

Unified Theory of Resistivity and Superconductivity

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Abstract

Without a comprehensive theory for the cause of superconductivity, physicists have been hunting for high-temperature superconductors blindly for the last century. To understand the nature behind superconductivity, we started from a different perspective by asking ourselves what causes electrical resistivity. For a long time, we might have been misled in the classical Drude model that suggests electrical resistivity is caused by collisions between electrons and crystal lattices in conductors. The model is based on an assumption that current is resulted from free-floating electrons in conductors. Our studies indicate that electrons cannot move freely in conductors. The Drude model is not consistent with observations that resistivity decreases with increasing pressure. We were forced to abandon the model and proposed new hypotheses for the movement of electrons and the cause of resistivity. Current is the result of electrons meandering along the bordering orbitals between molecules. Each electron is relayed from one molecule to the next in the electric field of the nearest nucleus. Electrical resistivity is a function of the distance between molecules. A large intermolecular distance requires more energy to lift electrons from their equilibrium orbitals to the bordering orbitals to create current. The required lifting energy is the fundamental cause of resistivity. Superconducting is a state predicted by this theory when there is zero distance between molecules. One approach to reduce the distance is to lower the temperature. The first superconductor was discovered in this way. Another approach is to apply pressure. Most of the high-temperature superconductors are found in this manner. The theory provides an alternative view for the cause of superconductivity that may lead to searching for superconductors from a different course with the provided guidelines.

Introduction

Initially discovered in 1911, superconductivity has been the subject of much research due to its extraordinary properties and promising applications, such as MRI and Maglev trains.^[1-2] Cooper pairs of electrons bound together at low temperatures were proposed to be responsible for superconductivity in BSC theory.^[3] Since 1986, more and more superconductive materials have been found at higher temperatures, substantially above the theoretical maximum of 30 K predicted by BCS theory.^[4-8] The theory cannot address the positive effect of pressure on superconductivity in certain materials and does not account for the Meissner effect.^[9] To reveal the mystery of superconductivity, we need to understand what causes electrical resistivity first.

Most modern theories can trace their origins back to the Drude model, which states that electrical resistivity is caused by collisions between free electrons and the crystal lattice of conductors.^[10] Each collision dissipates some of the electron's energy, resulting in electrical resistance. Assuming that the Drude model were true, one would expect high density materials to have high resistivity. As pressure increases, molecules/particles are packed more densely, therefore increasing the odds of a collision and resulting in higher resistivity. However, observations indicate just the opposite. A new theory is in order, and a better understanding of the mechanics of electric current and resistivity may enhance our understanding of superconductivity.

How Current Flows

One of the assumptions of the Drude model is that electrons can move freely within conductors.^[11] It disagrees with our studies. An electron is a charged particle. Its movement is controlled by the electric force described in Coulomb's law.^[12-13] According to Coulomb, a free electron is one that is infinitely far away from its nucleus. Floating electrons in plasma may be approximately considered to be free electrons. Normally, an electron is bound to its nucleus in a molecule. The molecule also attracts any nearby electrons of adjacent molecules or ions.^[14] It is this attractive force that binds molecules together in solid. Intermolecular forces have been modeled and estimated using helium atoms.^[15] The attractive force between two helium atoms at a distance of 140 pm may be up to 1.03 nano N. To get a sense of the scale of this force, that is equivalent to accelerating a kilogram mass with 1.548×10^{17} N force. This is why a thin iron wire can be used to hang a large amount of weight. In general the attraction between molecules decreases as temperatures increase, causing phase transitions from solid to fluid. At very high temperatures, electrons may even get free, forming plasma. Thus, free electrons are only observable in plasmas not solids. Note that the attractive force is caused primarily by the attractions between nuclei and the electrons of adjacent molecules. That same attraction will also affect any nearby electrons. So, in a close range with nuclei in a solid, electrons cannot float freely between molecules, but are always affected by the attractions of nearby molecules.

Then how does an electron move in a conductor? We propose an alternative: the **orbital crossing** model.^[16] In the attraction of a nucleus, an electron is normally confined in an orbital corresponding its energy level and cannot move freely. In this state there is no current. Nevertheless, current is still possible if there are electrons in the bordering orbitals between adjacent atoms. Because there is an infinite number of orbitals for each atom, orbital overlap exists between any adjacent atoms. **Bordering orbitals** are defined as the lowest pair of orbitals between two atoms that both have the same energy level and share some overlap. Even at such a bordering orbital, an electron cannot move freely. Where the two orbitals meet, the attraction created by the two adjacent nuclei is the same. A minor advantage from the far side will cause the electron to cross over from one atom to the other, completing an orbital crossing. Essentially, the electron is relayed from one atom to the next in the attraction of the nearest nucleus. During the whole process, the electron remains at the same energy level,

which does not consume any energy. This is critical to superconductivity which requires free current flow.

