Phase diagram of the excitonic insulator

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Abstract

Motivated by recent experiments, which give strong evidence for an excitonic insulating phase in TmSe$_{0.45}$Te$_{0.55}$, we developed a scheme to quantitatively construct, for generic two-band models, the phase diagram of an excitonic insulator. As a first application of our approach, we calculated the phase diagram for an effective mass two-band model with long-range Coulomb interaction. The shielded potential approximation is used to derive a generalized gap equation controlling for positive (negative) energy gaps the transition from a semi-conducting (semi-metallic) phase to an insulating phase. Numerical results, obtained within the quasi-static approximation, show a steeple-like phase diagram in contrast to long-standing expectations.

Key words: excitonic insulator, phase transition
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The possibility of an excitonic insulator (EI) phase, separating, below a critical temperature, a semiconducting from a semi-metallic phase, has been predicted by theorists more than three decades ago [1]. However, experimental efforts to establish this phase in actual materials largely failed. It is only until recently, that detailed experimental investigations of TmSe$_{0.45}$Te$_{0.55}$ suggested the existence of an EI phase in this compound [2,3]. The pressure dependence of the electrical resistivity below 270K, for instance, strongly points towards an emerging EI phase [2]. Further evidence for collective behavior which may have its origin in an EI phase comes from the linear increase of the thermal conductance and diffusivity at very low temperatures [3].

Under the assumption that the external pressure controls the energy gap $E_g$, the resistivity data have been used to construct a phase diagram for TmSe$_{0.45}$Te$_{0.55}$ in the $E_g$-T plane [2]. Although experimental data strongly suggest that this phase diagram is the phase diagram of an EI, to unambiguously decide if this interpretation is correct requires further theoretical examination, taking the relevant parts of the electronic structure of the material into account. However, even for the simplest two-band models, a quantitative phase diagram for an EI has never been calculated. As a first step towards a theoretical scrutiny of the phases of the Tm[Se,Te] system it is therefore appropriate to present here such a calculation.

In close analogy to the strong-coupling theory of superconductivity, we employed a matrix propagator formalism. Within a two-band model, the anomalous or off-diagonal (in the band indices $i = 1, 2$) self-energy $\Sigma_{12}(k, i\omega_n)$ describing the pairing between conduction and valence band electrons serves as an order parameter: $\Sigma_{12}(k, i\omega_n) \neq 0$ signals the existence of the EI phase. Our selfconsistent approximation enables us to take a variety of physical processes into account and results in a nonlinear functional equation for $\Sigma_{12}(k, i\omega_n)$. Linearizing this equation in the vicinity of the phase boundary, where $\Sigma_{12}(k, i\omega_n)$ is small, yields a generalized “gap equation”. The phase boundary $T_c(E_g)$ can...
then be found by mapping out the T-E_g range for which
the “gap equation” has nontrivial solutions.

We applied this scheme to an isotropic, effective mass
two-band model for valence and conduction band elec-
trons interacting via the long-range Coulomb potential
V_0(q) = 4\pi e^2/q_0 q^2. The energy gap E_g is indirect (Γ-
X) and can be positive or negative. Within the screened
potential approximation the generalized gap equation
for the real part of the interband self-energy reads
\[ \Delta(k, \tilde{\epsilon}_i) = \int \frac{dk'}{(2\pi)^3} \left[ V(k - k', \tilde{\epsilon}_i, \tilde{\epsilon}_i') B_2(\tilde{\epsilon}_i', \tilde{\epsilon}_i) \Delta(k', \tilde{\epsilon}_i') 
+ V(k - k', \tilde{\epsilon}_i, \tilde{\epsilon}_2) B_1(\tilde{\epsilon}_1', \tilde{\epsilon}_2') \Delta(k', \tilde{\epsilon}_2') \right], \tag{1} \]
where \( \tilde{\epsilon}_i(k) = e_i(k) - \mu_i \), \( B_i(x, y) = (x - y)/(x - y)^2 + \gamma_i |k|^2 \), and \( V(k - k', \tilde{\epsilon}_i, \tilde{\epsilon}_i') = Re V'_r(k - k', \tilde{\epsilon}_i - \tilde{\epsilon}_i') \).

