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Aromaticity in Superconducting Solids: Kohn-Sham Density Functional Theory Based on Correlated Electron Pairs in Oscillatory Resonant Quantum States

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Research Article

Keywords:

Posted Date: February 26th, 2026

DOI: https://doi.org/10.21203/rs.3.rs-8905573/v1

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Additional Declarations: No competing interests reported.

TITLE

Aromaticity in Superconducting Solids: Kohn-Sham Density Functional Theory Based on Correlated Electron Pairs in Oscillatory Resonant Quantum States

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ABSTRACT

Aromaticity in heteroatomic metal clusters has been studied. The issue is that most researchers evaluate aromaticity in solids based on the specific geometry the solid adopts under certain conditions. For small clusters with well-defined geometries, the concept of aromaticity is more applicable, but it becomes less effective for larger clusters. Understanding aromaticity is important because these compounds exhibit unusual properties, including superconductivity. In this work, we explain how the model of correlated electron pairs in oscillatory resonant quantum states converges in aromaticity and superconductivity in solids. Hückel's 4n+2 rule, which requires a minimum of two electrons, supports the theoretical model. The coordinated oscillatory motion of the pairs, through the exchange of a boson, represents a two-time process of the 2n+1 rule. Applying Density Functional Theory for pair diagnosis cannot be performed under the Born-Oppenheimer approximation, since it is the motion of the nuclei that creates the quantization of vibrations or the exchange bosons during the electron pair correlation. The boson is responsible for the combined spin change of the paired electrons and their oscillation in resonant quantum states. The pairs maintain their fermionic identity despite having opposite spins. They never condense and always have antisymmetric wave functions.

INTRODUCTION

The term "aromaticity" is among the most commonly used in organic chemistry and related fields. The concept rests on different theoretical foundations. The electronic, energetic, magnetic, and geometric aspects have been described to ascertain a molecule's aromatic character, but these ideas can't explicitly define aromaticity[1]. We have recently described a model of aromaticity based on the formation of correlated electron pairs in oscillatory resonant quantum states [2,3]. Also, in recent years, the concept of aromaticity has been extended to the solid state [4,5]. It can be applied to describe chemical bonding in transition-metal systems. Features commonly used to identify sigma-aromatic/antiaromatic compounds—such as stability, reactivity, and electron delocalization—are similar to those of typical π-aromatic/antiaromatic species [6,7], and therefore should be recognized and applied in the same way.

Simultaneously, gaining a thorough understanding of how dislocation motion occurs in non-metallic materials is becoming more crucial. Dimensionality reduction is essential because two-dimensional (2D) and one-dimensional (1D) systems often exhibit unusual magnetic properties and, in particular, can give rise to distinct types of phase transitions [8,9]. In an orbitally driven Peierls distortion, a 1D metallic system can alternate between short and long bonds, with large and small inter-site hopping. This dimerization opens a gap in the Fermi surface, thereby lowering the energies of the occupied electron states. Transitions to partially filled 1D bands running along all chains in solid lattices have led to more complex interaction structures [10–12]. For example, in $MgTi_2O_4$, the Peierls effect explains the high-temperature cubic-to-tetramerization transition, which involves alternating short−intermediate−long−intermediate bonds [13,14]. The transition from a regular to a dimer structure under pressure has also been well documented in some solids [15,16]. The metal-metal distance in such dimers is usually shorter than in the original material.

However, some materials are nonmagnetic at low temperatures due to Peierls dimerization [17]. The dimer state is often insulating, whereas the starting material is metallic. Thus, the

system exhibits orbital-selective behavior [18,19], with different orbitals responding differently to an external perturbation. For example, the temperature dependence of the magnetic susceptibility is revealed, where some orbitals are responsible for the high-temperature behavior. Still, in response to lower temperatures, other orbitals start to contribute [20]. This indicates that a dimensional change must be accompanied by specific conditions that are conducive to electron-correlation effects and exceptional properties for these phenomena to be observed. Moreover, in some solids, dimer clusters exist because of the crystal structure itself [21,22]. Orbitals directed toward neighbors may behave as delocalized and should be described by molecular orbitals, whereas the electrons in other orbitals may still be localized [23]. This is important because orbital-orbital hopping creates a state with opposite spins (S = 0 states), whereas the spin at localized orbitals is only ½. The physical mechanism of the slip process, which is closely related to the atomic structure, remains unexplained. The strong correlations at low temperatures in solids largely depend on the electronic structure, which is further affected by nontrivial topologies and symmetries. For example, 1D lattices, including tunnel geometries, have been shown to spontaneously develop structural instabilities below the critical temperature as electron–phonon interactions increase, thereby promoting a Peierls transition. Moreover, electron-phonon coupling (vibrational effects) is seen to be necessary in carbon nanotubes [24–26]. The same electron–phonon interactions could also lead to superconductivity. The role of correlated electron pairs oscillating in resonant quantum states, induced by inter-phonon exchange within aromatic structures and in superconductivity, was recently clarified through theoretical studies [2,3,27].

Quantum effects are typically associated with degeneracy arising from these spin-ordering mechanisms. Coulomb repulsion reduces collective charge fluctuations and causes electrons to localize on specific clusters. In transition metals with a honeycomb lattice, electrons hopping between p- or d-orbitals form structures that retain hexagonal symmetry [28–31], a state very similar to that of benzene, with the same molecular orbitals. In fact, as in a benzene molecule, six of such molecular orbitals form not levels but bands in a solid. Aromaticity in several heteroatomic metal clusters has been described [32–34].

