

Electrical polarizability of a few electrons in a parabolic potential in the presence of a pairing interaction

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Abstract

We examine the electrical polarizability of a few electrons confined in a one dimensional parabolic potential in the presence of an effective pairing interaction. We use Richardson's model to first determine the energies and wavefunctions, and then use perturbation theory to treat the effect of the electric field. In the cases studied, it is found that the polarizability decreases with respect to the normal state.

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Introduction

The hallmark of superconductivity is zero electrical resistivity [1], but there are other effects that occur in superconducting samples, such as the expulsion of magnetic fields (The Meissner effect [2]), the changes in the electronic heat capacity and heat conductivity below the transition temperature and the presence of an energy gap at the Fermi level. There are counterexamples to all these manifestations of superconductivity, as pointed out recently by Leon Cooper [3], so a more modern definition of superconductivity focuses on the associated phase transition [4]. We understand that a pairing interaction affects electrons that are close to the Fermi Surface producing a *macroscopic* effect and forming a new wavefunction. In light of this understanding, it is interesting to investigate what happens when the size of a superconducting sample becomes so small that it stops being macroscopic. This would cause the energy levels to be few and discrete, and band theory would no longer describe the behavior of electrons.

The critical size for which superconductivity still exists has been deemed the most fundamental problem of superconducting particles [5]. Theoretically, in Anderson's famous paper [6] about dirty superconductors, he suggested the criterion for the critical size in which superconductivity still exists is when the energy gap is comparable to the separation between energy levels at the Fermi surface. Experiments done at Harvard in the 1990s [7][8] showed that the energy gap was still present in aluminum particles of diameter $\approx 5nm$, where the gap is larger than the average level spacing, for smaller particles it was not possible to distinguish between the level separation and the gap.

A single atom cannot have zero resistivity, so superconductivity in the usual sense should disappear when the size of the sample gets too small, but what happens to the pairing interaction? At least in principle, there could be manifestations of superconductivity in small particles other than zero resistivity. For example, the odd-even alternation in the binding energy observed in nuclei has been explained by pairing interactions between nucleons [9].

Another possible manifestation might be the transition to a state that behaves like a ferroelectric. This was observed at Georgia Tech in 2002 [10] in clusters of niobium, vanadium, and tantalum, which are superconductors in the bulk. This effect is absent in other non superconducting metals. Other clues that point towards an explanation based on superconductivity are the spin decoupling observed in niobium [11], the effect of magnetic dopants, the enhancement of the effect with aluminum, the odd-even alternation that favors clusters that have even number of electrons, and the similarity in the transition temperatures [12].

The effects observed at Georgia Tech are complex and require more than a simple model based on permanent dipole moments attached to the frame of the cluster [13]. According to our present understanding, the superconducting wavefunction behaves as a “frozen crust” (as Victor Weisskopf described it back in 1981 [14]), meaning that a finite energy is required to change the quantum state. Could this explain a ferroelectric-like response? This question prompted us to study the polarizability of small particles with a few electrons in the presence of a pairing interaction. We use Richardson’s model to first find the energies and wavefunctions, and then treat the electric field as a perturbation as explained below. We do not pretend to approach a realistic approximation, but rather to gain insight in how the pairing interaction might affect the electrical polarizability.

Richardson’s Model

The model was originally intended to study the pairing interaction in nuclei, but it has been successfully applied to small superconducting particles like the ones studied experimentally by the Harvard group. We are guided by the tutorial written by F. Braun and J. von Delft [15], and the original work published by Richardson cited therein especially reference [16].

In the absence of a pairing interaction the Hamiltonian we will consider is simply:

$$H = \sum_{i,\sigma} \epsilon_i c_{i\sigma}^+ c_{i\sigma} \quad \text{Equation 1}$$

Here $c_{i\sigma}^+$ is the operator that creates an electron that occupies level i with spin σ when acting on the vacuum. This Hamiltonian corresponds to only diagonal elements. Its solutions are anti-symmetric wavefunctions that can be expressed as Slater determinants, where the swapping of two electrons changes the sign of the determinant. In compact form, the solution can be expressed as occupation numbers, which specify whether a level is occupied or not. Following the review written by von Delft [17], we can use a cartoon representation of this wavefunction as shown in equation 2:

$$|\psi\rangle = \left| \begin{array}{c} \text{---} \\ \bullet\bullet \\ \bullet\bullet \end{array} \right\rangle \quad \text{Equation 2}$$

We could call this the “normal” state, where the electron-electron interaction is ignored and the electrons in the ground state occupy levels up to the Fermi surface. But in the presence of an attractive interaction between electrons the Hamiltonian has to include an additional term that describes the pairing interaction:

$$H = \sum_{i,\sigma} \varepsilon_i c_{i\sigma}^+ c_{i\sigma} - g \sum_{i,j} c_{i\uparrow}^+ c_{i\downarrow}^+ c_{j\downarrow} c_{j\uparrow} \quad \text{Equation 3}$$

The second term in equation 3 is due to the attraction between electrons. It has the consequence of scattering pairs of electrons, reducing the energy of the system.

The resulting wavefunction for the Hamiltonian of equation 3 will be a product of two operators acting on the vacuum. One factor contains all the single-electron creation operators and the other contains pair creation operators.

$$|\psi\rangle = \left(\prod_{i \in B} c_{i\sigma}^+ \right) \left(\sum_{j_1, j_2, \dots, j_n \in U} \left(C(j_1, j_2, \dots, j_n) \cdot \prod_{v=1}^n b_{j_v}^+ \right) \right) |0\rangle \quad \text{Equation 4}$$

Once an energy level is occupied by a single electron it is not available for pair scattering, so it will not participate in the attractive interaction. In equation 4, B stands for the set of all levels that are blocked due to single occupancy, and U stands for the set of all unblocked levels available for pair scattering. The number of electron pairs is n , so the total number of electrons is $2n+b$, where b is the number of electrons that make up the blocked states. The pair creation operator $b_{j_v}^+$ is defined as $b_{j_v}^+ = c_{j_v\uparrow}^+ c_{j_v\downarrow}^+$ and C is a numerical coefficient. We can define the wavefunction of paired electrons as $|\psi\rangle_U$ as follows:

$$|\psi\rangle_U = \sum_{j_1, j_2, \dots, j_n \in U} C(j_1, j_2, \dots, j_n) \prod_{v=1}^n b_{j_v}^+ |0\rangle \quad \text{Equation 5}$$

Note that the paired wavefunction is invariable under an exchange of two pairs. In that sense, it follows Bose statistics. However, the pair creation operator is made out of two fermion creation operators, so $(b_{j_v}^+)^2 = 0$. This differs from normal Bose statistics and must be taken into account in the solution.

