Superconductivity and Ferromagnetism in Nanomaterial $NbSe_2$

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Abstract. Finding of superconductivity (SC) in ultra thin layer of Niobium diselenide ($NbSe_2$) caught the attention of each condensed matter physicist in the era of nanotechnology. The coexistence of SC and magnetism have been a topic of interesting research in solid-state physics since the discovery of superconductivity. Ferromagnetism induced in any compound could destroy superconductivity by disturbing the cooper pairing of electrons of the atoms. The interplay between ferromagnetism (FM) and SC in nanomaterial $NBSe_2$ impressed to study and to know the exact mechanism behind this coexistence which can lead to a very interesting research: superconductivity at room temperature. In this paper, I have theoretically studied the coexistence of SC and FM in $NbSe_2$ and how this material could be useful in finding many high T_c nanomaterials.

INTRODUCTION

Superconductivity (SC) and Magnetism (M) are said to[1,2] be antagonistic to each other since its discovery but scientists found the coexistence of ferromagnetism (FM) & SC[3,4,5] ,coexistence of antiferromagnetism (AFM) & SC[6,7] and also the coexistence of all three interactions[8] in a single system for more than half several decades. The coexistence of SC & FM in newly discovered nanomaterial $NbSe_2$[9,10,11] renewed the interest to know the exact mechanism responsible for pairing of cooper pairs and localization of ferromagnetic electrons in $NbSe_2$. It has been seen that niobium(Nb) atoms are sandwiched between two selenium atomic layers and the density or arrangement of Nb atoms of the ultrathin superconducting $NbSe_2$ by polar hydrazine molecules enhances a slight elongation of the covalent Nb–Se bond, which will weak the covalent interaction and increases the ionicity of the Nb^{4+} atoms with unpaired electrons, resulting in ferromagnetic ordering. There is one possibility that the induced ferromagnetic momentum couples with conduction electrons of Nb atoms generate correlated effects to form cooper pairs in $NbSe_2$. In this work an attempt is made to develop the microscopic theory of coexistence of superconductivity and ferromagnetism by writing a system Hamiltonian for $NbSe_2$ having ferromagnetic interactions of selenium layers with Nb conduction electrons.

MATHEMATICAL FORMULATION

The model Hamiltonian for the system having superconducting and ferromagnetic interactions is given below:

$$H=\sum_{q\sigma}\xi_q c^+_{q\sigma} c_{q\sigma} - V\sum_{qq'} c^+_{q\uparrow} c^+_{-q\downarrow} c_{-q'\downarrow} c_{q'\uparrow} + \sum_m E_m c^+_{m\sigma} c_{m\sigma} + \sum_{\substack{m\,n\\ \sigma\sigma'}} \eta_{mn} c^+_{m\sigma} c^+_{n\sigma'} c_{m\sigma'} c_{n\sigma}$$
$$+\sum_{\substack{l\,n\\ q}} \mu^{mn}_q \left(c^+_{m\uparrow} c^+_{n\uparrow} c_{-q\downarrow} c_{q\uparrow} + h.c.\right) \qquad (1)$$

where $c^+_{q\sigma}\left(c_{q\sigma}\right)$ and $c^+_{l\sigma}\left(c_{l\sigma}\right)$ denote creation (annihilation) operators for conduction and localized electrons respectively, V is the electron phonon interaction and E_m is the energy of the localized electrons of Se atoms. η_{mn} is the exchange interaction energy of localized Se atoms located at neighboring sites and the last term describes the interaction between the localized ferromagnetic moments of Se atoms and with the Nb electrons.

MATHEMATICAL CALCULATIONS

Using Green Function Technique [12], the Hamiltonian given by the equation (1) has been solved and the following equations of motion are obtained:

$$\left(\omega - \xi_{q_1}\right)\left\langle\left\langle c_{q\uparrow} \middle| c^{+}_{q\uparrow}\right\rangle\right\rangle_{\omega} = \frac{1}{2\pi} - \Delta\left\langle\left\langle c^{+}_{-q\downarrow} \middle| c^{+}_{q\uparrow}\right\rangle\right\rangle_{\omega} - \phi_{\uparrow\uparrow}\left\langle\left\langle c^{+}_{-q\downarrow} \middle| c^{+}_{q\uparrow}\right\rangle\right\rangle_{\omega} \tag{2}$$