In general, the interplay between covalent bond formation, spin-orbit coupling, and intra-atomic exchange interactions is essential for understanding the specific physical properties observed in transition-metal oxides. The unique significance of density functional theory (DFT) in the modern quantum chemical toolkit, particularly for modeling structures, properties, and processes, strengthens the validity of these conclusions. A strong link between theory and experiment often offers crucial insights into the geometric, electronic, and spectroscopic properties of the studied systems. Every day, DFT is widely used for computational modeling of molecules and materials with the expectation of high accuracy. However, in some instances, popular density-functional approximations (DFAs) can produce significant quantitative and even qualitative errors. Common issues have been identified, including systems with highly delocalized electron densities, charge-transfer complexes, transition states of radical reactions, band gaps, and extended conjugation [35–39].

This paper offers a theoretical approach to modeling dislocation processes in solids within the framework of conceptual density functional theory. It explains patterns of aromaticity change in solids using the model of correlated electron pairs in oscillatory resonant quantum states. Our model explicitly incorporates two-fermion correlation via a boson, unlike previous approaches in which the electron pair condenses. This can lead to new insights into reducing the inherent brittleness of materials and exploring compositions with unusual

properties. The developed framework for precise calculations will improve understanding of electronic and magnetic properties and can be utilized by both computational chemists and experimentalists.

AROMATIC CLUSTER IN SOLIDS. DFT THEORETICAL METHOD

Analyzing the orbital dependence. The electron density in the nucleus for the $2p$ orbitals is zero because the p orbitals have a "node" in the nucleus, meaning the probability of finding an electron there is zero. Unlike s orbitals, p and d orbitals have nodes at the nucleus. The "dumbbell" shape of the p orbitals indicates that the electron density is concentrated in two lobes on either side of the nucleus, not in the nucleus itself. The np orbitals become more diffuse as n increases, spreading the electron density over a larger area around the nucleus. As a result, the bonds formed with these orbitals weaken progressively as n increases. The square of the wave function indicates the density of probability of finding an electron in a specific region of space. In the nucleus, for p orbitals, the square of the wave function vanishes, implying that the electron density is zero.

According to Huckel's rule, a molecule needs at least two electrons to be aromatic $(4n + 2)$. In a way, the rule supports the concept of correlated electron pairs associated with aromaticity [2,3]. It usually begins with benzene, the prototype of aromaticity, which has six π-electrons. Although the Kekulé structure depicts localized double bonds, benzene's actual structure is delocalized, with the electron cloud above and below the ring plane (three electrons up ↑ and three electrons down ↓).

If we define an oscillation as the periodic motion of a system around an equilibrium position, we can better understand additional properties of aromatic compounds related to the formation of correlated electron pairs (Figure 1). The node of the p or d orbital creates an equilibrium position for the oscillating electron. Because the node carries a higher positive charge, it allows the electron to oscillate from a lower-energy node to a higher-energy node, thereby gaining kinetic energy, likely due to lattice vibrations. Self-oscillation is a property of certain dynamic systems. In a self-oscillator, the driving force is governed by the oscillation itself, so it remains in phase with the velocity: there is no need to adjust an external frequency to match resonance [40]. Self-oscillators differ from forced- and parametric-resonant systems, in which an externally modulated power source drives oscillations. Resonance is a phenomenon in which a system’s amplitude reaches a maximum when the driving frequency matches its natural frequency, resulting in a significant increase in energy and vibration. That is why we previously stated that one condition for the formation of correlated electron pairs in resonant quantum states was that the energy of the exchange phonon (boson) exactly matches the energy difference between the two electrons [2,3].

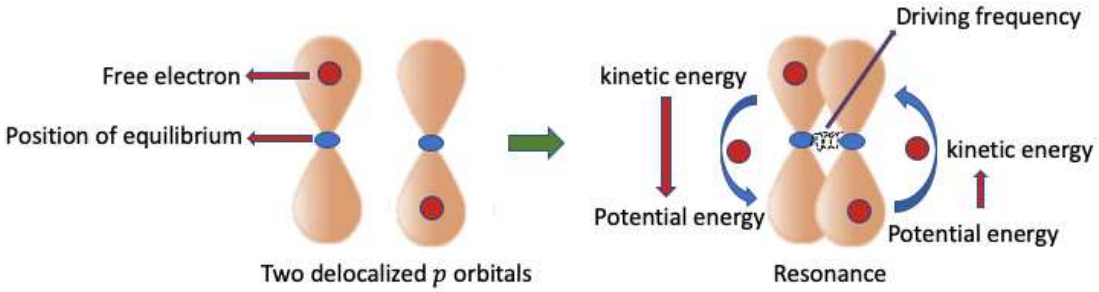


Figure 1: Self-oscillation of electrons in orbitals, considering the node as the equilibrium reference. When two orbitals of the same type and direction converge laterally at the same oscillation frequency, this results in a significant increase in energy and vibration, leading to resonance.

The concepts of delocalization, resonance, and aromaticity, although closely related, lack a concrete real-space definition that is independent of orbitals or specific wave-function expansions. We agree with Reuter et al. on defining delocalization as electron arrangements connected through paths of high probability density in the many-electron real space, and resonance as the consideration of additional electron arrangements that provide alternative pathways [41]. In contrast, we develop in this article an extension of the probability density analysis for the probabilistic quantification of “electron sharing arrangements” using the model of correlated electron pairs in ORQS.

