Instability of Metals under Strong Electron–Phonon Interaction and the Prospect of Room-Temperature Superconductivity

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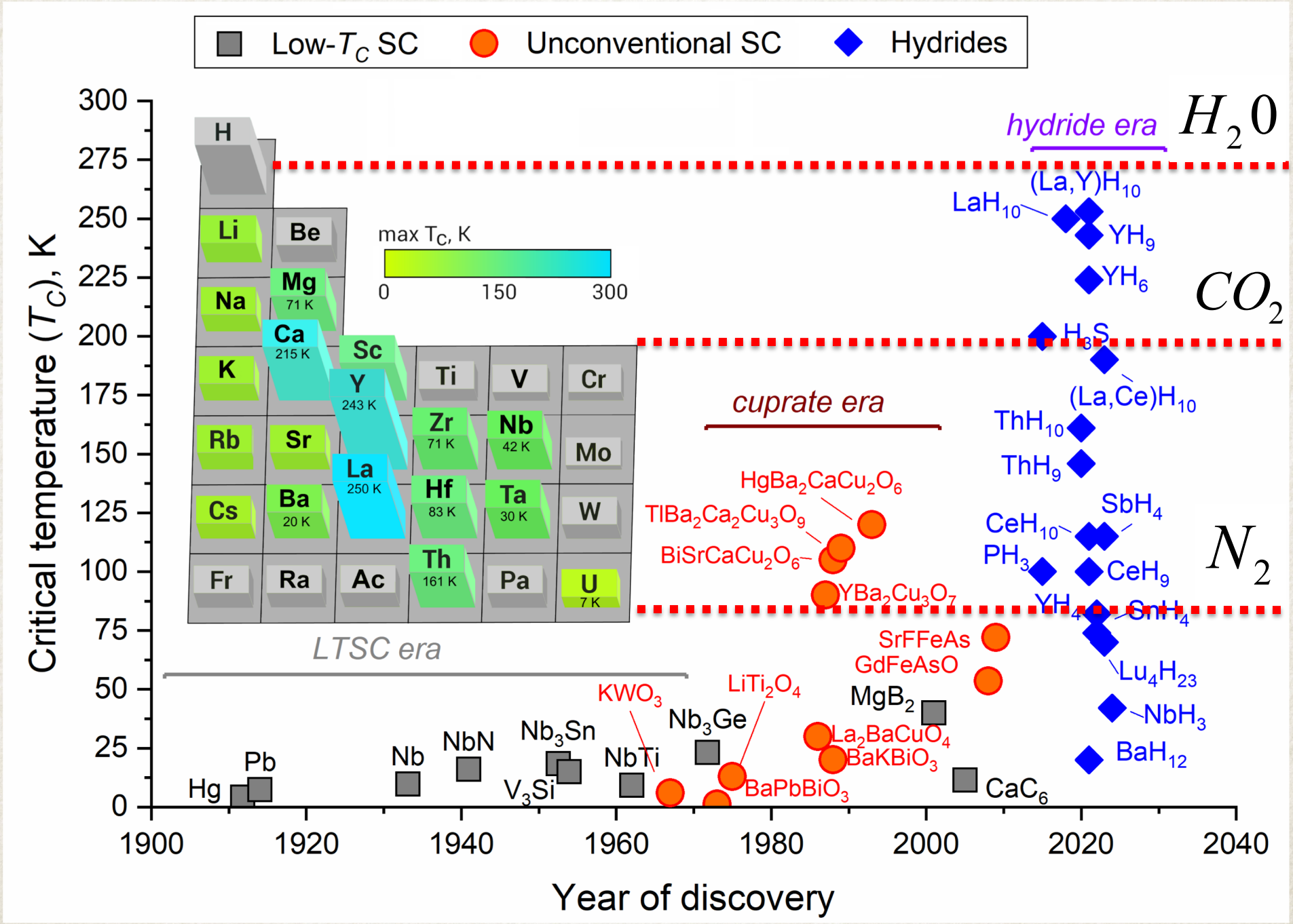
RUTGERS–NEW BRUNSWICK
School of Arts and Sciences


Low-T_C SC
Unconventional SC
Hydrides
Critical temperature (T_C), K
Year of discovery
max T_C, K
0
150
300
H
Li
Be
Na
Mg
71 K
K
Ca
215 K
Sc
Y
243 K
Ti
V
Cr
Rb
Sr
Zr
71 K
Nb
42 K
Mo
La
250 K
Hf
83 K
Ta
30 K
W
Cs
Ba
20 K
Th
161 K
U
7 K
Fr
Ra
Ac
Pa
LTSC era
cuprate era
hydride era
$H_2 0$
CO_2
N_2
Hg
Pb
Nb
NbN
Nb_3Sn
V_3Si
NbTi
KWO_3
Nb_3Ge
$LiTi_2O_4$
$BaPbBiO_3$
MgB_2
La_2BaCuO_4
$BaKBiO_3$
CaC_6
SrFFeAs
GdFeAsO
$HgBa_2CaCu_2O_6$
$TlBa_2Ca_2Cu_3O_9$
$BiSrCaCu_2O_6$
$YBa_2Cu_3O_7$
LaH_{10}
$(La,Y)H_{10}$
YH_9
YH_6
H_3S
$(La,Ce)H_{10}$
ThH_{10}
ThH_9
SbH_4
CeH_{10}
PH_3
CeH_9
YH_4
SnH_4
Lu_4H_{23}
NbH_3
BaH_{12}
1900
1920
1940
1960
1980
2000
2020
2040
0
25
50
75
100
125
150
175
200
225
250
275
300

History of superconductivity in metallic hydrogen

Prediction of metallic hydrogen:

E. Wigner, H. B. Huntington,

On the possibility of a metallic modification of hydrogen,

J. Chem. Phys., **3**, 764 (1935).

Pressure needed: > 25 GPa. Now: 450-500 GPa

Prediction of the superconductivity:

N. W. Ashcroft,

Metallic Hydrogen: A High-Temperature Superconductor?

Phys. Rev. Lett., **21**, 1748 (1968).

Now:
T_c=374K

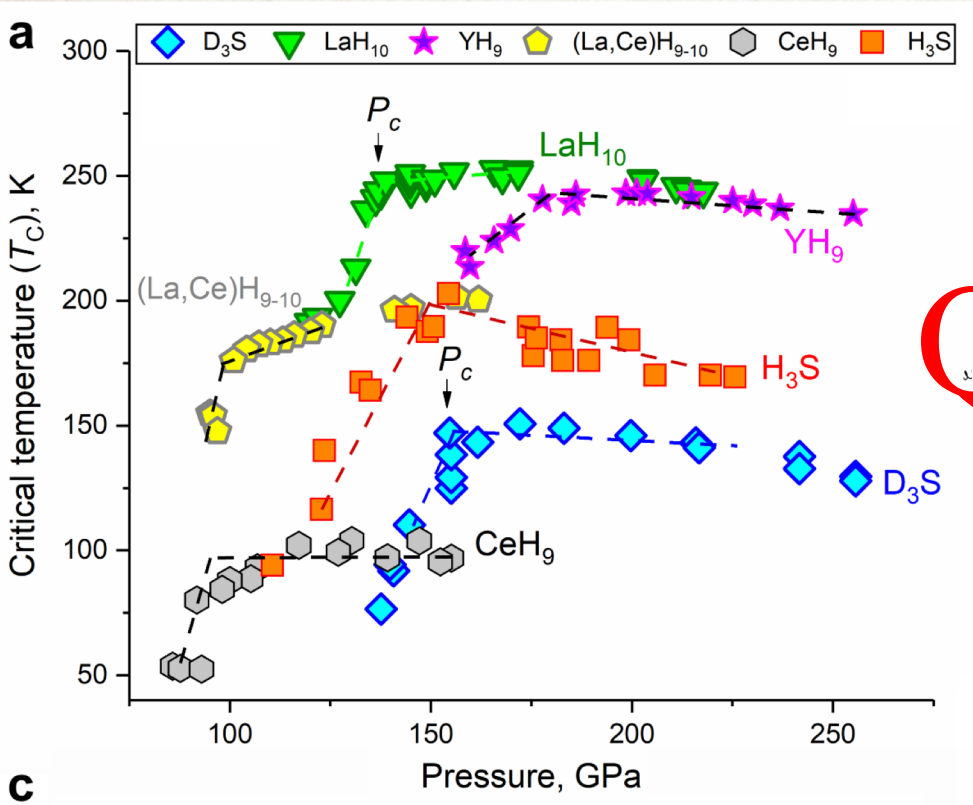
Chemical pressure:

