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In search for near-room-temperature superconducting critical temperature of metal superhydrides under high pressure: A review

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Abstract

An overview and the latest status of the superconductivity of metal superhydrides under high pressure are discussed in this review article. The searching for near-room-temperature superconductors have been one of the most enthusiastic fields in physics. This is because of several key factors in both theoretical and experimental sides. By advanced experiment innovation, pressure exceeded that of the earth's core can be generated in laboratories. This allows scientists to explore new physics of materials under high pressure. In the synergy form, the theoretical calculation gives accountable predictions on the structural and electronic properties which can be served as a practical map for experimentalists. In this review, I also give a brief overview on the existing theory of superconductivity which leads to the calculation of the superconducting critical temperature, T_c. The key element for calculating T_c is stemmed from the so-called spectral function, which can now be evaluated from the density functional theory. In order to obtain insight information and gain deeper understanding, I model the spectral function with a simple constant function. This analysis gives a powerful suggestion on the way to search for a higher value of T_c.

1. Introduction

A superconductor is a phase of materials which exhibit zero electrical resistivity and perfect diamagnetism at temperature lower than a critical value, called the superconducting critical temperature, T_c. The external applied magnetic field is expulsed from a superconductor. This is the so-called Meissner-Ochsenfeld effect [1]. The first known superconductor is Hg with T_c = 4.15 K, discovered in 1911 by Onnes [2]. He received the Nobel prize in 1913. Since then, large number of materials, such as a number of metals [3] and intermetallic compounds [4], had been discovered to be a superconductor. In 1957, Bardeen, Cooper and Schriffer announced the theory that gives the convincing explanation to the superconducting phenomenon [5]. This is the so-called BCS theory. They received the Nobel prize in 1972. The BCS theory gives many powerful predictions, such as the superconducting gap and the critical temperature, T_c, which can be expressed as

$$T_c = \frac{\theta_D}{1.14}\exp\left(-\frac{1}{N_F V_{eff}}\right). \quad (1)$$

The BCS prediction of T_c is based on three key physical quantities, such as the Debye temperature, θ_D, the density of electrons at the Fermi energy, N_F, and the effective electron interaction, V_{eff}. The condition for the BCS theory to be valid is that the normal state of materials needs to be a metal. This type of materials is called a conventional superconductor. However, there are also some metals, such as calcium and strontium, which are not a superconductor at ambient pressure. The search for a high value of T_c is to look for large θ_D and large N_F. Sometimes, large N_F can be found if van Hove singularity [6] occurs around the Fermi level. However, V_{eff} is hard to be identified in practice. The BCS theory valids for the weak electron-phonon coupling regime only. Before the new millennium, the highest T_c in the conventional superconductors was found just below 39 K [3]. At the turning of the new millennium, MgB_2 was discovered to be a convention superconductor with T_c = 39 K [7]. This gave a boost in the field of superconductors as MgB_2 can be easily synthesized and non-toxic. It opens large number of possibilities in terms of superconducting technology and applications. Despite of a large number of modifications, MgB_2 had been a T_c champion in the class of the conventional superconductors for more than a decade.

There is another class of superconductors, called non-conventional or high- T_c superconductors. Surprisingly. they are mostly a ceramic, of which normal state is an insulator. The first known superconductor of this class is a BaLaCuO compound with T_c = 35.1 K, discovered in 1986 by Bednorz and Müller [8]. They were awarded the Nobel Prize in Physics in 1987. Since then, large number of ceramic compounds have been found to be a high- T_c superconductors. The famous examples are a YBaCuO compound with T_c = 93 K [9] and a HgBaCaCuO compound with T_c = 130 K [10]. In Thailand, the theory for high-T_c superconductors has been pioneered by Prof.Suthat Yoksan [11]. In 2010, Udomsamuthirun *et. al.* [12] have discoveried new

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composition of YBaCuO compounds with T_c = 94 K [12]. Up till now, the highest Tc of this class of superconductors is around 150 K. Unfortunately, the BCS cannot give a complete description of this class of materials. The applicable theory for this class of materials is really complicated and far from complete. This is beyond the scope of this review.