Richardson established that the solution could be found exactly by assuming wavefunctions of the form:

$$|\psi_n\rangle_U = C \prod_{v=1}^n \left(\sum_j \frac{b_j^+}{2\varepsilon_j - E_v} \right) |0\rangle \quad \text{Equation 6}$$

Where the energies E_v satisfy the equations:

$$1 - \sum_j \frac{g}{2\varepsilon_j - E_v} + \sum_{\mu=1(\neq v)}^n \frac{2g}{E_\mu - E_v} = 0, \text{ for } v = 1, \dots, n \quad \text{Equation 7}$$

Thus, this model not only provides the wavefunction, but also the energy of the system given by the sum:

$$E = \sum_{i \in B} \varepsilon_i + \sum_{v=1}^n E_v \quad \text{Equation 8}$$

Proof of these results can be found in the original papers by Richardson and in an alternative, simpler form in the tutorial written by von Delft and Braun [15].

Solving the problem for two electrons:

Following Richardson's model [16], we assume that the single particle states are equally separated energy levels. We take the separation as the unit of energy, and start this ladder at $\varepsilon_1 = 1$. This hypothetical system could correspond to a one dimensional parabolic potential well, $V = \frac{1}{2}m\omega^2x^2$, where the ground state has been arbitrarily set to unity. The unit of energy is defined as $\hbar\omega$. In the simplest possible case, we can assume that the number of energy levels is truncated at two. This is the simplest case because the third term in Equation 7 does not exist, so the equation becomes:

$$1 - \frac{g}{2-E} - \frac{g}{4-E} = 0 \quad \text{Equation 9}$$

With only one variable, the equation can be solved numerically for every value of g , or by using the approach suggested by Richardson [18] by mapping the problem into a two dimensional electrostatic problem.

Using the latter approach, the energy E represents an equilibrium position, x , of an infinite long rod that can only move along the x -axis with a uniform linear density of charge in a region of space where there are potentials of the form:

$$V_1 = -\int 1 dx = -x \quad \text{Equation 10a}$$

$$V_2 = -\int -\frac{g}{2-x} dx = -g \ln|2-x| \quad \text{Equation 10b}$$

$$V_3 = -\int -\frac{g}{4-x} dx = -g \ln|4-x| \quad \text{Equation 10c}$$

As an example, Figure 1 shows the potential for the case when $g=0.5$ and the solid arrow indicates the equilibrium position for the ground state. The pair can also exist in an excited state, which is indicated in the figure with a dashed arrow. Besides this, there is an excited state of a *split* pair, where one electron occupies the lowest level and the other occupies the highest one. In this case, the energy would simply be $3\hbar\omega$ regardless of the value of g , because both electrons occupy blocked states. A similar situation was suggested by Cooper in his seminal paper about pairing in superconductors [19] when he suggested that the splitting of a pair was the most likely channel for excitation.

Plotting the ground state energy as a function of g is shown in Figure 2 as the solid line. And the first excited pair state as a dashed line. The split state energy is represented with the dotted line.

The ground state wavefunction will be given by:

$$|\psi_n\rangle_U = C \cdot \left(\frac{b_1^+}{2\varepsilon_1 - E} + \frac{b_2^+}{2\varepsilon_2 - E} \right) |0\rangle = \left| \frac{C}{2-E}, \frac{C}{4-E} \right\rangle = \frac{|4-E, 2-E\rangle}{\sqrt{(4-E)^2 + (2-E)^2}} \quad \text{Equation 11}$$

The consequence of having a pairing interaction is that the electron pair occupies higher energy levels to take advantage of the second term in the Hamiltonian (equation 3), and reduce the overall energy.

Introducing an Electric Field

We want to ask ourselves what would happen if we put this small system in an electric field. With e being the absolute value of the charge of the electron and F being the strength of the electric field, we consider an additional term in the Hamiltonian:

$$H_1 = -eF\hat{x} \quad \text{Equation 12}$$

In this equation, \hat{x} is the position operator acting on all the electrons. Writing this expression with the usual definition of raising, $a^+|n\rangle = \sqrt{n+1}|n+1\rangle$, and lowering, $a|n\rangle = \sqrt{n}|n-1\rangle$, operators becomes:

$$H_1 = -eF\sqrt{\frac{\hbar}{2m\omega}}(a^+ + a) \quad \text{Equation 13}$$

We need to be aware that in principle an error is introduced because the ladder is truncated to only two levels. For that reason, we later extend the calculations to more levels.

We can try first order perturbation theory to calculate the shift in energy as follows:

$$\Delta E_F = \langle \psi_n | -eF\sqrt{\frac{\hbar}{2m\omega}}(a^+ + a) | \psi_n \rangle = -eF\sqrt{\frac{\hbar}{2m\omega}} \langle \psi_n | (a^+ + a) | \psi_n \rangle \quad \text{Equation 14}$$

However, the position operator acts on one electron at a time. When acting on the ground state ket it will break the pair, so the resulting wavefunction will be orthogonal to the ground state bra. Thus, first order perturbation theory gives a null result.

