International Journal of Engineering Research & Management Technology
ISSN: 2348-4039
Volume 9, Issue-2 March-april 2022
Email: editor@ijermt.org www.ijermt.org

# FORMATION OF A LARGE SINGLE BIPOLARON

**Vijay Kumar Pancholi**

**Department of physics , M.L.V Government college**

**Bhilwara, Rajasthan, India**

## ABSTRACT

It is possible to have large-bipolaron superconductivity with carrier densities that are far lower than those of typical metals. Carriers that self-trap in pairs give rise to the formation of bipolarons. For massive bipolarons to move coherently, the ratio of their static dielectric constants to their optical dielectric constants has to be exceedingly high. The mutual Coulomb repulsion experienced by the paired carriers of a planar big bipolaron causes the structure to assume a four-lobed configuration. Condensation of large-bipolarons into a liquid is driven by an attraction mediated by phonons between the bipolarons. The excitations of this liquid travel very slowly and have a very large effective mass. A modest dc resistivity at low temperatures is produced by the simultaneous mild scattering of phonons by excitations. This resistance rises linearly with increasing temperature. As the temperature drops, an energy gap develops between the excitations of big bipolarons and those of the carriers of their self-trapped electronic states.

***Keywords:*** *polaron, bipolaron, small-bipolaron, large-bipolaron, superconductivity, optical conductivity, resistivity, Seebeck coefficient*

## INTRODUCTION

It has been hypothesized that He could possess a superconductivity similar to that of superfluidity. Continuing with the analogy of 4He atoms, electronic charge carriers in appropriate condensed matter would then unite to generate bosons, which are mobile realspace singlet-paired carriers. Continuing on with the example of liquid helium, these mobile real-space couples would then need to condense into a liquid state in order to function properly. In conclusion, for this kind of superconductivity to exist, it is necessary for the liquid to experience a Bose condensation as a result of further cooling in order to establish a limited occupancy of a ground state that is fluid. The lack of measureable spins in some semiconducting materials with large densities of carriers that move incoherently through low-mobility thermally aided hopping is evidence that carriers pair with one another. This phenomenon is seen in materials with high carrier densities. It is not anticipated that charge carriers that have incoherent transit, such as tiny bipolarons, would offer a viable foundation for superconductivity.

This section addresses the conditions for the formation of coherently moving paired carriers, sometimes known as big bipolarons. The formation of large-bipolarons is possible in semiconductors that have highly displaceable ions, which are characterized by very high ratios of the static to high-frequency dielectric constants, 0/ > 2. The pair of electronic carriers inside a large-bipolaron are able to make adjustments in response to phonon-induced changes in the potential well within which they are self-trapped. The related atoms' stiffness constants are decreased as a result of this electronic polarization's effect. This action, when it is powerful enough, will cause the introduction of local vibration modes, such as the short-wavelength "ghost modes" that occur in cuprates when doping is performed. Additionally, the cooperative reactions of different pairs of self-trapped electronic carriers reduce the frequencies of phonons whose wavelengths are greater than the spacing between big bipolarons. This occurs because the phonons are self-trapped. Because of this mechanism, attractive interactions between big bipolarons are caused through phonon-mediated interactions. When the static dielectric constant is very high, the attractive interactions between big bipolarons are strong enough to overcome the direct repulsions that exist between them, allowing the huge bipolarons to condense into a liquid.

If the ground state of big bipolarons stays liquid rather of condensing more into a solid, then large-bipolaron superconductivity will be the consequence. In contrast, if the ground state of a big bipolaron becomes globally commensurate with the underlying square planar lattice of a CuO2 plane, then superconductivity will unavoidably be inhibited. Doping levels 2/(44), and are shown to be ineffective in preventing massive bipolaron superconductivity. This property is in agreement with the fact that the superconductivity of La2CuO4 was found to be suppressed when the material was doped to a level of 1/8 in the middle of its superconducting region. Large-bipolaron liquids may be distinguished from traditional conductors by their anomalous frequency-dependent conductivity as well as their low-temperature dc resistivity. The frequency-dependent conductivity results from the combination of two distinct contributions.