Pressure is an important thermodynamic variable. A device that controls high pressure in experiments is the so-called anvil cell, pioneered by Bridgman [13]. His device can produce pressure as high as 10 GPa, 100,000 times higher than the ambient pressure. He was awarded the Nobel Prize in Physics in 1946. In 1959, the first diamond anvil cell (DAC) was invented [14]. Since then, high pressure has become a powerful tool for studying the new physics of materials. For example, pressure can induce structural phase transitions, and some physical properties are dependent on the crystal structure of materials. The more explicit example is calcium, which is not a superconductor at ambient pressure, but was found to be a superconductor under high pressure [15-17]. Its highest T_c of 29 K was found at 216 GPa [16]. This is so far the highest T_c among the elemental metals. Likewise, strontium is not a superconductor at ambient pressure, but becomes a superconductor under high pressure [18,19]. Strontium has been shown to exhibit series of structural phase transitions [20] and some specific structures under high pressure are responsible for its superconductivity [21]. At the present time, the periodic table included T_c of all elements both at ambient and under pressure is almost fully constructed [22].

Apart from experimental studies, the theoretical methods have also been developed. These theories are based on the quantum behavior of materials. One of the most powerful tools for calculating the quantum effects in many-body systems is the so-called density functional theory (DFT), pioneered by Hohenberg, Kohn and Sham [23,24]. Kohn received his Nobel prize in 1998. However, the practical DFT calculations were realized by several superb state-of-the-art softwares, such as the Vienna Ab initio Simulation Package (VASP) [25], the Cambridge Serial Total Energy Package (CASTEP) [26], and the Quantum Espresso (QE) [27]. Together with a powerful structure searching algorithm, such as Universal Structure Predictor: Evolutionary Xtallography (USPEX) [28] and Ab initio random structure searching (AIRSS) [29], the search for the most energetically favorable structure at each pressure and its associating physical properties, such as superconductivity becomes computationally feasible. As of now, we enter into the era of machine learning, some useful outputs that involving structural properties and their superconductivity have also emerged from the combination of DFT and machine learning [30-31].

The most explicit example of the long-term interplay between experiments and theoretical calculations is the search for metallic hydrogen. Wigner and Huntington predicted the existence of metallic hydrogen in 1935 [32]. At that time, its correct structure at high pressure was unknown. Since then, there have been a large number of experimental and theoretical developments in order to identify the correct structure and the precise transition pressure of the metallic hydrogen [33]. Only recently, the experiments have just observed a possible candidate of the metallic hydrogen at pressure between 425-495 GPa [34,35]. From Eq. (1), the BCS theory suggested that high θ_D could also give high T_c. As H is the lighest atom, it has a potential to give the highest θ_D. In 1968, Ashcroft predicted that the metallic hydrogen could become a high-temperature superconductor [36]. Up till now, the closest realization of Ashcroft's prediction is the hydrogen-rich compounds. In 2014, a H_3S compound was predicted to be a conventional superconductor at 200 GPa with $T_c \approx 200\ K$ [37,38]. In 2015, the H_3S compound was observed in a high-pressure experiment [39]. It was confirmed that it is a conventional superconductor with $T_c = 203\ K$ at 155 GPa [39]. These researches have opened a new direction of searching for new hydrogen-rich compounds which exhibit a high value of T_c under high pressure.

I conclude this section with Table 1 which summarizes T_c of several metals and compounds from experiments. In the next section, I will give a brief overview of a new class of compounds, called metal superhydrides. Some of these compounds exhibit T_c that is exceeding those of the non-conventional superconductors, and the classification word "high-Tc" is about to be disrupted.

Table 1. T_c of some selected metals and compounds from experiments.

Superconductors	**P (GPa)**	T_c^{EXP}**(K)**	**Reference(s)**
Hg	0	4.16	[1]
V_3Si	0	17.1	[4]
MgB_2	0	39	[7]
$Ba_xLa_{5-x}Cu_5O_{5(3-y)}$	0	30	[8]
$YBaCuO_{7-x}$	0	93	[9]
HgBaCaCuO	0	130	[10]
Sr	58	8.0	[19]
Ca	216	29	[16]
ThH_{10}	175	161	[45]
H_3S	155	203	[39]
YH_6	166	224	[50]
YH_6	237	227	[51]
YH_9	201	243	[51]
LaH_{10}	180-200	260, 280	[48], [49]