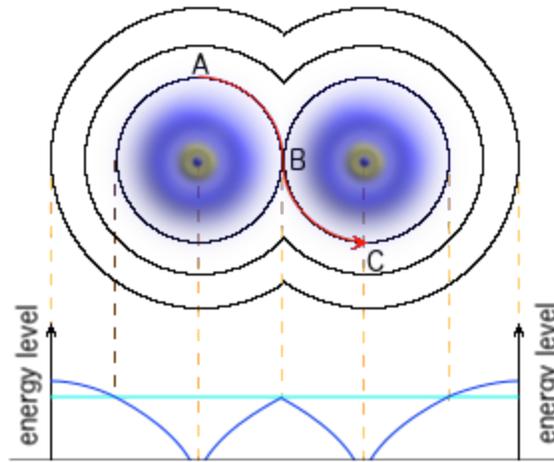


Figure 1, Electron crossing over atom boundary along bordering orbitals.

As an example, consider a system of two atoms next to each other. Figure 1 depicts a plane through the centers of the nuclei. The contours in the plane indicate the potential/energy levels created by the attractions of the nuclei to electrons. At the intersection of the bordering orbitals, point *B*, the attractions with respect to the nuclei on both sides are the same. Suppose the right atom is a positively charged ion. Normally, an electron at location *A* circulates in its orbital on the left atom. However, the missing an electron gives the ion an advantage to pull the electron over, causing it to cross the orbital border at *B* and continue to *C* along the red path. This type of potential advantage may also arise when there is an extra electron in one of the atoms, which is a negative ion. There is no gain or loss in energy during the orbital crossing process. The blue curve in the lower part of Figure 1 indicates the attractive force (vertical) created by each nucleus as a distance from the nucleus (horizontal). During the entire orbital crossing process, the electron stays at the same potential level indicated by the blue horizontal line.

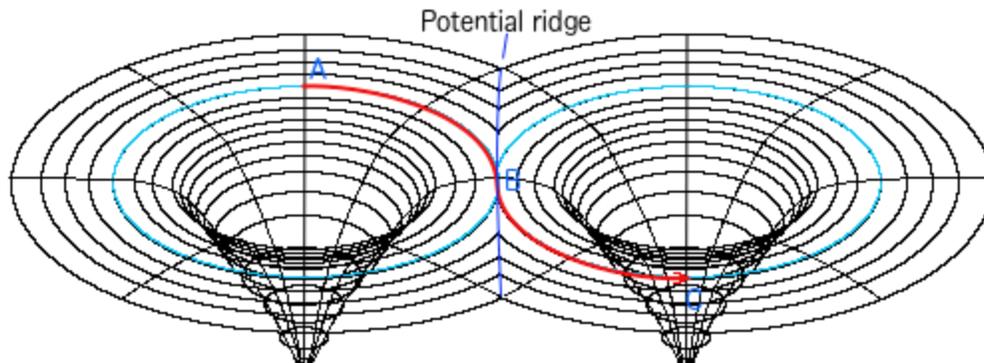


Figure 2, A 3D terrain of potential created by attractions to electrons of two nuclei.

To visualize the potential fields created by the two nuclei, a 3D terrain is presented in Figure 2. A funnel shaped potential field is created by each nucleus with a minimum centered at the nucleus, increasing outwards. In this model, the potential field is like topography. Moving to a higher orbital means going uphill in the terrain. To move a heavy object from left side to the right, energy is required to overcome the gravity/potential. To save energy, the best point to cross over the ridge (indicated by the blue curve) between the two funnels is at the location *B* in the middle of the field. For an orbital crossing from *ABC*, *B* is not only the lowest point to cross the ridge, but also the only location that the entire path can be at the same potential level. To an electron in a solid, the space between molecules is not just empty space, but mountain ranges of electric potential. An electron cannot just move up and down hills freely. Current is only possible by electrons moving at bordering orbitals where electrons are relayed from one molecule to the next through orbital crossing.

Even though the orbital crossing model illustrated in the example above use two of the same atoms, the concept works the same for complicated inhomogeneous atoms or molecules because bordering orbitals exist between any two atoms no matter what element they are.

