Theory of coexistence of superconductivity and ferroelectricity

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A new investigation of the coexistence and competition of ferroelectricity and superconductivity is reported. In particular we show that the starting Hamiltonian of a previous study by Birman and Weger (2001) can be exactly diagonalized. The result differs significantly from mean-field theory. A Hamiltonian with a different realization of the coupling between ferroelectricity and superconductivity is proposed. We report the results for mean-field theory applied to this Hamiltonian. We find that the order parameters are strongly affected by this coupling.

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In the present paper we report two related results from a reexamination of previous work on nearly ferroelectric superconductors. In that paper a coupling term was introduced into the original Hamiltonian (Eq. 27 of Ref. 1). An investigation of that coupling term shows that it only gives a squeezing of the phonons and no coupling to the electronic pairs, and therefore the Hamiltonian can be diagonalized exactly. However, the double mean-field approximation does result in an effective coupling between the two subsystems. (Eq. 34 of Ref. 1). Therefore the results of the analysis of that equation remain valid. Our second result follows from introducing a different bi-quadratic coupling term in the Hamiltonian of Eq. 27 of Ref. 1 which satisfies gauge and inversion symmetries. This term does couple the two subsystems. We will treat this new Hamiltonian in mean-field approximation.

We start with the model of coexistence of superconductivity and ferroelectricity proposed by Birman and Weger. For convenience we include its main features here. Birman and Weger start with two separate Hamiltonians for the superconducting and ferroelectric sectors. The superconducting sector is a mean-field reduced BCS pseudo-spin model (we corrected a misprint in Ref. 1)

\[ H_{SC} = -2 \sum_k (\varepsilon_k \hat{j}_{3k} + 2 \Delta_k \hat{j}_{2k}) \]

where \( \varepsilon_k \) is the single-electron energy and \( \Delta_k \) is the pairing interaction energy. The pseudo-spin operators \( \hat{j}_{pk} \) obey \( SU(2) \) commutation relations and are defined as

\[
\begin{align*}
\hat{j}_{1k} &= (-i/2) (\hat{b}^\dagger_k - \hat{b}_k) \\
\hat{j}_{2k} &= (1/2) (\hat{b}^\dagger_k + \hat{b}_k) \\
\hat{j}_{3k} &= (-1/2) (\hat{n}_k + \hat{n}_{-k} - 1)
\end{align*}
\]

where \( \hat{b}_k \) and \( \hat{b}^\dagger_k \) are pair operators defined by

\[
\hat{b}^\dagger_k = \hat{a}^\dagger_{k\uparrow} \hat{a}^{-\dagger}_{-k\downarrow}, \quad \hat{b}_k = (\hat{b}^\dagger_k)^\dagger, \quad \hat{n}_k = \hat{a}^\dagger_{k\uparrow} \hat{a}_{k\uparrow}
\]

and \( \hat{a}_{k\uparrow} \) and \( \hat{a}^\dagger_{k\uparrow} \) are the electron annihilation and creation operators for wave vector \( \vec{k} \), spin (\( \uparrow \)) , etc.

The Hamiltonian of the ferroelectric sector of the model is simply a Hamiltonian of a displaced harmonic oscillator

\[ H_{FE} = \omega_0 \left( \hat{N}_B + \frac{1}{2} \right) + \gamma_1 \left( \hat{B}_0^\dagger + \hat{B}_0 \right) \]

where \( \hat{B}_0^\dagger, \hat{B}_0 \) have boson commutation relations.

Combining those two sectors together and introducing a gauge invariant coupling between them, Birman and Weger obtain the following Hamiltonian (Eq. 27 of Ref. 1)

\[
\hat{H} = -2 \sum_k (\varepsilon_k \hat{j}_{3k} + 2 \Delta_k \hat{j}_{2k}) + \omega_0 \left( \hat{N}_B + \frac{1}{2} \right) + \gamma_1 (\hat{B}_0^\dagger + \hat{B}_0) + \sum_k \gamma_2 \hat{j}_{2k}^2 (\hat{B}_0^\dagger + \hat{B}_0)^2
\]

If a single \( k \) mode is isolated

\[
\hat{H} = -2 (\varepsilon_\delta + 2 \Delta_\delta) + \omega_0 \left( \hat{N}_B + \frac{1}{2} \right) + \gamma_1 (\hat{B}_0^\dagger + \hat{B}_0) + \gamma_2 \hat{j}_2^2 (\hat{B}_0^\dagger + \hat{B}_0)^2
\]

Here we notice that the structure of the pseudo-spin operators in terms of the pair operators implies

\[
\hat{j}_1^2 = \hat{j}_2^2 = \hat{j}_3^2
\]

and therefore \( \hat{j}_1^2, \hat{j}_2^2 \) and \( \hat{j}_3^2 \) are invariant to any rotation of the form \( \exp \left[ i \hat{n} \cdot \vec{\mathbf{j}} \right] \).

