Excitonic versus electron-hole liquid phases in $TmSe_{0.45}Te_{0.55}$: A theorists' point of view $^{(*)}$

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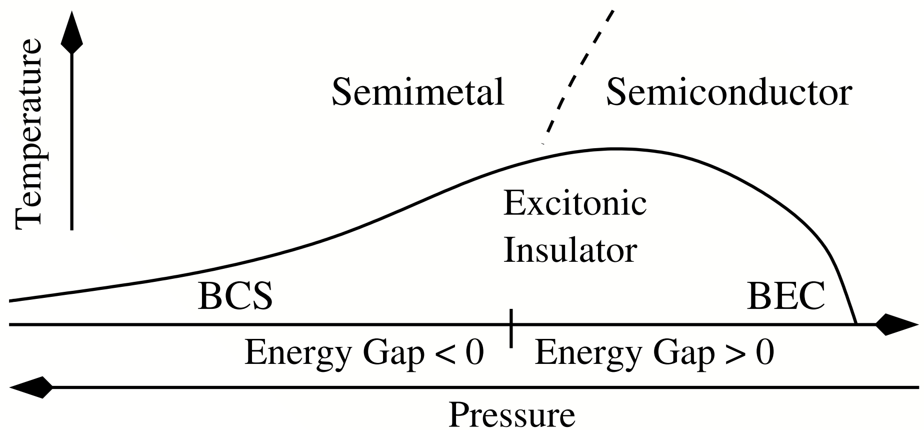
Outline

- pressure-induced SC/SM transition in $\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}$ (experiment)

  $\rho(p,T)$, $\lambda(p,T) \Rightarrow$ X phases, excitonic insulator ($\equiv$ X condensation)?

- theoretical analysis & sorting out $^{(*)}$

  generic model $\Rightarrow T_c(E_g), T_M(E_g)$, halo, EI vs. EHL



- conclusions & outlook

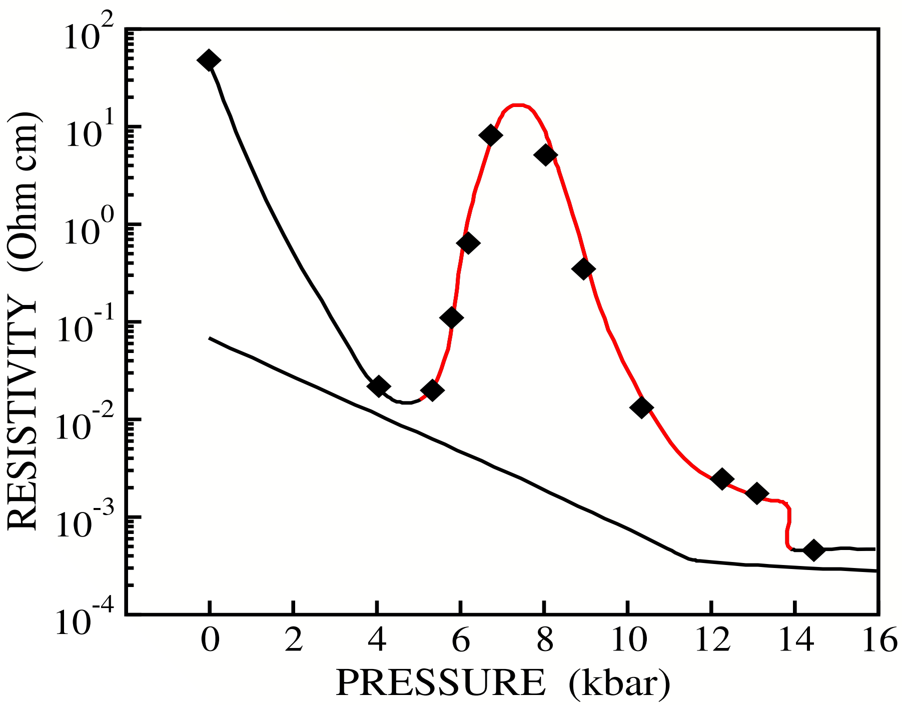
  EI in $\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}$ plausible (!) but further studies (exp. & theory) required