We move onto second order perturbation theory:

$$\Delta E_F = \sum_{m \neq n} \frac{\left| \langle \psi_m | -eF\sqrt{\frac{\hbar}{2m\omega}}(a^+ + a) | \psi_n \rangle \right|^2}{E_n - E_m} = \frac{e^2 F^2 \hbar}{2m\omega} \sum_{m \neq n} \frac{\left| \langle \psi_m | (a^+ + a) | \psi_n \rangle \right|^2}{E_n - E_m} \quad \text{Equation 15}$$

Given the solution found above in Richardson's Model we get for the summation:

$$\sum_{m \neq n} \frac{\left| \langle \psi_m | (a^+ + a) | \psi_n \rangle \right|^2}{E_n - E_m} = - \frac{\left| \langle \psi_{split-pair-state} | (a^+ + a) | 4-E, 2-E \rangle \right|^2}{(3-E)((4-E)^2 + (2-E)^2)} \quad \text{Equation 16}$$

The expression in equation 16 can be simplified to give the shift in energy:

$$\Delta E_F = - \frac{e^2 F^2 \hbar}{2m\omega} \frac{8(3-E)}{(4-E)^2 + (2-E)^2} \quad \text{Equation 17}$$

Notice that the shift in energy is proportional to the electric field squared. This indicates a behavior that mimics a polarizability α :

$$\alpha = \frac{-2\Delta E_F}{F^2} = \frac{e^2}{m\omega^2} \frac{8(3-E)\hbar\omega}{(4-E)^2 + (2-E)^2} \quad \text{Equation 18}$$

This result is shown in figure 3, where we notice that when $g \rightarrow 0$ the system approaches the normal state where $E = 2\hbar\omega$ and then the polarizability is equal to the normal value $\alpha = 2e^2 / m\omega^2$. The normal value can be obtained directly from the Hamiltonian by noticing that it can be written as:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + eFx = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \left(x + \frac{eF}{m\omega^2} \right)^2 - \frac{1}{2} \frac{e^2}{m\omega^2} F^2 \quad \text{Equation 19}$$

The last term in equation 19 shifts the bottom of the potential well downwards, but doesn't change its shape, so the consequence is a polarizability of $e^2 / m\omega^2$ per electron. The trend when the value of g increases, as shown in figure 3, is a decrease in the polarizability.

Considering the problem with more energy levels

Truncating the spectrum at two levels might be an extreme simplification. Then, it is a fair question to ask for the consequences of having more energy levels. To examine the other extreme we can treat the problem for two electrons in a ladder of 16 energy levels. This time the equation to solve will be:

$$1 - \frac{g}{2-E} - \frac{g}{4-E} - \frac{g}{6-E} - \frac{g}{8-E} \dots - \frac{g}{32-E} = 0 \quad \text{Equation 20}$$

Like before, this equation can be numerically approached to get E as a function of g . The resulting function is shown in figure 4. We observe a much faster drop in the overall energy as g increases as compared to the case with two levels. This is not surprising, because the extra levels are now available for more scattering.

With C as the normalizing coefficient, the wavefunction becomes:

$$|\psi_n\rangle_U = C \cdot \left(\frac{b_1^+}{2-E} + \frac{b_2^+}{4-E} \dots + \frac{b_{16}^+}{32-E} \right) |0\rangle = \left| \frac{C}{2-E}, \frac{C}{4-E}, \dots, \frac{C}{32-E} \right\rangle \quad \text{Equation 21}$$

Once again, we use second order perturbation theory to calculate the shift in energy as a response to an electric field by:

$$\Delta E_F = e^2 F^2 x_o^2 \sum_{m \neq n} \frac{\left| \langle \psi_m | (a^+ + a) | \psi_n \rangle \right|^2}{E_n - E_m} \quad \text{Equation 22}$$

We also need to apply the operator to each electron and add all terms. In each case, the operator will break the pair, and the resulting ket will need to be multiplied by its corresponding bra to find its contribution. The shift in energy is given by equation 23:

$$\Delta E_F = \frac{e^2 F^2 x_o^2}{4} \sum_{m \neq n} \frac{\left| \langle \psi_m | (a^+ + a) \left| \frac{C}{2-E}, \frac{C}{4-E}, \dots, \frac{C}{32-E} \right\rangle \right|^2}{E_n - E_m} \quad \text{Equation 23}$$

And consequently the polarizability is given by equation 24:

$$\alpha = -\frac{e^2 x_o^2}{2} \sum_{m \neq n} \frac{\left| \langle \psi_m | (a^+ + a) \left| \frac{C}{2-E}, \frac{C}{4-E}, \dots, \frac{C}{32-E} \right\rangle \right|^2}{E_n - E_m} \quad \text{Equation 24}$$

The polarizability as a function of g for this case is shown in figure 5. We observe again a decrease in the polarizability as g increases, similar to the case of two states, but the decrease is slower in the present case.

Solving the Problem for Four Electrons

Let's consider four electrons in a three energy level system. This is the simplest non-trivial case where we can consider the pair-pair interaction expressed in the third term of equation 7. The equations become:

$$1 - \frac{g}{2-E_1} - \frac{g}{4-E_1} - \frac{g}{6-E_1} + \frac{2g}{E_2-E_1} = 0 \quad \text{Equation 25a}$$

$$1 - \frac{g}{2-E_2} - \frac{g}{4-E_2} - \frac{g}{6-E_2} + \frac{2g}{E_1-E_2} = 0 \quad \text{Equation 25b}$$

Like before, we use the approach of mapping the problem to an electrostatic configuration, the energies represent equilibrium positions of two infinite long rods in a region of space where the potential is given by:

$$V = -x - g \ln|2-x| - g \ln|4-x| - g \ln|6-x| \quad \text{Equation 26}$$

And the rods attract each other, according to the force

$$F_{12} = \frac{2g}{E_1 - E_2} \quad \text{Equation 27}$$

Because of this attractive force, this time, the equilibrium positions will not be at the bottom of the potential wells. Figure 6 illustrates this situation for $g=0.5$, the attraction brings the two positions closer together.

An analysis of the energies E_1 and E_2 as a function of g shows that the value of E_1 first decreases, but then starts to increase, while E_2 decreases monotonically (see figure 7). More importantly, the sum of the energies decreases monotonically. (The figure shows the average energy as a dotted line).

