## Study of band structure renormalization of tight-binding model semiconductor by incorporating GW self-energy

A. R. Hayyu, A. Azhar, and M. A. Majidi

Citation: AIP Conference Proceedings **2023**, 020053 (2018); doi: 10.1063/1.5064050 View online: https://doi.org/10.1063/1.5064050 View Table of Contents: http://aip.scitation.org/toc/apc/2023/1 Published by the American Institute of Physics

#### Articles you may be interested in

Density functional theory (DFT) - based GW+BSE calculations to investigate the influence of substitution of Ga with Al on the band gap and the optical spectra of  $Al_XGa_{1-X}N$  (x = 0, 0.125, 0.25, 1) AIP Conference Proceedings **2023**, 020038 (2018); 10.1063/1.5064035

Study on the formation of DNA adduct 8-hydroxy-2'-deoxyguanosine (8-OHdG) in vitro with bisphenol a through Fenton reaction AIP Conference Proceedings **2023**, 020056 (2018); 10.1063/1.5064053

CoFe<sub>2</sub>O<sub>4</sub> magnetic catalyst assisted a facile one-pot multicomponent construction of 2,4,5-trisubstituted-1Himidazole derivatives AIP Conference Proceedings **2023**, 020057 (2018); 10.1063/1.5064054

Isobar model for  $K^+\Sigma^0$  photoproduction AIP Conference Proceedings **2023**, 020002 (2018); 10.1063/1.5063999

Neutron star stability within Eddington-inspired Born Infeld gravity AIP Conference Proceedings **2023**, 020001 (2018); 10.1063/1.5063998

I-V characteristics of a four-chain DNA model in environment disorder AIP Conference Proceedings **2023**, 020045 (2018); 10.1063/1.5064042

# **AP** Conference Proceedings

Enter Promotion Code PDF30 at checkout

Get 30% off all print proceedings!

### Study of Band Structure Renormalization of Tight-Binding Model Semiconductor by Incorporating *GW* Self-Energy

#### A. R. Hayyu, A. Azhar, and M. A. Majidi<sup>a)</sup>

Department of Physics, Faculty of Mathematics and Natural Sciences (FMIPA), Universitas Indonesia, Depok 16424, Indonesia

a)Corresponding author: aziz.majidi@sci.ui.ac.id

Abstract. In semiconductors containing transition metal elements having d orbitals in their valence and/or conduction band(s), which we consider as strongly correlated semiconductors, electron-electron (*e-e*) interactions may play a more significant role. We hypothesize that such kind of semiconductors would have band structures, including their band gaps, being rather sensitive to temperature change due to *e-e* interactions. We construct the model Hamiltonian through tight-binding approximation incorporating *e-e* interactions in the self energy. We solve the model within *GW* method. The *GW* self-consistent calculation is performed numerically in the Matsubara frequency domain. Then, we do analytic continuation using Padé approximant to obtain the retarded Green function defined in the real frequency domain. Using this retarded Green function, in principle, we can calculate and analyze the density of states (DOS) at various temperatures for short-range as well as long-ranged repulsive Coulomb interactions. However, in this paper we only present our calculation results for short-range interactions. Our results show that the correlation effects become stronger as temperature is decreased, which reflect in the fact that the band gap increases and chemical potential shifts to a higher energy due to the presence of *e-e* repulsive interactions.

**Keywords:** strongly-correlated systems, band-structure renormalization, semiconductors, electron-electron interactions, *GW* method

#### INTRODUCTION

Almost in all first-principles or modeling calculations of semiconductors that do not take into account e-e interactions the resulting band gap is too much underestimated as compared to experimental data. Most conventional semiconductors, such as Ge, Si, or GaAs, may be classified into non-correlated systems or weakly correlated systems in which e-e interactions do not play any significant role. For such semiconductors, their band gaps may be insensitive to temperature change. Meanwhile, in semiconductors containing transition metal elements having d orbitals in their valence and/or conduction band(s), which we consider as strongly-correlated semiconductors, the e-e interactions may play a more significant role. To remedy this problem, e-e interactions need to be incorporated.