2. Metal Superhydrides

There is a large class of metal polyhydrides, MH_x, where M is a metal element and $x > 2$. If x is large, sometimes the compounds are called metal superhydrides. There were several excellent theoretical and experimental reviews led by Peng *et al.* [40], Zurek and Bi [41], Semenok *et al.* [42], and Flores-Livas *et al.* [43]. They gave a comprehensive overview of the current achievement on the structural prediction of these metal superhydrides and their superconducting properties under high pressure. Some of these compounds appear to be a metal in their normal states at room temperature and a conventional superconductor at temperature below T_c. Also, there have been many metal superhydrides that can be synthesized under high pressure by using DAC. Furthermore, there are several members of this metal superhydride class that exhibit superconductivity with Tc > 150 K, see Table 2 for theoretical prediction, and some have been confirmed by experiments, see Table 1. Thus, we have arrived at the age of synchronizing interplay between experiments and theory. The most surprising finding is that T_c is now getting closer to the room temperature.

A large number of metal superhydrides share common host-guest clathrate structures. In these structures, hydrogen atoms form a hydrogen cage which hosts a metal atom inside. The first example is ThH_{10} with an Fm-3m structure. It was predicted that T_c = 176-241 K at 100 GPa and T_c = 166-228 K at 200 GPa [44]. The Fm-3m-ThH_{10} was confirmed by an experimental observation, and it was reported that T_c =159-161 K at 170-175 GPa [45] in excellent agreement with the previous prediction. The most famous examples are the prediction of superconducting LaH_{10} and YH_{10}, as the predicted T_c is approaching the room temperature. In LaH_{10}, it was predicted that T_c = 274-286 K at 210 GPa [40,46,47] and it was reported by experiments that LaH_{10} is indeed a conventional superconductor with T_c of 260 K at 180-200 GPa [48], and the latest report has shown the evidence that its T_c could be as high as 280 K [49]. In YH_{10}, it was predicted that T_c could be as high as 305-326 K at 250 GPa [46]. This theoretical prediction has been very fascinating as, at around 300 K, it is the so-called room temperature. The YH_x compounds have been synthesized under high pressure [49-51]. The existence of superconducting YH_6 and YH_9 compounds have been confirmed with T_c = 227 K at 237 GPa [51] and T_c = 243K at 201GPa [51], respectively. However, YH_{10} and its superconductivity are yet to be confirmed.

Another example is the CeH_x compounds which have been synthesized by Salke *et al.* [52] using a laser-heated DAC. They obtained the CeH_2, CeH_3 and CeH_9 compounds at different pressures. The structure of CeH_9 was identified as a hexagonal clathrate structure with the $P6_3$/mmc space group at 80 GPa. Its T_c has not been measured but it was estimated to be 117 K at 200 GPa [52]. At the same time, the existence of CeH_9 has been confirmed by another independent experiment by Li, *et al.* [53]. However, its superconductivity is yet to be confirmed by experiments.

There are a large number of metal polyhydrides that were predicted to be a superconductor but experimental confirmation is still awaiting. I give here only a limited list of examples. The first examples are the MgH_x compounds. The MgH_2 compound has attracted much of attention as its application on the hydrogen storage [54,55]. Its phase transitions under high pressure have been studied [56,57] and a phase with superconductivity was found at 180 GPa with T_c = 23 K [57]. Its superhydride cousin, MgH_6, was predicted to have a sodalite-like structure and exhibit superconductivity with T_c as high as 263-384 K [58-60], depending on the models of T_c. Another close cousin of MgH_6 is CaH_6. It was reported to be a superconductor with a similar lattice structure as of MgH_6. At 150 GPa, CaH_6 was predicted with T_c = 235 K [61]. More of the CaH_x compounds have been studied [62] and the existence of CaH_6 is still debatable. The last of my list is the real example of the word "superhydride". It is the family of actinium superhydrides, AcH_x, where x = 10-16 [63]. The AcH_{10} compound exhibits T_c = 204-251 K at 200 GPa, and the AcH_{16} compound exhibits T_c = 199-241 K at 150 GPa [63].

The binary hydride compounds have been diligently investigated for a few decades. A nearly complete periodic table of the stable binary hydrides under high pressure has been established. The next step is the making of ternary hydride compounds, $A_xB_yH_z$. It seems like a straightforward modification but some tedious works must also be resolved. A large number of possibilities of how to combine xA and yB and zH is a handful computational task. Nevertheless, some examples have already been theoretically investigated. The first few examples are $MgGeH_6$ which is a superconductor with T_c = 66.6 K at 200 GPa [64], $CaYH_{12}$ with T_c = 226-258 K at 200 GPa [65], and $MgCaH_{12}$ with T_c = 205-288 K at 200 GPa [66]. In 2019, there was a theoretical suggestion on the increment of the electron density of states at the Fermi level by using a metal substitution method. The most famous example is the substitution of Li into the MgH_{16} clathrate structure [67]. Its T_c was reported to be as high as 473 K at 250 GPa. This finding has coined the term "hot superconductors", which are yet to be confirmed by experiments.