E. Zurek et. al.,

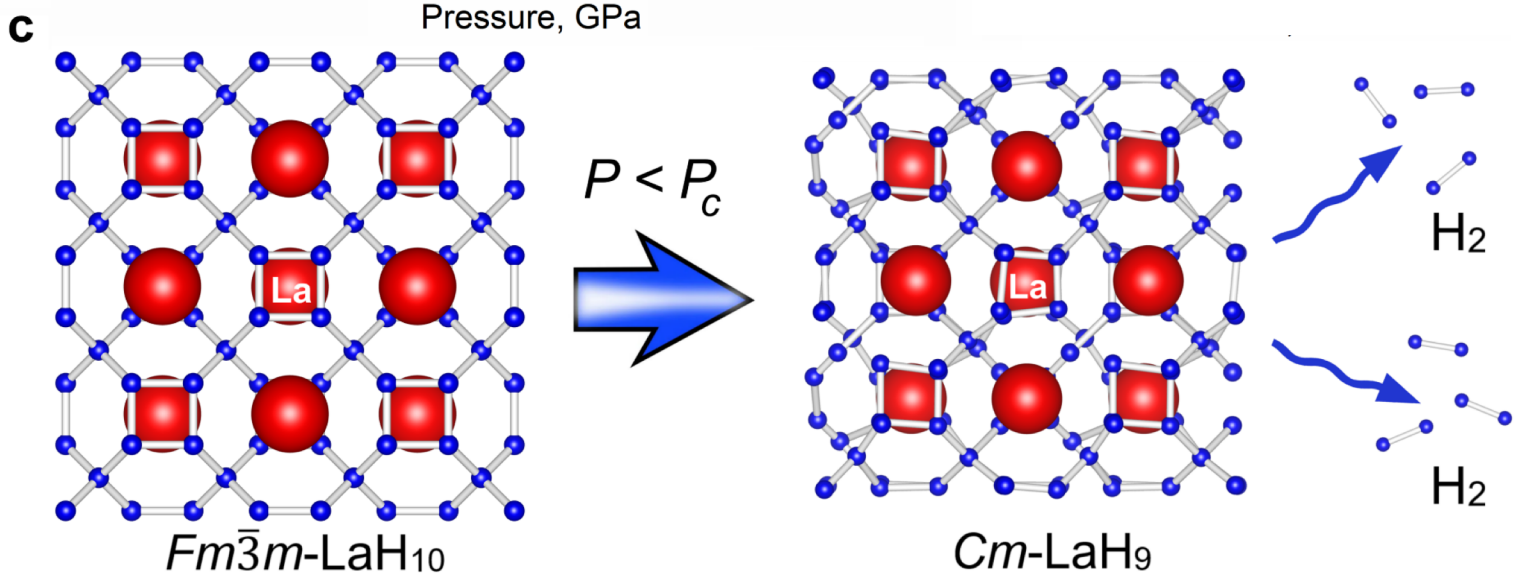
A little bit of lithium does a lot of hydrogen,

PNAS, **106**, 17640 (2009).

Pressure needed:
450 GPa ⟸ 150 GPa



Q: What happens at P_c? Why do T_c and the electron-phonon coupling suddenly drop ?



Migdal-Eliashberg Theory

INTERACTION BETWEEN ELECTRONS AND LATTICE VIBRATIONS IN A NORMAL METAL

A. B. MIGDAL

J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 1438-1446 (June, 1958)

INTERACTIONS BETWEEN ELECTRONS AND LATTICE VIBRATIONS IN A SUPERCONDUCTOR

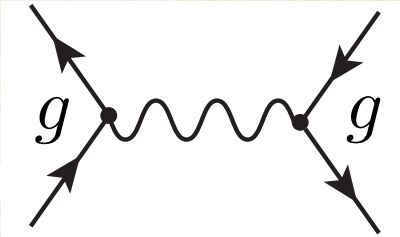
G. M. ELIASHBERG

J. Exptl. Theoret. Phys. (U.S.S.R.) **38**, 966-976 (March, 1960)

A. B. Migdal G. M. Eliashberg

1. Retarded electron-electron interaction mediated by phonons

$$V_{\rm int}(\omega) = \frac{g^2}{\omega^2 + \Omega^2}$$ (assume Einstein phonons for now)



2. Mean-field theory controlled by a small parameter $\frac{\Omega}{E_F} \sim 10^{-3}$. Quantitatively accurate predictions for T_c and other properties.

3. BCS theory is the weak-coupling limit $\lambda \to 0$ of the ME theory

$$V_{\rm int}(t - t') \to \lambda\, \delta(t - t')$$

Dimensionless electron-phonon coupling: $\lambda = \frac{g^2}{\Omega^2}$

Total specific heat in the normal (metallic) state

$$C_{\mathrm{tot}} = C_{\mathrm{el}} + C_{\mathrm{ph}}$$

Specific heat of electrons interacting via virtual phonons

Specific heat of physical phonons

Einstein phonons: $$C_{\mathrm{ph}} = \left(\frac{\Omega}{2T}\right)^2 \sinh^{-2}\left(\frac{\Omega}{2T}\right)$$

$$\frac{C_{\mathrm{ph}}}{C_{\mathrm{el}}} \sim \frac{E_F}{\Omega} \to \infty$$

Phonons serve as a heat bath with infinite heat capacity for electrons

Electronic specific heat in the normal state

Electronic specific heat: $C_{\rm el} = \dfrac{2\pi^2 \nu_0 T}{3}\left[1 - \lambda g\left(\dfrac{\Omega}{2\pi T}\right)\right]$

$\psi(x)$ – digamma function

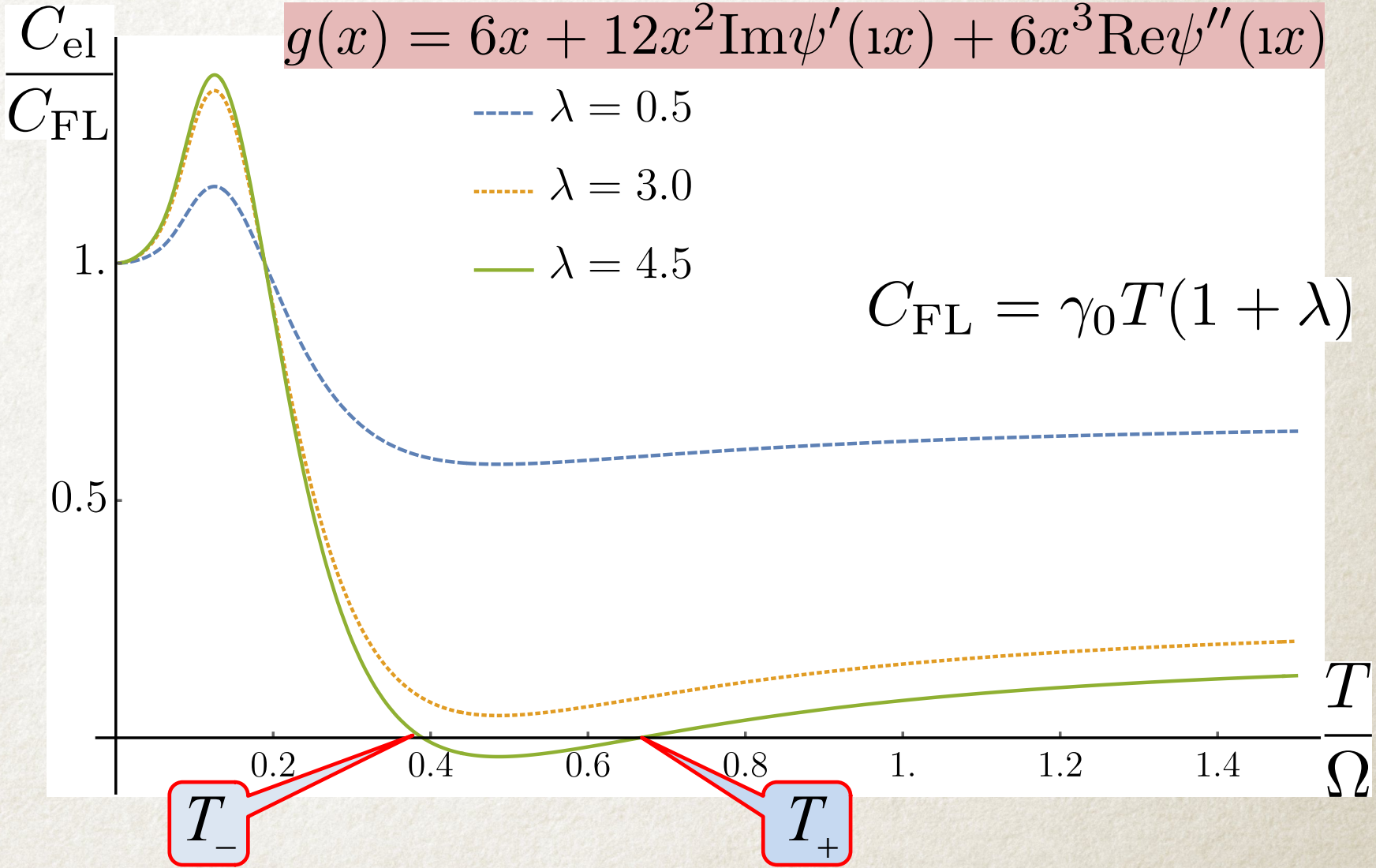
$C_{\rm el} < 0$ for $\lambda > 3.69$ and $T_- < T < T_+$

