Chapter 2

Theory

In several works [6-8], the electric potentials of weakly nonlinear composites have been obtained only up to the second order by using the perturbation expansion method. In order to obtain a more accurate solution of the electric potential, we extend the derivation for the field equations and the boundary conditions from base on the second-order to the third-order perturbation expansion.

2.1 Linear dielectrics

A linear dielectric has a property of which the response to an external electric field is linear. Thus, we can write the relation between the electric displacement (**D**) and the electric field (**E**) of a linear dielectric as

$$\mathbf{D} = \varepsilon \mathbf{E} \ , \tag{2.1}$$

where ε is a linear coefficient or a dielectric constant.

2.2 Nonlinear dielectrics

A nonlinear dielectric has the property of which the response to an external electric field is nonlinear. Thus, we consider the relation between the electric displacement (**D**) and the electric field (**E**) of nonlinear dielectric as [8]

$$\mathbf{D} = \varepsilon \mathbf{E} + \chi |\mathbf{E}|^2 \ \mathbf{E} + \eta |\mathbf{E}|^4 \ \mathbf{E} \ , \tag{2.2}$$

where ε, χ, and η are linear, nonlinear dielectric coefficients in the third and the fifth-orders, respectively. In this research, we will focus on the nonlinear dielectric composite in the case of weak nonlinearity which nonlinear properties are that $\eta |\mathbf{E}|^4 \ll \varepsilon$ and $\chi |\mathbf{E}|^2 \ll \varepsilon$.

2.3 Basic equations of electrostatics

The basic equations of electrostatics are Maxwell's equations, the first one is that

$$\nabla \cdot \mathbf{D} = \rho_f, \tag{2.3}$$

where ρ_f is the free electric charge density.

For the electrostatic problem in which there is no free electric charge (or $\rho_f = 0$). Thus, we can reduce Eq. (2.3) in to

$$\nabla \cdot \mathbf{D} = 0. \tag{2.4}$$

Another one of the four Maxwell's equations for electrostatics is

$$\nabla \times \mathbf{E} = 0. \tag{2.5}$$

From this equation, the electric field ($\mathbf{E}$) can be written in terms of the scalar electric potential (ϕ), which is

$$\mathbf{E} = -\nabla\phi. \tag{2.6}$$

Eqs. (2.2), (2.4) and (2.6) are the basic equations to be used to solve for the electric potential.

Because the nonlinear relation between the electric displacement and the electric filed of the composite so that the equation for the electric potential is a very nonlinear differential equation which cannot be solved exactly in an analytic form. Thus, many approximation methods have been developed to solve this problem such as variational method [1,19], decoupling approximation [10] and perturbation expansion method [6-8,15,16]. Each approximation method has its own advantages and drawbacks. In this research, we use the perturbation expansion method to solve this problem.

2.4 The perturbation expansion method

In theoretical physics, there are several forms of equation that the exact solutions cannot be obtained. Therefore, the approximate methods are required to get the solutions in order to explain these problems to the accurate level that is acceptable. The perturbation expansion method is based on the assumption that the system being considered is not much different from the system that has an exact solution. For example, problems of hydrogen atom and nonlinear harmonic oscillator [16]. By using the perturbation expansion method, the solution for each order is solved separately and the approximate solution is obtained by combining the solutions of all orders.

2.5 Field equations and boundary conditions

In this work, we first extend the derivation for the field equations and the boundary conditions from the second order previously published [6-8] to base on the third-order perturbation expansion for weakly nonlinear dielectric composites with the electric displacement (**D**) and the electric field (**E**) relation including the fifth-order nonlinear coefficient as shown in Eq. (2.2).

We begin with writing the electrostatic potentials in the inclusion (ϕ^i) and host medium (ϕ^m) using the perturbation expansion method up to the third order as follows:

$$\phi^i = \phi_0^i + \lambda\phi_1^i + \lambda^2\phi_2^i + \lambda^3\phi_3^i \ , \tag{2.7}$$

$$\phi^m = \phi_0^m + \lambda\phi_1^m + \lambda^2\phi_2^m + \lambda^3\phi_3^m \ , \tag{2.8}$$

where the superscripts i and m denote, respectively, the quantities in the inclusion region and in the host medium region. λ is the expansion parameter that represents how much the nonlinearity of the composite is. We will call ϕ_0^α, ϕ_1^α, ϕ_2^α

and ϕ_3^α are the zeroth, the first, the second and the third orders electric potentials, respectively and $\alpha = i$ or m.