In our model, orbital contraction increases the overall kinetic energy. However, the core of resonance remains essentially kinetic. Therefore, for simplicity, resonance can be viewed as two steps: contraction of the wave function at the nuclei and the actual resonance (Figure 2). The antisymmetry of fermionic wave functions must be considered; swapping two spin electrons changes the sign of the wave function, but the probability density remains the same, preserving the electrons' indistinguishability. Additionally, we should examine the effect of the phonon. The alternating spin structure is not independent since the rotation of one electron occurs when it absorbs a phonon that is subsequently destroyed within it and absorbed by the other electron. The combined rotation in opposite directions yields permutations of opposite sign, consistent with our model of correlated electron pairs in ORQS.

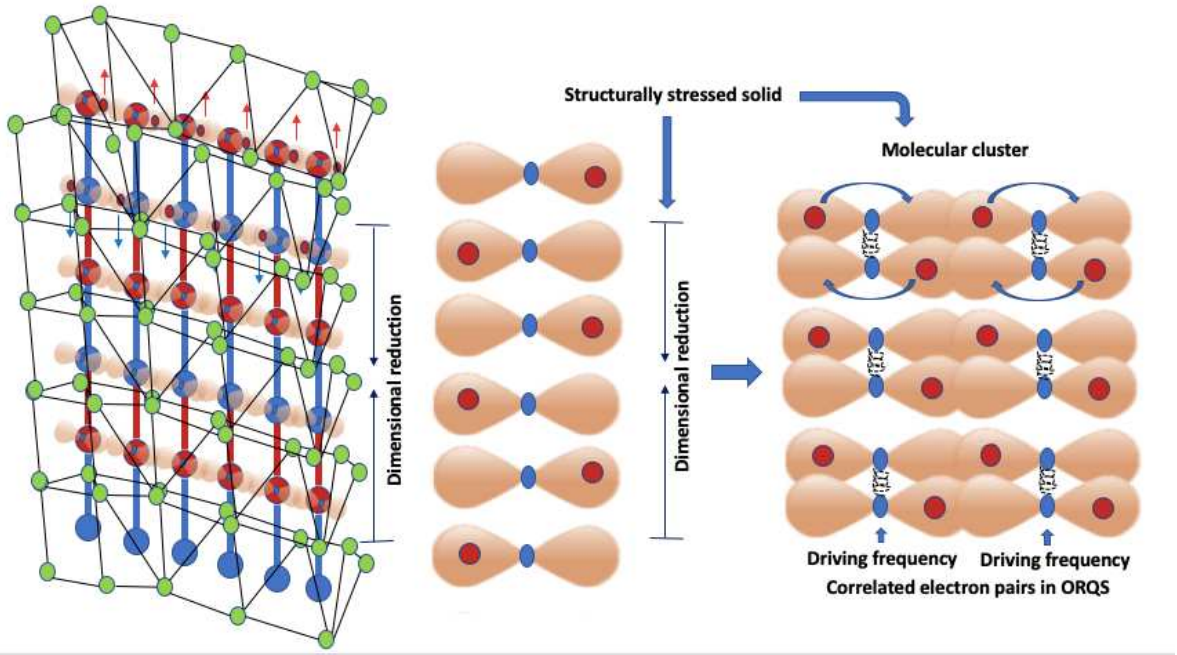


Figure 2: The orbital rearrangement induced by an external stimulus, such as a change in temperature or pressure, leads to the formation of molecular clusters within the crystal structure. These clusters resemble the geometry of aromatic compounds and are formed by correlated electron pairs in oscillatory, resonant quantum states.

The internal resonance, associated with nonlinearity in a multi-degree-of-freedom system, leads to the formation of correlated electron pairs in ORQS. Fermion pairs can only correlate through boson exchange. The pair carries the boson along, but each particle keeps its identity. There is a conversion in the quantization of oscillations due to the driving frequency. The combination of ionic contributions mainly results in kinetic stabilization. Spin-up and spin-down electrons can only move independently when both are odd-numbered because even numbers add extra nodes. This directly explains the Hückel rule of aromaticity $(4n + 2)$ and the pairing of electrons. To identify them, one must evaluate the spin functions (with $\alpha(m_s) = 1/2 + m_s$ and $\beta(m_s) = 1/2 - m_s$) and arrange the indices, which then yields block-diagonal Slater matrices. The determinants of these matrices are products of spin-up and spin-down determinants influenced by a boson. Therefore, we are compelled to modify the standard Kohn-Sham DFT, which often struggles to accurately describe noncovalent interactions.

The Kohn-Sham method yields a set of self-consistent orbitals and eigenvalues, corresponding to orbital energies. The operator that defines the movement of electron i (e_i) is $\hat{O}_i$. The following expression gives the operator Ô with $\hbar = m_e = e = 1$:

$$\hat{O}_i \emptyset_i = \varepsilon_i \emptyset_i$$

$$\hat{O} = -\frac{1}{2}\hat{\nabla}^2 + \hat{V}(r) + \int \left[\frac{\rho(r')}{|r - r'|} + \frac{\delta E_{xc}[\rho]}{\delta \rho(r)}\right] dr$$

Where E_{xc} is the exchange-correlation energy or potential, the electronic density $\rho(r)$ is constructed from the occupied orbital f_i:

$$\rho = \sum_{i}^{N} |\phi_i|^2$$

The chemical potential (m), molecular hardness (h), and polarizability (a) are electronic properties that define the reactivity of a chemical system. Physically, m describes the tendency of electrons to escape from the equilibrium system; it is associated with the electronic charge redistribution involved in any chemical process. Molecular hardness can be seen as a resistance to charge transfer. In Kohn–Sham density functional theory, the total energy of a system is represented as a functional of the charge density:

$$E[\rho] = T_s[\rho] + \int dr v_{ext}(r)\rho(r) + E_H[\rho] + E_{xc}[\rho]$$

Where:

v_{ext} is the electron–nuclei interaction (an electron in system S with nuclei in system S1)