We encounter a problem at $g=0.78$. The two energies coalesce at $E=2$, so the solutions to the equations diverge. Richardson attacked this problem by considering complex energies [16]. We can do this by substituting $E_1 = \varepsilon - i\eta$ and $E_2 = \varepsilon + i\eta$. The energies must be complex conjugates of each other because the total energy, E_1+E_2 , must be real.

Therefore, the equations become:

$$1 - \frac{g}{2-\varepsilon+i\eta} - \frac{g}{4-\varepsilon+i\eta} - \frac{g}{6-\varepsilon+i\eta} + \frac{2g}{\varepsilon+i\eta-\varepsilon+i\eta} = 0 \quad \text{Equation 28a}$$

$$1 - \frac{g}{2-\varepsilon-i\eta} - \frac{g}{4-\varepsilon-i\eta} - \frac{g}{6-\varepsilon-i\eta} + \frac{2g}{\varepsilon-i\eta-\varepsilon-i\eta} = 0 \quad \text{Equation 28b}$$

Notice that equation 28b is the complex conjugate of 28a; therefore we only need to solve one. However, we still have to make sure that both real and imaginary parts equal zero. The new equations become:

$$1 - \frac{g(2-\varepsilon)}{(2-\varepsilon)^2 + \eta^2} - \frac{g(4-\varepsilon)}{(4-\varepsilon)^2 + \eta^2} - \frac{g(6-\varepsilon)}{(6-\varepsilon)^2 + \eta^2} = 0 \quad \text{Equation 29a}$$

$$\rightarrow g = \frac{1}{\frac{(2-\varepsilon)}{(2-\varepsilon)^2 + \eta^2} + \frac{(4-\varepsilon)}{(4-\varepsilon)^2 + \eta^2} + \frac{(6-\varepsilon)}{(6-\varepsilon)^2 + \eta^2}} \quad \text{Equation 29b}$$

$$\frac{\eta^2}{(2-\varepsilon)^2 + \eta^2} + \frac{\eta^2}{(4-\varepsilon)^2 + \eta^2} + \frac{\eta^2}{(6-\varepsilon)^2 + \eta^2} = 1 \quad \text{Equation 29c}$$

Equation 29b is the same as equation 29a, but solved for g . Since equation 29c does not involve g , we can use it to solve for η given a value of ε and then use equation 29b to find g . Using this approach, the trend in figure 7 for $g < 0.78$ can be extended to larger values as shown in the figure.

The resulting wavefunction can be calculated as expressed in equations 30:

$$|\psi_n\rangle_U = C \left(\frac{b_1^+}{2-E_1} + \frac{b_2^+}{4-E_1} + \frac{b_3^+}{6-E_1} \right) \left(\frac{b_1^+}{2-E_2} + \frac{b_2^+}{4-E_2} + \frac{b_3^+}{6-E_2} \right) |0\rangle \quad \text{Equation 30a}$$

$$|\psi_n\rangle_U = C \left(\begin{aligned} &\frac{b_1^+ b_2^+}{(2-E_1)(4-E_2)} + \frac{b_1^+ b_3^+}{(2-E_1)(6-E_2)} + \frac{b_2^+ b_3^+}{(4-E_1)(6-E_2)} \\ &+ \frac{b_2^+ b_1^+}{(4-E_1)(2-E_2)} + \frac{b_3^+ b_1^+}{(6-E_1)(2-E_2)} + \frac{b_3^+ b_2^+}{(6-E_1)(4-E_2)} \end{aligned} \right) |0\rangle \quad \text{Equation 30b}$$

Using a cartoon representation of this wavefunction we get equation 31.

$$|\psi_n\rangle_U = c_{12} \begin{vmatrix} - - \\ \bullet \bullet \\ \bullet \bullet \end{vmatrix} + c_{13} \begin{vmatrix} \bullet \bullet \\ - - \\ \bullet \bullet \end{vmatrix} + c_{23} \begin{vmatrix} \bullet \bullet \\ \bullet \bullet \\ - - \end{vmatrix} \quad \text{Equation 31}$$

Where:

$$c_{12} = \frac{C}{(2-E_1)(4-E_2)} + \frac{C}{(4-E_1)(2-E_2)}$$

$$c_{13} = \frac{C}{(2-E_1)(6-E_2)} + \frac{C}{(6-E_1)(2-E_2)}$$

Equations 32

$$c_{23} = \frac{C}{(4-E_1)(6-E_2)} + \frac{C}{(6-E_1)(4-E_2)}$$

To find the response to an electric field, we calculate the shift in energy using perturbation theory. In first order, we notice that the application of the position operator will split pairs in the wavefunction, so we again obtain a null result. In second order perturbation theory, we need to consider excited states.

$$\alpha = -\frac{e^2 x_o^2}{2} \sum_{m \neq n} \frac{|\langle \psi_m | (a^+ + a) | \psi_n \rangle|^2}{E_n - E_m} \quad \text{Equation 33}$$

The excited states that include a split pair are simple to calculate in this case because the two blocked states will not be available for the remaining pair to scatter. Regardless of the value of g, the energy of the following excited states will be constant:

$$|\psi_{m=1}\rangle = \begin{vmatrix} - \bullet \\ \bullet - \\ \bullet \bullet \end{vmatrix} \quad E_{m=1} = 7$$

$$|\psi_{m=2}\rangle = \begin{vmatrix} \bullet - \\ \bullet \bullet \\ - \bullet \end{vmatrix} \quad E_{m=2} = 8$$

$$|\psi_{m=3}\rangle = \begin{vmatrix} \bullet \bullet \\ - \bullet \\ \bullet - \end{vmatrix} \quad E_{m=3} = 9$$

Equations 34

The ket resulting from the application of the position operator on the ground state is:

$$(a^+ + a)|\psi_n\rangle = c_{12}\sqrt{2}|\psi_{m=1}\rangle + c_{13}\sqrt{2}|\psi_{m=1}\rangle + c_{13}|\psi_{m=3}\rangle + c_{23}|\psi_{m=3}\rangle \quad \text{Equation 35}$$