From Eq. (2.6), the electric field can also be written in the form of perturbation expansion as

$$\mathbf{E}^\alpha = -(\nabla\phi_0^\alpha + \lambda\nabla\phi_1^\alpha + \lambda^2\nabla\phi_2^\alpha + \lambda^3\nabla\phi_3^\alpha), \tag{2.9}$$

or

$$\mathbf{E}^\alpha = \mathbf{E}_0^\alpha + \lambda\mathbf{E}_1^\alpha + \lambda^2\mathbf{E}_2^\alpha + \lambda^3\mathbf{E}_3^\alpha. \tag{2.10}$$

Again, $\mathbf{E}_0^\alpha$, $\mathbf{E}_1^\alpha$, $\mathbf{E}_2^\alpha$ and $\mathbf{E}_3^\alpha$ are the zeroth, the first, the second and the third orders electric fields, respectively.

For convenient, it is defined

$$G^\alpha = |\mathbf{E}^\alpha|^2 = (\nabla\phi^\alpha)\cdot(\nabla\phi^\alpha), \tag{2.11}$$

to denote the square of the electric fields in each region. From Eqs. (2.10) and (2.11), we obtain

$$\begin{aligned} G^\alpha &= (\mathbf{E}_0^\alpha + \lambda\mathbf{E}_1^\alpha + \lambda^2\mathbf{E}_2^\alpha + \lambda^3\mathbf{E}_3^\alpha)\cdot(\mathbf{E}_0^\alpha + \lambda\mathbf{E}_1^\alpha + \lambda^2\mathbf{E}_2^\alpha + \lambda^3\mathbf{E}_3^\alpha), \\ G^\alpha &= |\mathbf{E}_0^\alpha|^2 + \lambda(2\ \mathbf{E}_0^\alpha\cdot\mathbf{E}_1^\alpha) + \lambda^2(2\ \mathbf{E}_0^\alpha\cdot\mathbf{E}_2^\alpha + |\mathbf{E}_1^\alpha|^2) + \lambda^3(2\ \mathbf{E}_1^\alpha\cdot\mathbf{E}_2^\alpha + 2\ \mathbf{E}_0^\alpha\cdot\mathbf{E}_3^\alpha) \\ &\quad + \text{higher order terms.} \end{aligned}$$

G^α can be written in the form of perturbation expansion as follows:

$$G^\alpha = G_0^\alpha + \lambda G_1^\alpha + \lambda^2 G_2^\alpha + \lambda^3 G_3^\alpha\ , \tag{2.12}$$

where

$$G_0^\alpha = |\nabla\phi_0^\alpha|^2, \tag{2.13}$$

$$G_1^\alpha = 2\ \nabla\phi_0^\alpha\cdot\nabla\phi_1^\alpha, \tag{2.14}$$

$$G_2^\alpha = |\nabla\phi_1^\alpha|^2 + 2\ \nabla\phi_0^\alpha\cdot\nabla\phi_2^\alpha, \tag{2.15}$$

$$G_3^\alpha = 2\ \nabla\phi_0^\alpha\cdot\nabla\phi_3^\alpha + 2\ \nabla\phi_1^\alpha\cdot\nabla\phi_2^\alpha\ . \tag{2.16}$$

From Eq. (2.2), the relation between the electric displacement and the electric field in the inclusion and host medium can be written as

$$\mathbf{D}^\alpha = \varepsilon_\alpha \mathbf{E}^\alpha + \chi_\alpha G^\alpha \ \mathbf{E}^\alpha + \eta_\alpha (G^\alpha)^2 \ \mathbf{E}^\alpha. \tag{2.17}$$