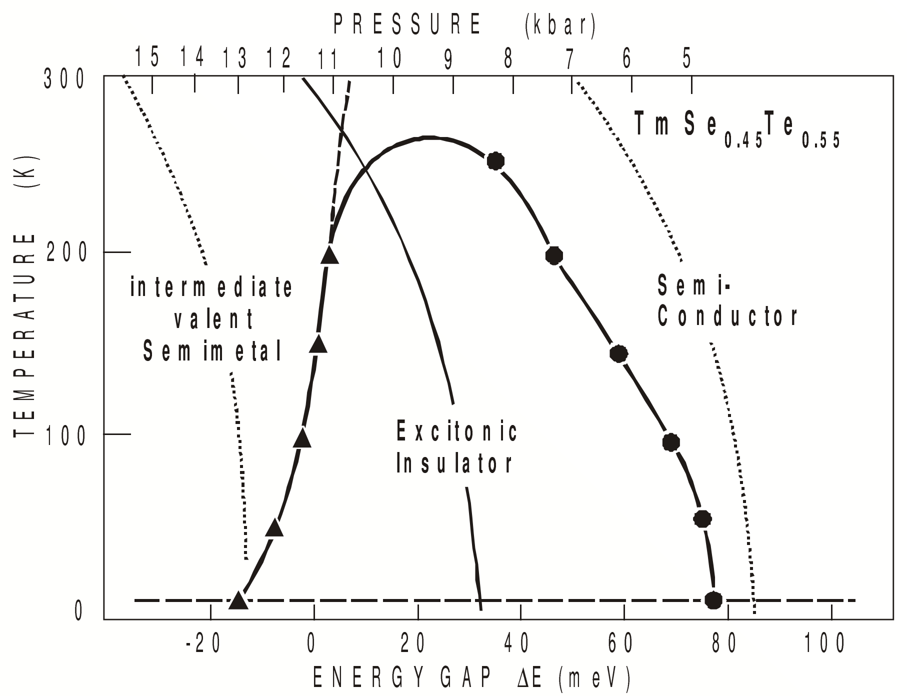
$^{(*)}$ Franz X. Bronold and Holger Fehske, PRB accepted, cond-mat/0605415

Experiment (1)

pressure-dependent electrical resistivity of $\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}$

(J. Neuenschwander et al. PRB 1990, B. Bucher et al. PRL 1991)





$\exists$ further experimental studies:

Hall resistivity and mobility

thermal transport

however

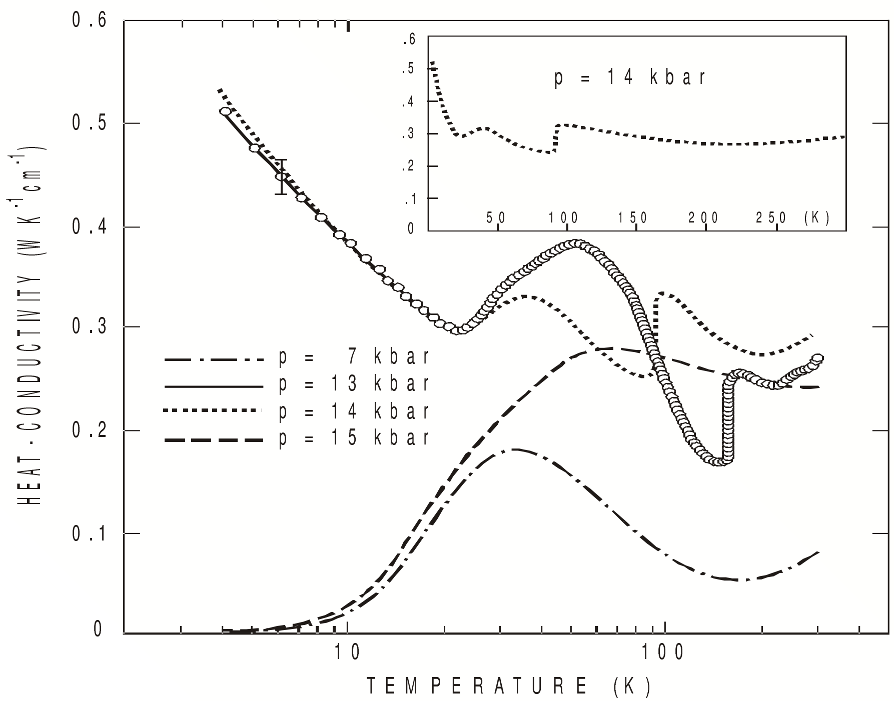
no optics, for instance,

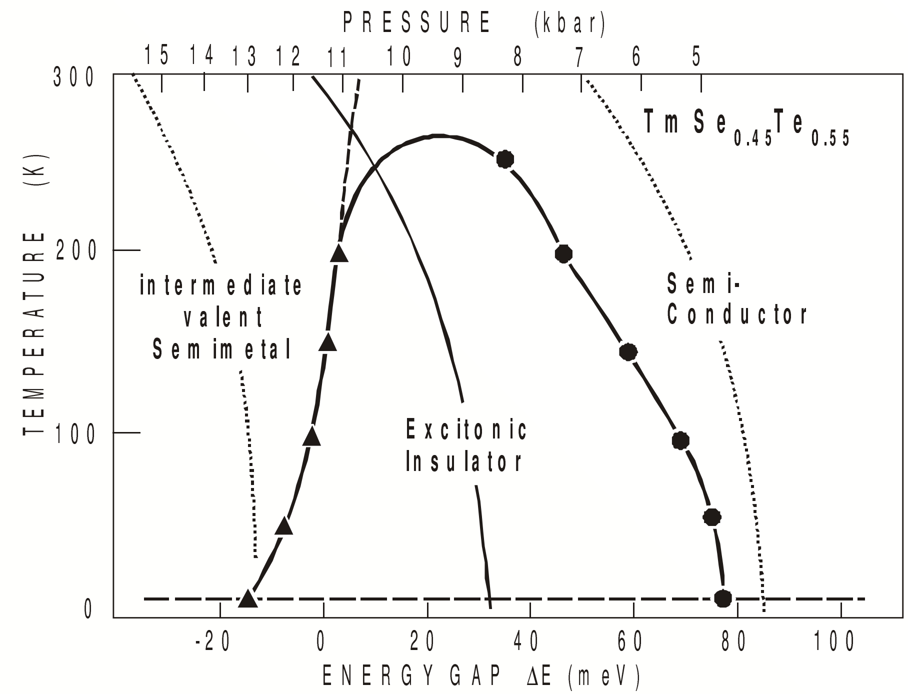
$\varepsilon(\omega)$ & THz-spectroscopy

Experiment (2)

temperature-dependent heat conductivity of $\mathrm{TmSe_{0.45}Te_{0.55}}$

(P. Wachter et al., PRB 2004)





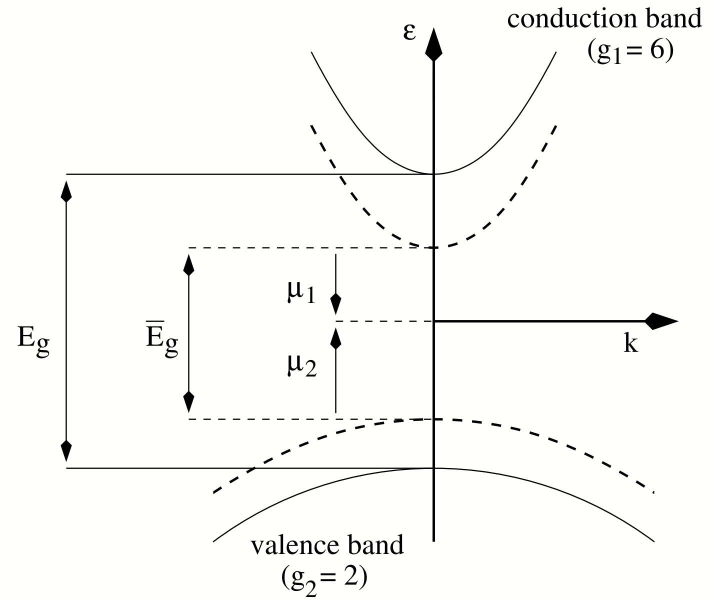
experimentalists' point of view:

1. ∃ X phases in vicinity of SC/SM transition
2. @ low enough T ∃ Bose condensate of X

Theory (1)

Model: indirect semiconductor with $m_1 \ll m_2$ & $E_g(p)$

$$
\begin{aligned}
H &= \sum_{\mathbf{k},i} e_i(\mathbf{k}) c^\dagger_{i,\mathbf{k}} c_{i,\mathbf{k}} \\
&+ \frac{1}{2} \sum_{\mathbf{q}} V_s(\mathbf{q}) \rho(\mathbf{q}) \rho(-\mathbf{q}) \\
e_1(\mathbf{k}) &= E_g + \varepsilon_1(\mathbf{k}) \\
e_2(\mathbf{k}) &= -\varepsilon_2(\mathbf{k}) - \Sigma_0(\mathbf{k}) \\
\varepsilon_i(\mathbf{k}) &= \mathbf{k}^2/2m_i \\
V_s(\mathbf{q}) &= \frac{4\pi e^2}{\varepsilon_0} \frac{1}{q^2 + q_s^2}
\end{aligned}
$$

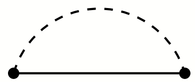


effective model for relevant electrons:

- $\mathbf{k}$ measured from band extrema
- isotropic bands
- static screening!