There are various approximate techniques to incorporate  $e \cdot e$  interactions in the calculations, such as mean-field approximations, perturbative approach, etc. GW method is among the well-known techniques for this purpose. However, its implementation has been mostly applied to the Density Functional Theory (DFT) based framework, which to some extent, not flexible to modify. In a previous study, we started the development of tight-binding based GW technique applied to graphene [1]. While our method applied to graphene still needs further improvement, here we would like to extend this development to apply to semiconductors, by developing GW method that is suitable for tight-binding based semiconductor Hamiltonian. We hypothesize that semiconductor properties including the band gap would be rather sensitive to temperature because of the  $e \cdot e$  interactions. Our results qualitatively confirm that  $e \cdot e$  interactions tend to increase the semiconductor band gap, and the correlation effects become stronger as we decrease temperature.

Proceedings of the 3rd International Symposium on Current Progress in Mathematics and Sciences 2017 (ISCPMS2017) AIP Conf. Proc. 2023, 020053-1–020053-6; https://doi.org/10.1063/1.5064050 Published by AIP Publishing, 978-0-7354-1741-0/\$30.00

#### 020053-1

#### **MODEL HAMILTONIAN**

To simplify our calculations while still expecting some meaningful qualitative results, we model the hypothetical semiconductor we study by considering only two bands separated with a band gap, with the chemical potential lying inside the band gap. The two bands are constructed through tight-binding approximation on a simple cubic lattice.

The non-interacting part of the model Hamiltonian  $H_0$  in **k**-space (momentum space) can be written as

$$H_0 = \sum_{\mathbf{k},\sigma} \begin{pmatrix} a_{\mathbf{k},\sigma}^{\dagger} & b_{\mathbf{k},\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} \epsilon_1(\mathbf{k}) & 0 \\ 0 & \epsilon_2(\mathbf{k}) \end{pmatrix} \begin{pmatrix} a_{\mathbf{k},\sigma} \\ b_{\mathbf{k},\sigma} \end{pmatrix}.$$
 (1)

× /

In Equation 1  $a_{\mathbf{k},\sigma}^{\dagger}$ ,  $b_{\mathbf{k},\sigma}^{\dagger}$  and  $a_{\mathbf{k},\sigma}$ ,  $b_{\mathbf{k},\sigma}$  are the creation and annihilation operators corresponding to the upper (conduction) band and the lower (valence) band, respectively, with **k** being the corresponding wave vector defined in the cubic Brillouin zone and  $\sigma$  the spin of the hopping electrons. The diagonal matrix in Equation 1 contains the energy dispersions of the two bands derived from tight-binding approximation a simple cubic lattice,

$$\epsilon_1(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a + \cos k_z a - 3) + E_c$$
  

$$\epsilon_2(\mathbf{k}) = 2t(\cos k_x a + \cos k_y a + \cos k_z a - 3) + E_y,$$
(2)

where  $E_c$  refers to the minimum energy of the conduction band, and  $E_v$  refers to the maximum energy of the valence band.

Incorporating the e-e interactions the full Hamiltonian reads as

$$H = H_0 + \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{aa}(\mathbf{q}) a^{\dagger}_{\mathbf{k}-\mathbf{q}} a^{\dagger}_{\mathbf{k}'+\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}} + U_{ab}(\mathbf{q}) b^{\dagger}_{\mathbf{k}-\mathbf{q}} a^{\dagger}_{\mathbf{k}'+\mathbf{q}} a_{\mathbf{k}'} b_{\mathbf{k}} + U_{bb}(\mathbf{q}) b^{\dagger}_{\mathbf{k}-\mathbf{q}} b^{\dagger}_{\mathbf{k}'+\mathbf{q}} b_{\mathbf{k}'} b_{\mathbf{k}}, \tag{3}$$

in which  $U_{aa}(\mathbf{q})$ ,  $U_{ab}(\mathbf{q})$ ,  $U_{bb}(\mathbf{q})$  are the *e-e* Coulomb interactions between two electrons coming from same and different bands defined in momentum space.