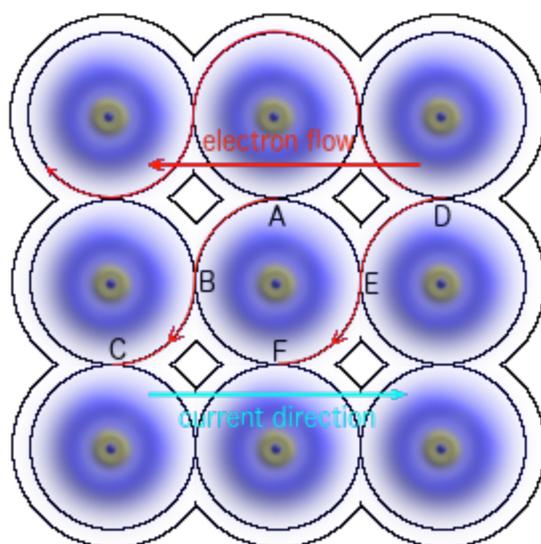


Figure 3, Currents created by orbital crossing.

As a result of orbital crossing, current is created as illustrated in Figure 3. Suppose there is an electron hole at atom *C*. An electron located at *A* tends to cross the orbital to *C* following the red contour *ABC*. Now the electron hole has shifted to the center atom *F*, causing an electron at *D* to move to *F* through *DEF*, and so on. The overall effect is that electrons flow to the left and the electron hole shifts to the right, creating a current to the right. Each electron meanders around atoms along a path at the same energy level, shown as the red path in up portion of Figure 3.

Currents created in this example assume the existence of electron holes, or positive ions. Similarly, currents may be created with negative ions, e.g. with the existence of extra electron.

What Causes Resistivity?

Orbital crossing does not have to be at a particular orbital level. It may occur at any shared border between two orbitals at the same energy level. Since an atom has an infinite number of orbitals, bordering orbitals may occur/overlap at different levels between two atoms depending on the distance between them. Figure 4 shows three different levels of orbital overlaps. With a large distance between the atoms, the bordering orbitals overlap at a higher energy level.

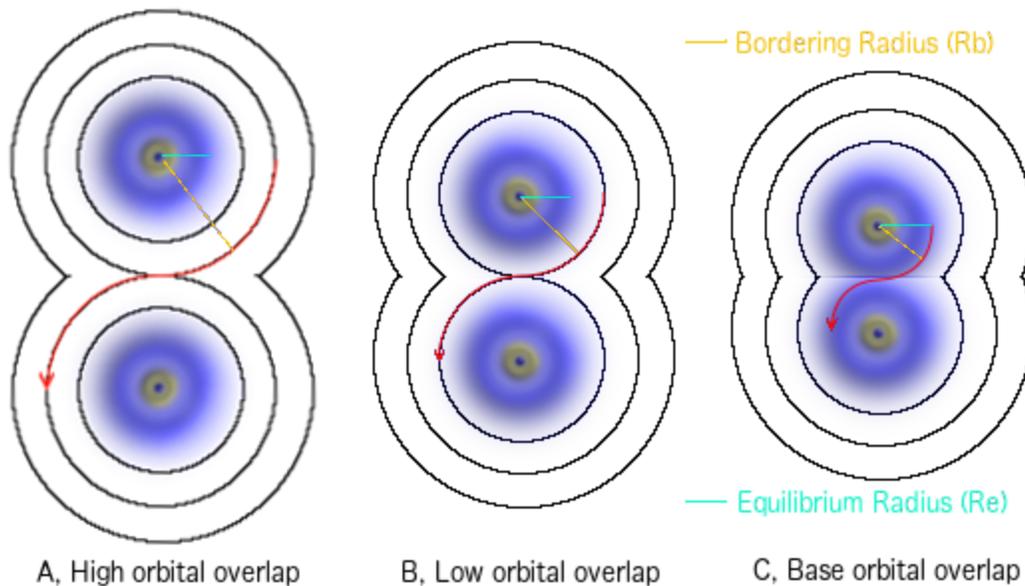


Figure 4, Orbital crossing at different levels.

An electron circulating around a nucleus in an orbital lower than the bordering orbital will be confined to the atom because of the potential barrier between atoms. Normally, current will not be created. To produce current, an electron has to be lifted to a bordering orbital as shown by red curves in Figure 4. This requires energy, which comprises the initial cost to create current. If the current is maintained at the bordering orbital level throughout the entire process, no energy is required further. However, electrons tend to step down to lower orbitals whenever there are electron holes. To maintain the current, energy has to be supplied constantly to relift the electron everytime it drops to a low level, which is the primary cause of electrical resistivity.