Theory (2)

excitonic insulator @ $T < T_c$: Nambu formalism for $G_{ij}(\mathbf{k}, i\omega_n)$

MFA, i.e. $\Sigma^X =$  & linearization with respect to $\Delta(\mathbf{k}) = \Sigma^X_{12}(\mathbf{k}) \Rightarrow T_c(E_g)$

$$\Delta(\mathbf{k}) = \int \frac{d\mathbf{k}'}{(2\pi)^3} V_s(\mathbf{k}-\mathbf{k}') \frac{1 - n_\mathrm{F}(\epsilon_2(\mathbf{k}') - \mu_2) - n_\mathrm{F}(\epsilon_1(\mathbf{k}') - \mu_1)}{\epsilon_1(\mathbf{k}') + \epsilon_2(\mathbf{k}') + \bar{E}_g} \Delta(\mathbf{k}')$$

$$q_s^2 = \frac{4\pi e^2}{\epsilon_0} \left(\frac{\partial}{\partial \mu_1} n_1 + \frac{\partial}{\partial \mu_2} \bar{n}_2 \right)$$

$$-\bar{E}_g = \mu_1 + \mu_2 = -E_g + \sum_i \int \frac{d\mathbf{k}}{(2\pi)^3} V_s(\mathbf{k}) n_\mathrm{F}(\varepsilon_i(\mathbf{k}) - \mu_i)$$

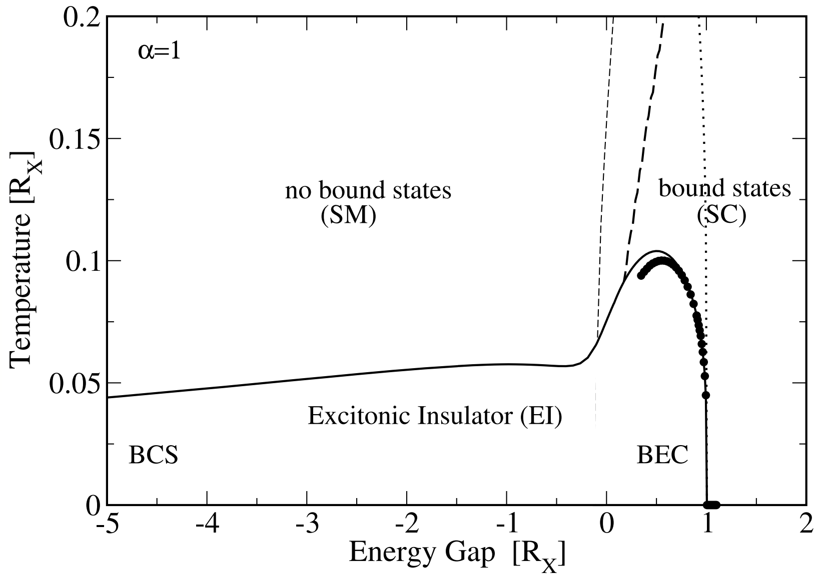
$$n_1 = \int \frac{d\mathbf{k}}{(2\pi)^3} n_\mathrm{F}(\varepsilon_1(\mathbf{k}) - \mu_1) \quad \bar{n}_2 = \int \frac{d\mathbf{k}}{(2\pi)^3} n_\mathrm{F}(\varepsilon_2(\mathbf{k}) - \mu_2)$$

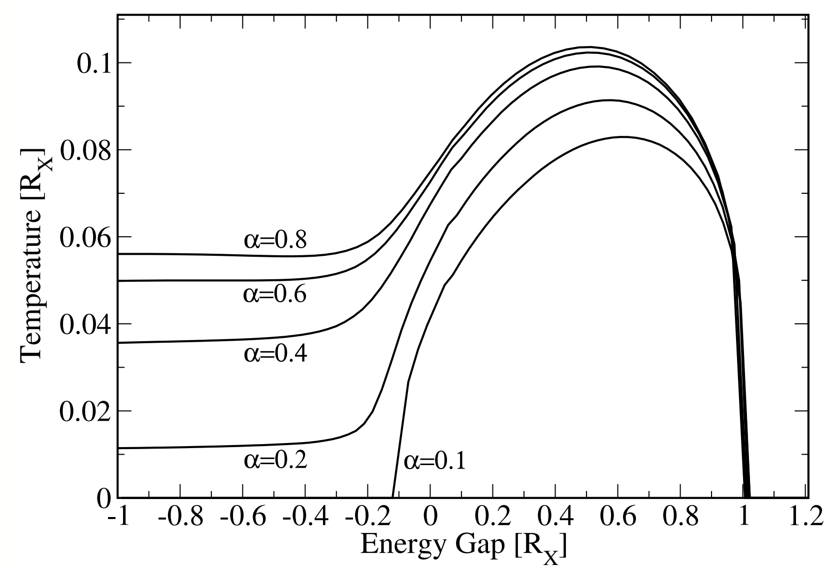
charge neutrality $\Rightarrow n_1 = \bar{n}_2$

