Optical conductivity calculation of a k.p model semiconductor gaas incorporating first order electron hole vertex correction = Perhitungan konduktifitas optis model k.p semikonduktor gaas dengan koreksi vertex orde pertama elektron-hole

Maryam Nurhuda, author

Abstrak

ABSTRACT
The role of excitons in semiconducting materials carries potential applications. Excitonic signals usually do not appear clearly in optical absorption spectra of semiconductor systems with narrow gap, such as Gallium Arsenide, which makes experimental analyses on excitons in such systems become very challenging. On the iii iv theoretical side, calculation of optical spectra based purely on Density Functional Theory DFT without taking electron hole interactions into account does not lead to the appearance of any excitonic signal. Meanwhile, existing DFT based algorithms that include a full vertex correction through Bethe Salpeter equation may reveal an excitonic signal, but the algorithm has not provided a way to analyze the excitonic signal further. Motivated to provide a way to isolate the excitonic effect in the optical response theoretically, we develop a method of calculation for the optical conductivity of a narrow band gap semiconductor GaAs within the k.p 8 band model, that includes electron hole interactions through first order electron hole vertex correction. The k.p model is chosen because it provides a description of 8 energy bands 2 conduction and 6 valence bands in which the role of spin orbit coupling is also taken into account. We expect that this first order vertex correction reveals how the optical spectral weight redistributes as a function of temperature.
<hr>
ABSTRAK
Peran eksiton pada material semikonduktor membawa banyak potensi aplikasi. Sinyal eksiton tidak terlalu jelas kemunculannya pada spektrum absorbsi optis semikonduktor bercelah sempit, seperti Gallium Arsenite, sehingga analisis keberadaan eksiton secara eksperimen menjadi cukup menantang. Dari segi teori, perhitungan dengan metode Density Functional Theory DFT yang tidak melibatkan interaksi electron-hole belum dapat menunjukan keberadaan eksiton. Sedangkan untuk perhitungan DFT yang mengikutsertakan koreksi vertex secara lengkap dengan metode Bethe-Salpeter equation BSE dapat memunculkan sinyal eksiton, namun algoritma yang ada belum dapat memberi cara untuk menganalisis eksiton lebih jauh. Dengan motifasi tersebut, kami mengembangkan metode perhitungan konduktifitas optis semikonduktor bercelah sempit material Gallium Arsenite dengan menerapkan model k.p 8 pita, dengan mengikutsertakan interaksi electronhole melalui koreksi verteks orde pertama. Metode k.p di pilih karena metode ini dapat menjelaskan 8 pita 2 pita konduksi dan 6 pita valensi dan turut melibatkan faktor spin orbit coupling.