Normally, electrons are in their **equilibrium orbitals**, the orbitals in which electrons are at their thermal equilibrium.^[15] So, the actual energy cost for current is to lift electrons from the equilibrium orbitals to the bordering orbitals. The level of bordering orbitals is determined by the distance between atoms. More specifically, the distance discussed in this context is the minimum distance between the outermost equilibrium orbitals of adjacent molecules, named

equilibrium distance (or De , short for equilibrium orbital distance).^[16] For single atom molecules as shown in Figure 4, the equilibrium radius Re is the radius of the outermost equilibrium orbital. The equilibrium distance De is twice the difference between bordering radius Rb and equilibrium radius Re :

$$De = 2(Rb - Re). \tag{1}$$

Essentially, electrical resistance is determined by the equilibrium distance De . A large De results in a greater bordering radius Rb and high resistivity. Thus, as the De increases, the resistivity of the material also increases.^[16] A large De has several effects on resistivity. It requires more energy to lift an electron to the bordering orbitals and also means more spaces for electrons to step down, which increases energy loss. The density of matter is inversely related to De . Hence, equilibrium distance theory predicts that electrical resistivity is inversely related to density. This insight is useful because density is much easier to measure than equilibrium distance. Furthermore the density of a substance increases with pressure and decreases with increasing temperature. Consequently, electrical resistivity increases with temperature and decreases with increasing pressure.

The predictions can also be understood from a different perspective. With increasing temperature, the distance between molecules increases as thermal expansion. Therefore, resistivity increases. As pressure increases, molecules are forced to be packed closely, which reduces the distance between molecules. Therefore, resistivity decreases. There is a large body of empirical evidence that supports equilibrium distance theory's predictions of the relationship between resistivity and temperature or pressure.^[17-19] Note, the Drude model predicts that resistivity increases with pressure, which contradicts the observations in the reports. Figure 5 indicates the general trend of resistance as a function of pressure.

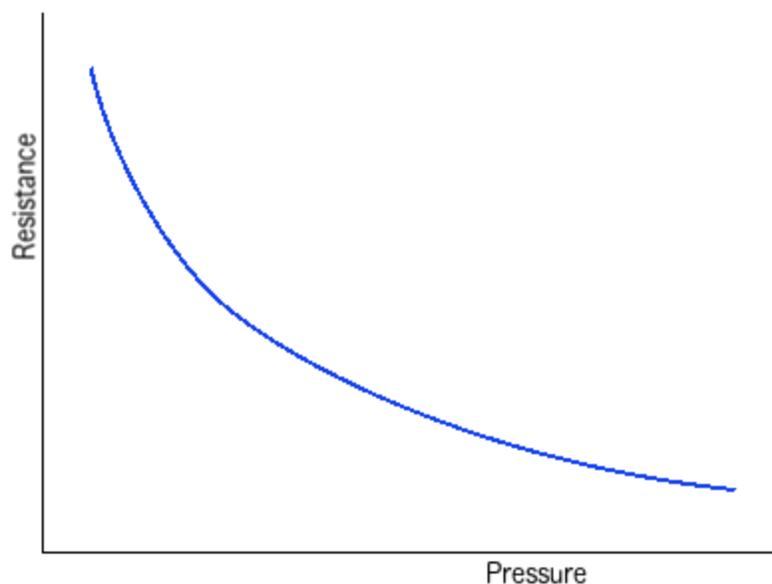


Figure 5, Resistance as a function of pressure.

For example, a research by Vaidya R., et al. reports that the electrical resistance decreases with increasing pressure on crystals of WSe₂, as shown in Fig. 2 of the paper.^[18] The electrical resistances were measured at pressures up to 8.5 GPa using Bridgman anvil setup and beyond it using diamond anvil cell (DAV) up to 27 GPa. There was no clear indication of any structural transition till 27 GPa, the highest pressure reached in the study. Another work published by Souza E., et al. also indicates that electrical resistance decreases with pressure for three different transmission joints, as shown in Fig. 2 of their paper. The study was conducted to search for better materials for transmission joints.^[19] All three types of materials in the comparison display the same negative relationship between electrical resistance and pressure, consistent with the prediction by the equilibrium distance theory.

Superconducting State

Equilibrium distance theory not only explains electrical resistivity but also predicts the existence of superconductivity. Based on its postulations, electrical resistivity decreases with equilibrium distance. At zero distance, there is no resistance, only superconductivity. In Figure 4, superconductivity is demonstrated to be a theoretical consequence of orbital bordering at the lowest orbitals, or base orbitals, typically for low temperature superconductors. As equilibrium distance decreases from Figure 4A to 4B to 4C, the bordering orbitals occur at lower and lower levels. In Figure 4C, since there is zero equilibrium distance, no lifting energy is required and electrons can propagate across atom border freely.