Results (1)

no spin, single-valley band structure $\Rightarrow g_1 = g_2 = 1$

$T_c(E_g)$ as a function of $\alpha = m_1/m_2$





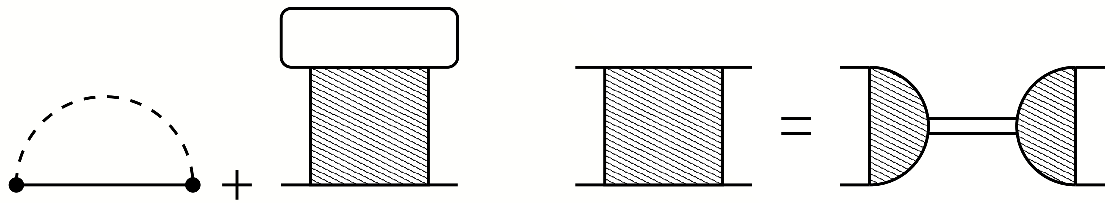
- steeple-like shape $\Rightarrow$ BEC vs. BCS
- BCS asymptotic @ $E_g < 0, |E_g| \gg 1$
- SC/SM (Mott) transition

- $\alpha \ll 1 \Rightarrow \mu_1 \neq \mu_2$ @ T>0
  - $\Rightarrow$ BCS suppressed
  - $\Rightarrow$ EI on SC side

Theory (3)

excitonic insulator @ $T > T_c$: ladder approximation, separable T-matrix

$\Sigma^X + \Sigma^L =$



$$\Lambda_{12}(\mathbf{k},\mathbf{k}';\mathbf{q},i\Omega_n) \;=\; g(|\mathbf{k}-\frac{m_1}{M}\mathbf{q}|)\cdot D_X(\mathbf{q},i\Omega_n-\bar{E}_g-\frac{q^2}{2M})\cdot g(|\mathbf{k}'-\frac{m_1}{M}\mathbf{q}|)$$

$$D_X^{-1}(0,-\bar{E}_g) \;=\; 0 \Leftrightarrow \bar{B}=\bar{E}_g=-\mu_1-\mu_2 \Rightarrow T_c(E_g)$$

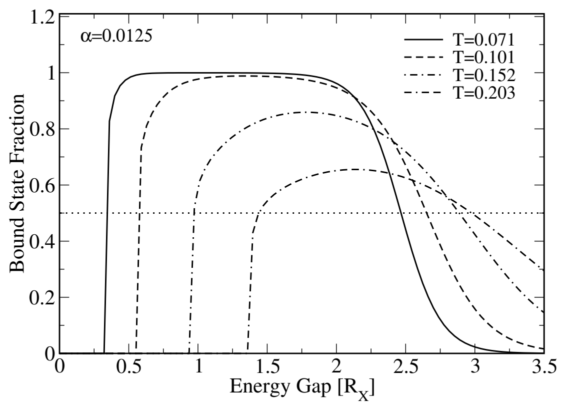
$$\bar{B} \;=\; 0 \Rightarrow T_M(E_g)$$ SC/SM (Mott) transition