I conclude this section with Table 2 which summarizes T_c of several metal hydride compounds from the theoretical predictions.

Table 2. The parameters ω_{ln} and λ, and T_c of some selected binary compounds and ternary compounds from theoretical predictions. In literature, T_c have been estimated using different models, i.e. McM is the McMillan equation (modified by Allen and Dynes, Eq. (13)), AD is the strong coupling Allen-Dynes equation (Eq. (15)) and E is from the numerically solved Eliashberg equation [71].

Compounds	P (GPa)	λ	ω_{ln} (K)	T_c (K)	(Model) Reference
MgH_2	180	0.58	1111	23	(McM) [57]
CaH_6	150	2.69	n/a	235	(E) [61]
YH_6	165	2.24	929	184 240	(AD) [50] (E) [50]
MgH_6	300	3.29	1450	263 384	(McM) [58] (AD) [59]
CeH_9	200	2.30	740	117	(McM) [52]
LaH_{10}	210	3.41	848	238 286	(McM) [46] (E) [46]
YH_{10}	250	2.58	1282	265 326	(McM) [46] (E) [46]
$MgGeH_6$	200	1.16	773	66.6	(McM) [64]
$CaYH_{12}$	200	2.2	1230	226 258	(AD) [65] (E) [65]
$MgCaH_{12}$	200	2.53	1400	205 288	(McM) [66] (AD) [66]
Li_2MgH_{16}	250	~4.0	n/a	473	(E) [67]

3. Electron-Phonon Interaction

Superconductivity is stemmed from the electron-phonon interaction. There are several excellent reviews on the subject [68,69]. I will only give a brief description.

Migdal [70] and Eliashberg [71] used quantum field theory to solve the system with FrÖlich Hamiltonian, which describes the interaction between electrons and phonons. The FrÖlich Hamiltonian can be written as

$$H = H_e + H_{ph} + H_{e-ph}, \tag{2}$$

where H_e describes electrons, H_{ph} describes phonons and H_{e-ph} describes the electron-phonon interaction via the electron-nucleus potential, $V(\boldsymbol{r}_i - \boldsymbol{R}_I^0)$, with the electron's coordinates, $\boldsymbol{r}_i$, and nuclear's coordinate, $\boldsymbol{R}_I^0$, and nucleus displacements, $\boldsymbol{u}_i$. Thus, H_{e-ph} can be explicitly written as

$$H_{e-ph} = \boldsymbol{u}_i \cdot \nabla V(\boldsymbol{r}_i - \boldsymbol{R}_I^0) \tag{3}$$

The lattice vibrations and hence all phonon modes are embeded in u_i. By treating H_{e-ph} as perturbation, the solution can be derived in terms of Green's function as

$$G(\boldsymbol{k}, \varepsilon) = \frac{1}{\varepsilon - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, \varepsilon) + i\eta}, \tag{4}$$

where the self-energy part, $\Sigma(\boldsymbol{k}, \varepsilon)$, can be written in terms of the so-called spectral function, $\alpha^2F(\omega)$, as follows;

$$\begin{aligned} \operatorname{Im} \Sigma(\boldsymbol{k}, \varepsilon) = -\pi \int_0^\infty d\omega \, (\alpha^2 F_{\boldsymbol{k}}^+(\omega)[b(\omega) \\ + f(\omega + \varepsilon)] \\ + \alpha^2 F_{\boldsymbol{k}}^-(\omega)[b(\omega) \\ + f(\omega - \varepsilon)]), \end{aligned} \tag{5}$$

where $b(\omega)$ and $f(\omega + \varepsilon)$ are boson's and fermion's number distribution, respectively. The spectral function can be calculated from