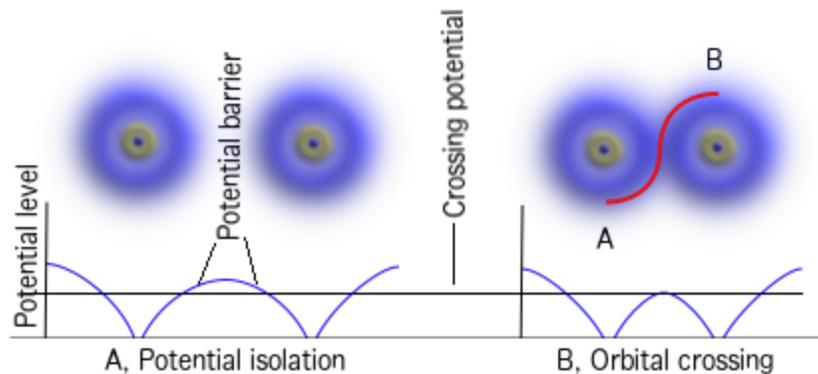


Figure 6, Potential barrier and superconductivity.

For instance, a normal equilibrium distance usually creates a potential barrier as shown in the lower part of Figure 6A, which prevents electrons from crossing over the border. The distance between atoms usually decreases as repulsion between them decreases with temperature.^[15] At low temperatures, the distance between atoms may decrease to a point where base orbitals overlap. At this point, there is no potential barrier between the atoms as shown in Figure 6B. Now the electrons in the outermost orbitals can flow from one atom to another without the need

superconductivity as shown in Figure 7A. With equation (1), the superconductivity condition can also be expressed as $De = 0$ or $Rb = Re$. Resistivity is a function of De which is affected by both temperature t and pressure p . The effect of pressure p is to reduce the distance between molecules. In other words, Rb is a function of p and $Rb(p)$ decreases with p . The distance between molecules also increases with temperature t . So, Rb is also a function of t and $Rb(t,p)$ increases with t . As t increases, equilibrium orbitals move higher, e.g. $Re(t)$ increases. Therefore, De is a function of both t and p . Equation (1) should be rewritten as:

$$De(t,p) = 2(Rb(t,p) - Re(t)). \quad (3)$$

The level of bordering orbitals $Rb(t,p)$ can be reduced by increasing p , potentially to the same level as equilibrium orbitals, e.g. $Rb(t,p) = Re(t)$, making it possible to achieve superconductivity by increasing p . Intermolecular separation also increases with t , which raises the level of bordering orbitals, e.g. $Rb(t,p)$ increases. Normally, the increasing speed of bordering orbitals $dRb(t,p)/dt$ is faster than that of equilibrium orbitals $dRe(t)/dt$, e.g. $dRb(t,p)/dt > dRe(t)/dt$. As t increases, eventually, $Rb(t,p) > Re(t)$, as shown in figure from 7A to 7B. This is why superconductivity is usually destroyed as temperature increases. With function (3), resistivity is a function of $De(t,p)$ representing a surface over t - p space. Superconductivity is a curve on the surface where $De(t,p) = 0$, which is equivalent to

$$Rb(t,p) = Re(t). \quad (4)$$

The so-called critical point of a superconductor is actually only a point along the phase transition line between superconductors and non-superconductors. In other words, t and p of the critical point is just one solution of equation (4). All the solutions to equation (4) is a continuous line in the space of t and p which draws the superconductivity phase transition curve as shown in the phase diagram by the blue line in Figure 8. In theory, solutions to equation (4) exist for almost any material. Many solutions are found in the space at high pressures. This explains why many high-temperature superconductors discovered recently are also under high-pressure. In a sense, high-pressures have been traded for high-temperatures.

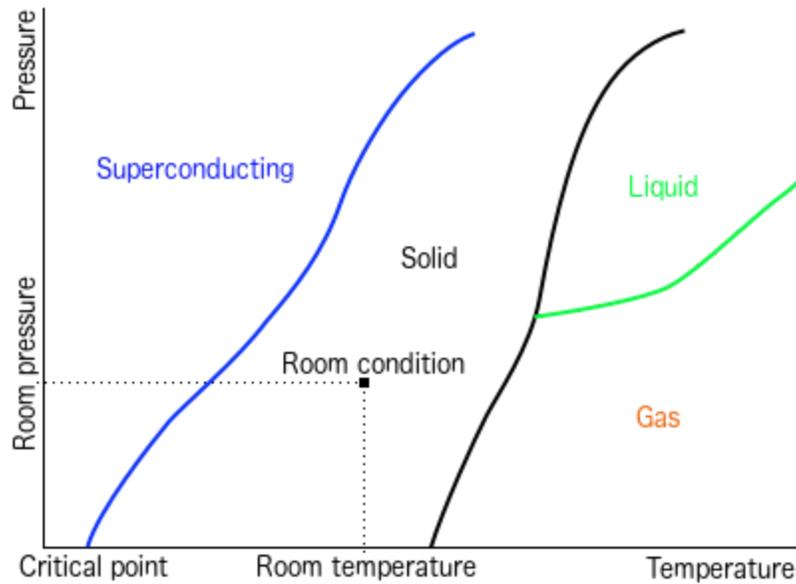


Figure 8, Phase diagram of superconductivity.