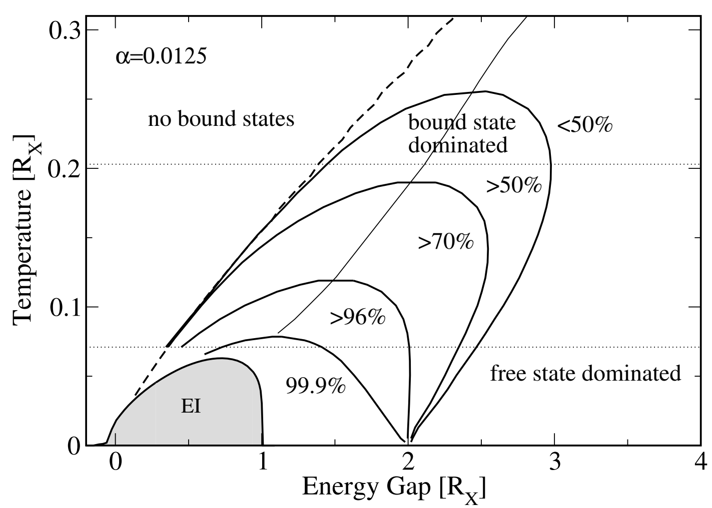
$$\bar{n}_2 = n_1 \;=\; \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{d\omega}{2\pi}A_{11}^{X+L}(\mathbf{k},\omega)n_{\mathrm{F}}(\omega) = n_1^f + n_1^b \Rightarrow \gamma = \frac{n_1^b}{n_1^f+n_1^b}$$

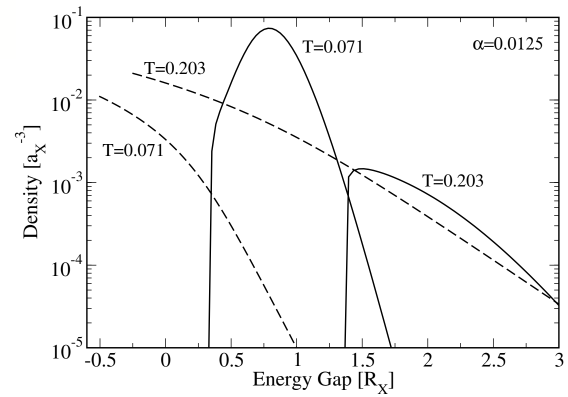
bound state fraction ($e + h \rightleftharpoons X$)

Results (2)

chemical equilibrium $e + h \rightleftharpoons X$ for $T > T_c(E_g)$







above $T_c(E_g)$ $\exists$ (E_g, T)-range where Xs prevail over unbound electrons and holes (halo) & give rise to additional scattering channel (e-X, h-X) $\Rightarrow$ resistivity anomaly

Confrontation with experiment (1)

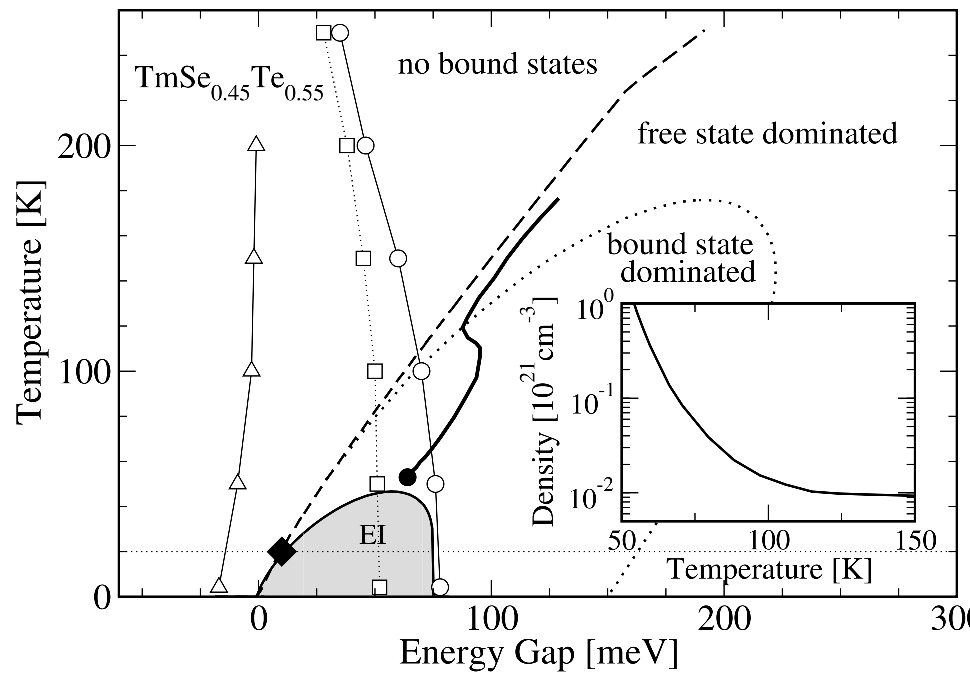
$\underline{\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}}$

$\alpha = 0.015$

$E_g = 135$ meV, $R_X = 75$ meV

fcc $\Rightarrow$ Γ-X gap

$g_1 = 6, g_2 = 2$ (spin, multi-valley CB)



theorists' point of view:

1. ρ-anomaly due to $e/h - X$ scattering in halo
2. λ-anomaly could be 2^{nd} sound of Bose-condensed Xs

however problems with E_g's $\rightarrow$ applicability of Wannier-type model?