The internal products become:

$$\langle \psi_{m=1} | (a^+ + a) | \psi_n \rangle = \sqrt{2}(c_{12} + c_{13})$$

$$\langle \psi_{m=2} | (a^+ + a) | \psi_n \rangle = 0$$

$$\langle \psi_{m=3} | (a^+ + a) | \psi_n \rangle = c_{13} + c_{23}$$

Equations 36

Therefore the resulting polarizability from perturbation theory is:

$$\alpha = -\frac{e^2 x_o^2}{2} \left[\frac{2(c_{12} + c_{13})^2}{E-7} + \frac{(c_{13} + c_{23})^2}{E-9} \right] \quad \text{Equation 37}$$

This is illustrated in figure 8. We observe once again that when $g \rightarrow 0$ the system approaches the normal state where $E = 6\hbar\omega$ and then the polarizability is equal to the normal value $\alpha = 4e^2 / m\omega^2$. The trend for increasing g is once again a reduction in the polarizability.

Four electrons and four levels

By adding more energy levels to the case of 4 electrons, the result becomes more realistic. Therefore we will examine the case of four energy levels. To find the energies, we need to solve two equations:

$$1 - \frac{g}{2-E_1} - \frac{g}{4-E_1} - \frac{g}{6-E_1} - \frac{g}{8-E_1} + \frac{2g}{E_2-E_1} = 0 \quad \text{Equation 37a}$$

$$1 - \frac{g}{2-E_2} - \frac{g}{4-E_2} - \frac{g}{6-E_2} - \frac{g}{8-E_2} + \frac{2g}{E_1-E_2} = 0 \quad \text{Equation 37b}$$

Once again, mapping the problem into an electrostatic problem works as long as the energies are real. If g is too large we will need to resort to a solution of energies that are complex conjugates of each other as previously performed. The solution for the energies as a function of g is shown in figure 9. We observe that the overall energy decreases monotonically, but E_1 first decreases and then increases to finally coalesce with E_2 at $g \approx 0.68$, which is similar to the result with 3 levels.

The wavefunction is calculated below:

$$|\psi_n\rangle_U = C \left(\frac{b_1^+}{2-E_1} + \frac{b_2^+}{4-E_1} + \frac{b_3^+}{6-E_1} + \frac{b_4^+}{8-E_1} \right) \left(\frac{b_1^+}{2-E_2} + \frac{b_2^+}{4-E_2} + \frac{b_3^+}{6-E_2} + \frac{b_4^+}{8-E_2} \right) |0\rangle$$

Equation 38a

$$|\psi_n\rangle_U = C \left(\begin{array}{l} \frac{b_1^+ b_2^+}{(2-E_1)(4-E_2)} + \frac{b_1^+ b_3^+}{(2-E_1)(6-E_2)} + \frac{b_1^+ b_4^+}{(2-E_1)(8-E_2)} + \frac{b_2^+ b_1^+}{(4-E_1)(2-E_2)} + \\ \frac{b_2^+ b_3^+}{(4-E_1)(6-E_2)} + \frac{b_2^+ b_4^+}{(4-E_1)(8-E_2)} + \frac{b_3^+ b_1^+}{(6-E_1)(2-E_2)} + \frac{b_3^+ b_2^+}{(6-E_1)(4-E_2)} + \\ \frac{b_3^+ b_4^+}{(6-E_1)(8-E_2)} + \frac{b_4^+ b_1^+}{(8-E_1)(2-E_2)} + \frac{b_4^+ b_2^+}{(8-E_1)(4-E_2)} + \frac{b_4^+ b_3^+}{(8-E_1)(6-E_2)} \end{array} \right) |0\rangle$$

Equation 38b

With a cartoon representation as follows:

$$|\psi_n\rangle_U = c_{12} \left| \begin{array}{c} - \\ - \\ \bullet \\ \bullet \end{array} \right\rangle + c_{13} \left| \begin{array}{c} - \\ \bullet \\ - \\ \bullet \end{array} \right\rangle + c_{14} \left| \begin{array}{c} \bullet \\ - \\ - \\ \bullet \end{array} \right\rangle + c_{23} \left| \begin{array}{c} - \\ \bullet \\ \bullet \\ - \end{array} \right\rangle + c_{24} \left| \begin{array}{c} \bullet \\ - \\ \bullet \\ - \end{array} \right\rangle + c_{34} \left| \begin{array}{c} \bullet \\ \bullet \\ - \\ - \end{array} \right\rangle \quad \text{Equation 39}$$

Where:

$$\begin{aligned} c_{12} &= \frac{C}{(2-E_1)(4-E_2)} + \frac{C}{(4-E_1)(2-E_2)} & c_{13} &= \frac{C}{(2-E_1)(6-E_2)} + \frac{C}{(6-E_1)(2-E_2)} \\ c_{14} &= \frac{C}{(2-E_1)(8-E_2)} + \frac{C}{(8-E_1)(2-E_2)} & c_{23} &= \frac{C}{(4-E_1)(6-E_2)} + \frac{C}{(6-E_1)(4-E_2)} \\ c_{24} &= \frac{C}{(4-E_1)(8-E_2)} + \frac{C}{(8-E_1)(4-E_2)} & c_{34} &= \frac{C}{(6-E_1)(8-E_2)} + \frac{C}{(8-E_1)(6-E_2)} \end{aligned} \quad \text{Equations 40}$$