The equilibrium distance theory is a unified theory for both electrical resistivity and superconductivity, where resistivity is a function $De(t,p)$ over $t-p$ space described by equation (3). The condition of superconductivity is $De(t,p) = 0$ or $Rb(t,p) = Re(t)$. The solutions to the equation is a continuous line in $t-p$ plane, which is the phase transition curve in the phase diagram.

The Cause of the Meissner Effect

A superconductor is not only a perfect conductor, but more significant because of its Meissner effect, a phenomenon where a magnetic field is expelled from the superconductor.^[9] Note, magnetic fields created by induction requires a change in magnetic flux according to Faraday's law of induction.^[19-20] The Meissner effect is observed during the transition to the superconducting state in an existing magnetic field where there is no change in magnetic flux. In other words, the Meissner effect is not because of induction. Rather, it is a result of existing currents in superconductors deflected by the Lorentz force.

According to the equilibrium distance theory, currents are created by electrons moving in bordering orbitals. Keep in mind, bordering orbitals and equilibrium orbitals are at the same level in superconductors. It does not require any additional energy to overcome resistivity. Free currents move in bordering orbitals, which exists naturally regardless of applied fields. If there is an external magnetic field, the currents rearrange their directions according to the Lorentz law.^[22-24] Lorentz force is described by $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$, where \mathbf{F} is the force, q is the electrical charge, \mathbf{v} is the velocity of the moving charge, \mathbf{B} is the magnetic field, and \mathbf{E} is the electric field (not applicable in this context). This force deflects a moving electron in superconductors. Looking in the direction of the applied magnetic field, the electron is deflected to circulate in a

clockwise direction. The circulating electrons, or currents, create an internal magnetic field that cancels the external field inside the superconductor and superimposes the applied field outside of the superconductor. The net result appears as if the applied field is expelled from the superconductor.

This is another challenge to BCS theory, which cannot explain the Meissner effect. At the time of the transition to the superconducting state, there is no external electrical field, e.g. $\mathbf{E} = \mathbf{0}$, to drive Cooper pairs. Cooper pairs cannot create current themselves without additional electrical fields. Motionless electrons cannot be deflected by an applied magnetic field because $\mathbf{v} = \mathbf{0}$ and the Lorentz force is also zero.

Effects of Critical Fields

When a superconductor is exposed to a magnetic field, it loses its superconductivity as the field passes a certain strength, known as the critical field. **Orbital deflection** theory addresses this phenomenon elegantly. Figure 9 shows both normal electron clouds and electron clouds deformed by an applied magnetic field. An electron in its normal orbital may be deflected by the field via the Lorentz force and its orbital plane turns to a direction perpendicular to the field. The outermost electrons have more freedom to change the orientation of orbital plane due to less tangling effect from other electrons in the same atom, which effectively flattens the clouds in the direction of the applied field. As the field is strong enough, the equilibrium distance between molecules may become large enough to separate the orbitals, causing the destruction of superconductivity. Keep in mind that only these outermost electrons are significant to superconductivity.

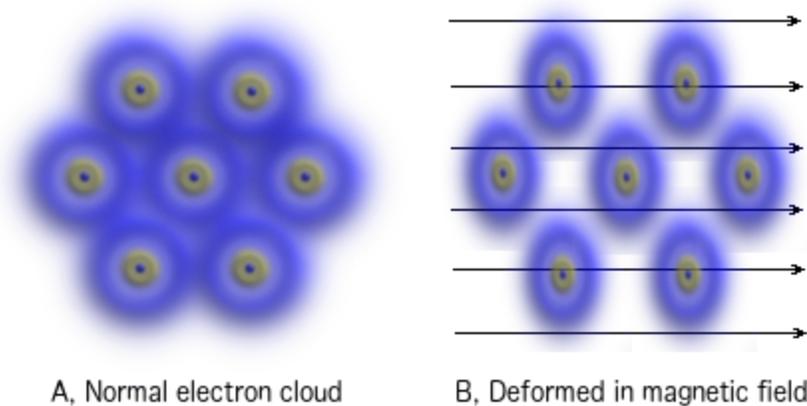


Figure 9, Deformed electron cloud in a magnetic field.

Figure 9 illustrates just one of many possible crystal structures. With a crystal structure made of large and complicated molecules, different deflection/flattening effects may be observed for fields applied from different directions. This could be why certain superconductors have different critical fields in different directions.

A type-II superconductor has two critical field: B_{c1} and B_{c2} .^[25-27] As an applied magnetic field is less than B_{c1} , normal superconductivity is observed. With the field greater than B_{c1} , some parts of the superconductivity are destroyed in the sample. These non-superconductive islands are called magnetic vortex. The density of vortex increases with the strength of applied magnetic field. When the field is greater than B_{c2} , superconductivity of the entire sample is destroyed. The peculiarities of type-II superconductors are the result of different equilibrium distances between different atoms in the compounds/alloys that make up type-II superconductors.