E_H is the Coulomb energy

T_s is the Kohn–Sham kinetic energy

$$E_H[\rho] = \frac{e^2}{2}\int dr \int dr_1 \frac{\rho(r)\rho(r_1)}{|r - r_1|}$$

$$T_s[\rho] = \sum_{i=1}^{N} \int dr \varphi_i^*(r)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\varphi_i(r)$$

The sum of the orbital energies is related to the total energy as:

$$E = \sum_{i}^{N} \varepsilon_i - E_H[\rho] + E_{xc}[\rho] - \int \frac{\delta E_{xc}[\rho]}{\delta\rho(r)}\rho(r)dr$$

DFT THEORETICAL METHOD FOR THE CORRELATED ELECTRON PAIR IN ORQS

To accurately apply DFT to the correlated electron pair in ORQS, we must treat molecular orbitals as bands rather than levels in a solid. In Figures 3 and 4, we highlight the differences between a good conducting metal and typical superconducting elements. In transition-metal compounds, the metal's p or d band is usually not fully filled; although band theory predicts that these materials should be metals, many do not conduct electricity.

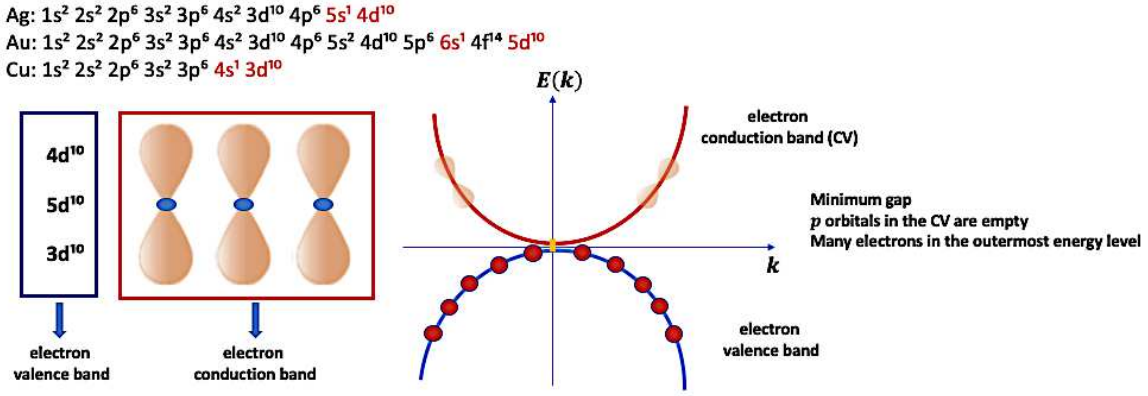


Figure 3: Schematic representation of a highly conductive material's band using its electronic structure and orbital arrangement.

The electronic structure of materials in which electron motion becomes correlated is markedly different from that of conventional band metals (Figure 4).

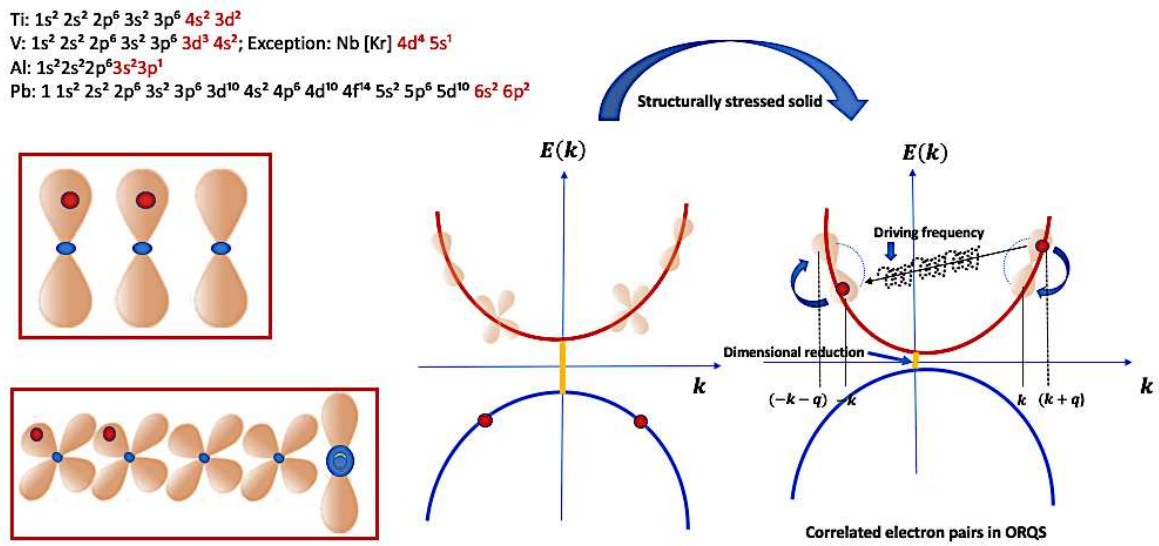


Figure 4. Schematic representation of a superconductor's band based on the model of correlated electron pairs in oscillatory resonant quantum states, when molecular clusters form due to the orbital rearrangement during a stimulus.

