which have been considered by solid state physicists:

Problem 1. Find critical values of α, η, etc. Namely, the border between existence and non-existence of ground state.

Problem 2. Estimate the size of a bipolaron.

Problem 3. Does the following hold?

$$\text{Binding Energy } \; 2E_{\rm SP} - E_{\rm BP} > 0 \iff \text{Bipolaron has a ground state}$$

where $E_{\rm SP}$ and $E_{\rm BP}$ are the ground state energy of Fröhlich single polaron and bipolaron, respectively.

Problem 4. Calculate the *renormalized mass* of bipolaron.

Problem 5. Does H tend to the Hamiltonian of 2 single polarons in a sense, when $U \gg \lambda$? Here $\lambda \equiv \hbar\omega_{\rm LO}\,(4\pi\alpha r_{\rm fp})^{1/2}$.

Problem 6. When translation invariance (symmetry) is broken to get a ground state, the Goldstone bosons appear to restore the symmetry following quantum field theory. Then, are such Goldstone bosons acoustic phonons?

In this talk I would like to make the prospects for the solution of Problem 1 brighter, in particular.