$$\alpha^2 F_{\boldsymbol{k}}^{\pm}(\omega) \propto \sum_{\boldsymbol{q}} \delta(\omega - \omega_{\boldsymbol{q}}) \sum_{\boldsymbol{k}'} \left| g_{\boldsymbol{q},\boldsymbol{k}',\boldsymbol{k}} \right|^2 \delta(\varepsilon - \varepsilon_{\boldsymbol{k}'} \pm \omega), \tag{6}$$

where $\boldsymbol{q}$ are the phonon modes, $\boldsymbol{k}', \boldsymbol{k}$ are the electron states, and the electron-phonon coupling matrix is given by

$$g_{\boldsymbol{q},\boldsymbol{k}',\boldsymbol{k}} = \langle \boldsymbol{k}' + \boldsymbol{q} | H_{e-ph} | \boldsymbol{k} \rangle. \tag{7}$$

The available electron states are confined in the vicinity of the Fermi surface only. This imposes a selection rule on the transfering states due to the interaction. From this theory, the largest superconducting gap is proportional to the quantity

$$\lambda = 2 \int d\omega \frac{\alpha^2 F(\omega)}{\omega}, \tag{8}$$

which is sometimes called the isotropic coupling constant, and $\alpha^2F(\omega)$ is closely related to Eq. (6). Most of all, the spectral function can be calculated by using DFT method [27]. Thus λ can be derived from the DFT results. Eq. (8) can be interpreted that λ measures the average strength of the electron-phonon coupling. Hopfield [72] analysed this equation and concluded the relation between λ and N_F, as

$$\lambda = \frac{N_F g_{eff}^2}{M\omega_{rms}^2}, \tag{9}$$

where g_{eff}^2 is the effective coupling related to $\left|g_{q,k',k}\right|^2$. This form of Eq. (9) already suggests that λ and ω_{rms}^2 are inversely proportional. This parameter λ can also be measured from the electronic specific heat, $C_{el}(T)$, as suggested by Allen [3]. The relation between $C_{el}(T)$ and λ can be written as

$$C_{el}(T) = N_F(1+\lambda)\frac{\pi^2 k_B^2}{3}T. \tag{10}$$

4. Empirical Formula of Tc

As discussed earlier, T_c from the BCS theory, Eq. (1), has some limitations. This is because Eq. (1) can be used in the weak electron-phonon coupling regime only. Furthermore, V_{eff} is very difficult to be evaluated. Thus, a more powerful model of T_c is needed. From section 3, it has been shown that λ can be evaluated in a more practical way, such as from DFT. Also, the effective interaction in the BCS theory can be related to λ as [3]

$$N_F V_{eff} \to \lambda - \mu^*, \tag{11}$$

where μ^* is effective Coulomb parameter, of which the value is limited in the range of 0.1-0.2 only. If we insert this relation into Eq. (1), the equation resembles

$$T_c = \frac{\theta_D}{1.14}\exp\left(-\frac{1}{\lambda-\mu^*}\right), \tag{12}$$

This led McMillan [73] and subsequent development of Allen and Dynes [74] to make a modification of Eq. (12) into an empirical formula of the form

$$T_c = \frac{\omega_{ln}}{1.20}\exp\left(-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right), \tag{13}$$

Eq. (13) is the so-called McMillan equation if the factor $\frac{\omega_{ln}}{1.20}$ is replaced by $\frac{\theta_D}{1.45}$. Subsequently, Allen and Dynes proposed that θ_D should be replaced by

$$\omega_{ln} = \exp\left(\frac{2}{\lambda}\int_0^\infty \frac{d\omega}{\omega}\ln(\omega)\,\alpha^2F(\omega)\right), \tag{14}$$

which measures the average frequency by using distribution function based on the spectral function. Eq. (13) has been widely accepted and also known as Allen-Dynes modified McMillan equation, denoted as McM in Table 2.

For the strong-coupling, in which $\lambda > 1.5$, the equation for T_c can be modified further to

$$T_c = f_1 f_2\frac{\omega_{ln}}{1.20}\exp\left(-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\ )}\right), \tag{15}$$

where the correction factor

$$f_1 f_2 = \left\{1+\left[\frac{\lambda}{2.46(1+3.8\mu^*)}\right]^{\frac{3}{2}}\right\}^{\frac{1}{3}} \left\{1+\frac{(\frac{\omega_{rms}}{\omega_{ln}}-1)\lambda^2}{\lambda^2+3.31(1+6.3\mu^*)\frac{\omega_{rms}}{\omega_{ln}}}\right\}, \tag{16}$$

and,

$$\omega_{rms} = \left\{\frac{2}{\lambda}\int_0^\infty d\omega\,\omega\,\alpha^2F(\omega)\right\}^{1/2}. \tag{17}$$

If we think of $\frac{\alpha^2F(\omega)}{\omega}$ as a distribution function, ω_{rms} is just the square root of the average ω^2 over the distribution function. Eq. (15) is known as the strong coupling Allen-Dynes equation, denoted as AD in Table 2.