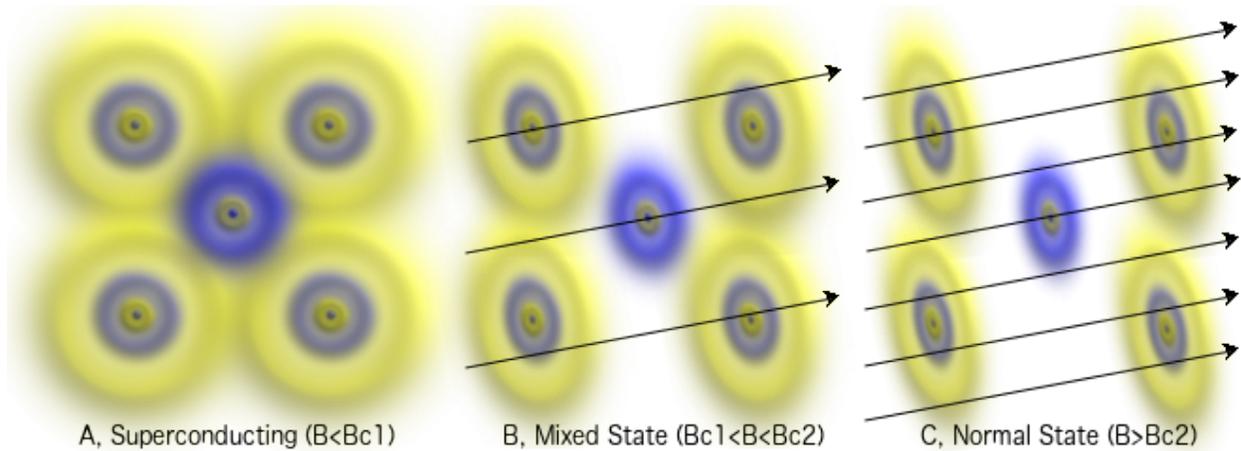


Figure 10, Type-II superconductors at different field strengths.

Figure 10 illustrates a type-II superconductor made of alloys. The normal superconductivity is observed at a magnetic field $B < B_{c1}$, Figure 10A, and the superconductivity is destroyed at the field $B > B_{c2}$, Figure 10C. With the field between B_{c1} and B_{c2} , Figure 10B, the equilibrium distance for the central molecule is large enough to destroy the superconductivity, while other molecules surrounding it are still in superconducting state. The center part becomes a non-superconductive island, known as a vortex, which allows magnetic flux to penetrate. The existence of vortex is responsible for flux pinning, also known as quantum locking or quantum levitation, which makes type-II superconductors more interesting and valuable for applications.

Searching for Superconductors

Scientists have been searching for high-temperature superconductors without a solid theoretical framework for over a century. With the equilibrium distance theory, we are optimistic that higher temperature superconductors will be discovered rapidly. As shown in Figure 8, superconducting is just another state of matter and not uncommon. Equilibrium distance theory predicts that high pressure environments are just as suitable for superconductors as low temperatures, presenting a new, larger attack surface on the problem of high-temperature superconductors.

Atom sizes increase as equilibrium orbitals rise with temperature. As atom sizes increase, the repulsion between atoms increases, so does the distance between them, which causes the rise

of bordering orbitals.^[15] Based on the equilibrium distance theory, the requirement of superconductivity is that the equilibrium orbitals meet the bordering orbitals. Equilibrium orbitals also rise with temperature. For equilibrium orbitals to keep up with rising bordering orbitals, the material needs to be less repulsive. Thus, the search should be focused on less repulsive materials. Less repulsive materials usually have higher melting or boiling points.^[16] That is to seek for materials with high melting or boiling points. So, let's turn to the periodic table to look for elements that are melting and boiling at high temperatures.