Introducing an Electric field

One more time, to find the response to an electric field we calculate the shift in energy using second order perturbation theory (equation 33). This time the excited states energies will be functions of g . The split pair of electrons blocks two levels, but the remaining pair will have two states to scatter. The excited states that contain one split pair are:

$$\begin{aligned} |\psi_{m=1}\rangle &= k_{11} \left| \begin{array}{c} - \\ \bullet \\ - \\ \bullet \end{array} \right\rangle + k_{12} \left| \begin{array}{c} \bullet \\ - \\ - \\ \bullet \end{array} \right\rangle & E_{m=1} &= 1 + 2 + \delta_1 \quad \text{where} \quad \delta_1 < 6 \\ |\psi_{m=2}\rangle &= k_{21} \left| \begin{array}{c} - \\ \bullet \\ - \\ \bullet \end{array} \right\rangle + k_{22} \left| \begin{array}{c} \bullet \\ - \\ - \\ \bullet \end{array} \right\rangle & E_{m=2} &= 1 + 2 + \delta_2 \quad \text{where} \quad 8 > \delta_2 > 6 \\ |\psi_{m=3}\rangle &= k_{31} \left| \begin{array}{c} - \\ \bullet \\ \bullet \\ - \end{array} \right\rangle + k_{32} \left| \begin{array}{c} \bullet \\ \bullet \\ - \\ - \end{array} \right\rangle & E_{m=3} &= 2 + 3 + \delta_3 \quad \text{where} \quad \delta_3 < 2 \\ |\psi_{m=4}\rangle &= k_{41} \left| \begin{array}{c} - \\ \bullet \\ \bullet \\ \bullet \end{array} \right\rangle + k_{42} \left| \begin{array}{c} \bullet \\ \bullet \\ - \\ - \end{array} \right\rangle & E_{m=4} &= 2 + 3 + \delta_4 \quad \text{where} \quad 8 > \delta_4 > 2 \end{aligned}$$

$$\begin{aligned}
|\psi_{m=5}\rangle &= k_{51} \begin{array}{|c} \bullet - \\ - \bullet \\ - - \\ \bullet \bullet \end{array} + k_{52} \begin{array}{|c} - \bullet \\ \bullet - \\ \bullet \bullet \\ - - \end{array} & E_{m=5} &= 3 + 4 + \delta_5 \quad \text{where} \quad \delta_5 < 2 \\
|\psi_{m=6}\rangle &= k_{61} \begin{array}{|c} \bullet - \\ - \bullet \\ - - \\ \bullet \bullet \end{array} + k_{62} \begin{array}{|c} - \bullet \\ \bullet - \\ \bullet \bullet \\ - - \end{array} & E_{m=6} &= 3 + 4 + \delta_6 \quad \text{where} \quad 2 > \delta_6 > 4
\end{aligned}$$

Equations 41

And the ket that results from applying the operator on the ground state is:

$$\begin{aligned}
(a^+ + a)|\psi_n\rangle &= \sqrt{2}(c_{12} + c_{13}) \begin{array}{|c} - - \\ - \bullet \\ \bullet - \\ \bullet \bullet \end{array} + \sqrt{3}(c_{13} + c_{14}) \begin{array}{|c} - \bullet \\ \bullet - \\ - - \\ \bullet \bullet \end{array} + (c_{13} + c_{23}) \begin{array}{|c} - - \\ \bullet \bullet \\ - \bullet \\ \bullet - \end{array} \\
&+ (c_{14} + c_{24}) \begin{array}{|c} \bullet \bullet \\ - - \\ - \bullet \\ \bullet - \end{array} + \sqrt{3}(c_{23} + c_{24}) \begin{array}{|c} - \bullet \\ \bullet - \\ \bullet \bullet \\ - - \end{array} + \sqrt{2}(c_{24} + c_{34}) \begin{array}{|c} \bullet \bullet \\ - \bullet \\ \bullet - \\ - - \end{array}
\end{aligned}$$

Equation 42

So, the matrix elements are:

$$\begin{aligned}
\langle \psi_{m=1} | (a^+ + a) | \psi_n \rangle &= (c_{13} + c_{23})k_{11} + (c_{14} + c_{24})k_{12} \\
\langle \psi_{m=2} | (a^+ + a) | \psi_n \rangle &= (c_{13} + c_{23})k_{21} + (c_{14} + c_{24})k_{22} \\
\langle \psi_{m=3} | (a^+ + a) | \psi_n \rangle &= \sqrt{2}(c_{12} + c_{13})k_{31} + \sqrt{2}(c_{24} + c_{34})k_{32} \\
\langle \psi_{m=4} | (a^+ + a) | \psi_n \rangle &= \sqrt{2}(c_{12} + c_{13})k_{41} + \sqrt{2}(c_{24} + c_{34})k_{42} \\
\langle \psi_{m=5} | (a^+ + a) | \psi_n \rangle &= \sqrt{3}(c_{13} + c_{14})k_{51} + \sqrt{3}(c_{23} + c_{24})k_{52} \\
\langle \psi_{m=6} | (a^+ + a) | \psi_n \rangle &= \sqrt{3}(c_{13} + c_{14})k_{61} + \sqrt{3}(c_{23} + c_{24})k_{62}
\end{aligned}$$

Equations 43

The polarizability as a function of g is shown in figure 10. We observe one more time a decrease as g increases, but the trend is slower than in the case of 3 levels. There is also a small sharp change around $g \approx 0.68$ where $E_1 = E_2$, but the main result remains that the pairing interaction reduces the polarizability.

Discussion and conclusions

The Richardson model has allowed us to find the energies and wavefunctions of the pairing Hamiltonian. The solution is simple for a few electrons, but the number of terms

in the solution is given by the Newton binomial $\binom{\# \text{ of Levels}}{\# \text{ of Pairs}}$, which grows very fast with the size of the sample.

Once the solution is found, to calculate polarizabilities using perturbation theory, it is necessary to find the matrix elements of all wavefunctions with the perturbing Hamiltonian. Obviously, these elements will depend on the shape of the potential used for the electrons. In this work, we used a simple parabolic potential and found that the polarizability decreases as the pairing interaction becomes stronger. However, preliminary calculations show a similar effect in the case of an infinite square potential (particle in a box problem). It seems that the effect is robust and although dependent on the exact potential used, the results shown here are general trends.