We use this property to diagonalize the Hamiltonian analytically by applying the following unitary transformation

\[
\begin{align*}
\hat{U} &= \frac{1}{\sqrt{2}} (B_0^\dagger - B_0) e^{i \theta_2} H e^{-i \theta_1} \hat{B}_0^\dagger - B_0) e^{-i \theta_1} (B_0^\dagger + B_0) e^{i \theta_2} \\
&= H_D + \hat{J}_2 (2 \varepsilon \sin \theta - 4 \Delta \cos \theta) + \left( \hat{B}_0^\dagger + \hat{B}_0 \right) \left( \omega_0 \alpha e^{-2 \beta} + \gamma_1 e^{-\beta} + 4 \alpha \gamma_2 e^{-2 \beta} + \gamma_2 \hat{j}_2 e^{-2 \beta} \right)
\end{align*}
\]

where \( \alpha, \beta, \gamma_1, \gamma_2 \) are fixed by the Hamiltonian.
Here $H_D$ is a Hamiltonian diagonal in the $|j_3, N_B\rangle$ basis:

$$H_D = 2\tilde{j}_3 (2\Delta \sin \theta - \varepsilon \cos \theta) +$$

$$+ \omega_0 \left( \hat{N}_B \text{ch} 2\hat{\beta} + \text{sh} 2\beta + \frac{1}{2} + \alpha e^{-2\beta} \right) +$$

$$+ 2\alpha \gamma_1 e^{-\beta} + \gamma_1^2 e^{-2\beta} \left( 2\hat{N}_B + 1 + 4\alpha^2 \right)$$

and if we want the non-diagonal parts to vanish we require

$$2\varepsilon \sin \theta = 4\Delta \cos \theta$$

$$\omega_0 \alpha e^{-2\beta} + \gamma_1 e^{-\beta} + 4\alpha \gamma_2^2 e^{-2\beta} = 0$$

$$\gamma_2 j_2 e^{-2\beta} = \frac{\omega_0}{2} \text{sh} 2\beta$$

These yield the following set of coupled equations for the parameters

$$\tan \theta = \frac{2\Delta}{\varepsilon}, \quad \alpha = -\frac{\gamma_1 e^{\beta}}{\omega_0 + \gamma_2}, \quad \varepsilon^{4\beta} = \frac{\omega_0 + \gamma_2}{\omega_0}.$$ 

Inserting them back into the transformed Hamiltonian gives

$$H_D = -2\tilde{j}_3 \frac{\varepsilon^2 - 4\Delta^2}{\sqrt{\varepsilon^2 + 4\Delta^2}} - \frac{\gamma_1}{\gamma_2 + \omega_0} +$$

$$+ \sqrt{\omega_0 (\omega_0 + \gamma_2)} \left( \hat{N}_B + \frac{1}{2} \right)$$

and this is the decoupled Hamiltonian of a squeezed and shifted harmonic oscillator and a spin of one-half in a magnetic field. The energy spectrum is given by

$$H_D (m, n) = -2m \frac{\varepsilon^2 - 4\Delta^2}{\sqrt{\varepsilon^2 + 4\Delta^2}} - \frac{\gamma_1^2}{\gamma_2 + \omega_0} +$$

$$+ \sqrt{\omega_0 (\omega_0 + \gamma_2)} \left( n + \frac{1}{2} \right)$$

We can now use the exact eigenstates of the Hamiltonian to compute the order parameters of the system:

$$\eta_{FE} \equiv \langle \hat{B}_0^\dagger + \hat{B}_0 \rangle = 2\alpha e^{-\beta} = -\frac{\gamma_1}{\omega_0 + \gamma_2} \quad (3)$$

$$\eta_{SC} \equiv \langle j_2 \rangle = -\frac{1}{2} \sin \theta = -\frac{\Delta}{\sqrt{\varepsilon^2 + 4\Delta^2}}$$

While the order parameter of the ferroelectric sector is affected by the SC-FE coupling strength, the order parameter of the superconducting sector is not. This occurs since in the coupling term $\gamma_2 j_2 \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2$, $j_2$ is a c-number and not an operator.