At frequencies of application lower than that of the characteristic phonons, the slow-moving collective excitations of large-bipolarons are a contributing factor. In contrast, when applied frequencies are greater than the characteristic phonon frequency, self-trapped carriers are stimulated from and inside their self-trapping potential well. This occurs when the frequency of the applied field is greater than the typical phonon frequency. As the temperature drops, the low-frequency responses move to lower frequencies, which creates a gap between those responses and the high-frequency ones. The production of a moderate mobility is brought about by the extremely weak scattering of huge, slowly moving collective large-bipolaron excitations by long-wavelength acoustic phonons. Even at temperatures that are far lower than the Debye temperature, the associated dc resistivity is shown to be proportional to temperature. In the end, the big-bipolaron method to understanding oxide superconductivity only depends on one essential physical trait. This feature is the unusually large ratio of the static to high-frequency dielectric constants of these materials that behave similarly to ferroelectric materials. The main portion of this article simply outlines the fundamental physical principles that underpin this hypothesis. Longer reviews and the publications that are mentioned below provide more content such as background information, technical computations, and analyses of experimental results.

## Self-Trapping and Polaron Formation

It is energetically beneficial for electronic charge carriers to self-trap, as shown in, provided that the interactions between electrons and phonons are strong enough. Next, there is a change in the equilibrium locations of the atoms that are around the carrier. Because these atoms have altered their equilibrium locations, a potential well has been established, which bonds the carrier with energy Est. A state of energetic stability is reached when the amount of energy lost by the carrier during this process is greater than the amount of energy needed to displace the related atoms. A (strong-coupling) polaron is the name given to the entity that consists of both the self-trapped electronic carrier as well as the accompanying atomic displacement pattern. When this happens, the frequency at which a self-trapped carrier circulates inside its self-trapping potential well becomes greater than that of the vibrations of its atoms:

## OBJEACTIVES

1. The study Large-bipolaron superconductivity is plausible with carrier densities.
2. The study Bipolarons form when carriers self-trap in pairs. Coherently moving large-bipolarons require.

## Electron-phonon interactions

The interaction between an electron and a phonon in an electronic carrier is what drives its self-trapping. The electron-phonon interaction defines the dependency of the electronic potential encountered by an electronic charge carrier on displacements of the atoms in a solid from their carrier-free equilibrium locations. This dependence is described by the electron-phonon interaction. In particular, it is generally accepted that the potential energy of the carrier, denoted by V(r), depends linearly on the atomic displacements:

$$V(\boldsymbol{r}) = \int d\boldsymbol{u}\, Z(\boldsymbol{r} - \boldsymbol{u})\, \Delta(\boldsymbol{u}),$$

where represents the translation of the atom whose carrier-free equilibrium position is u and where u specifies the location of the atom. After then, the function will be used to represent the extent of the electron-phonon interaction as well as its intensity. In a broad sense, the electron-phonon interaction is described as the sum of its short-range and long-range components. The short-range component of the electron-phonon interaction illustrates the dependency of the energy of a carrier on the displacements of atoms that are near to it. This component is analogous to the deformation potential of a covalent semiconductor. ZSR equals F for a deformable continuum, where stands for the Dirac delta function and F stands for the short-range force that exists between the carrier and the atoms that are nearby to it. Because the electronic energies of oxides are particularly sensitive to oxygen-cation separations, this force has a particularly powerful effect on those molecules. In point of fact, as seen in the simplified diagram, the outermost electron of an O2+ anion gets liberated after the cations that surrounded it have been removed.

## Self-trapped carrier’s non-linear wave

equation the potential well that binds a self-trapped carrier is the consequence of the atoms around it being moved to new equilibrium locations; this is shown by the equation. In addition, the wavefunction of the self-trapped carrier affects the atomic equilibrium positions that have been moved as a result. This feedback is shown to exist when the ground state of the self-trapped carrier satisfies a nonlinear wave equation. In order to simplify the process of obtaining this non-linear equation, it is assumed that the displacements of atoms from their carrier-free equilibrium locations adhere to Hooke's law. Additionally, it is assumed that the potential energy of a carrier that is self-trapped depends linearly on the displacements of the atoms that are in its immediate environment. The appropriate pattern of displaced atomic equilibrium locations is obtained by minimizing the sum of the expected value of the potential energy of the self-trapped carrier and the potential energy of the displaced atoms. These atomic displacements result in the production of the potential well that binds the self-trapped carrier of the ground-state polaron. To be more specific, the unique non-linear waveequation for this self-trapped electronic carrier is.

$$\left[\frac{-\hbar^2}{2m^*}\nabla_r^2 - \frac{V_c}{k}\int d\mathbf{r}'\ |\varphi(\mathbf{r}')|^2 \int d\mathbf{u}\ Z(\mathbf{r}-\mathbf{u})Z(\mathbf{r}'-\mathbf{u})\right]\varphi(\mathbf{r}) = E\varphi(\mathbf{r}).$$

This equation illustrates the potential well that binds the self-trapped carrier in a manner that is dependent on the wave function of the carrier as well as the interaction between electrons and phonons. As a consequence of this non-linearity, the self-trapped state is qualitatively dependent on the range of the electron-phonon interaction as well as the dimensionality of the electronic structure.