It is interesting that the polarizability decreases as the interaction gets stronger. This result might explain some of the observations made at Georgia Tech. Figure 2 in reference [10] shows a clear decrease in the polarizability (before stronger effects are observed at even lower temperatures), signaling an inability of the electrons to screen external fields. But in order to explain the ferroelectric effect we would need to consider additional factors since we cannot reproduce them in the present model.

Acknowledgements

We thank Dr. Vitaly Kresin and Dr. Vladimir Kresin for their helpful comments on a first version of this work. We also thank Dr. Xiaoshan Xu, who shared with us his unpublished calculations where he attacks this problem using a different approach.

FIGURES

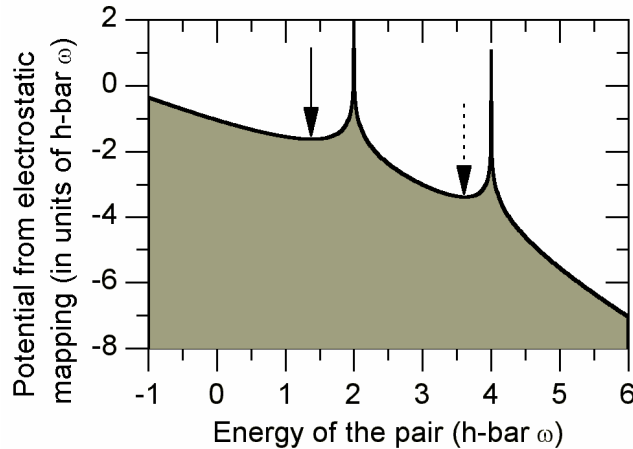


Figure 1: The problem of 2 electrons in the presence of a pairing interaction with strength $g = 0.5\hbar\omega$ mapped into a 2-dimensional electrostatic problem. The y-axis is the potential and the x-axis represents the energy of the pair in units of $\hbar\omega$. The solid arrow indicates the energy of the ground state and the dotted arrow indicates the energy of the excited state of the pair.

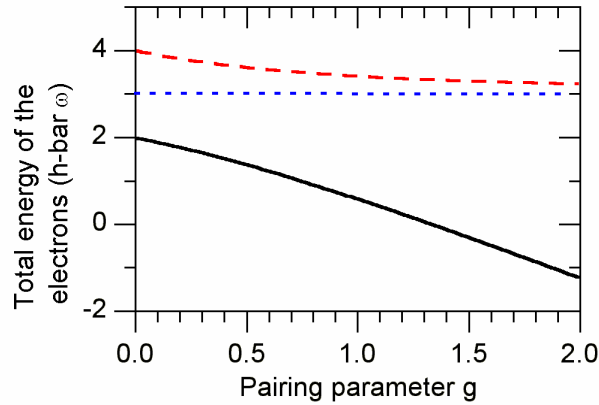


Figure 2: Ground state energy of a pair of electrons as a function of the pairing parameter “g” in the case of 2 levels available for scattering (solid line). Also shown, is the energy of an excited pair state (dashed line) and an excited split pair (dotted line).

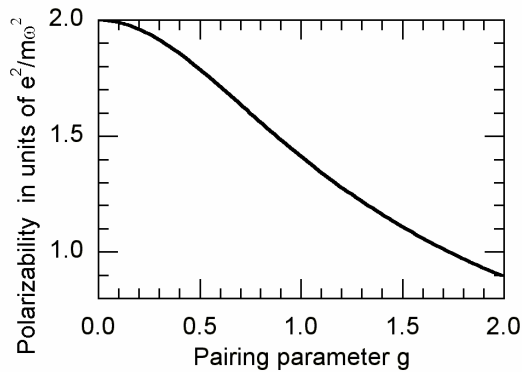


Figure 3: Polarizability of 2 electrons in a parabolic potential well truncated at 2 levels as a function of the pairing parameter “g”. We observe a decrease in the polarizability as g increases. The maximum value happens when $g=0$.

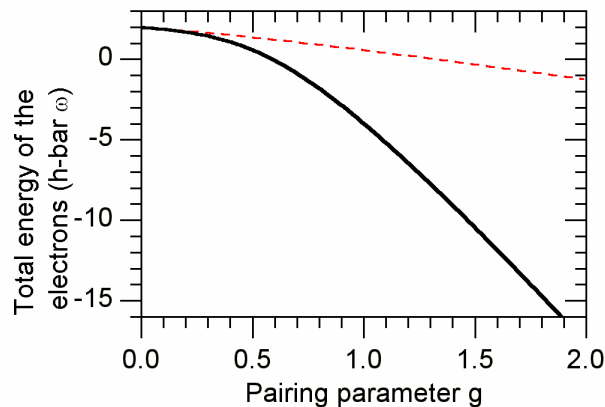


Figure 4: Ground state energy of 2 electrons in a parabolic potential well truncated at 16 levels as a function of the pairing parameter “g” (solid line). For comparison, the ground state energy of 2 electrons when only 2 levels are available for scattering is shown in the figure as the dashed line.

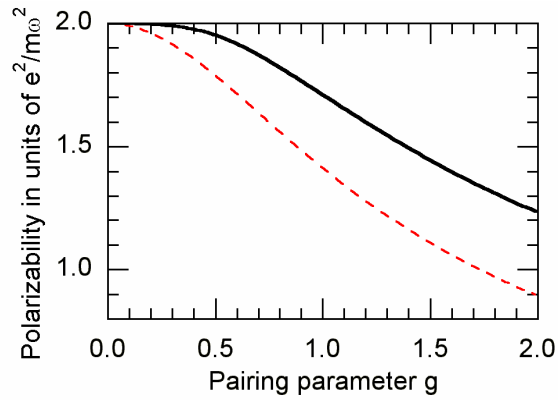


Figure 5: Polarizability of 2 electrons in a parabolic potential well truncated at 16 levels as a function of the pairing parameter “g” (solid line). The polarizability when only 2 levels are available for scattering is shown as a dashed line for comparison.