$\rightarrow$ experimental determination of E_g?

Theory (4)

multi-valley CB $\Rightarrow$ electron-hole liquid phases?

need: thermodynamics of EHL

$\mu_{eh}(n,T) = -E_g(n,T)$ with $n = n_1 = \bar{n}_2$

however static screening partly suppresses correlation energy $\Rightarrow$ X phases favoured

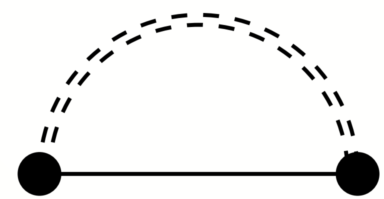
thus: quasi-static screening, i.e. $\Sigma^X + \Sigma^C \rightarrow \Sigma^{SX}|_{no\ recoil} + \Sigma^{CH}_{no\ recoil}$

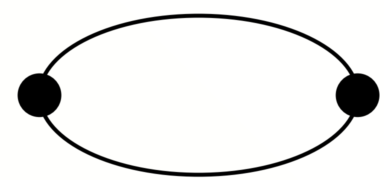
$$\Sigma^{SX}_{ii}(\mathbf{k}) = -\int \frac{d\mathbf{k}'}{(2\pi)^3} V_{qs}(\mathbf{k}-\mathbf{k}') n_{\mathrm{F}}(\epsilon_i(\mathbf{k}') - \mu_i)$$

$$\Sigma^{CH}_{ii}(\mathbf{k}) = \frac{1}{2}\int \frac{d\mathbf{k}'}{(2\pi)^3} \left[V_{qs}(\mathbf{k}') - V_0(\mathbf{k}')\right]$$

$$V_{qs}(\mathbf{q}) = V_0(\mathbf{q})\left[1 + \frac{\omega_{pl}^2}{(\omega+i\eta)^2 - \omega(\mathbf{q})^2}\right]$$

$$\omega(\mathbf{q})^2 = \omega_{pl}^2\left[1 + \left(\frac{q}{q_s}\right)^2\right] + \frac{Cq^4}{16m^2}$$