The full analysis of Eq. (1) is the subject of a forth-
coming publication [4]. Here, we focus on the quasi-
static approximation, \( V'_r(k - k', \tilde{\epsilon}_i - \tilde{\epsilon}_i') \sim V'_r(0) \),
which simplifies the gap equation enormously. Ex-
cept for very small band overlaps (very small Fermi
surfaces), we expect this approximation to work rea-
sonably well, as it does for interband self-energies.

For equal band masses and temperature independent
screening, the quasi-static approximation reduces Eq.
(1) to \[ \Delta(u) = \int_0^{\infty} du' V(u, u') \frac{\tanh u'}{u'} \Delta(u') \tag{2} \]
\[ V(u, u') = \frac{1}{4\pi^2 k_B T} \log \left[ \frac{\sqrt{k + k'} - u'}{\sqrt{k - k'} + u'} \right] \tag{3} \]
with \( k = \sqrt{u - u_1}, k' = \sqrt{u' - u_1}, u_1 = E_g/4k_B T \), and
\( \kappa^2 = (2\sqrt{E_g}/\pi k_B T) \theta(-E_g) \).

To construct the phase boundary \( T_c(E_g) \), we discretize Eq. (2) and determine,
for fixed \( E_g \), the temperature \( T = T_c \) for which
the determinant of the coefficient matrix of the resulting
system of linear equations vanishes. For \( E_g > 0 \) this
approach can be directly applied, whereas for \( E_g < 0 \),
the logarithmic singularity of the kernel has to be
removed first [4].

The phase boundary \( T_c(E_g) \) is presented in Fig. 1,
measuring energy and temperatures in units of the
exciton Rydberg \( R_0 \). Above \( T_1 \approx 0.45 \), the EI phase is
unstable. Below \( T_1 \), we find a steeple-like phase bound-
ary which strongly discriminates between \( E_g > 0 \) and

\[ E_g < 0. \text{ For } E_g > 0, T_c(E_g) \text{ smoothly decreases to zero at } E_g = 1, \text{ the critical band gap, above which the}
\text{ EI phase cannot exist. For } E_g < 0, \text{ in contrast, } T_c(E_g) \text{ initially drops extremely fast, within a few percent of}
\text{ } R_0, \text{ to a second critical temperature } T_2 \approx 0.04. \text{ Below } T_2 \text{ the EI phase is stable with an almost constant}
\text{ } T_c \text{, which, however, for larger band overlaps slowly decreases (see inset). The steeple-like shape of the phase diagram reflects the different phases from which the EI is approached: semi-conducting for } E_g > 0 \text{ and semi-metallic for } E_g < 0. \text{ Entering the EI phase from the semi-conductor side leads to formation of strongly bound excitons. On the other hand, when the EI phase is approached from the semi-metal, exciton formation is strongly suppressed due to the free carrier’s screening of the Coulomb potential. In that case, loosely bound Cooper-type pairs emerge, resulting in a rather fragile EI phase. The crossover from excitons to Cooper-type pairs occurs at } E_g \approx -0.3, \text{ the band overlap, where the screening}
\text{ length becomes roughly equal to the exciton radius. For } |E_g| \ll 4k_B T, \text{ the critical temperature is exponen-
tially small and approximately given by } k_B T_c \approx \gamma |E_g|/\pi \exp (-\pi |E_g|/\sqrt{E_g}/2), \text{ with } \gamma = \exp (0.577) \text{ (dashed line in the inset). Anisotropies in the band structure and other pair breaking effects would easily destroy this part of the phase diagram.}

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Phase diagram for an excitonic insulator with equal band masses.}
\end{figure}

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