Metals that are poor conductors can become superconducting under certain conditions because, unlike good conductors, their electronic structures have fewer valence electrons and more vacant intraorbital spaces. These spaces act like holes or available sites. When orbital entanglement occurs, the nucleus-nucleus interaction appears stronger, and the quantization of this vibration facilitates the exchange of electron spin. When two neighboring orbitals are entangled, each containing an electron and a hole, two oscillators at the same frequency become coupled, resulting in correlated electron pairs in ORQS (Figure 5).
Given two electrons e_i and e_j with wave vector k+q and -k, and energies E(k+q) and E(-k), the wave function for the first oscillation is: $|k+q;-k;q\rangle$, and for the second oscillation is: $|-k-q;k;-q\rangle$. The Dispersion Law for a correlated pair of electrons in CEP-ORQS is:

$$H_{INT} = H_{e_i e_j} + U_{e_i B e_j} = U_{e_i(k+q)e_j(-k)} + U_{e_i(k+q)Be_j(-k)}$$

The momentum of the boson is q and the energy difference of the electrons pair is equal of the boson energy. The sum of their momentum is q:

$$k + q - k = q$$

When $e_i(k+q)$ emits a boson to $e_j(-k)$ with momentum q, e_i changes its position to $h_2(k)$. $e_j(-k)$ absorbs the boson (momentum q) and moves to $h_1(-k-q)$. A new pair is formed in $\left(e_j(-k), e_i(k+q)\right)$. Then, there is a complete oscillation.
Let's then find the wave function of a complete oscillation, considering only the internal state of the correlated pair. First, we need to define the Hamiltonian for each half-oscillation of the correlated pair:
For the first half-oscillation $\left(e_i(k+q), e_j(-k)\right)$:

$$H_{INT1} = U_{e_i(k+q)e_j(-k)} + U_{e_i(k+q)Be_j(-k)}$$

For the second half-oscillation $e_j(-k) = h_1(-k-q)$:

$$H_{INT2} = U_{e_j(-k-q)e_i(k)} + U_{e_j(-k-q)Be_i(k)}$$

If $k+q = P_1$ and $-k = P_2$, and $-k-q = -P_1$ and $k = -P_2$, then,
The total Hamiltonian is:

$$H_T = H_{INT1}H_{INT2} = \left[U_{e_j(-P_1)e_i(-P_2)} + U_{e_j(P_1)Be_i(-P_2)}\right]\left[U_{e_i(P_1)e_i(P_2)} + U_{e_i(P_1)Be_i(P_2)}\right]$$

The total wave function will be the momentum representation:

$$\psi(P) = |-k-q,k\rangle|k+q,-k\rangle = |-P_1,-P_2\rangle|P_1,P_2\rangle$$

The internal energy for a correlated pair after a complete oscillation is:

$$E_T^2 = E_{e_ie_j}^2 - E_{e_iBe_j}^2$$

For the complete oscillation, the functional density of the correlated pair $(e_i - e_j)$ with P impulse is:

$$\rho_{ij}(P) = |\psi(P)\rangle|^2$$

And the probability of finding a correlated pair at a point with momentum P is:

$$W_{ij}(P) = \int \rho(P)d^3P$$

Where $d^3P = dP_xdP_ydP_z$
If we want to represent the wave function in the coordinate-dependent Hilbert space, we need to apply the Fourier Transform, which allows us to transition from the infinite Hilbert space in F to the infinite space in P. The wave function in position space $\psi(\vec{r})$ is obtained from the wave function in momentum space $\phi(P)$ by means of the integral:

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int_{r^3}\phi(P)e^{i\vec{P}.\vec{r}/\hbar}d^3P$$

And

$$\psi(\vec{P}) = \frac{1}{(2\pi\hbar)^{3/2}}\int_{R^3}\psi(\vec{r})e^{-i\vec{P}.\vec{r}/\hbar}d^3r$$

Where $\vec{P} = \hbar\vec{k}$ and $\vec{r}$ is the real space.
Then, the probability density can be generalized:

$$\rho = \sum_{ij} c_{ij}\left|\psi_i(r)\psi_j(r)\right|^2$$

In general, the wave function is the tensor product of the wave functions in Hilbert spaces.

$$\rho = \sum_{ij} c_{ij}\psi_i(r) \otimes \psi_j(r)$$

The Kinetic energy of the correlated electron pair:

$$\hat{E} = -\frac{\hbar^2\nabla^2}{2m}$$

With $m = m_{e1}+m_{e2}$
In atomic units:

$$E_c = -\frac{\hbar^2}{4m_e}\nabla^2$$

$$T(\rho) = \sum_{i=1}^{N}\int d\vec{r}\psi_i^*(\vec{r})\left(-\frac{\hbar^2}{4m_e}\nabla^2\right)\psi_i(\vec{r})$$

$$E_H(\rho) = 2e/ze \int dr \int dr_1 \frac{\rho(r)\rho(r_1)}{|\vec{r} - \vec{r}_1|}$$

To determine the wave function of the already formed correlated pair, we will examine the formation of a π orbital. Two orbitals are aligned parallel to each other, with the two lobes of one orbital overlapping laterally with the two lobes of the other (Figure 1). They are characterized by the absence of electron density along their intermediate axis.