Using a double mean-field approximation for the Hamiltonian (Eq. 34 of Ref. H) and variational coherent state wave function, Birman and Weger obtained the following relations for the order parameters

$$\eta_{FE} = 2\xi \quad \eta_{SC} = \frac{m (\Delta' / \varepsilon + \xi \Gamma_2 / \varepsilon)}{\sqrt{1 + (\Delta' / \varepsilon + \xi \Gamma_2 / \varepsilon)^2}}$$

with

$$\xi = [-\Gamma_1/\omega_0 - \Gamma_2 (1 - m \sin \theta)] / \omega_0$$

$$\Delta' = \Delta (1 - \gamma_2 P^2)$$

$$\Gamma_1 = \gamma_1 - 2\gamma_2 P\Delta^2 \quad \Gamma_2 = 4\gamma_2$$

Here both order parameters are affected by the SC-FE coupling strength ($\gamma_2$).

To sum up this part, we have obtained an exact analytical solution of the ferroelectricity and superconductivity coexistence model, used in Ref. H. We showed here that contrary to the mean-field results, an exact solution of the model demonstrates that the ferroelectric order parameter is affected by the coupling, but the superconducting order parameter is not. If one were to initially model the SC-FE system by Eq. 34 of Ref. H the results reported in Ref. H would remain valid.

Returning to the original question of the proper coupling term in a quantum mechanical Hamiltonian, we need to respect gauge and inversion symmetry. Since the superconducting gap parameter is a complex quantity the added term should correspond to the bilinear $|\Delta|^2$. We now take this as $j_+ j_-$. The coupling term for the ferroelectric polarization, which respects inversion symmetry will correspond to $P^2$ and can be taken as $\left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2$.

Thus the bilinear coupling becomes $j_+ j_- \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2$.

We note that $j_+ j_- = j_1^2 + j_2^2 + j_3 = 1 + j_3$ (Using $j_+ j_-$ would have changed $j_3$ into $-j_3$). The coupling becomes $\gamma_2 \left( j_3 + \frac{1}{2} \right) \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2$. The Hamiltonian is now

$$\hat{H} = -2 (\varepsilon j_3 + 2\Delta j_2) + \omega_0 \left( \hat{N}_B + \frac{1}{2} \right) +$$

$$+ \gamma_1 \left( \hat{B}_0^\dagger + \hat{B}_0 \right) + \gamma_2 \left( j_3 + \frac{1}{2} \right) \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 \quad (4)$$

The interaction term in this Hamiltonian differs from the corresponding term (Eq. 27) in Ref. H. This Hamiltonian is not exactly solvable, therefore we make a mean-field approximation in the form

$$j_3 \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 \simeq \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 \langle j_3 \rangle +$$

$$+ \langle j_3 \rangle \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 - \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 \langle j_3 \rangle \quad (5)$$

Inserting Eq. K into Eq. H results in a solvable bilinear Hamiltonian

$$\hat{H}_{MF} = \varepsilon' j_3 - 4\Delta j_2 + \omega_0 \left( \hat{N}_B + \frac{1}{2} \right) + \gamma_1 \left( \hat{B}_0^\dagger + \hat{B}_0 \right) +$$

$$+ \gamma_2 \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 - \gamma_2 \left( \hat{B}_0^\dagger + \hat{B}_0 \right)^2 \langle j_3 \rangle \quad (6)$$
This set of equations can be reduced to a polynomial equation, which we solved numerically. Using these numerical results we investigate the behavior of the order parameters

\[ \eta_{FE} \equiv \langle \hat{B}_0^+ + \hat{B}_0 \rangle = 2 \alpha e^{-\beta} \]

\[ \eta_{SC} \equiv \langle j_2 \rangle = -\frac{1}{2} \sin \theta \]

Fig. 1 shows the dependence of the two order parameters on the coupling coefficient between the ferroelectric and superconducting subsystems. There is a smooth evolution of each of the order parameters with the coupling coefficient \( \gamma_2 \). Both order parameters are non-vanishing at \( \gamma_2 = 0 \). We note that \( \gamma_2 \) is bounded by two critical values, beyond which there are no real solutions for the set of self-consistent equations (7). At the positive critical value the superconducting gap parameter \( \eta_{SC} \) reaches its maximum, and the polarization order parameter \( \eta_{FE} \) reaches its minimum. For negative values of \( \gamma_2 \) the superconducting order parameter vanishes very rapidly, while the ferroelectric order parameter sharply diverges, when \( \gamma_2 \) approaches its negative critical value.

In conclusion we note that our new model for SC-FE coexistence/competition does agree with the spirit of the Matthias conjecture that each of these cooperative effects tends to exclude or suppress the other.

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