$T_+ > T_c$ for all λ

$T_c \approx 0.18\sqrt{\lambda}\Omega$

$T_+ \approx 0.38\sqrt{\lambda}\Omega$

$g(x) = 6x + 12x^2 \mathrm{Im}\psi'(1x) + 6x^3 \mathrm{Re}\psi''(1x)$



Electronic specific heat in the normal state

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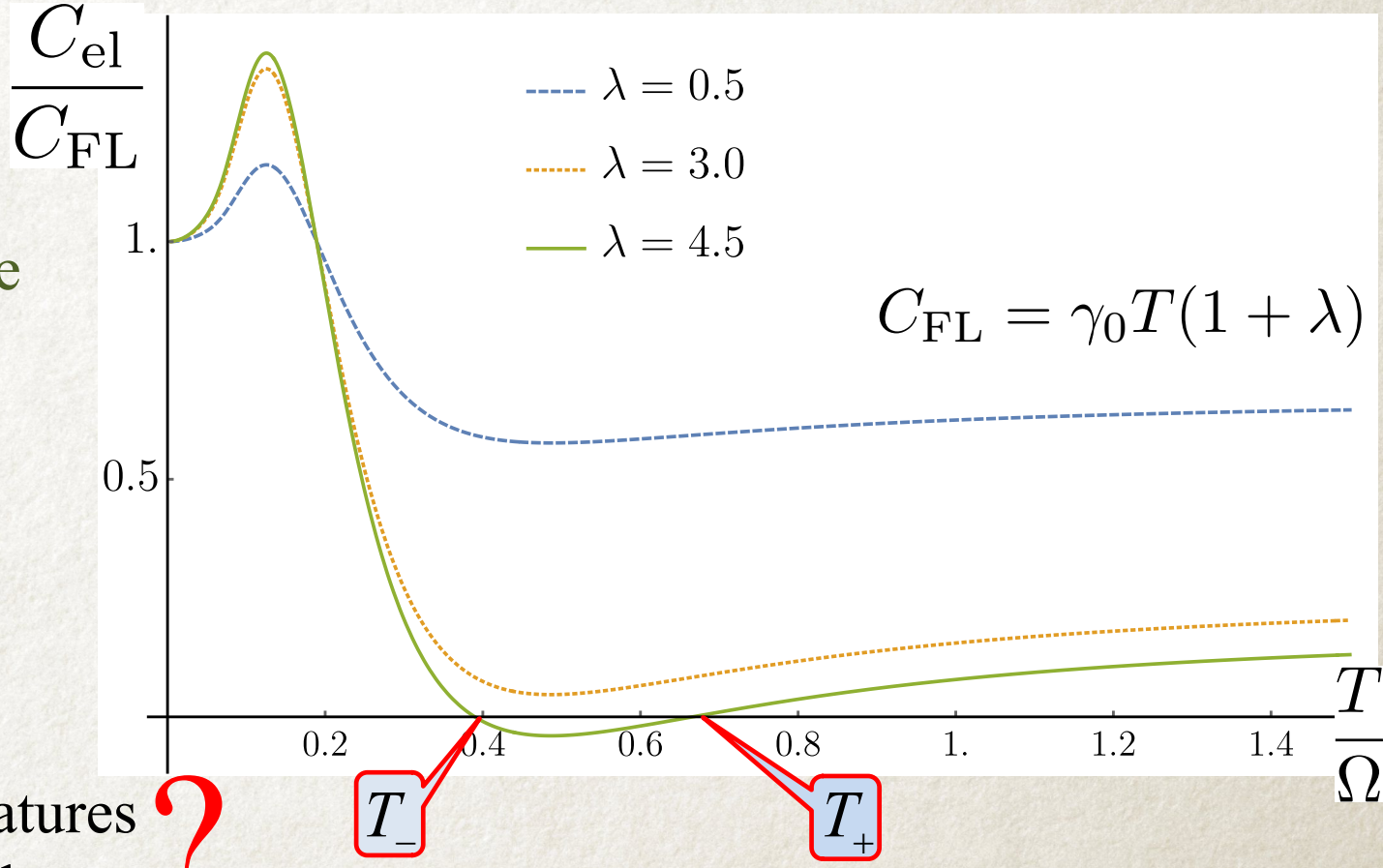
$\psi(x)$ – digamma function

$C_{\rm el} < 0$ for $\lambda > 3.69$
and $T_- < T < T_+$

$g(x) = 6x + 12x^2 {\rm Im}\psi'(\imath x) + 6x^3 {\rm Re}\psi''(\imath x)$

A system with negative heat capacity **weakly coupled** to a system with positive and much larger heat capacity (bath) is unstable.

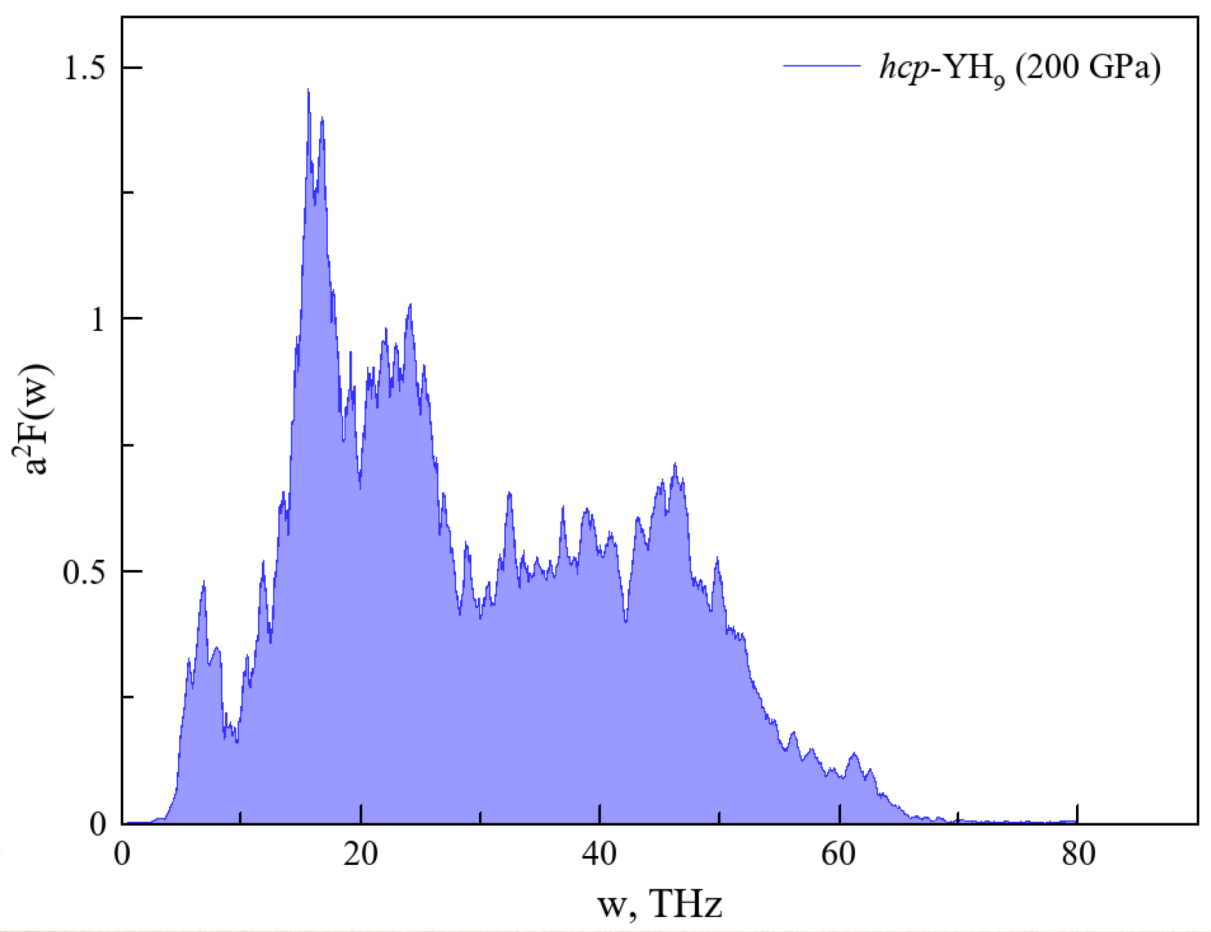
But nominal coupling between electrons and phonon bath **isn't weak**…



Q: Is the state with equal temperatures of electrons and phonons stable ?

Dispersing phonons: Eliashberg function

$$\alpha^2 F(\omega) = \frac{1}{N} \sum_k \frac{\lambda_k \omega_k}{2} \delta(\omega - \omega_k)$$