For a pair of electrons that occupy the same spatial orbital (ψ_π) with opposite spins, the total wave function (ψ_T) is a determinant of the orbital-spin products ensuring antisymmetry:

$$\psi(\vec{r}_1, m_{s1}; \vec{r}_2, m_{s2}) = \frac{1}{\sqrt{2}}[\psi_\pi(\vec{r}_1)\alpha(m_{s1})\psi_\pi(\vec{r}_2)\beta(m_{s2}) - \psi_\pi(\vec{r}_2)\alpha(m_{s2})\psi_\pi(\vec{r}_1)\beta(m_{s1})]$$

Where $\psi(\vec{r}, m_s)$ is the field operators of electrons and $\vec{r}$ and m_s are the spatial and spin coordinates, respectively ($\vec{r}_1$ and $\vec{r}_2$ are the positions of each electron, m_{s1} and m_{s2} are their respective spins), and α and β are the parameters of opposite spins. Exchanging the two electrons changes the function's sign, thereby satisfying the antisymmetry principle. The square of this function represents the probability density of finding the electron pair within a given region of space, forming a probability density cloud centered on the nucleus.

$$\rho(\vec{r}_1, m_{s1}; \vec{r}_2, m_{s2}) = \sum_i^N \left| \frac{1}{\sqrt{2}}[\psi_\pi(\vec{r}_1)\alpha(m_{s1})\psi_\pi(\vec{r}_2)\beta(m_{s2}) - \psi_\pi(\vec{r}_2)\alpha(m_{s2})\psi_\pi(\vec{r}_1)\beta(m_{s1})] \right|^2$$

In superconductivity, electrons cannot condense into a single state because of Pauli's principle; they are forced to oscillate (Figure 5). Oscillations can significantly influence the properties of natural electron fluxes. When two oscillators are coupled, they periodically exchange oscillations. If their natural frequencies are identical, this exchange becomes perfect, producing oscillations with maximum amplitude and resonance. A system of coupled oscillators closely mimics the oscillation characteristics when interactions are taken into account. It is the motion of the nuclei that produces the quantization of vibrations (bosons), and it is the bosons that carry the energy that electrons exchange in order to oscillate in resonant quantum states.

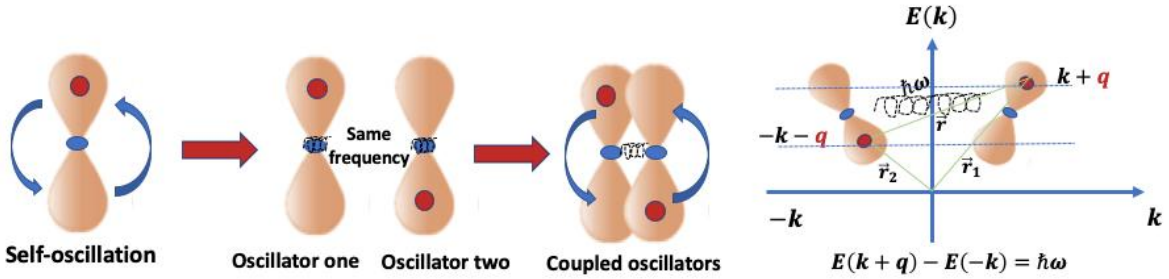


Figure 5. Formation of correlated electron pairs in oscillatory resonant quantum states. The node-node interaction generates the quantization of vibrations (bosons). The boson's energy is used by the pairs for the combined exchange of spin during each half-oscillation. Since nucleus-nucleus vibrations occur when specific physical conditions—such as temperature or pressure—are met, the final process yields a resonance frequency. Fermions maintain their identity and are correlated through a boson. It is evident that electrons occupy different energy levels, which is why they do not condense.

To get $\psi(e_i, e_j)$ the necessary condition is: $(Ee_i - Ee_j = \hbar\omega;\ m_{s1} \uparrow \rightarrow m_{s2} \downarrow)$
In general, if $\vec{r} = \vec{r}_2 - \vec{r}_1$: $\psi = \psi(\vec{r})$ depends on $\left(e_i, e_j; Ee_i - Ee_j = \hbar\omega; m_{s1e_i} \uparrow m_{s2e_j} \downarrow ; \uparrow\rightarrow\downarrow\right)$

$$\psi(e_i, e_j) = |k+q, -k, k+q-k = q, m_{s1} \uparrow m_{s2} \downarrow\rangle$$

The difference of the electron pair momentum is $\pm(2k+q)$ and the sum of the electron pairs is the phonon moment $\pm q$.

$$k + q = P_1, k = P_2$$

$$\psi(e_i, e_j) = |P_1, -P_2, P_1 + P_2 = q;\ m_{s2} \uparrow m_{s1} \downarrow\rangle$$

Self-oscillation of $(e_i, h_i) = |k+q, k, -q, m_{s1} \uparrow\rightarrow m_{s2} \downarrow\rangle$, with h_i the permissible space in the same orbital.
Self-oscillation of $(e_j, h_j) = |-k, -k-q, -q, m_{s2} \downarrow\rightarrow m_{s1} \uparrow\rangle$, with h_j the permissible space in the same orbital.

$$\psi(e_j, e_i) = |-P_2, -P_1, +q, m_{s2} \downarrow\rightarrow m_{s1} \uparrow\rangle$$

$$\psi\begin{pmatrix} e_i & e_j \\ e_j & e_i \end{pmatrix} = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi(e_i e_j) & \psi(e_j e_i) \\ \psi(e_j e_i) & \psi(e_i e_j) \end{vmatrix}$$

$$\widetilde{H}_{int1}\widetilde{H}_{int2} = \Delta^2 = E^2_{e_i e_j} - E^2_{e_i B e_j}$$

$$\Delta(e_i, e_j) = \sqrt{E^2_{e_i e_j} - E^2_{e_i B e_j}} = \hbar\omega_B;\ \text{B is the boson.}$$