Substituting $\mathbf{E}^\alpha$ from Eq. (2.10) and G^α from Eq. (2.12) into Eq. (2.17), we obtain

$$\begin{aligned}\mathbf{D}^\alpha = & -\varepsilon_\alpha(\nabla\phi_0^\alpha + \lambda\nabla\phi_1^\alpha + \lambda^2\nabla\phi_2^\alpha + \lambda^3\nabla\phi_3^\alpha) - \chi_\alpha(G_0^\alpha + \lambda G_1^\alpha + \lambda^2 G_2^\alpha + \lambda^3 G_3^\alpha) \\ & [\nabla\phi_0^\alpha + \lambda\nabla\phi_1^\alpha + \lambda^2\nabla\phi_2^\alpha + \lambda^3\nabla\phi_3^\alpha] - \eta_\alpha(G_0^\alpha + \lambda G_1^\alpha + \lambda^2 G_2^\alpha + \lambda^3 G_3^\alpha)^2 \\ & [\nabla\phi_0^\alpha + \lambda\nabla\phi_1^\alpha + \lambda^2\nabla\phi_2^\alpha + \lambda^3\nabla\phi_3^\alpha] \,.\end{aligned}$$

To perform the grouping of terms in the above equation according to their magnitudes, we first note that the perturbation parameter λ is just a fictitious parameter introduced in such a way that a term multiplied by λ^n has its size of the nth order correction to the corresponding unperturbed quantity. Since ε_α, $\chi_\alpha|\mathbf{E}^\alpha|^2$ and $\eta_\alpha|\mathbf{E}^\alpha|^4$ correspond to the order of λ^0, λ^1 and λ^2, respectively, we define χ_α and η_α in terms of λ^n as $\chi_\alpha = \lambda\beta_\alpha$ and $\eta_\alpha = \lambda^2\gamma_\alpha$. Consequently, the grouping of terms according to their sizes can be done without any confusion, with the result

$$\begin{aligned}\mathbf{D}^\alpha = & -\varepsilon_\alpha\nabla\phi_0^\alpha - \lambda(\varepsilon_\alpha\nabla\phi_1^\alpha + \beta_\alpha G_0^\alpha \ \nabla\phi_0^\alpha) - \lambda^2(\varepsilon_\alpha\nabla\phi_2^\alpha + \beta_\alpha(G_0^\alpha \ \nabla\phi_1^\alpha \\ & + G_1^\alpha \ \nabla\phi_0^\alpha) + \gamma_\alpha(G_0^\alpha)^2 \ \nabla\phi_0^\alpha) - \lambda^3(\varepsilon_\alpha\nabla\phi_3^\alpha + \beta_\alpha(G_0^\alpha \ \nabla\phi_2^\alpha + G_1^\alpha \ \nabla\phi_1^\alpha \\ & + G_2^\alpha \ \nabla\phi_0^\alpha) + \gamma_\alpha((G_0^\alpha)^2 \ \nabla\phi_1^\alpha + 2 \ G_0^\alpha G_1^\alpha \ \nabla\phi_0^\alpha)) + \text{higher order terms.}\end{aligned} \tag{2.18}$$

Comparing Eq. (2.18) with

$$\mathbf{D}^\alpha = \mathbf{D}_0^\alpha + \lambda\mathbf{D}_1^\alpha + \lambda^2\mathbf{D}_2^\alpha + \lambda^3\mathbf{D}_3^\alpha \tag{2.19}$$

yields

$$\mathbf{D}_0^\alpha = -\varepsilon_\alpha \nabla \phi_0^\alpha \,, \tag{2.20}$$

$$\mathbf{D}_1^\alpha = -\varepsilon_\alpha \nabla \phi_1^\alpha - \beta_\alpha G_0^\alpha \; \nabla \phi_0^\alpha \,, \tag{2.21}$$

$$\mathbf{D}_2^\alpha = -\varepsilon_\alpha \nabla \phi_2^\alpha - \beta_\alpha (G_0^\alpha \; \nabla \phi_1^\alpha + G_1^\alpha \; \nabla \phi_0^\alpha) - \gamma_\alpha (G_0^\alpha)^2 \; \nabla \phi_0^\alpha \,, \tag{2.22}$$