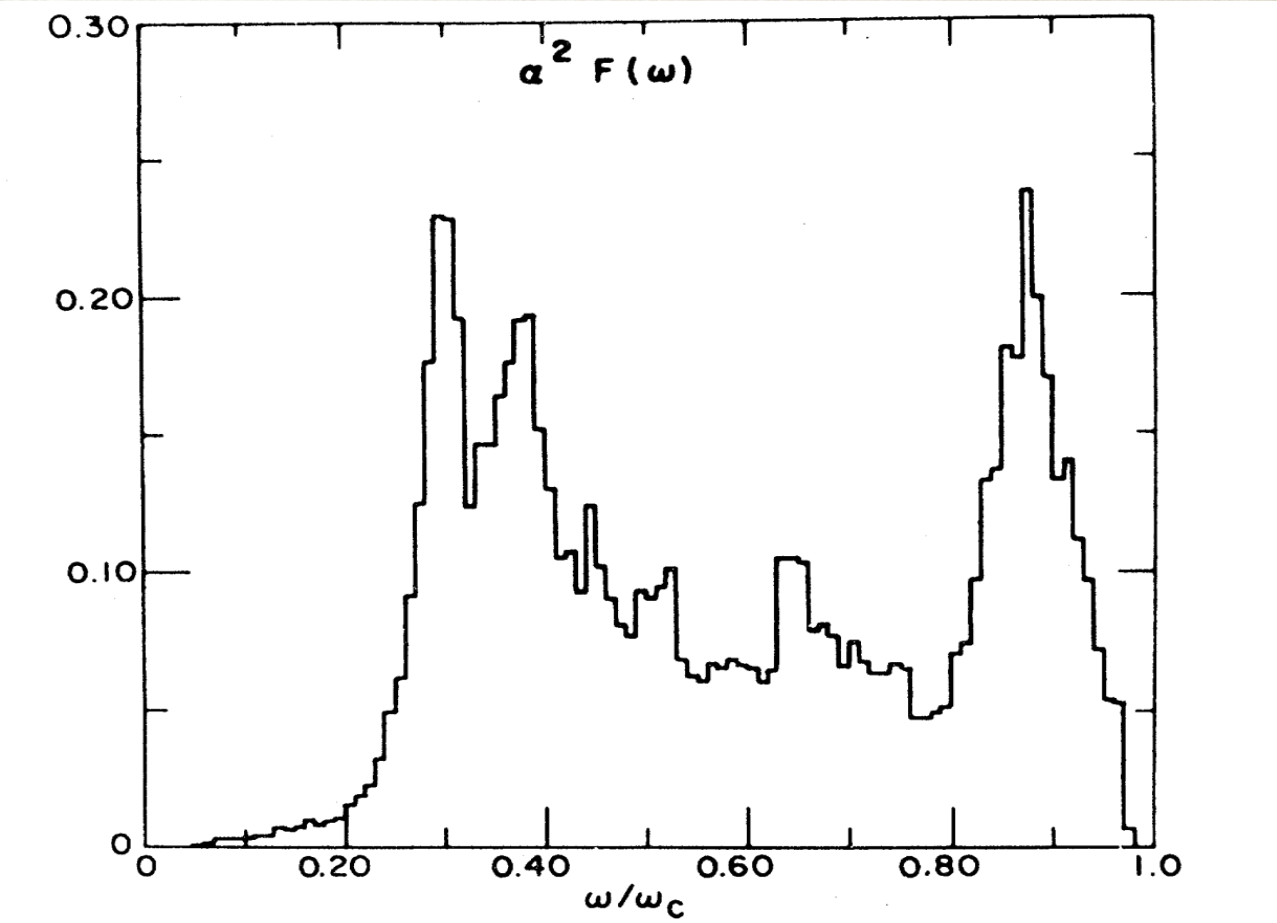


FIG. 20. Calculated isotropic $\alpha^2 F(\omega)$ function for Zn as a function of reduced frequency ω/ω_c with $\omega_c = 4.178 \times 10^{13}$ rad/sec, the maximum phonon frequency in the crystal. Multiple plane waves with a fitted pseudopotential and measured phonons were employed [Tomlinson and Swihart (1979)].

Dispersing phonons: Eliashberg function

$$\alpha^2 F(\omega) = \frac{1}{N}\sum_k \frac{\lambda_k \omega_k}{2}\delta(\omega - \omega_k)$$

$$\lambda = \frac{1}{N}\sum_k \lambda_k = \frac{1}{N}\sum_k \frac{g_k^2}{\omega_k^2}$$

Electronic specific heat: $$C_{\rm el} = \frac{2\pi^2 \nu_0 T}{3}\left[1 - \int_0^\infty g\left(\frac{\omega}{2\pi T}\right)\frac{2\alpha^2 F(\omega)}{\omega}d\omega\right]$$

$$g(x) = 6x + 12x^2 {\rm Im}\psi'(\imath x) + 6x^3 {\rm Re}\psi''(\imath x)$$

Compare with Einstein phonons: $$C_{\rm el} = \frac{2\pi^2 \nu_0 T}{3}\left[1 - \lambda g\left(\frac{\Omega}{2\pi T}\right)\right]$$

$$\lambda = \frac{g^2}{\Omega^2}$$

Q: Is the state with equal temperatures of electrons and phonons stable?

Suppose phonons and electrons have slightly different temperatures and analyze resulting dynamics

Kinetic equation for electron distribution function $f(E,t)$: $(1-\Sigma')\dot{f} + f'\dot{\Sigma} = I_{\rm ep}$

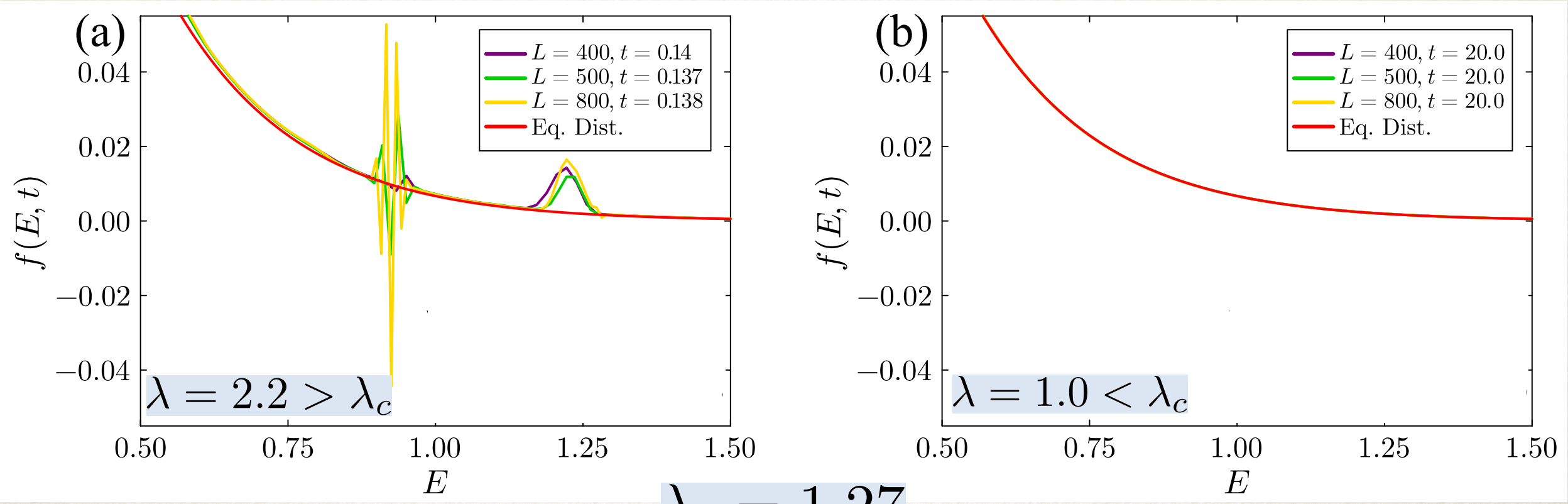
$$\Sigma[f] = \int dx \int_0^\infty d\omega \alpha^2 F(\omega) \frac{f(x+\omega) - f(x-\omega)}{E-x}$$ – electron self-energy

$$I_{\rm ep} = 2\pi \int_0^\infty d\omega \alpha^2 F(\omega) \left[N_0(T_{\rm ph})(f_+ + f_- - 2f) - f(f_+ - f_-) + f_+ - f \right]$$

Phonons stay in equilibrium serving as a thermal bath, because: $\dfrac{\tau_{\rm ph}}{\tau_{\rm el}} \sim \dfrac{C_{\rm ph}}{C_{\rm el}} \sim \dfrac{E_F}{\omega_{\max}} \to \infty$

$f_\pm = f(E \pm \omega, t)$

Kinetic equation: Direct simulation



$$\lambda_c = 1.27$$

Time evolution of fermion distribution for small deviations from thermal equilibrium for Einstein phonons

EY, Altshuler, Patra, Phys. Rev. Lett. (2025)

Kinetic equation: Strong coupling limit (any phonon dispersion)

$$\lambda = \frac{1}{N}\sum_k \frac{g_k^2}{\omega_k^2} \to \infty$$ equivalent to $\omega_k \to 0$

(strong coupling limit is universal)

$$g^2 \equiv \frac{1}{N}\sum_k g_k^2$$

(single energy scale)

$$I_{\rm ep} = 2\pi \int_0^\infty d\omega \alpha^2 F(\omega)\left[N_0(T_{\rm ph})(f_+ + f_- - 2f) - f(f_+ - f_-) + f_+ - f\right]$$

$$f_\pm = f(E \pm \omega, t)$$

$$I_{\rm ep} \to \pi g^2 (T_0 f'' - 2ff' + f')$$

$$T_0 \equiv T_{\rm ph}$$

Kinetic equation: $(1-\Sigma_0')\dot{f} + f_0'\dot{\Sigma} = T_0 f'' - 2ff' + f'$

$$(1-\Sigma_0')\dot{f} = T_0 f'' - 2ff' + f'$$

Fixed point: Fermi distribution at temperature T_0: $f_0 = \frac{1}{e^{E/T_0}+1}$

EY, Altshuler, Patra, Phys. Rev. Lett. (2025)