## Condensation To a Large-Bipolaron Liquid

Condensation of big bipolarons into a liquid requires an interaction between them that is both appealing and mutually beneficial. This attractive interaction arises from the movement of electronic carriers in response to the vibrations of atoms, much as the BCS superconductivity phenomenon does. BCS views these electronic carriers as being provided at no cost. However, in this case, these carriers are the electronic elements that are self-trapped inside enormous bipolarons.

After passing the adiabatic limit, in which atoms are held in place at their equilibrium locations, the relaxation of self-trapped carriers as a reaction to the vibrations of atoms results in a decrease in the stiffness constants of the atoms.3 This dynamic effect, which is illustrated in, may even create local vibration modes, such as ghost modes, which mostly arise at wavelengths that are shorter than the spatial extent of the self-trapped charges. These modes can be seen in. In addition to this, as shown in the self-trapped carriers react coherently when the phonon wavelengths are greater than the separations between large-bipolarons. This coherent effect creates an attraction between big bipolarons that is phonon-mediated throughout an intermediate range. The strength of this attraction ranges approximately as (Rst/s), where signifies the relevant phonon zeropoint energy and Rst and s, respectively, signify the typical radius and spacing of large bipolarons. Repulsions that occur across short distances between bipolarons prohibit them from merging together to form larger polarons, such as quad-polarons. Because the Pauli principle necessitates boosting their electronic carriers over their self-trapping potential well's lowest energy level, they become energetically unfavorable. Large bipolarons also exhibit mutual Coulomb repulsions over extended distances, denoted by the expression (2e) 2 /0s. On the other hand, as shown in an illustration of a net attraction, this only occurs when the static dielectric constant is sufficiently great. The reciprocal attraction that exists between large-bipolarons is what ultimately causes them to condense into a liquid state.

## A Large-Bipolaron Liquid's Distinctive Transport and Optical Properties

Only when these atoms move will a huge bipolaron, which is a composite quasi-particle consisting of a pair of extended self-trapped electronic carriers and their associated pattern of atomic displacements, move. As a consequence of this, the effective bandwidth of a large-bipolaron is very limited, denoted by the notation (/Ebp), and its velocity is much lower than the velocity of a typical phonon. In point of fact, the effective mass of a big bipolaron, denoted by Ebp/ 2Rbp 2, is enormous in comparison to the mass of a free electron.3,6 In addition, the excitations of a large-bipolaron liquid have their own unique characteristics. Take, for instance, the excitations that are present in a square-layered large-bipolaron liquid E(k).15,16 In the limit of long wavelengths, these excitations are governed by the mutual Coulomb repulsions that are present between big bipolarons. If this is the case, the "plasma-energy" that is produced is a significant amount lower than the phonon energy: E(0) = [16(n2a 3 /b)(/0]1/2, where n2 signifies the planar density of big bipolarons and a and b respectively represent the lattice constant of a square-layer and the interlayer spacing, and /0 1 (for example, 0.03 in cuprate insulators). In addition to this, the breadth of the excitation spectrum of big bipolarons is much lower than the typical phonon energy. In the same vein, the group velocity of these excitations, denoted by the symbol is much lower than the typical phonon velocity. The effective mass associated with these excitations, denoted by the symbol mbpl, is likewise much more than the mass of the free electrons. Unusual electronic transport features are generated as a result of these particular characteristics of the excitation spectrum of a large-bipolaron liquid. The dc resistivity and the frequency-dependent conductivity that result from the interaction of a large-bipolaron liquid with ambient acoustic phonons are both detailed here as examples.

**Bipolaronic Superconductivity**

When mutually interacting mobile particles go through a Bose condensation, they enter a collective ground state that allows non-dissipative irrotational flow. This is the condition that leads to super-flow, superfluidity, or superconductivity. The Bose condensation guarantees that there will be a limited number of occupants in this ground state. The fact that the ground state of the system predominates over all of its other features guarantees that it has no entropy. since of this, the Seebeck coefficient of a superconducting state disappears since it is related to the entropy that is being transferred. When excitations that would impart resistance to the flow of the collective groundstate are repressed, a phenomenon known as non-dissipative flow occurs as a consequence. The "rigidity" of the ground state of interacting particles is what ensures that the flow does not rotate.