and

$$\begin{aligned} \mathbf{D}_3^\alpha \; &= \; -\varepsilon_\alpha \nabla \phi_3^\alpha - \beta_\alpha (G_0^\alpha \; \nabla \phi_2^\alpha + G_1^\alpha \; \nabla \phi_1^\alpha + G_2^\alpha \; \nabla \phi_0^\alpha) \\ &\quad - \gamma_\alpha ((G_0^\alpha)^2 \; \nabla \phi_1^\alpha + 2 \; G_0^\alpha G_1^\alpha \; \nabla \phi_0^\alpha). \end{aligned} \tag{2.23}$$

Substituting Eqs. (2.20)-(2.23) into Eq. (2.4), we obtain

$$\varepsilon_\alpha \nabla^2 \phi_0^\alpha \; = \; 0, \tag{2.24}$$

$$\varepsilon_\alpha \nabla^2 \phi_1^\alpha + \beta_\alpha (G_0^\alpha \; \nabla^2 \phi_0^\alpha + \nabla G_0^\alpha \cdot \nabla \phi_0^\alpha) \; = \; 0, \tag{2.25}$$

$$\begin{aligned} &\varepsilon_\alpha \nabla^2 \phi_2^\alpha + \beta_\alpha (G_0^\alpha \; \nabla^2 \phi_1^\alpha + \nabla \phi_1^\alpha \cdot \nabla G_0^\alpha + G_1^\alpha \; \nabla^2 \phi_0^\alpha \\ &+ \nabla \phi_0^\alpha \cdot \nabla G_1^\alpha) + \gamma_\alpha ((G_0^\alpha)^2 \; \nabla^2 \phi_0^\alpha + 2 \; G_0^\alpha \; \nabla \phi_0^\alpha \cdot \nabla G_0^\alpha) \; = \; 0, \end{aligned} \tag{2.26}$$

and

$$\begin{aligned} &\varepsilon_\alpha \nabla^2 \phi_3^\alpha + \beta_\alpha (G_0^\alpha \; \nabla^2 \phi_2^\alpha + \nabla \phi_2^\alpha \cdot \nabla G_0^\alpha + G_1^\alpha \; \nabla^2 \phi_1^\alpha + \nabla \phi_1^\alpha \cdot \nabla G_1^\alpha \\ &+ G_2^\alpha \; \nabla^2 \phi_0^\alpha + \nabla \phi_0^\alpha \cdot \nabla G_2^\alpha) + \gamma_\alpha ((G_0^\alpha)^2 \; \nabla^2 \phi_1^\alpha + 2 \; G_0^\alpha \; \nabla \phi_1^\alpha \cdot \nabla G_0^\alpha \\ &\quad + 2 \; G_0^\alpha G_1^\alpha \; \nabla^2 \phi_0^\alpha + 2 \; G_0^\alpha \; \nabla \phi_0^\alpha \cdot \nabla G_1^\alpha + 2 \; G_1^\alpha \; \nabla \phi_0^\alpha \cdot \nabla G_0^\alpha) = 0. \end{aligned} \tag{2.27}$$

Eqs. (2.24), (2.25) and (2.26) are the zeroth, the first and the second order equations, describing the electrostatic potential, which have been reported by several authors [6-8]. We obtain more general results that are the equations for determination of ϕ_3^α (Eq. (2.27)) and the equation for fitting the boundary condition (Eq. (2.23)). We also note that the electrostatic potential, including the third-order potential, was generally more accurate than the result having only the first and the second-orders [15]. This is the reason why we expanded the electric potential up to the third order.

In order to solve for each order electrostatic potential, the following boundary conditions are applied:

1. the electrostatic potential in the host medium at remote distance.

2. the electrostatic potential at the center of the inclusion.

3. the continuity of the tangential of the electric field at the inclusion surface.

4. the continuity of the normal component of the electric displacement at the inclusion surface.

We will discuss each boundary condition in details in the next chapter.