Kinetic equation in strong coupling limit: Burgers/Diffusion equation

$$(1-\Sigma_0')\dot{f} = T_0 f'' - 2ff' + f'$$

Variable change: $u = 2f - 1, \quad y = E - \Sigma[f_0]$

Within the same approximation $u\frac{du}{dy} \approx -\frac{du}{dy}$

$$\dot{u} = \frac{d}{dy}\left(D\frac{du}{dy}\right) - u\frac{du}{dy}$$

Burgers' equation

$$\dot{u} = \frac{d}{dy}\left(D\frac{du}{dy}\right) - u\frac{du}{dy}$$

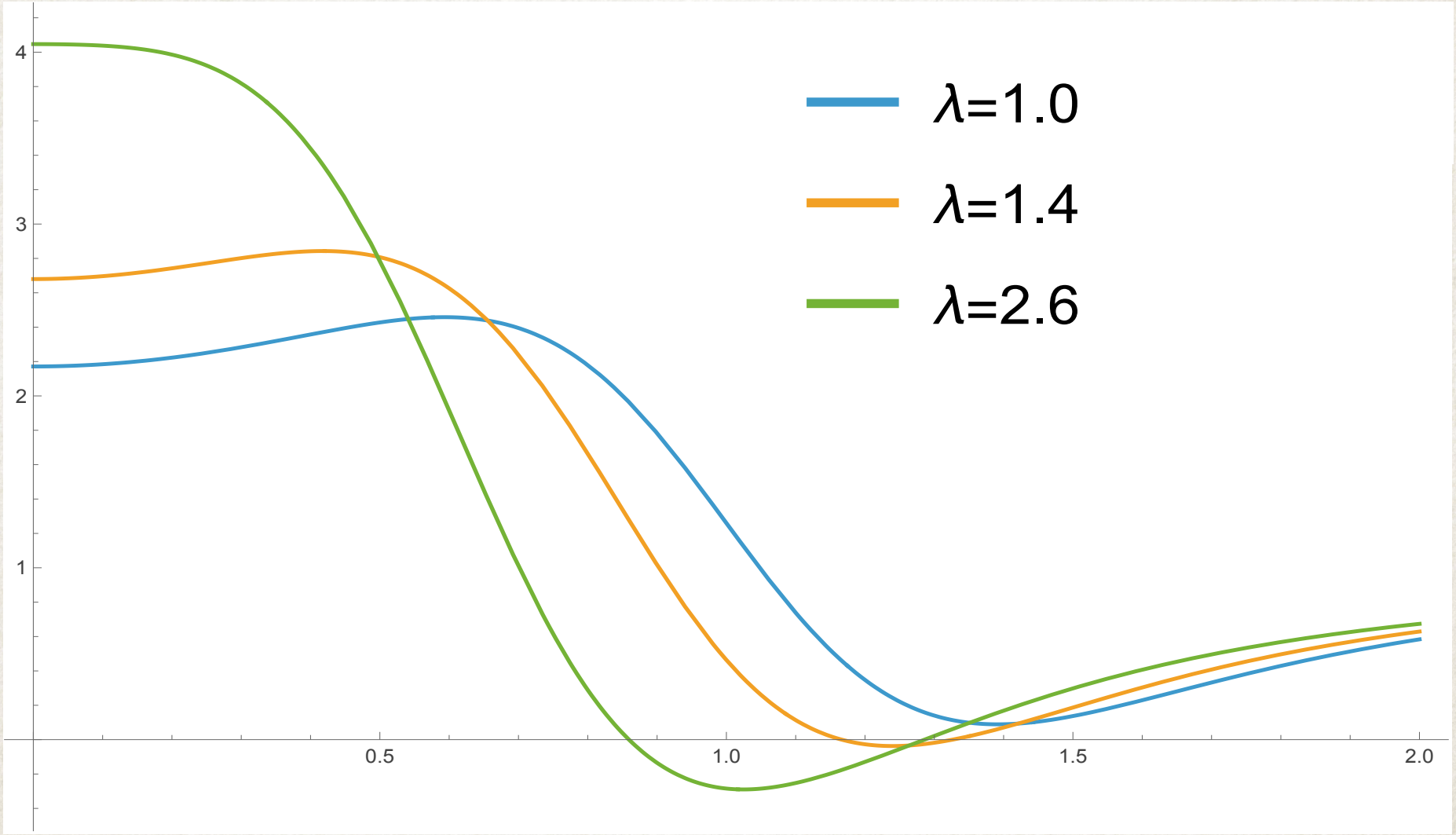
1D diffusion-convection equation

Position-dependent diffusion coefficient: $D(E) = T_0(1-\Sigma_0')$

$D(E) < 0$ same as reversing the time arrow – deviations grow and aggregate instead of becoming smaller and dispersing. Maxima increase and minima decrease. System moves away from rather than toward the equilibrium.

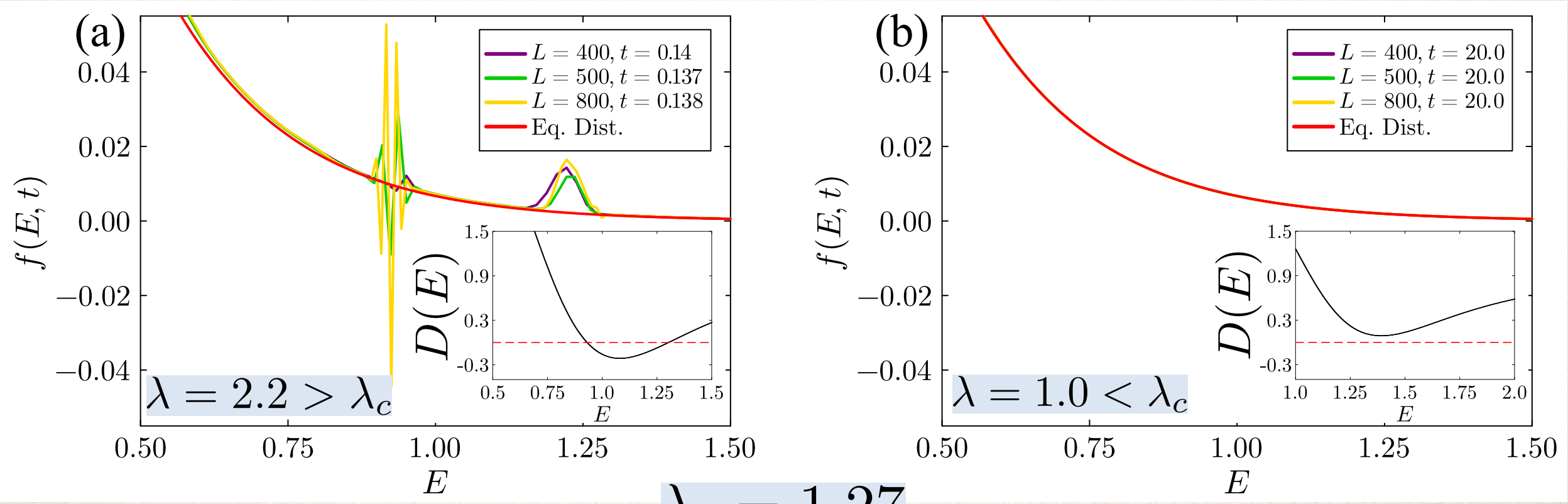
The kinetic equation is unstable if $\min_E D(E) < 0$

The minimum of $D(E)$ decreases as λ increases and dips below zero for $\lambda > \lambda_c$



Plots of $D(E) = T_0(1 - \Sigma_0')$ for Einstein phonons at $T = 0.2g > T_c$

Kinetic equation: Direct simulation



$$\lambda_c = 1.27$$

Time evolution of fermion distribution for small deviations from thermal equilibrium for Einstein phonons. Insets show $D(E)$

The instability develops in the region where $D(E) < 0$ and is most prominent near the points where $D(E) = T_0(1 - \Sigma_0') = 0$

Linear stability analysis

Kinetic equation for electron distribution function $f(E,t)$

$$(1-\Sigma')\dot{f} + f'\dot{\Sigma} = a_{\rm ep} I_{\rm ep} + a_{\rm ee} I_{\rm ee}$$

$$\Sigma[f] = \int dx \int_0^\infty d\omega \alpha^2 F(\omega) \frac{f(x+\omega) - f(x-\omega)}{E-x}$$ – electron self-energy

Coefficients $a_{\rm ep} > 0$ and $a_{\rm ee} > 0$ added for argument sake; in the actual system, $a_{\rm ep} = a_{\rm ee} = 1$

Linearized kinetic equation $\delta f = f - f_0 = -f_0' \varphi$ – miraculous substitution from LL v. X

$$A \cdot \dot{\varphi} = -M \cdot \varphi \qquad M = a_{\rm ep} M_{\rm ep} + a_{\rm ee} M_{\rm ee} \qquad A \cdot \dot{\varphi} = \int d\tilde{E} A_{\tilde{E}E} \dot{\varphi}(\tilde{E})$$

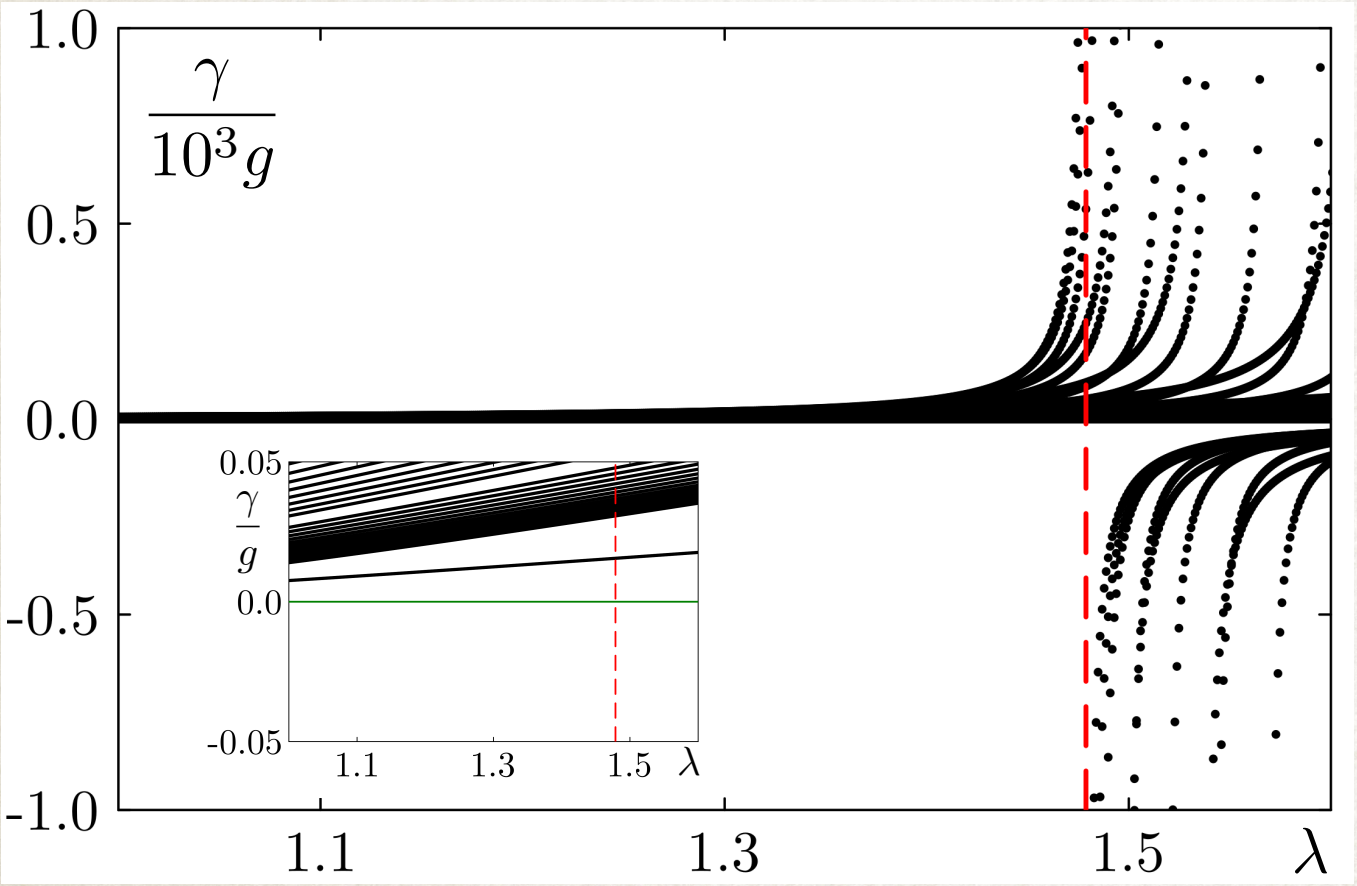
Separable solutions $\varphi(E,t) = e^{-\gamma t} h(E)$ form a basis. The metal is stable if all $\gamma > 0$