The analytic equation of T_c is now explicitly related to two important quantities, λ and ω_{ln}. In order to find a high value of T_c, it seems that we need both large λ and large ω_{ln}. However, from Eq. (14), they are not independent. Thus if we need to improve T_c, we might need to look into one step deeper. The next section, I will discuss the spectral function from which both λ and ω_{ln} are derived.

5. Simple Model of Spectral Function

For any system, if we look for a high value of T_c, it is natural to search for conditions that give large ω_{ln} and λ. However, from Eq. (8) and (14), λ and ω_{ln} are not entirely independent. There is no guarantee that λ and ω_{ln} will always be large at the same time. This led us to make a deeper detail analysis. As both λ and ω_{ln} are stemmed from $\alpha^2F(\omega)$, we need to elucidate its impacts in more detial. In order to give a simplest view of $\alpha^2F(\omega)$ and to gain insight into the improvement of T_c, Allen and Dynes proposed the Einstein Model for analyzing the spectral function [74], written as

$$\alpha^2F_E(\omega) = \frac{\lambda\theta_E}{2}\delta(\omega-\omega_E). \tag{18}$$

It can be shown easily that Eq. (18) gives $\omega_{ln} \to \theta_E$, where θ_E is the celebrated Einstein temperature. It turns out that the model in Eq. (18) is too simple.
In this review, I assume that $\alpha^2F(\omega)$ can be estimated by a constant function

$$\alpha^2F(\omega) = \begin{cases} c_H; & \omega_a \le \omega \le \omega_b \\ 0; & elsewhere \end{cases}. \tag{19}$$

This is a straightforward modification of Eq. (18). It can be thought of as a sum of a series of many different Einstein oscillators, instead of just one type of the Einstein oscillator as in Eq. (18). This is because, by inspection, I find that the spectral function in most metal hydrides under high pressure is dominated by the oscillation part of the hydrogen atoms. A typical spectral function from DFT [66] is shown in Figure 1, where the yellow line shows the contribution from the metal atoms and the green line shows the contribution from the hydrogen atoms. Let us call the function in Eq. (19) as the bandwidth function. The constant c_H can be related to the average magnitude of the electron-phonon interaction, and subscript H emphasises the importance of the hydrogen atoms. Typically, the bandwidth function starts at $\omega_a > 0$ as the low-frequency vibrations of metal atoms contribute much less to $\alpha^2F(\omega)$, comparing with the high-frequency vibration of hydrogen atoms, and ω_b has a cutoff roughly around the order of 70 THz (equivalent to approximately 3,500K). For a pure hydrogen lattice, ω_b could be as high as 85 THz (equivalent to approximately 4,100K) [43]. Table 3 gives the values of ω_a , ω_b and c_H of several compounds, roughly extracted from the DFT calculations [43,66].

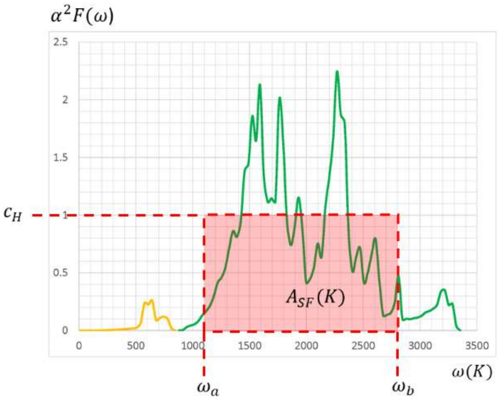

Figure 1. Shows a typical spectral function of MgCaH$_{12}$ at 250 GPa, calculated from DFT [66]. The yellow line shows the contribution from metal atoms and the green line shows the contribution from hydrogen atoms. The red dashed lines show the definition of model parameters of Eq. (19). These parameters are chosen in order to conserve the area under the original spectral function curve, denoted by A_{SF}.

