Pseudogap, Quantum Harmonic Oscillation and Confinement in High-Temperature Superconductors


Abstract

For a 1-dimensional array of equidistant particles with equal masses the concepts of quantum harmonic oscillation (QHO) and particle-in-the-box (PiB) have been applied in a general form. It turns out that the lowest PiB energy level is lower than the lowest QHO energy level by \( \frac{E_{\text{PiB}}}{E_{\text{QHO}}} = \frac{\pi}{4} \). Comparing the results with experimental facts/data of high-temperature superconductors (HTSC) it might shed light on fundamental characteristics of HTSCs like the transition temperature \( T_c \), the energy level of the superconducting state and the existence of a pseudogap \( \Delta E_{pg} = 7.9k_B T_c \) above \( T_c \).

Keywords: superconducting phase transition, pseudogap, current channels in high-temperature superconductors, quantum harmonic oscillation
1. Introduction

For several types of high-temperature superconductors (HTSC) resonant Raman Scattering [1 and references therein], scanning tunnelling and high resolution angle-resolved photoemission spectroscopy (ARPES) measurements [2-4] show prominent absorption at an energy of $\Delta E_{px} = (7.9 \pm 0.5)k_B T_c$. $T_c$ is the critical transition temperature and $k_B$ the Boltzmann constant. It has also been shown, that this energy gap in the electronic density of states - so called pseudogap - exists above $T_c$ which probably originates from a state other than superconductivity [5 and references therein, 6].

Parallel to the experimental evidence of the existence of a pseudogap several research groups performed quantum oscillation experiments in p- and n-type HTSCs. They suggest that quantum oscillations in HTSCs are associated with the opening of the pseudogap [7-8 and references therein].

Very recently the authors have found a correlation between the optimum doping density of HTSCs and maximum transition temperature, which might be explained by the confinement concept of a 1-dimensional (1-D) particle-in-a-box (PiB) system [9].

This paper is an attempt to look for relations between the prominent absorption at $\Delta E_{px} = 7.9k_B T_c$, the effect of quantum harmonic oscillation (QHO), and the 1-D PiB concept.

2. Quantum harmonic oscillation and pseudogap

For cuprates the superconducting highway is in the CuO$_2$ plane of the crystal unit cell. Additionally, resistivity measurements in HTSC have been mostly performed by investigating a 1-D superconducting carrier flow. Therefore we will consider - as a simplified approximation - superconducting current channels as a 1-D system.

A simplified 1-dimensional quantum harmonic oscillator model assumes a very long chain of equal and equidistant particles with mass $M_{eff}$ forming a perfect straight line. For HTSCs the effective mass is given by $M_{eff} = 2m_e$. For a linear QHO the maximum displacement of each particle should be given by $\Delta l = \pm x/2$. The vibrational energy levels $E_n(QHO)$ with $n = 1, 2, ..$ have equidistant quantized energies (Fig. 1)

$$E_n(QHO) = (n-1/2)\hbar \omega \quad (1)$$

$$E_1(QHO) = \frac{\hbar \omega}{2} = \hbar \sqrt{\frac{k_r}{M_{eff}}} \quad (2)$$

The coupling constant $k_r$ corresponds to a linear restoring force $F_R = -k_r \Delta l$. The expression $\omega = 2\sqrt{k_r/M_{eff}}$ is derived from the nearest neighbour approximation for a very long chain of masses [10-12]. As a first approximation the total energy of the QHO is equal to the QHO potential energy at maximum displacement. In the classical sense the energy of the particle in the QHO is all potential energy and the kinetic energy is zero

$$E_{pot}(QHO) = \frac{1}{2} k_r \left( \frac{x}{2} \right)^2 \quad (3)$$

A more precise formulation can be achieved by using one important consequence of the uncertainty principle: a particle is confined to occupy a limited region of space and therefore has a minimum average kinetic energy $\langle E_{kin} \rangle$. It is considered that the particle is confined in 1-D and that the uncertainty in knowledge of the particle position is $\Delta x = x$. With the following relations [13]
\[ \Delta p > \frac{\hbar}{2\Delta x} \quad \text{and} \quad \langle E_{\text{kin}} \rangle > \frac{(\Delta p)^2}{2M_{\text{eff}}} \quad (4) \]

it yields

\[ \langle E_{\text{kin}} \rangle > \frac{\hbar^2}{8M_{\text{eff}} x^2} \quad (5) \]

With this correction, the total energy will be described by the Hamiltonian of a 1-D harmonic oscillator and results in [9]

\[ E_{\text{tot}}(\text{QHO}) = \frac{\hbar^2}{8M_{\text{eff}} x^2} + \frac{1}{2} k_R \left( \frac{x}{2} \right)^2 \quad (6) \]

Note that at \( T = 0 \) K a QHO remains at the energy level \( E_1 \). Equation (2) describes the lowest QHO energy level but does not give any information concerning the temperature at which most of the QHO energy is represented by the lowest level.