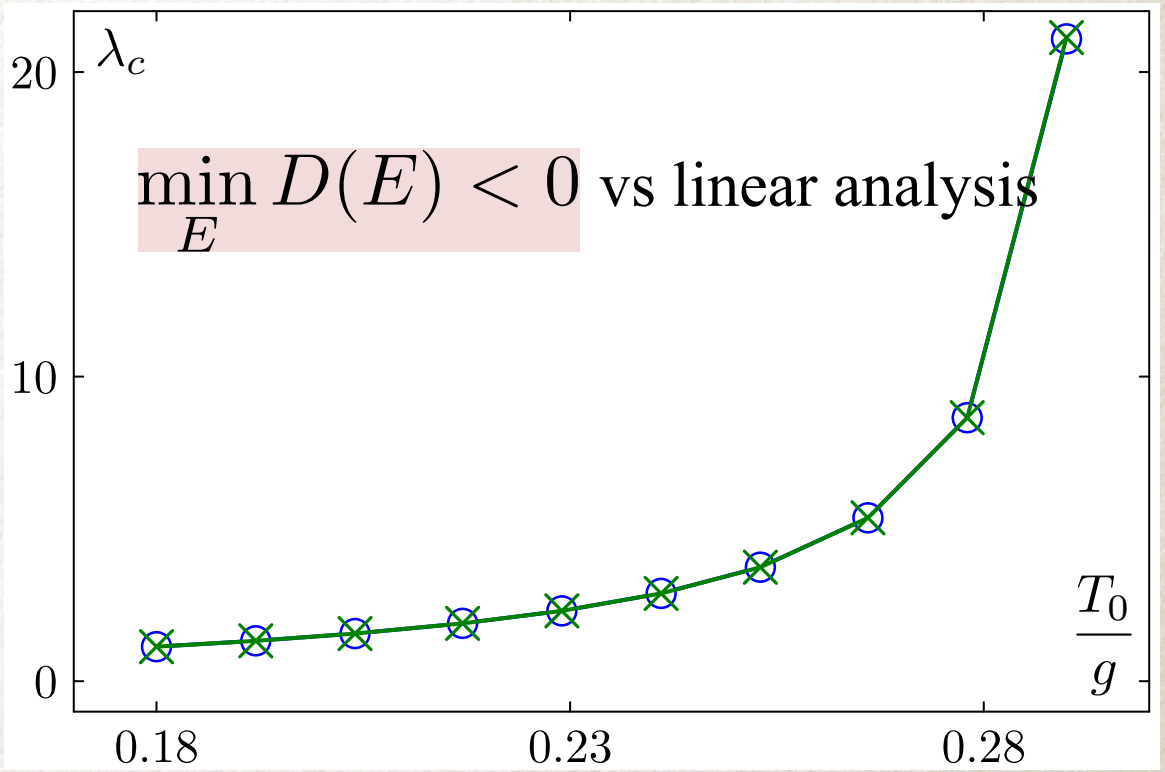
Generalized eigenvalue equation: $\gamma A \cdot \varphi = M \cdot \varphi$

Linear stability analysis

Generalized eigenvalue equation: $\gamma A \cdot \varphi = M \cdot \varphi$

The metal is stable if all $\gamma > 0$





Eigenvalues as functions of λ for a generic Eliashberg function

Linear stability analysis

Linearized kinetic equation $\delta f = f - f_0 = -f_0' \varphi$ – miraculous substitution from LL v. X

$$A \cdot \dot{\varphi} = -M \cdot \varphi \qquad M = a_{\rm ep} M_{\rm ep} + a_{\rm ee} M_{\rm ee} \qquad A \cdot \dot{\varphi} = \int d\tilde{E} A_{\tilde{E}E} \dot{\varphi}(\tilde{E})$$

Separable solutions $\varphi(E,t) = e^{-\gamma t} h(E)$ form a basis. The metal is stable if all $\gamma > 0$

Generalized eigenvalue equation: $\gamma A \cdot \varphi = M \cdot \varphi$

Matrices $M_{\rm ep}$ and $M_{\rm ee}$ are positive definite $\Rightarrow$ $a_{\rm ep} M_{\rm ep} + a_{\rm ee} M_{\rm ee} > 0$ for any $a_{\rm ep}, a_{\rm ee} > 0$

$\Rightarrow$ System is stable iff $\mathrm{A} > 0$ and then it is stable for all $a_{\rm ep}, a_{\rm ee} > 0$

Assume system is stable and $a_{\rm ep} \gg a_{\rm ee} > 0$. Then, electrons equilibrate among themselves at instantaneous temperature $T_{\rm el}$ much faster than they equilibrate with phonons

$$f = f_0[T_{\rm el}(t)] = \frac{1}{e^{E/T_{\rm el}(t)} + 1}$$

Linear stability analysis

Kinetic equation for electron distribution function

$$(1-\Sigma')\dot{f} + f'\dot{\Sigma} = a_{\rm ep} I_{\rm ep} + a_{\rm ee} I_{\rm ee}$$

$$f = f_0[T_{\rm el}(t)] = \frac{1}{e^{E/T_{\rm el}(t)}+1}$$

Suppose $C_{\rm el} < 0$ and initially $T_{\rm el} > T_{\rm ph}$

Multiply both sides of the kinetic eq. by E and integrate over E

$$C_{\rm el}\dot{T}_{\rm el} = 4\nu_0 a_{\rm ep}\int_0^\infty d\omega \alpha^2 F(\omega)\omega^2 \left[N_0(T_{\rm ph}) - N_0(T_{\rm el})\right] \qquad \alpha^2 F(\omega) > 0$$

Phonon distribution function $N_0(T)$ is a monotonically increasing function of T

⇨ RHS < 0. If also $C_{\rm el} < 0$, heat flows from hot to cold, but $T_{\rm el}$ increases instead of decreasing and the system never equilibrates

⇨ Thermal equilibrium between electrons and phonons is unstable

EY, Altshuler, Patra, Phys. Rev. Lett. (2025)

Stability condition

$$\alpha^2 F(\omega) = \frac{1}{N}\sum_k \frac{\lambda_k \omega_k}{2}\delta(\omega - \omega_k)$$

$$\lambda = \frac{1}{N}\sum_k \lambda_k = \frac{1}{N}\sum_k \frac{g_k^2}{\omega_k^2}$$

Electronic specific heat: $$C_{\rm el} = \frac{2\pi^2 \nu_0 T}{3}\left[1 - \int_0^\infty g\left(\frac{\omega}{2\pi T}\right)\frac{2\alpha^2 F(\omega)}{\omega}d\omega\right]$$

$$g(x) = 6x + 12x^2 {\rm Im}\psi'(\imath x) + 6x^3 {\rm Re}\psi''(\imath x)$$

Stability condition: $$C_{\rm el} > 0 \iff \xi \equiv \max_T \left\{\int_0^\infty g\left(\frac{\omega}{2\pi T}\right)\frac{2\alpha^2 F(\omega)}{\omega}d\omega\right\} < 1$$

Stability parameter

Semenok, Altshuler & EY, Adv. Mater. (2025)

Compound	T_c, K	λ	ξ
Experimental Materials			
Ga (amorph.)[54]	8.6	2.25	0.16
Pb (amorph.)[54]	7.2	1.91	0.29
Bi (amorph.)[54]	6.1	1.84 – 2.46	0.19
Hg[54]	4.2	1.0 – 1.6	0.14
Nb[54]	9.2	0.82 – 1.05	0.2
Nb_3Sn[55]	17.9	1.6 – 1.8	0.27
MgB_2[56]	40	0.87	0.16
PbBi (amorph.)[57]	7.0	3.0	0.26
PbBi3 (amorph.)[57]	6.8	2.78	0.23
H_3S (157 GPa)[41]	190	1.84	0.32
LaH_{10} (214 GPa)[58, 59]	245	2.06	0.43
YH_6 (165 GPa)[60]	224	1.71	0.39
ThH_9 (150 GPa)[61]	146	1.73	0.32
ThH_{10} (170 GPa)[61, 62]	161	1.65	0.31
YH_9 (205 GPa)[39, 52]	235	2.66	0.36
$(La,Y)H_{10}$ (180 GPa)[63]	253	3.87	0.47
$(La,Ce)H_9$ (123 GPa)[43, 64]	190	2.27	0.33
DFT Calculations			
CaH_6 (172 GPa)[65]	215	2.69	0.58
LaH_{16} (250 GPa)[66]	141	1.89	0.31
ScH_{12} (200 GPa)[67]	325	2.85	0.47
Li_2MgH_{16} (250 GPa)[68]	473	3.30	0.49
MgH_6[65]	263	3.29	0.58
Hydrogen ($I41/amd$, 500 GPa)[69]	374	2.85	0.45