Considering that if $\hat{b}_q^+$ and $\hat{b}_q^-$ are the creation and annihilation operators respectively of a phonon (boson) in the states q, and $\hat{c}_k^+$ and $\hat{c}_k^-$ are the creation and annihilation operators of a fermion (an electron) in the states k. Using the spin-polarized states and the operator of creation and annihilation, the field operators for correlated electron pair in ORQS is:
With χ_e the spin function, since χ_e depends on b_q ($m_s \uparrow\rightarrow C_k b_q;\ m_s \downarrow\rightarrow C_k$):

$$\Delta = (r_1 m_{s1} b_q; r_2 m_{s2} b_q)$$
$$= \frac{1}{2}\sum_{e_i}\sum_{e_j}\langle\left(C_{k_i} b_q \uparrow\right)\left(C_{k_j} b_q \uparrow\right)\rangle\begin{vmatrix} \varphi_{e_i\uparrow(r_1)b_q} & \varphi_{e_j\downarrow(r_2)} \\ \varphi_{e_j\uparrow(r_2)b_q} & \varphi_{e_i\downarrow(r_2)} \end{vmatrix}\{[(\chi_e$$
$$\uparrow(m_{s1})b_q)(\chi_e \downarrow(m_{s2}))] + [(\chi_e \downarrow(m_{s1}))(\chi_e \uparrow(m_{s2})b_q)]\}$$

The sum of the orbital energies in the molecular aromatic cluster inside a solid is related to the total energy as:

$$E = \sum_{e_i e_j}^{N} \varepsilon_{e_i e_j} - E_H[\rho] + E_{xc}[\rho] - \int \frac{\delta E_{xc}[\rho]}{\delta\rho(r)}\rho(r)dr$$

Where:
E_H is the Coulomb energy interaction between the correlated pair and the nucleus
The total energy for a correlated electron pairs in ORQS and a two-nucleus system is the sum of several energy components:

$$E_H = E_{e_i e_j} + V_{e_i e_j n_1} + V_{e_i e_j n_2} + V_{n_1 n_2}$$

The potential energy of interaction between the pair and the sigma electrons is omitted, considering the valence approximation where they are treated as part of the nuclei.
These terms represent:
$E_{e_i e_j}$: the energy of the correlated pair in ORQS

$V_{e_ie_jn_1}$: the potential energies of attraction between the pair and the nucleus one
$V_{e_ie_jn_2}$: the potential energies of attraction between the pair and the nucleus two
$V_{n_1n_2}$: the nuclear-nuclear repulsion potential energy
Using the formalism of the second quantization:

$$E_{e_ie_j} = K_p = \sum_k \varepsilon_p(k) P_k^+ P_k$$

Where P_k^+ and P_k are the operators of creation and annihilation of the electron pair. With

$$P_{k+q,-k}^+ = C_{-k}^+ C_{k+q}^+ b_q^+; P_{k+q,-k} = C_{-k} C_{k+q} b_q$$

For the interaction between the electrons and the nuclei, considering two identical nuclei, we modified Equation 2 in reference [42]:

$$V_{e_ie_jn} = -\sum_{e_ie_j} \int d^3r \int d^3R \Psi_{e_ie_j}^*(r)\, \Phi^*(R)\, \frac{Z}{|r-R|} \Phi(R)\, \Psi_{e_ie_j}(r)$$

Where $\Psi_{e_ie_j}(r)$ and $\Phi(R)$ are the electron pair and the nuclear wave function, respectively, and the atomic position is R.

$$V_{e_ie_jn_1} = -\sum_{e_ie_j} \int d^3r \int d^3R_1 \Psi_{e_ie_j}^*(r)\, \Phi^*(R_1) \frac{Z_1}{|r-R_1|} \Phi(R_1) \Psi_{e_ie_j}(r)$$

$$V_{e_ie_jn_2} = -\sum_{e_ie_j} \int d^3r \int d^3R_2\, \Psi_{e_ie_j}^*(r)\, \Phi^*(R_2) \frac{Z_2}{|r-R_2|} \Phi(R_2) \Psi_{e_ie_j}(r)$$

For nuclei-nuclei interactions:

$$V_{n_1n_2} = \frac{Q_1Q_2}{4\pi\varepsilon_0|R_1-R_2|}$$

$$V_{n_1n_2} = \frac{1}{4\pi\varepsilon_0} \int d^3R_{n1} \int d^3R_{n2} \frac{\rho(R_{n1})\rho(R_{n2})}{|R_{n1}-R_{n2}|}$$

Kohn and Sham presented an approximation of $E_{xc}[\rho]$ (functional of exchange and correlation) [43] as:

$$E_{xc}[\rho] = \int \rho(r) \varepsilon_{xc}\big(\rho(r)\big) d^3r$$

Where $\varepsilon_{xc}\big(\rho(r)\big)$ is the total exchange and correlation energy per electron of a uniform electron gas of density ρ. This is known as the local density approximation (LDA). The generalized gradient approximations (GGA) functionals have an integral formula similar to this Equation, with the addition that they can also depend on local gradients of ρ. Including information on correlated electron pairs in the Kohn–Sham equation will improve our understanding of solids.

DISCUSION

The directional nature of orbitals often effectively reduces the dimensionality of systems with orbital degrees of freedom. This can sometimes directly lead to the formation of well-defined clusters in solids. Descriptions of such clusters indicate that intracluster distances are shorter and that electrons are often delocalized, consistent with the molecular orbital picture [44–46]. The concepts of electron localization and delocalization, derived from the analysis of

the electronic structure of benzene, are crucial not only for understanding the molecular structures of aromatic compounds but also for modern chemistry as a whole. The delocalization of π-electrons has long been used to explain the molecular structure, stability, magnetic properties, and chemical reactivity of π-conjugated molecules. A state very similar to that of benzene is found in some solids, where electrons hop within "molecular orbitals", creating structures with hexagonal arrangements symmetry [28–31]. Aromaticity in metal clusters has been described [32–34].