From the bandwidth function, Eq. (19), we can integrate Eq. (8) and (14) analytically for λ and ω_{ln} respectively. The results are

$$\lambda = 2c_H \int_{\omega_a}^{\omega_b} \frac{d\omega}{\omega} = 2c_H \ln\left(\frac{\omega_b}{\omega_a}\right), \tag{20}$$

and

$$\begin{aligned} \omega_{ln} &= \exp\left(\frac{2c_H}{\lambda}\int_{\omega_a}^{\omega_b}\frac{d\omega}{\omega}\ln(\omega)\right) \\ &= \exp\left(\frac{c_H(\ln^2(\omega_b) - \ln^2(\omega_a))}{2c_H \ln\left(\frac{\omega_b}{\omega_a}\right)}\right) \\ &= \sqrt{\omega_a\omega_b}. \end{aligned} \tag{21}$$

The analytic solutions give us some insight information as follows;

1. According to Eq. (20), λ will be large if c_H is large and the bandwidth function is wide, i.e. $\omega_b \gg \omega_a$.

2. According to Eq. (21), ω_{ln} will be large if both ω_a and ω_b are large. Hence, ω_{ln} will be largest for a given set of parameters if $\omega_a = \omega_b$. In the other words, ω_{ln} will be large if the bandwidth function is narrow with a large value of ω_a and ω_b. In addition, ω_{ln}, derived from Eq. (21), is independent of c_H.

3. Under some influential factors, i.e. under high pressure, sometimes c_H is only slowly varying in a given compound. If the influential factors tend to make a higher ω_{ln} by narrowing the bandwidth function, λ will definitely tend to reduce. Figure 2 shows typical plots between ω_{ln} and λ . For comparison, ω_{ln} and λ of some selected compounds, calculated from DFT [60], are shown in Table 4. It clearly shows the inverse proportion between ω_{ln} and λ. By further analyzing Eq. (17) and (21), the relation between ω_{ln} and ω_{rms} can be established and they are positively correlated. Figure 2 also shows the positive correlation between ω_{ln} and ω_{rms}. This implies that increasing of ω_{rms} will also tends to diminish λ. This finding is also in fair agreement with Hopfield analysis, Eq. (9) in that λ and ω_{rms}^2 are inversely proportional.

4 The limitation of the above analysis is that c_H is assume to be slowly varying. If it is largely varied between different compounds, or different structures of the same compound, the above analysis might be invalid.

Table 3. Parameters for the model of the spectral function, Eq. (19), of several compounds, roughly extracted from the DFT calculations of Ref. [43] and [66].

Compounds	ω_a (K)	ω_b (K)	c_H	λ Eq. (20)	ω_{ln} (K) Eq. (21)	A_{SF} (K)	T$_c$ (K)
H$_3$S [43]	812.32	2901.13	0.64	1.63	1535.13	1336.84	214
LaH$_{10}$ [43]	580.23	2669.04	0.72	2.20	1244.45	1503.95	234
MgCaH$_{12}$ [66]	1100	2800	1	1.87	1754.99	1700	277
H [43]	928.36	4061.58	0.56	1.65	1941.81	1754.60	282

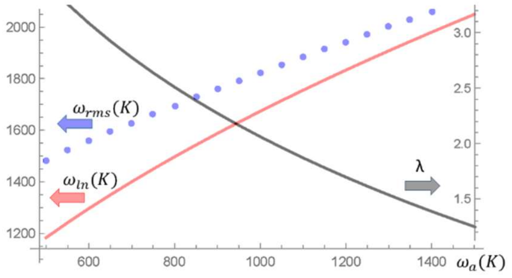

Figure 2. shows typical plots between ω_{ln} (light red line) and λ (light grey line), and also shows the positive correlation between ω_{ln} and ω_{rms} (light purple dots).

Table 4. The inverse proportion between ω_{ln} and λ in several compounds. All data are taken from Ref. [60].