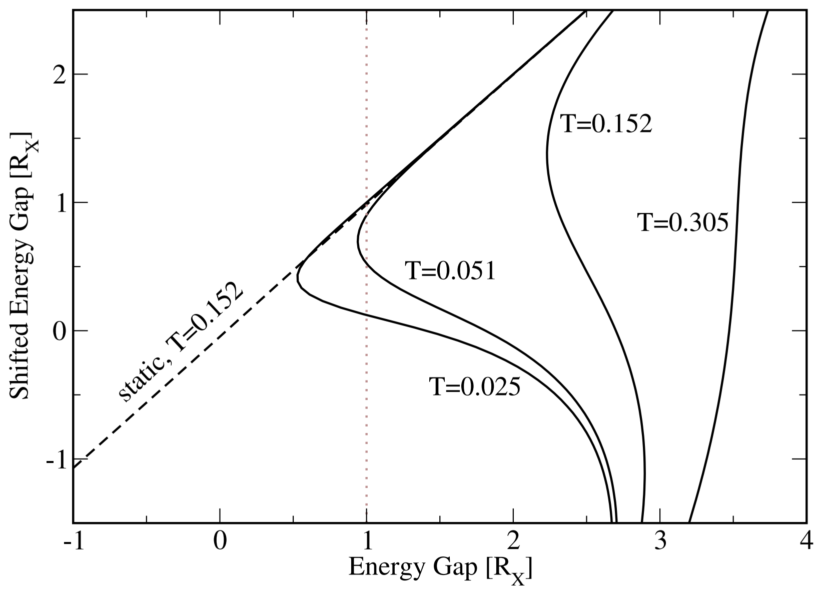


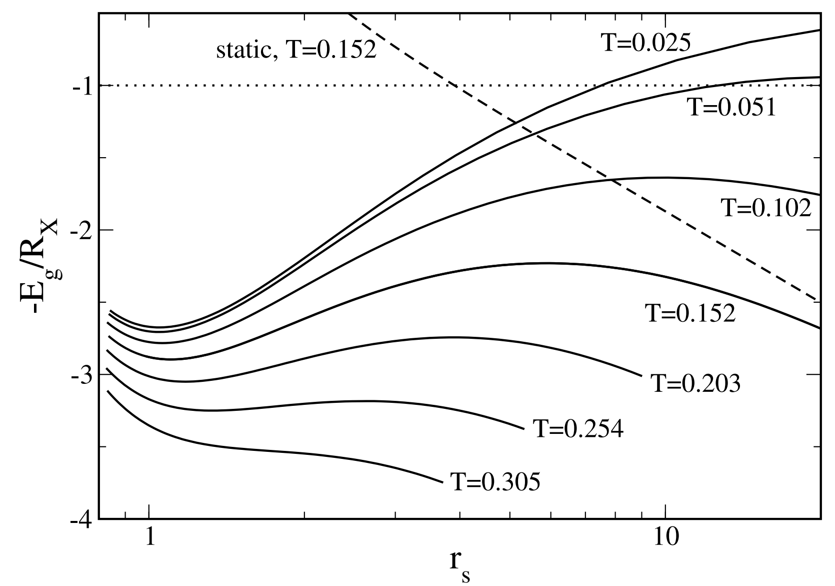


note: only intraband selfenergies $\&$ X ignored

Results (3)

$\underline{\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}}$ parameters: $g_1 = 6, g_2 = 2, \alpha = 0.015$



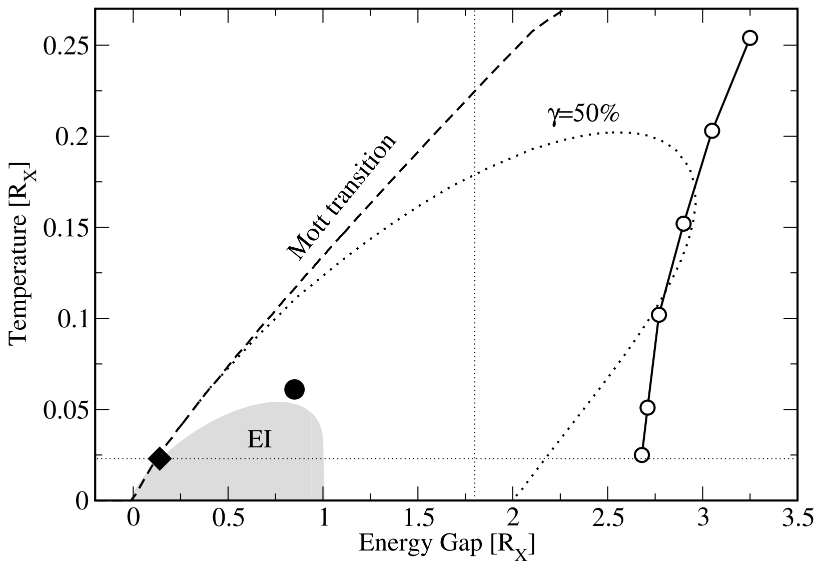


$R_X > \min[\mu_{eh}(r_s, T)] = \min[-E_g(r_s, T)] \Rightarrow$ X phases unstable against EHL

note, however, $\mu_{eh} = -E_g$ calculated without X

improved theory has to take X into account, that is, ladder corrections to RPA

Confrontation with experiment (2)



multi-valley CB & QS screening ⇒

no X phases ∼ SC/SM transition (which would be @ the solid line)

however metallic EHL in conflict with resistivity data

ρ-anomaly cannot be explained by EHL

thus, X phases must be stabilised by

- multi-valley scattering
- electron-phonon coupling (narrow VB band)
- ?

Conclusion & Outlook

X condensation (EI) in $\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}$ plausible

- $\alpha \ll 1 \Rightarrow$ EI on SC side of SC/SM transition (favourable for condensation)
- ρ-anomaly because of EI's halo
- ρ- and λ-anomaly in expected temperature range

but further experimental & theoretical studies necessary to clarify

- EHL vs. EI (multi-valley CB)
- electron-lattice coupling, density waves
- mixed-valence $f^n \rightleftharpoons f^{n-1} + e^-$
- $(p, T) \leftrightarrow (E_g, T)$ mapping

in particular, optical response should be investigated in great detail

note: so far, X condensation not seen in optically pumped SC (problem: Xs not in TD equilibrium)

pressure-sensitive mixed-valence materials, such as $\mathrm{TmSe}_{0.45}\mathrm{Te}_{0.55}$, offer a promising alternative (advantage: Xs in TD equilibrium)