This irrotational flow prevents the carriers' orbital paramagnetism from occurring, which results in the Meissner effect occurring in superconductors. In the theory of bipolaronic superconductivity, electronic carriers are envisioned as being able to self-trap and generate mobile individual singlet pairs. To put it another way, the electrical carriers of bipolarons are non-overlapping singlet pairs in real space. As a consequence of this, bipolarons are comparable to the individual atoms that make up the superfluid phase of liquid He. Since the mobility of bipolarons needs substantial motion from the atoms in their surroundings, this results in very sluggish movement for the bipolarons and extraordinarily large effective masses. In general, bipolaronic superconductivity is considered to be comparable to the superfluidity of He, despite the fact that it involves charged particles.

Similar to polarons, bipolarons may be broken down into two separate categories. The electronically charged carriers that are self-trapped inside a tiny bipolaron condense into a single location. On the other hand, the self-trapped electrical carriers of a big bipolaron stretch across a number of different locations. When regulated by their short-range interactions with the atoms around them, self-trapped carriers in multi-dimensional electronic systems will always collapse to a single site. This phenomenon is analogous to the deformation potential of covalent semiconductors.

Therefore, electron-phonon interactions on short distances promote the creation of tiny bipolarons. On the other hand, the Coulomb interaction-based long-range interactions that self-trapped carriers have with the ions in their surroundings often stimulate the creation of massive bipolarons. In most cases, the motion of tiny bipolarons, similar to the motion of small polarons, is incoherent. When the amount of energy that must be changed in order to move between locations is greater than the amount of energy that must be transferred, coherence is lost. Therefore, it has been found that minuscule polarons and bipolarons travel with a very low mobility (less than one centimeter squared per unit of time) by way of a series of hops that are supported by thermal forces. When temperatures are high enough to regard atomic vibrations as classical, pairs of smallbipolarons even split and hop independently. This occurs when the temperature is high enough.20 Even the slightest amount of disorder is enough to destroy coherence, making it impossible for tiny polarons and bipolarons to move around in the crystal. This is true even if a perfect crystal will sustain coherent motion at the low-temperature limit. The collective resistance-less flow of a superconducting condensate cannot be supported by immobile carriers, since this would not be an appropriate foundation.

Since Shafroth1 demonstrated that bipolaronic superconductivity occurs at temperatures below that of Bose-Einstein condensation, the subject of whether or not bipolarons may be created has drawn an ever-increasing number of investigations. In particular, this has been the case ever since Shafroth1. Over the course of the last several decades, there has been growing interest in this issue from the perspective of high-temperature superconductors. In this piece of work, we are going to center our attention on the consistency of the production of big bipolarons. Within a three-dimensional crystal, we will examine the behavior of two electrons that are connected with longitudinal optical (LO) phonons. In most cases, the interaction between an electron and a phonon wraps the electron in a cloud of phonons. The polaron is the name given to this kind of clothed electron. We make the assumption that the newly proposed second quantization adequately describes the electron-phonon interaction. If the two electrons are pushed so far apart from one another by the Coulomb repulsion that exists between them, then there will be no exchange of phonons between the two electrons. This is because each electron will have dressed itself in its own distinct phonon cloud. To be more specific, the only kind of repulsion that exists between them is the Coulomb type, and as a result, the crystal can only generate two distinct single polarons. On the other hand, if the distance between the two electrons is so close that the phonon-exchange takes place, then there is a probability that attraction will arise between them, and as a result, they will be bonded to each other. This is because the distance between them was so close that the phonon-exchange took place. The unified state of two polarons is referred to as a bipolaron.

A significant number of investigations on the big bipolaron have been carried out in light of superconductivity. Concerning the tiny Frohlich polaron, Alexandrov and Kornilovich elucidated its many physical features. In their research, Alexandrov and Ranninger demonstrated that it is possible for tiny bipolarons to exhibit superconductivity. In addition, Alexandrov and Mott, as well as Alexandrov, drew attention to the mobility of both the small and the big bipolarons. Mott was the first to make this observation. As a result, we are likewise curious in the process through which huge bipolarons expand in size. By using the traditional model presented in, we are able to provide an explanation for the phenomenon of attraction that takes place between the two electrons. The fact that an electron has a negative charge causes it to leave a deformation trail in the crystal lattice as it moves through it. This trail causes the locations of the ion centers to be altered. The presence of the ion cores is responsible for the higher density of positive charge that may be seen along this route. As a consequence of this, it exerts an attractive force on a second electron. To be more specific, the distortion of the lattice is what creates the attraction that exists between the first and second electrons. Therefore, the question that has to be answered is whether or not the attraction is strong enough to bind the two electrons together.