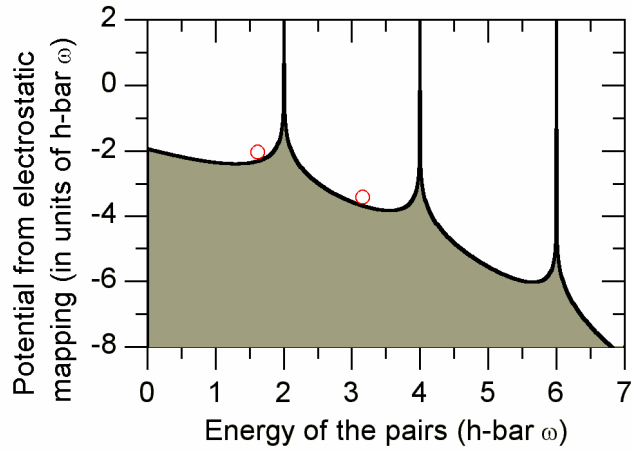


Figure 6: Electrostatic mapping of the problem of four electrons in a three level system in the presence of a pairing interaction of strength $g = 0.5\hbar\omega$. The attractive pair-pair interaction maps into an attractive force that causes the two electron pairs to move from the bottom of each well as represented by the circles.

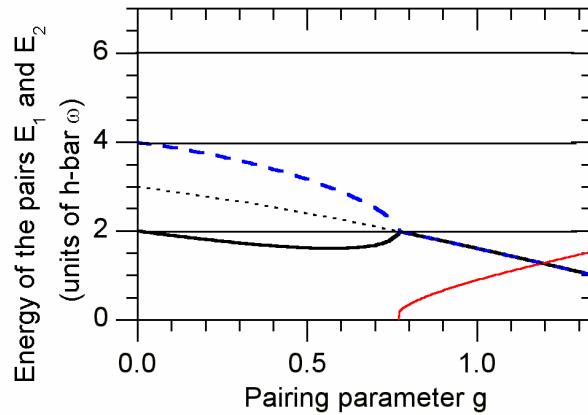


Figure 7: Energies of the two electron pairs E_1 (solid line) and E_2 (dashed line) with 3 levels available for scattering shown as a function of the pairing parameter g . When $g=0$ they adopt the lowest levels with energies of $2\hbar\omega$ and $4\hbar\omega$, as g increases the energies show an initial decrease, but as the attractive pair-pair force exceeds the repulsive force caused by the potential well, the two pairs coalesce on a single real energy (equal to $2\hbar\omega$) when $g \approx 0.78$. The dotted line represents the average energy of the two pairs. Continuing from the coalescing point, the pairs have complex energies that are conjugates (only the real part is shown for $g > 0.78$). The total energy is real, as it must be, and monotonically decreases with g . The magnitude of the imaginary component is represented by the thin line emerging from zero at $g=0.78$.

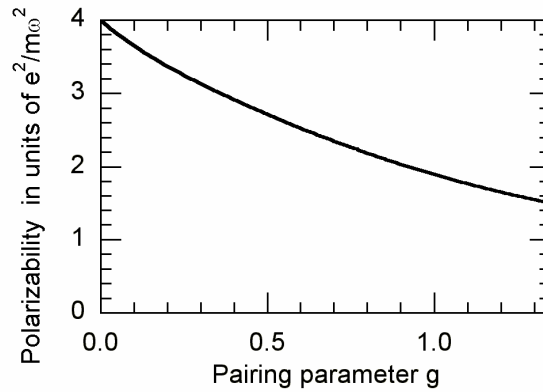


Figure 8: Polarizability of 4 electrons in the presence of a pairing interaction with 3 unblocked levels available for scattering. The value decreases with respect to the normal state as g increases.

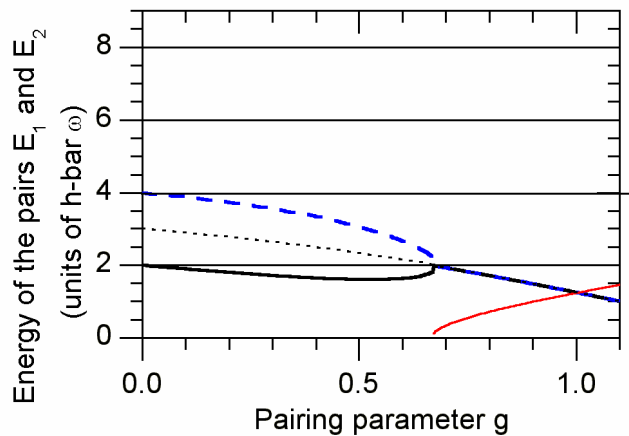


Figure 9: Extending from figure 7, the introduction of another energy level causes the coalescing point to happen at a lower value of g (here at 0.68) and the energy to drop more quickly as g increases. This is because another energy level increases the opportunity for pairs to scatter, reducing the energy of the system.

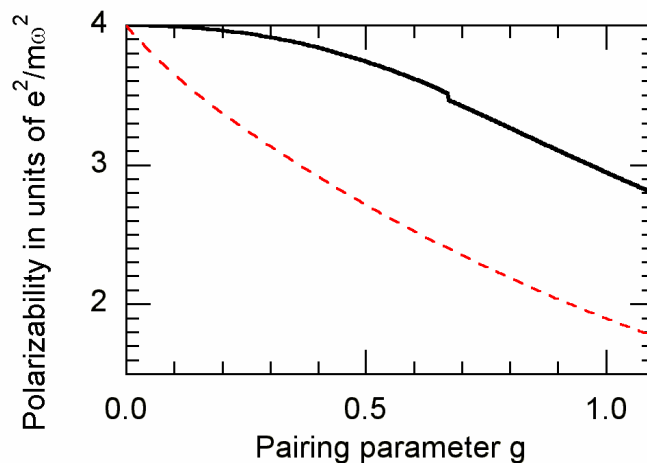


Figure 10: Polarizability of 4 electrons in the presence of a pairing interaction with 4 unblocked levels available for scattering (solid line). The value decreases with respect to the normal state as seen in the case of 3 levels (dashed line), but the decrease is slower here.

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