Stability condition:

$$C_{\rm el} > 0 \iff \xi < 1$$

Recall: for Einstein phonons this is equivalent to $\lambda \leq 3.69$

Since strong coupling limit is universal, expect the upper bound on λ for other phonon spectra to be close to 3.69

Semenok, Altshuler & EY, Adv. Mater. (2025)

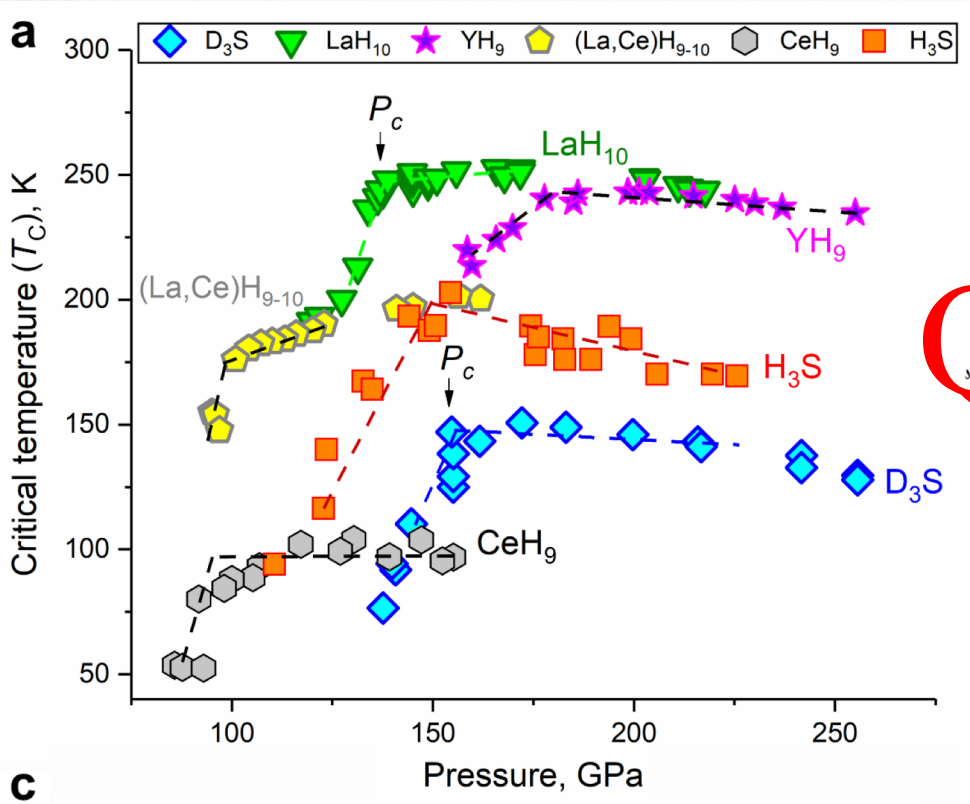
Table ___. Calculated ξ and λ values for various superconductors.

Compound	$\xi \equiv \max_T \left\{ \int_0^\infty g\left(\frac{\omega}{2\pi T}\right) \frac{2\alpha^2 F(\omega)}{\omega} d\omega \right\}$	λ
LaH_{16} (250 GPa)	0.31	1.89
$LaYH_{12}$ (180 GPa)	0.47	3.88
MgB_2	0.16	1.3
ScH_{12} (200 GPa)	0.47	2.85
ThH_{10} (100 GPa)	0.46	2.56
YH_9 (200 GPa)	0.36	2.76
H_3S (200 GPa)	0.32	1.52

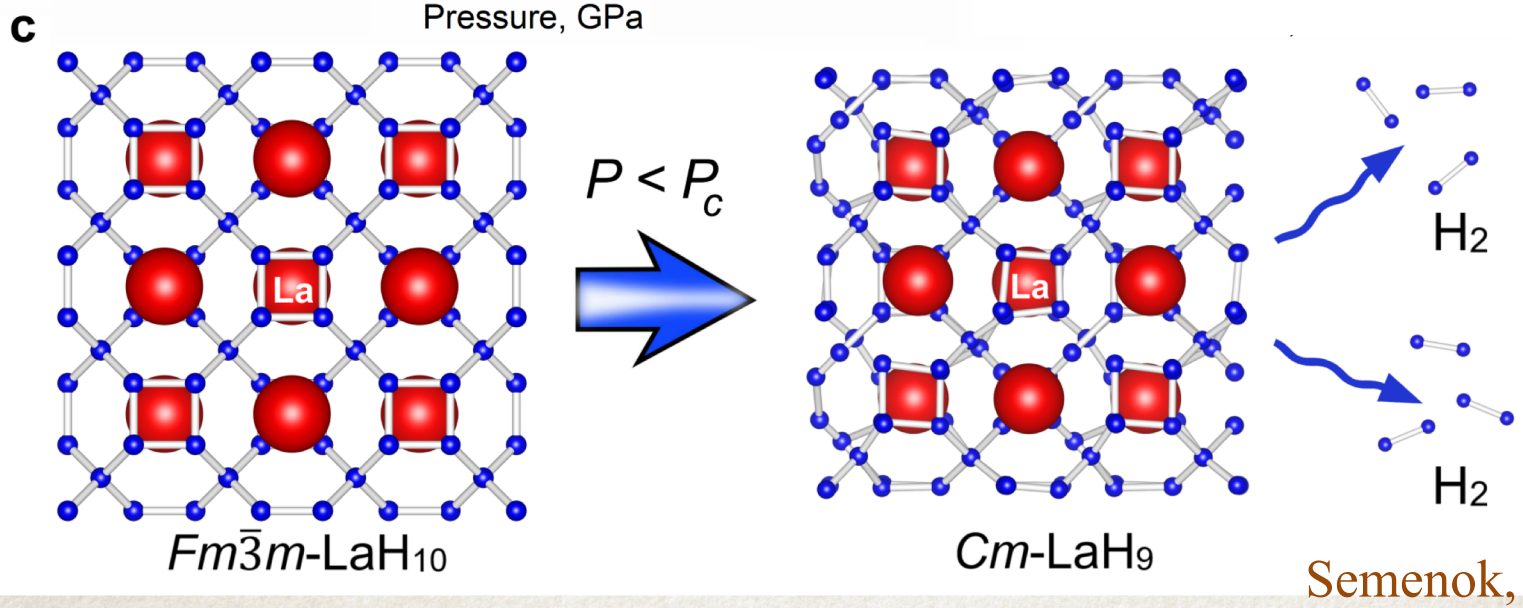
Stability condition: $C_{\rm el} > 0 \iff \xi < 1$

Recall: for Einstein phonons this is equivalent to $\lambda \leq 3.69$

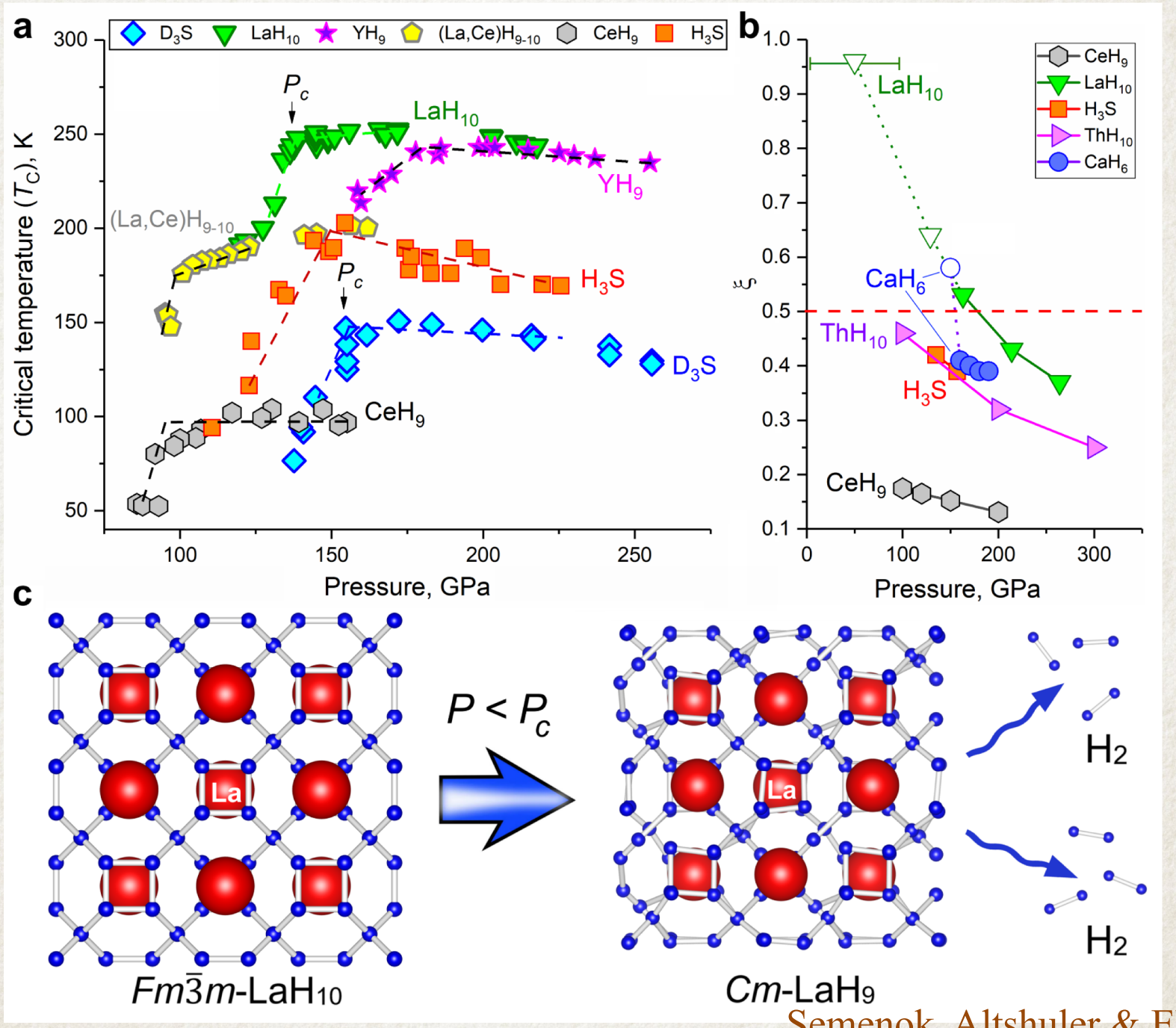
Semenok, Altshuler & EY, Adv. Mater. (2025)