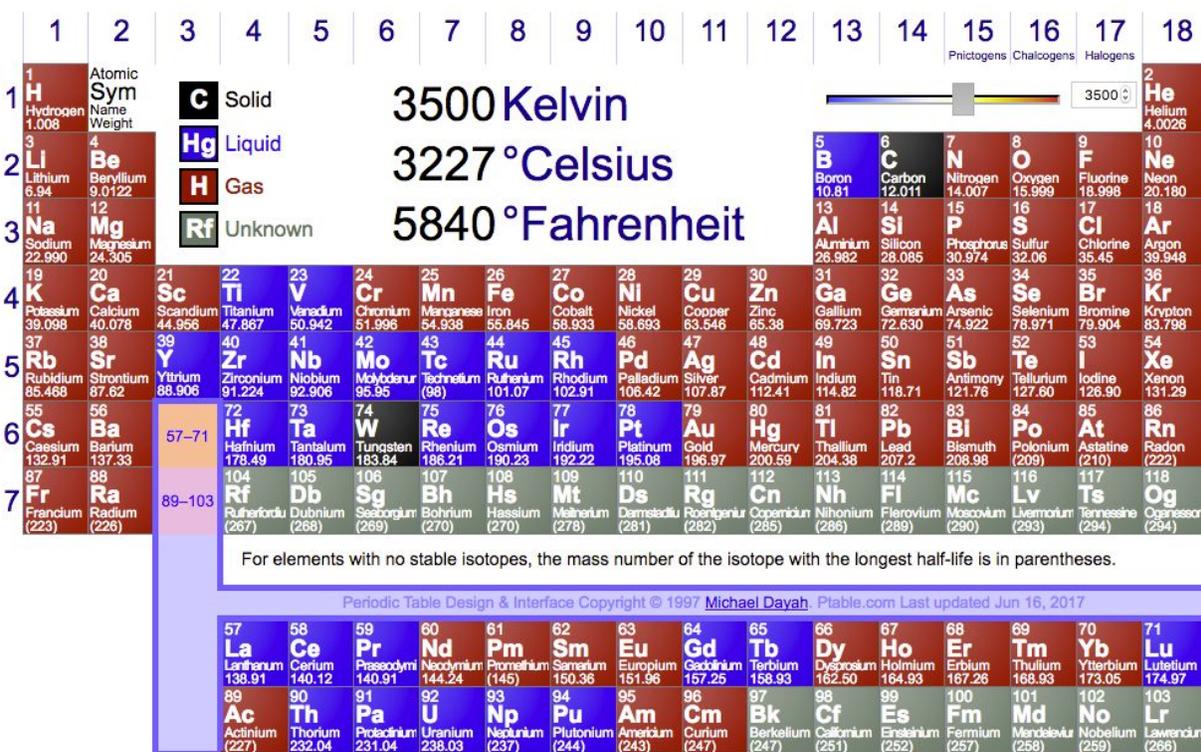


Figure 11, The states of elements at 3500 K (screenshots from [ptable site](http://ptable.com)).

Figure 11 shows the states of elements at 3500 K in different colors. In general, melting points decrease to the right in each row, indicating that the repulsion between molecules increases when more electrons are in the outer shell, leading to lower melting and boiling points. In each column of elements, there are the same number of electrons in the outermost shell. The element in the lower row has one more inner shell compared with the upper element, which makes its outermost electrons less significant than that in the upper row in terms of repulsion. Thus, the lower elements are less repulsive. overall, repulsion decreases from the top right to bottom left. All of the elements in two left columns, such as hydrogen, boil at low temperatures because of their relatively large radii compared with elements to the right in the same row. This trend is consistent with the helium model's prediction that a larger radius produces a greater repulsion.^[15] As a result, the least repulsive elements are found to the left of the lower center in the table. Of note is the fact that these elements match the low temperature superconductors discovered so far as shown in Figure 12.

molecules in natural crystals is the primary challenge for high-temperature superconductors. Artificial superconductors are trying to solve the problem from a different perspective. This alternative direction may hold the solution to high-temperature superconductors.

It would be interesting to investigate the superconducting/non-superconducting phase transition curves for some materials, such as mercury. This would not only verify the equilibrium distance theory, but more importantly provide understanding and insight to the trends of phase transition for superconductors. This will reveal some hints on how to search for high-temperature superconductors.

Conclusions

The Drude model for electrical resistivity cannot account for pressure and density tests, nor does BCS theory. BCS theory fails to explain high-temperature/high-pressure superconductors, the Meissner effect, and critical field, too. With the equilibrium distance theory, both superconductivity and electrical resistivity are explained in a unified theory.

- Electrical resistance is a function of equilibrium distance, which is the energy cost to lift electrons from equilibrium orbitals to bordering orbitals. Resistivity increases with temperature and decreases with pressure.
- Superconductivity is predicted by the equilibrium distance theory wherever the equilibrium distance is zero.
- The theory predicts the existence of a superconducting state for all materials. Superconducting temperature increases with pressure, which explains the occurrence of high-temperature/high-pressure superconductors.

Orbital crossing provides a better model of electron movements in conductors. Under the attraction of atoms in conductors, an electron cannot move freely, but meanders between atoms along the bordering orbitals. Currents created by orbital crossing in superconductors exist naturally regardless of external fields, which makes it possible for the Meissner effect. Orbital deflection theory provides an explanation to critical fields for both type-I and type-II superconductors. Based on the equilibrium distance theory some guidelines are provided for searching high temperature superconductors more effectively.

Acknowledgements

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