In the following it is assumed - as already suggested in [7,8] - that the relatively sharp pseudogap [2] is a result of a 1-D quantum harmonic oscillation in the form

\[ \hbar \omega = \Delta E_{\text{pg}} = (7.9 \pm 0.5)k_B T_c \quad (7) \]

So that the lowest energy level is given by

\[ E_1(\text{QHO}) = 3.95k_B T_c = 4\gamma_Q k_B T_c \quad (8) \]

The constant \( \gamma_Q = 0.9875 \) has been introduced for convenience. This assumption will be verified in section 4. For this consideration the most prominent energy transition is given by the equidistant energy levels \( \hbar \omega = hf_Q = 8\gamma_Q k_B T_c \) which results in a frequency of \( f_Q \approx 164.6 \times T_c \text{[GHz]} \) and a HTSC displacement constant similar to Wien’s displacement law:

\[ \frac{hf_Q}{k_B T_c} = 8\gamma_Q = \frac{hc}{\lambda_Q k_B T_c} \quad \Rightarrow \lambda_Q T_c \approx 1.8 \times 10^{-7} \text{[}m \times K\text{]} \quad (9) \]

Although we do not know the absolute value of maximum displacement \( \Delta l = \pm x/2 \), it is possible to calculate the coupling constant \( k_R \) by using equations (2) and (8). If the pseudogap in HTSCs represents the 1-D QHO transition \( \hbar \omega \), then this real existing pseudogap [2, 3] might provide a characteristic estimate of the electron coupling for pairing in HTSCs using equations (2) and (8)

\[ k_R = 4.87 \times 10^{-7} \times T_c^2 \text{[}Nm^{-1}\text{]} \quad (10) \]

For a HTSC with about \( T_c \approx 100K \) the coupling constant would be in the range of \( k_R \approx 5 \times 10^{-3} \text{[}Nm^{-1}\text{]} \).

**Fig. 1**

The energy levels of a linear array of equidistant particles with equal mass can be described by quantum harmonic oscillation and particle-in-a-box concept.
3. HTSC and particle-in-a-box concept

For more than 20 HTSC materials the authors have found a strong correlation between the uniform doping density distance $x$ in the superconducting plane and the inverse of the transition temperature $T_c$ in the range $20K \leq T_c \leq 135K$ as illustrated in Figure 2. Using the concept of a 1-D PiB system the correlation curve can be written in the form

$$ (2x)^{3} n^{-2/3} 2M_{eff} \pi k_{B} T_c \approx h^2 $$ (11)

where $n$ is the number of superconducting planes, e.g. CuO$_2$ planes in cuprates, per chemical formula within a unit cell [9 and references therein]. For $n = 1$ equation (11) transforms into

$$ \pi k_{B} T_c = \frac{h^2}{8M_{eff} x^2} = E_i(PiB) $$ (12)

which is equivalent to the lowest energy level of a 1-D PiB system (Figure 1) and is a solution of the time-independent Schrödinger wave equation. According to this result the superconducting state has an energy level of $\pi k_{B} T_c$.

4. Confinement by PiB and QHO

Now, sections 2 and 3 permit to examine if the pseudogap is a result of QHO by analysing in a general form the theoretical concept of a 1-D QHO system combined with a PiB system [13]:

The two physical phenomena are describing the same system. Therefore it is justified to assume that for very low temperatures the lowest PiB energy level should be equal to the QHO energy at maximum displacement given by equation (6). In other words, the stationary solution for the energy of a confined particle with mass $M_{eff}$ will be compared with the energy of the Hamiltonian of a 1-D QHO.

With this relation $E_{10}(QHO) = E_i(PiB)$ the coupling constant $k_R$, the restoring force $F_R$ and the energy ratio of the lowest energy levels $E_i(PiB)/E_i(QHO)$ can be determined by

$$ \frac{1}{(2\pi)^2} \frac{h^2}{8M_{eff} x^2} + \frac{1}{2} k_R \left( \frac{x}{2} \right)^2 = \frac{h^2}{8M_{eff} x^2} $$ (13)

$$ k_R = \left( 1 - \frac{1}{(2\pi)^2} \right) \frac{h^2}{M_{eff} x^2} = \gamma_Q \frac{h^2}{2M_{eff} x^2} $$ (14)

$$ F_R = k_R \left( \frac{x}{2} \right) = \gamma_Q \frac{h^2}{2M_{eff} x^2} $$ (15)

$$ E_i(QHO) = h \sqrt{ \frac{k_R}{M_{eff}} } = \gamma_Q \frac{h^2}{2\pi M_{eff} x^2} $$ (16)

$$ \frac{E_i(PiB)}{E_i(QHO)} = \frac{\pi}{4\gamma_Q} \approx \frac{\pi}{4} $$ (17)

by introducing the constant $\gamma_Q \approx 0.98725$.