#### **GW ALGORITHM**

The *GW* algorithm has the purpose of finding the Green function self-consistently along with the self-energy defined in Matsubara frequency domain. The algorithm is derived from Feynman diagrams describing the Dyson equation, the electron-hole polarization, and the renormalized Coulomb interaction [2, 3], depicted as the following

We can start *GW* algorithm with the construction of Green function matrix  $[G(\mathbf{k}, i\omega_n)]$  through the Dyson equation in matrix form as

$$[G(\mathbf{k}, i\omega_n)] = \left[ [G_0(\mathbf{k}, i\omega_n)]^{-1} - [\Sigma(\mathbf{k}, i\omega_n)] \right]^{-1},$$
(4)

where the bare Green function matrix is defined as  $[G_0(\mathbf{k}, i\omega_n)] = [(i\omega_n + \mu)[I] - [H_0(\mathbf{k})]]^{-1}$ , with  $[H_0(\mathbf{k})]$  being the non-interacting part of the Hamiltonian matrix (the middle matrix on the r.h.s. of Equation 1), and  $\mu$  being the chemical potential. Customarily, we can initialize the self energy matrix with  $[\Sigma^{\text{initial}}(\mathbf{k}, i\omega_n)] = 0$ , and  $\mu$  with some guessed value.

Next, we compute the polarization bubble  $\Pi^{\alpha\beta}(\mathbf{q}, i\omega_n)$ ,

$$\Pi^{\alpha\beta}(\mathbf{q},i\omega_x) = T \sum_{\omega_n} \sum_{\mathbf{k}} G^{\alpha\beta}(\mathbf{k},i\omega_n) G^{\alpha\beta}(\mathbf{k}-\mathbf{q},i\omega_n-i\omega_x)$$
(5)

where **k** and **q** represents the electron and the virtual photon momenta, respectively. Here, the scatterings involve umklapp processes, namely, if the resulting  $\mathbf{k} - \mathbf{q}$  vector falls out of the Brillouin Zone (BZ), it must be brought back to the BZ by adding or substracting it with the shortest corresponding **G** vector.

Once the polarization bubble has been obtained, we can calculate the dressed interaction  $W(\mathbf{q}, i\omega_x)$  from the bare interaction  $V(\mathbf{q})$  within Random Phase Approximation (RPA), as described by the diagrams in Fig. 1b, for which the mathematical formulation can be recast into a matrix equation

$$[W(\mathbf{q}, i\omega_x)] = \left[ [I] - [V(\mathbf{q})] [\Pi(\mathbf{q}, i\omega_x)] \right]^{-1} [V(\mathbf{q})], \tag{6}$$



FIGURE 1. Feynman diagrams describing GW algorithm: (a) Dyson equation showing the relation between the dressed Greens function G (shown as bold arrows, the self-energy Σ, and bare Green function G<sub>0</sub> (shown as thin arrows); (b) Random Phase Approximation (RPA) process, where thin wiggly lines represent the bare interaction V, bold wiggly lines represent the dressed interaction W, and the pair of arrows with opposite directions is the polarization bubble Π. (c) Self energy, Σ that consists of direct (tadpole) and exchange (shell) terms.

with

$$[V(\mathbf{q})] = \begin{pmatrix} U(\mathbf{q}) & U(\mathbf{q}) \\ U(\mathbf{q}) & U(\mathbf{q}) \end{pmatrix}.$$
(7)

Further, using the bare and the dressed interactions we compute the direct ( $\omega_n$ -independent) self energy,  $\Sigma_{\alpha\beta}^{\text{direct}}(\mathbf{k})$ , and the exchange ( $\omega_n$ -dependent) self-energy,  $\Sigma_{\alpha\beta}^{\text{exchange}}(\mathbf{k}, i\omega_n)$ , which also involves umklapp processes through  $\mathbf{k} + \mathbf{q}$ , as

$$\Sigma_{\alpha\alpha}^{\text{direct}}(\mathbf{k}) = T \sum_{\omega_m} \sum_{\mathbf{k}'} \sum_{\lambda} G_{\lambda\lambda}(\mathbf{k}', i\omega_m) e^{i\omega_m 0^+} V_{\alpha\lambda}(\mathbf{q} = 0, i\omega_x = 0), \tag{8}$$

$$\Sigma_{\alpha\beta}^{\text{exchange}}(\mathbf{k}, i\omega_n) = -T \sum_{\omega_x} \sum_{\mathbf{q}} G_{\alpha\beta}(\mathbf{k} + \mathbf{q}, i\omega_n + i\omega_x) W_{\alpha\beta}(\mathbf{q}, i\omega_x).$$
(9)

The resulting calculated self-energy matrix  $[\Sigma^{\text{calc}}(\mathbf{k}, i\omega_n)] = [\Sigma^{\text{direct}}(\mathbf{k})] + [\Sigma^{\text{exchange}}(\mathbf{k}, i\omega_n)]$  is to be compared with  $[\Sigma^{\text{initial}}(\mathbf{k}, i\omega_n)]$ . If the difference between them is still larger than some tolerance value, the initial self-energy matrix is replaced by the mixture of the previously initialized and calculated self-energy matrices, and the calculation must be iterated until the self-energy matrix is converged.