## CONCLUSION

The pair of electronic carriers inside a large-bipolaron are able to make adjustments in response to phonon-induced changes in the potential well within which they are self-trapped. The related atoms' stiffness constants are decreased as a result of this electronic polarization's effect. This action, when it is powerful enough, will cause the introduction of local vibration modes, such as the short-wavelength "ghost modes" that occur in cuprates when doping is performed. Additionally, the cooperative reactions of different pairs of self-trapped electronic carriers reduce the frequencies of phonons whose wavelengths are greater than the spacing between big bipolarons. This occurs because the phonons are self-trapped. Because of this mechanism, attractive interactions between big bipolarons are caused through phonon-mediated interactions. When the static dielectric constant is very high, the attractive interactions between big bipolarons are strong enough to overcome the direct repulsions that exist between them, allowing the huge bipolarons to condense into a liquid. If the ground state of big bipolarons stays liquid rather of condensing more into a solid, then large-bipolaron superconductivity will be the consequence. In contrast, if the ground state of a big bipolaron becomes globally commensurate with the underlying square planar lattice of a CuO2 plane, then superconductivity will unavoidably be inhibited.

## REFERENCES

1. Emin, D., “Formation, phase separation and superconductivity of large bipolarons,” [Polarons and bipolarons in high-Tc superconductors and related materials], eds. Salje, E. S. H., Alexandrov, A. S. and Liang, W. Y., Cambridge University Press, Cambridge, 80-109 (1995).

2. Emin, D., “Overview of the theory of the superconductivity of large bipolaron,” [Models and methods of high-Tc superconductivity: Some frontal aspects, Vol. 2], eds. Srivastava, J. K., and Rao, S. M., Nova Science Publishers Inc., New York, 343-367 (2003).

3. Emin, D., “Superconductivity of large bipolarons,” [Polarons], Cambridge University Press, Cambridge, 163-172 (2013).

4. Emin, D. and Holstein, T., “Adiabatic theory of an electron in a deformable continuum,” Phys. Rev. Lett. 36, 323- 326 (1976).

5. Emin, D., “Formation, motion and high-temperature superconductivity of large bipolarons,” Phys. Rev. Lett. 62, 1544-1546 (1989).

6. Emin, D. and Hillery, M. S., “Formation of a large singlet bipolaron, Application to high-temperature superconductivity,” Phys. Rev. B 39, 6575-6593 (1989).

7. Emin, D., “Effect of electronic correlation on the shape of a large bipolaron: Four-lobed planar large bipolaron in an ionic medium,” Phys. Rev. B 52, 13874-13882 (1995).

8. Emin, D., “Seebeck effect,” [Wiley encyclopedia of electrical and electronics engineering, online], ed. Webster, J. G., New York, Wiley, 1-44 (2002).

9. Emin, D., “Determining a hopping polaron’s bandwidth from its seebeck coefficient: Measuring the disorder energy of a non-crystalline semiconductor,” J. Appl. Phys. 119, 045101 (2016).

10. Bardeen, J., Cooper, L. N. and Schrieffer, J. R. "Microscopic theory of superconductivity," Phys. Rev. 106, 162-164 (1957).

11. Bardeen, J, Cooper, L. N. and Schrieffer, J. R. "Theory of superconductivity," Phys. Rev. 108, 1175-1204 (1957).

12. Emin, D., "Additional short-wavelength vibratory modes of a large (bi)polaron," Phys. Rev. B 43, 8610-8612 (1991).

13. Emin, D., "Phonon-mediated attraction between large bipolarons: Condensation to a liquid," Phys. Rev. Lett. 72, 1052-1055 (1994).

14. Emin, D., "Large bipolaron transport and cuprate superconductors," Phys. Rev. B 45, 5525-5529 (1992).

15. Schüttler, H.-B. and Holstein, T., "Dynamics and transport of a large acoustic polaron in one dimension," Ann. Phys. (N.Y.) 166, 93-163 (1986).