$$\left(\omega + \xi_{q_1}\right)\left\langle\left\langle c^{+}_{q\downarrow} \middle| c^{+}_{q\uparrow}\right\rangle\right\rangle_{\omega} = - \Delta\left\langle\left\langle c_{-q\uparrow} \middle| c^{+}_{q\uparrow}\right\rangle\right\rangle_{\omega} - \phi_{\uparrow\uparrow}\left\langle\left\langle c_{-q\uparrow} \middle| c^{+}_{q\uparrow}\right\rangle\right\rangle_{\omega} \tag{3}$$

where $\Delta = V\sum_{q'} \left\langle c_{-q'\downarrow}\, c_{q'\uparrow}\right\rangle = V\sum_{q'} \left\langle c^{+}_{q'\uparrow}\, c^{+}_{-q'\downarrow}\right\rangle$ (Superconducting Order Parameter) (4)

$$\phi_{\uparrow\uparrow} = \sum_{mn} \mu^{mn}_{q}\left\langle c_{n\uparrow}\, c_{m\uparrow}\right\rangle = \sum_{mn} \mu^{mn}_{q}\left\langle c^{+}_{m\uparrow}\, c^{+}_{n\uparrow}\right\rangle \quad \text{(Ferromagnetic Order Parameter)} \tag{5}$$

Thus, on using Poisson summation formulas and contour integration over ω, superconducting order parameter((Δ) can be recast in the form:

$$\Delta = N(o)V\int_0^{\hbar\omega_D}\left(\Delta - \phi_{\uparrow\uparrow}\right)\frac{\tanh\frac{\beta}{2}\sqrt{\tilde{\xi}_q^{\,2} + \left(\Delta - \phi_{\uparrow\uparrow}\right)^2}}{\sqrt{\tilde{\xi}_q^{\,2} + \left(\Delta - \phi_{\uparrow\uparrow}\right)^2}}\, d\tilde{\xi}_q \tag{6}$$

Similarly $\phi_{\uparrow\uparrow}$ can be obtained by solving the following equations of motion

$$\left(\omega - \tilde{E}m\right)\left\langle\left\langle c_{m\uparrow} \middle| c^{+}_{n_1\uparrow}\right\rangle\right\rangle_{\omega} = \frac{1}{2\pi} + \eta^{mn}_{q}\left\langle\left\langle c^{+}_{n\downarrow} \middle| c^{+}_{m\uparrow}\right\rangle\right\rangle \tag{7}$$

$$\left(\omega + \tilde{E}m\right)\left\langle\left\langle c^{+}_{m\uparrow} \middle| c^{+}_{n\uparrow}\right\rangle\right\rangle_{\omega} = \eta^{mn}_{q}\left\langle\left\langle c_{n\downarrow} \middle| c^{+}_{m\uparrow}\right\rangle\right\rangle \tag{8}$$

$$\phi_{\uparrow\uparrow} = \sum_{\ln} \mu^{mn}_{q}\frac{\phi_{mn}}{2}\left[1 - \frac{\tilde{E}m}{\tilde{E}^2_m - \phi^2_{m_1}}\tanh\frac{\beta}{2}\sqrt{\tilde{E}^2_m - \phi^2_{mn}}\right] \tag{9}$$

I have calculated the superconducting order parameter (Δ) and the ferromagnetic order Parameter (φ ↑↑) and both are related to each other by single equation (6).

RESULTS AND DISCUSSION

The expression for superconducting order parameter (Δ) and ferromagnetic order parameter(φ ↑↑) of $NbSe_2$ are calculated and found the dependence of Δ on ferromagnetic ordering. It is not hard to see that both two order parameters are interrelated to each other by single equation (6) and in the particular temperature regime, they exist together which supports the coexistence of these two phenomena in $NbSe_2$. Theoretical microscopic calculations gave a solid base to extend our study to calculate the magnetization by using equation (9), density of states and specific heat of $NbSe_2$ which would further help in finding many unsolved phenomena like exact pairing mechanism responsible for cooper pairing, exact critical temperature etc. Though transition temperature of $NbSe_2$ is quite low but these materials are unconventional ones like high T_c cuprates which are anti ferromagnetic insulators in pure state. Hence coexistence of SC & FM in ultrathin monolayer of $NbSe_2$ excited the therotists and experimentalists from all over the world to study and develop new nano materials which could conduct even at room temperature.

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