Compounds	P (GPa)	ω_{ln} (K)	λ	T_c (K)
H_3S	220	1415.75	2.08	229
H_3S	250	1531.80	1.82	218
H_3S	280	1589.82	1.61	199
CaH6	150	1044.41	2.53	200
CaH6	200	1241.68	1.95	190
CaH6	250	1357.73	1.69	180
CaH6	300	1415.75	1.59	175
LaH10	250	1067.62	2.46	206
LaH10	300	1334.52	1.80	189

At this stage, I can now discuss the impact of the bandwidth function, Eq. (19), on the value of T_c. For $c_H = 1$ and $\mu^* = 0.1$, The contour plot of T_c, Eq. (15), as a function of ω_a and ω_b is shown in Figure 3. Some special cases can be discussed as follows;

1. If the path A (green arrow A) in Figure 3 is taken, where ω_a is fixed and ω_b increases, T_c will increase accordingly.
2. If the path B (green arrow B) in Figure 3 is taken, where ω_b is fixed and ω_a increases, T_c will appear to decrease.
3. If the path C (green arrow C) in Figure 3 is taken, where both ω_a and ω_b increases, there exists a special path that T_c appears to be a constant.
4. Surprisingly, in order to achieve a highest T_c, the present model favors a widest bandwidth function, as shown at the end point of the path A in Figure 3. This finding also implies that a large λ is more favorable than a large ω_{ln}. This is also in good agreement with the data in Table 4. If we look at the same compound, the highest T_c comes from the largest λ. However, for different compounds, a more careful analysis must be taken into account.

As searching for the largest T_c is related to searching for the widest bandwidth function. If c_H is not varied much, such as in the same compound with the same structure but slightly different thermodynamic conditions, we would arrive at searching for the largest area under the $\alpha^2F(\omega)$ curve, A_{SF}. In the other words, A_{SF} must be positively correlated with T_c. Tables 3 and 4 show the values of ω_{ln} and λ, and T_c. The relation among these three quantities is rather ambiguous. However, the relation between A_{SF} and T_c is clearly established, as shown in Figure 4. According to the Leavens-Carbotte analysis, they suggested that $T_c = T_0 + S \times A_{SF}$ [60,75]. In Figure 4, the red dotted line is the Leavens-Carbotte prediction with $S = 0.148$ [60,75]. The open triangles are the results taken from ref [60]. The open circles are the results from Table 3. The blue dashed line is the best linear fitting with $S = 0.172$. The discrepancy is possibly from the crudeness of the model, Eq. (19), and also from the different methods of finding T_c. Surprisingly, the correlation between T_c and A_{SF} also establishes across different compounds.

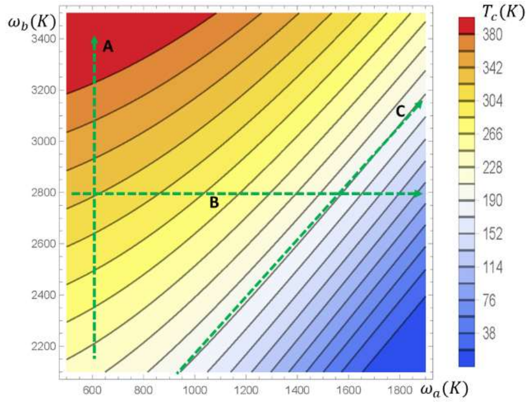

Figure 3. shows contour plot of T_c, Eq. (15), as a function of ω_a and ω_b, all in units of Kelvin.

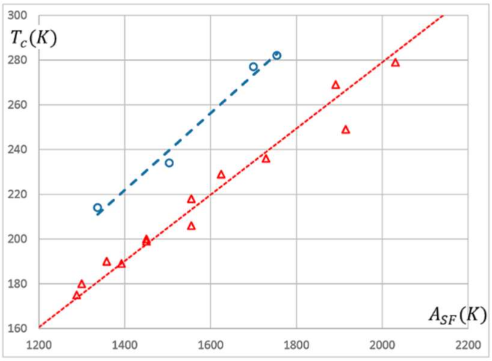

Figure 4. Shows Leavens-Carbotte analysis of T_c, i.e. $T_c = T_0 + S \times A_{SF}$ [60,75]. The red dotted line is the Leavens-Carbotte prediction with $S = 0.148$ [60,75]. The open triangles are the results taken from ref [60]. The open circles are the results from Table 3. The blue dashed line is the best linear fitting with $S = 0.172$.

6. Conclusions

I gave a brief review on the superconductivity in general in both experimental observation and theoretical prediction. Then, I focused on a limited list of metal superhydrides under high pressure and their near-room-temperature T_c. I also emphasised on the important of the spectral function in order to give a prediction on T_c. I proposed a simple model that provides insight information in the behavior of ω_{ln} and λ. Finally I pointed out where to look for a higher T_c.

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