Electron localization is also essential in descriptive chemistry because it helps identify the location of local electron distributions, such as core or valence electrons, electron pairs, bonding pairs, unpaired electrons, or π-electron systems. In particular, suitable auxiliary tools that enable electron pair localization also play a key role in analyzing electronic fluctuations and electron correlation effects. Therefore, this concept is relevant to the development of new density functionals. Since electron pair formation depends on the probability of finding two electrons simultaneously at two nearby positions, most methods used to determine electronic localization and delocalization are based on the two-electron density or pair density, which is the simplest quantity describing pair behavior, along with related functions such as the exchange correlation density, the Fermi hole, or the conditional pair probability. The concept of paired electrons was justified by and connected to the real-space picture presented in Reuter's work: the electron pair is the smallest multi-electron system abiding by the "two times $2n + 1$" rule [41].

Two years ago, our group introduced a model of aromaticity based on the correlation of electron pairs in ORQS [2]. This concept not only presents a new form of aromaticity derived from ORQS but also clarifies the properties of these compounds, including superconductivity. In classical superconductivity, there are always two types of interactions or forces. If the electron does not interact with the lattice vibration field, superconductivity cannot occur. In other words, phonons are essential for electron pairing. The interaction of lattice vibrations (phonons) with electrons causes the electrons to transition to different states. Recently, we explained how the same orbital effects that underlie aromaticity also account for superconductivity in solids [27]. Since aromaticity and superconductivity both involve the correlation of electron pairs in ORQS, transition metals can exhibit superconductivity when orbital effects—induced by a stimulus—create structures that resemble the delocalized orbitals of benzene. The orbital interaction must transmit lattice vibrations seamlessly, and electrons need available space in the opposite lobe of their orbitals to oscillate by exchanging phonons with neighboring electrons.

Oscillations can significantly influence the properties of natural electron fluxes. Oscillations are repetitive processes not related to the quantum nature of particles. Generally, the potential for self-oscillation is identified as an instability in the linearized equation of motion for perturbations about an equilibrium, manifesting as the limiting cycle of the self-oscillator [40]. Coupling between two oscillators results in a periodic transfer of oscillations from one to the other [47]. When the natural frequencies of the oscillators are matched, energy transfer is complete, resulting in oscillations with maximum amplitude. The driving force reaches its maximum amplitude when the driving frequency is tuned to the undriven oscillator's natural frequency [40]. A system of coupled oscillators reproduces nearly all the features of the oscillations when interactions are considered.

In contrast, when the frequencies differ, only part of the oscillations is transferred. Interactions between the system and the medium alter the appearance of the oscillations. If the medium's effect results from differences in elastic forward-scattering amplitudes, it

produces waves with different refractive indices, since the medium's energies, phase, and group velocities differ from those of the system. As a result, the system oscillates relative to the new states. The depth, period, and nature of the oscillations change because of this, compared to the "vacuum" quantities. That is why systems exhibit orbital-selective behavior [18,19].

There are two conditions essential for vigorous oscillatory transformations in matter: the resonance condition and the adiabatic or weakly nonadiabatic condition. Vigorous oscillatory transformations within the medium are therefore called resonance transformations (resonance oscillations). When the orbital rearrangement promotes the formation of correlated electron pairs in ORQS, the quantum geometry of the cluster within the solid mimics that of aromatic compounds, and all the properties of these compounds are exhibited. Density functional theory is intrinsically accurate. However, standard Kohn-Sham DFT often struggles to accurately describe certain structures and interactions [35–39]. Its success relies on the continual improvement and refinement of exchange-correlation functionals. In this work, we offer a different perspective on density and energy contributions based on electron pairings in ORQS to identify aromaticity and superconductivity. Many aspects of experimental data can be understood physically without the need for an unnecessarily large number of repetitions (shots) that scale intractably with system size.

CONCLUSIONS

The transition between the two main alternating spin structures occurs only when the spin-up and spin-down electrons rotate in opposite directions, consistent with our model of correlated electron pairs in ORQS, which explains aromaticity and superconductivity. A pair of fermions never condenses; they are forced to oscillate by correlating through the exchange of a boson. In this paper, the mechanism of aromatic cluster formation in solids is elucidated. In a self-oscillator, the driving force is regulated by the oscillation itself so that it remains in phase with the velocity. The unique structure of the p and d orbitals allows electrons to self-oscillate, with the node serving as the center of equilibrium. The coupling of two orbitals in the same direction, mediated by the environment, leads to the transfer of periodic oscillations between them, producing oscillations with maximal amplitude and a resonant behavior. Two or more coupled self-oscillators can spontaneously synchronize, forming molecular clusters in solids and thereby explaining their exceptional superconducting properties.

Hückel's rule requires at least two electrons, which supports the theoretical model of correlated electron pairs in ORQS. The application of DFT to correlated electron pairs cannot be done under the Bohr-Oppenheimer approximation because the motion of the nuclei creates the quantization of vibrations, i.e., bosons.

The boson, as a quantification of the vibrational motion of nuclei in molecules or of the crystal lattice in solids, accounts for the convergence of spin changes between paired electrons oscillating in resonant quantum states. Electron pairs maintain their fermionic identity despite having opposite spins. The pairs are never found in the same energy level, as they would be if they were bosons. They never condensate. The resulting wave function is antisymmetric. The boson mediates electron spin transitions and their oscillations in resonant quantum states. A study of internal resonance in a multi-degree-of-freedom system, grounded in underlying principles and mechanisms, assesses the state of the art in correlated electron pairs in ORQS and provides tentative guidance for future investigations of internal-resonance vibratory energy.

DECLARATIONS

Ethical Approval: not applicable
Funding: not funding
Availability of data and materials: All data and materials are included in the text

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The authors declare no competing financial interest.

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The authors declare no competing financial interest.