At each iteration process, however, we need to update the chamical potential ( $\mu$ ). To do this, we first need to obtain the density of states (DOS), which is related to the imaginary part of the retarded Green function matrix defined in the real-frequency domain,  $[G^R(\mathbf{k}, \omega)]$ . In order to construct  $[G^R(\mathbf{k}, \omega)]$  through the Dyson equation  $[G^R(\mathbf{k}, \omega)] = [[G_0^R(\mathbf{k}, \omega)]^{-1} - [\Sigma^R(\mathbf{k}, \omega)]]^{-1}$ , we need to transform  $[\Sigma^{calc}(\mathbf{k}, i\omega_n)]$  to  $[\Sigma^R(\mathbf{k}, \omega)]$  by means of analytic continuation. Formally, this process is to change the argument of the function from  $z = i\omega_n + \mu$  to  $z = \omega + i0^+$ . However, since we only have the function  $[\Sigma^{calc}(\mathbf{k}, \omega)]$  available as numerical data, there is no exact way for doing such an analytic continuation. Alternatively, we may use an approximate way. Here, we choose to use Padé approximation [4] in which a rational function [P(z)] is constructed as the approximant to the **k**-averaged self-energy matrix  $[\Sigma^{ave}(z)] = \frac{1}{N} \sum_{\mathbf{k}} [\Sigma^{calc}(\mathbf{k}, z)]$ , with *z* a complex energy variable. Each element of the Padé approximant matrix can, in principle, be obtained through

$$P(z) = \frac{\sum_{i=0}^{n} a_i z^i}{1 + \sum_{j=1}^{m} b_j z^j},$$
(10)

where the Padé algorithm searches for the fittest sets of coefficients  $a_i$  and  $b_j$ . Having obtained the desired coefficients  $a_i$  and  $b_j$ , we can define the approximate **k**-averaged self energy as  $[\Sigma_{ave}^R(\omega)] = [P(\omega + i0^+)]$ , and then take this into the Dyson equation to obtain  $[G^R(\mathbf{k}, \omega)]$ .

The DOS can then be obtained through

$$DOS(\omega) = -\frac{1}{\pi} \frac{1}{N} \sum_{\mathbf{k}} \operatorname{Im} \operatorname{Tr}[G^{R}(\mathbf{k}, \omega)].$$
(11)

From the obtained DOS function, for the given electron filling value,  $n_{\text{filling}}$ , we update the chemical potential ( $\mu$ ) by requiring that

$$n_{\text{filling}} = \int_{-\infty}^{\infty} d\omega \operatorname{DOS}(\omega) f(\omega, \mu, T),$$
(12)

where  $f(\omega, \mu, T)$  is the Fermi-Dirac distribution function for temperature T.

In this work, we aim to observe how the DOS varies with temperature for the case of no spin symmetry-breaking. We take several temperature values (T = 200 K, 300 K, and 400 K). The original form of the Coulomb long-ranged interaction in momentum space reads as

$$U(\mathbf{q})_{LR} = \frac{1}{V_{\text{unit cell}}} \frac{e^2}{\epsilon_0 \epsilon_r} \frac{1}{q_x^2 + q_y^2 + q_z^2 + \kappa^2},$$
(13)

with  $\epsilon_r$  and  $\kappa$  are to be chosen some presumably realistic values. From here, we take the value of the corresponding short-ranged Coulomb interaction by averaging  $U(\mathbf{q})_{LR}$  over all  $\mathbf{q}$  values in the BZ