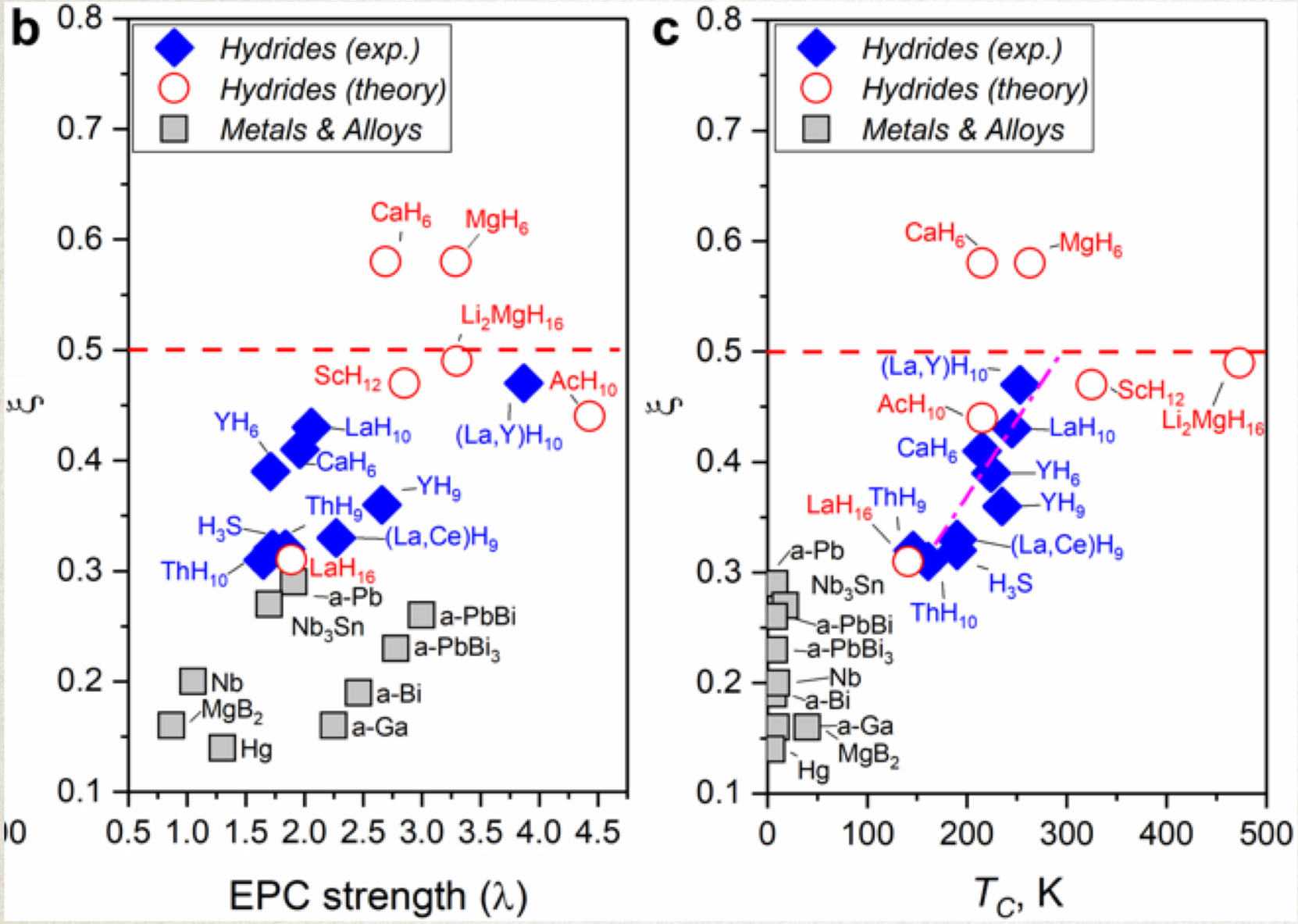
Q: What happens at P_c? Why do T_c and the electron-phonon coupling suddenly drop ?



Semenok, Altshuler & EY, Adv. Mater. (2025)



Semenok, Altshuler & EY, Adv. Mater. (2025)



$$\xi = 1$$

is the point of absolute instability of the original lattice

The lattice becomes metastable much earlier at a certain

$$\xi_c < 1$$

Empirically: $\xi_c = 0.5$

Semenok, Altshuler & EY, Adv. Mater. (2025)

Fundamental limit on superconducting T_c

Migdal-Eliashberg theory ⇨ $T_c < 0.18\sqrt{\lambda\langle\omega^2\rangle}$

Let $\omega_{\max}$ be the maximum phonon frequency. $\lambda\langle\omega^2\rangle$ is maximized by concentrating entire phonon weight at $\omega = \omega_{\max}$, i.e., for Einstein phonons with frequency $\Omega = \omega_{\max}$

Stability condition for Einstein phonons: $\lambda \leq 3.69$

⇩

$$T_c^{\max} = 0.31\,\omega_{\max}$$

Semenok, Altshuler & EY, Adv. Mater. (2025)

Kiessling, Altshuler, EY, J. Stat. Phys. (2025)

Fundamental limit on superconducting T_c

Observation: maximum phonon frequency $\leq$ *ionic* plasma frequency: $\omega_p \propto \frac{1}{\sqrt{A}}$

Interactions will only renormalize $\omega_{\max}$ down

Lebedev-Stepanov, J. Phys. Chem. Solids **75**, 903 (2014).

⇨ Assume $\omega_{\max}$ is highest in metallic hydrogen

Sharp maximum below 3000 K with quick drop from maximum to zero

Note: $\omega_{\max}$ increases somewhat when pressure is increased beyond 500 GPa, but λ decreases leading to an overall decrease in T_c

⇨ Safe to take $\omega_{\max} \leq 3000K$

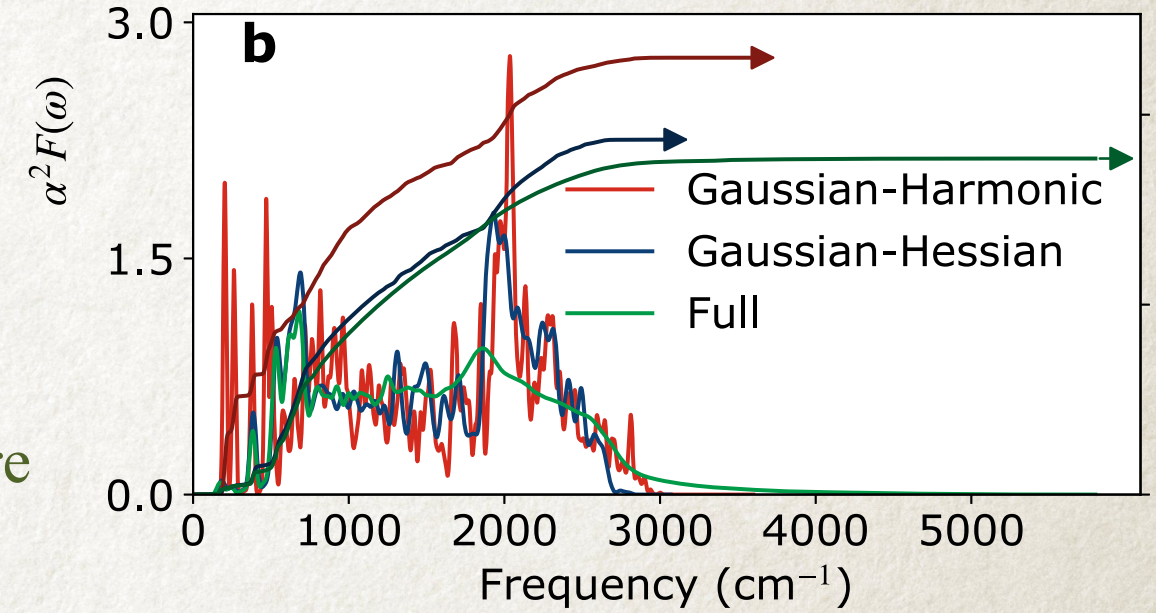


Fig. 3 | Eliashberg spectral function $\alpha^2F(\omega)$ for solid hydrogen in atomic tetragonal $I4_1/amd$ -2 phase at 500 GPa

Dangić. *et al., Commun Phys* **7**, 150 (2024).

Semenok, Altshuler & EY, Adv. Mater. (2025)

Fundamental limit on superconducting T_c

$$\omega_{\max} \leq 3000K \Rightarrow T_c^{\text{stable}} < \frac{600\,\text{K}}{\sqrt{A}}, \quad T_c^{\text{metastable}} < \frac{950\,\text{K}}{\sqrt{A}}$$

Using $\xi_c \leq 0.5$

Using $\xi \leq 1$

Atomic mass

Conclusion: Stable room-temperature superconductivity can only be achieved in hydrogen and deuterium compounds. At the same time, there are no fundamental reasons why T_c cannot exceed room temperature in hydrides, at least at sufficiently high pressure.

Semenok, Altshuler & EY, Adv. Mater. (2025)