With equal effective masses for both physical descriptions, $E_i(PiB)$ is lower than $E_i(QHO)$. This might be a chance for a 1-D equidistant particle system at low temperatures to “go” or to “condensate” from the lowest energy level $E_i(QHO) = 1/2\hbar \omega$ into a somewhat lower energy level if all boundary conditions are fulfilled.

Using the result of the correlation curve in Figure 2 with the appropriate equation (12) for $n = 1$ and combining it with equation (17) the lowest QHO energy level results in $E_i(QHO) = 4\gamma_Q k_{B} T_c$, which is in agreement with our assumption in equation (8) including the value of the constant $\gamma_Q$. 


Fig. 2
Correlation between the inverse of $T_c$ and the doping distance $x$ for maximum transition temperature of different HTSC materials [9]. The value $n$ is the number of superconducting CuO$_2$ planes per chemical formula within a unit cell. The straight line can be considered as a phase transition line between the normal conducting and superconducting state.

Fig. 3
Boltzmann population ratio of a two level energy system when using the lowest energy levels of QHO and PiB.
5. Relative population of energy levels $E_1(QHO)$ and $E_1(PiB)$

In this section the density of states and occupation probability will be considered for the special case at low temperature. When a large collection of particles is in thermal equilibrium at a temperature $T$, the relative populations of any two energy levels must be related by the Boltzmann ratio [14]. Applying the Boltzmann ratio to $E_1(QHO)$ with $N_1(QHO)$ particles and $E_1(PiB)$ with $N_1(PiB)$ respectively figure 3 leads to

$$\frac{N_1(QHO)}{N_1(PiB)} = \exp\left(-\frac{(4\gamma_0 - \pi)k_B T_c}{k_B T}\right)$$

$$\approx \exp\left(-0.81 \frac{T_c}{T}\right) \quad (18)$$

At $T = T_c$ equation (18) results in $N_1(QHO)/N_1(PiB) = 0.45$. This means that the majority of ~55% is at $E_1(PiB)$. An estimation shows that the population for energy levels $E_2(QHO)$ and $E_2(PiB)$ at $T_c$ is negligible because

$$\frac{N_2(QHO)}{N_1(QHO)} \approx \frac{N_2(PiB)}{N_1(PiB)} = 10^{-4} \quad (19)$$

Therefore the two-level consideration for equation (18) is justified. Below $T_c$ physical effects are dominated by the PiB description because the majority of particles are at energy level $E_1(PiB)$, whereas above $T_c$ these effects disappear, because the majority of particles are at energy level $E_1(QHO)$. Equation (18) explains why at $T_c/T \approx 1$, the superconducting phase is starting for $T \leq T_c$, or ending for $T \geq T_c$.

6. Transitions

Confinement and quantum harmonic oscillation in a 1-D system have been illustrated qualitatively in figure 1. With the results of equations (8, 12, 17) appropriate energy level diagrams for QHO and PiB can now be drawn with relative energy levels in values of $[k_B T_c]$ as shown in figure 4 and tabulated in figure 5. The critical temperature $T_c$ describes the physical temperature at which the physical effects caused by particles at $E_1(PiB)$ will dominate. Figure 4 explains why the pseudogap transition exists above $T_c$.

![Energy level diagram of a 1-dimensional quantum harmonic oscillator (QHO) of equidistant particles with equal/same mass separated by x and a particle-in-a-box (PiB) system with width x.](image)

**Fig. 4**

Energy level diagram of a 1-dimensional quantum harmonic oscillator (QHO) of equidistant particles with equal/same mass separated by x and a particle-in-a-box (PiB) system with width x.
Energy levels and energy differences between different levels for 1-dimensional quantum harmonic oscillator (QHO) and particle-in-a-box (PiB) systems.

Another result is the relation between the pseudogap frequency and the doping distance by combining equations (9) and (12)

\[(x^2 \pi) f_Q = \gamma_q \frac{h}{2m_e} \approx 3.59 \times 10^{-4} \left[ m^2 s^{-1} \right] \quad (20)\]

It looks like that the quantum of circulation for two electrons/holes is given by the product of the unit area of paired electrons/holes \((x^2 \pi)\) times the QHO frequency \(f_Q\).

7. Conclusions

This paper is an attempt to compare a 1-D quantum harmonic oscillator and a particle-in-a-box system with 1-D current channels in superconducting CuO planes in cuprates. Although the concept is a very simplified model for superconducting current channels it offers several interesting aspects for the understanding of different phenomena in high-temperature superconductors. Much more work has to be done in particular applying the concept also to conventional superconductors. Maybe figure 1 gives a hint to a possible explanation for the isotope effect on unconventional superconductors.

The search for a comprehensive theory of superconductivity is one of the central unsolved problems in modern physics. The ultimate goal is a recipe that would enable the growth of new HTSC crystals for operation at much higher temperatures than at present. Their application would prove revolutionary in several areas. In space technology for instance, electrical power systems would become more efficient and capable, heat shields would be better capable of rejecting re-entry heat loads, and propulsion systems could be made with material coatings capable of surviving higher engine temperatures.

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References