$$U_{SR} = \frac{1}{N} \sum_{\mathbf{q}} U_{LR}(\mathbf{q}). \tag{14}$$

#### **RESULTS AND DISCUSSION**

#### **Bare DOS**

All our calculation results are presented in Fig. 2a, 2b, and 2c. The non-interacting (bare) density of states (DOS) is shown as the black curves. According to the energy dispersion relation defined in Equation 2, where we choose the parameters t = 1 eV,  $E_v = 0$ , and  $E_c = E_g - E_v = 3 \text{ eV}$ , the bare DOS is symmetric with respect to 0 eV where the chemical potential lies, as the system is considered to be at half electron filling. The splitting of the DOS into two bands of width 12t = 12 eV, is to mimic the splitting of  $\pi$  (bonding) and  $\pi^*$  (anti-bonding) bands usually occurs in actual semiconductors. Here we choose the initial band gap value to be  $E_g = E_c - E_v = 3 \text{ eV}$ , mimicking the band gap value of some typical wide-band-gap oxide semiconductor containing some transition metal elements. That the chemical potential lies in the band gap ( $\mu = 0 \text{ eV}$ ) assurs that the material represented by this model is an insulator or a semiconductor. Due to not carrying any electron-electron interactions, the bare DOS profile is independent of temperature.

#### **Temperature Dependence of the Dressed DOS**

Upon incorporation of the *GW* sel energy, the corrected or the dressed DOS becomes sensitive to temperature. The red, green, and blue curves in Fig. 2a shows the whole DOS profile shifts to a higher energy due to the Coulomb repulsive interactions, but each curve remains symmetric with respect to its own shifted chemical potential value as this is the characteristic of a half-filled system. As expected, the general profile of each DOS curve modifies as compared to that of the bare DOS [5, 6]. Nevertheless, the accuracy of the detailed structure of the dress DOS may quite depend on the accuracy of the Padé approximant. Figure 2b displays basically the same sets of DOS curves as already shown in Fig. 2a, but with abscissa being changed from *E* to  $E - \mu$ . This is to emphasize that all the curves stay symmetric with respect to its own chemical potential. Now, if we look closer around the energy gap region (see Fig. 2c), the gap region gets widen as temperature decreases, or conversely, the gap tends to get destroyed as temperature increases. It is theoretically expected that at very high temperatures the gap would completely disappear, and the system becomes a metal. This is understandable because statistically the effect of temperature is to make higher energy states become more accessible by electrons, which eventually would make the electrons be more mobile.



**FIGURE 2.** Bare and GW-dressed DOS: (a) The black curve shows the non-interacting (bare) DOS with energy gap of 3 eV, while the red, green, and blue curves show the evolution (the right shift and the gap widening) of DOS with respect to temperature as the GW self-energy is incorporated. ; (b) The same curves as in (a) but plotted with respect to energy minus the chemical potential  $(E - \mu)$ ; (c) The zoomed-in version of (b) highlighting the bandgap widening as temperature decreases.

#### **CONCLUSION**

We have developed tight-binding based GW method applied to a model semiconductor and perform calculations to test the method. Our calculation results for short-ranged interaction confirm that the semiconductor band gap increases with the inclusion of *e-e* interactions. In addition, the chemical potential shifts to a higher energy. By varying

temperature value, we demonstrate that the correlation effects become stronger as we decrease the temperature, which reflect in the band gap widening. Apart from possible errors and lack of accuracy in our present results, we believe that the method we have developed will be useful for further studies dealing with modeling of materials having strong e-e interactions.

#### ACKNOWLEDGMENTS

This project was funded in full by Universitas Indonesia via PITTA research grant No. 666/UN2.R3.1/HKP.05.00/2017.

#### REFERENCES

- 1. M. A. Majidi, M. A. Naradipa, W. Y. Phan, A. Syahroni, and A. Rusydi, AIP Conf. Proc. 1729, 020013 (2016).
- 2. G. D. Mahan, *Many-Particle Physics*, 3<sup>rd</sup> Edition (Plenum Publishers, New York, 2000).
- 3. A. Syahroni, "Formulation of Tight-Binding Based GW Algorithm for Graphene," B.Sc. Project, Universitas Indonesia, Depok, 2014.
- 4. G. A. Baker and P. Graves-Morris, Padé Approximants (Cambridge University Press, New York, 1996).
- 5. Z. J. Yao, J. X. Li, and Z. D. Wang, Phys. Rev. B. 76, 212506 (2007).
- A. Avella and F. Mancini, *Strongly Correlated Systems: Theoretical Methods* (Springer-Verlag, Berlin Heidelberg, 2012).