Chapter 2

Introduction to Angular Spectrum Representation and Tight Binding Model

In this chapter, we introduce two important concepts which we have used extensively in the rest of the thesis in order to describe the field profile and dispersion relation of SSP in the high frequency limit. The first concept is that of angular spectrum representation of spatial electromagnetic field. This is the 2D Fourier transform of the spatial representation of the field to the spatial frequency domain [73, 72]. The other concept is the tight binding model which was developed originally to describe the electronic band structure of solids [50]. Given a 2D slice of field at some reference plane, angular spectrum representation is a very useful tool to quatify diffracted field at any other plane which is parallel to the reference plane. This approach will be useful to us when we try to quantify the SSP near-field in Ch. 3. On the other hand, the remarkable concept of photonic crystal came into existence from a question which is closely related to Condensed Matter Physics [**?**, **?**]. More specifically, Anderson [**?**] had theoretically predicted the localization of electrons in disordered solids. In analogy, the possibility of localization of photons in disordered dielectric lattices was investigated by John [**?**] paving the way to photonic crystal. Since then, analogy with Solid-state Physics has been proven to be a very important tool in order to understand several concepts of light propagation and trapping inside photonic crystals. In general, metallic photonic crystal, used in SSP, lacks the important property of being able to be formulated as a Hermitian eigenvalue problem [?]. Nevertheless, it shares great deals of similarities in band-structure and associated phenomena (such as, self-collimation). From this view-point, it seems quite possible to gain deeper insight into the dispersion relation of SSP (and photonic crystals, in general) using tight binding model (this problem will be addressed in Ch. 4). To this end, starting with Rayleigh-Sommerfeld formulation for diffraction [?] we discuss the angular spectrum representation of a 2D field distribution and its relation with propagating and evanescent field components. Next, we review the basics of tight binding model for a solid state crystal.

2.1 Rayleigh-Sommerfeld formulation for diffraction

Let us consider the following problem of diffraction of electromagnetic field from an aperture:

At $z = 0$, there is an aperture Σ of arbitrary shape on an infinite screen oriented along $xy-$plane (shown in Fig.). Given the field distribution $u(x', y', 0)$ over the aperture, where, $(x', y', 0)$ denotes the coordinate of a point on the aperture, we are interested in finding out the diffracted field $u(x, y, z)$ for $z > 0$ under the assumption that $u(x', y', 0)$ vanishes everywhere on the screen except the aperture.

To solve this problem, we start with the scalar wave equation:

$$\nabla^2 u + k^2 u = 0 \tag{2.1}$$

If G is the Green's function corresponding to Eq. 2.1, we can write the following:

$$\nabla^2 G + k^2 G = -4\pi\delta^3(r - r_0) \tag{2.2}$$

In order to get an integral representation for the field, we consider the following vector identities:

$$\vec{\nabla}.(u\vec{\nabla}G) = (\vec{\nabla}u.\vec{\nabla}G) + u\nabla^2 G \tag{2.3}$$

and

$$\vec{\nabla}.(G\vec{\nabla}u) = (\vec{\nabla}u.\vec{\nabla}G) + G\nabla^2 u \tag{2.4}$$

Subtracting Eq. 2.4 from Eq. 2.3:

$$\left(u\nabla^2 G - G\nabla^2 u\right) = \vec{\nabla}.\left(u\vec{\nabla}G - G\vec{\nabla}u\right) \tag{2.5}$$

Taking volume integral of both sides of Eq. 2.5 and applying divergence theorem, we get:

$$\iiint_V \left(u\nabla^2 G - G\nabla^2 u\right) = \oiint_S \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\overrightarrow{dS} \tag{2.6}$$

Multiplying Eq. 2.1 by G and multiplying Eq. 2.2 by u and subtracting we find that the surface integral on the right hand side of Eq. 2.6 vanishes when the closed surface over which the integral is carried out does not contain r_0:

$$\oiint_S \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\overrightarrow{dS} = 0 \tag{2.7}$$

However, when the surface S encloses the point r_0 this surface integral term does not vanish due to the singularity of the Dirac delta function at $r = r_0$. In this case the surface integral can be calculated by considering an infinitesimal ball of radius ε around $r = r_0$ (shown in Fig.), where $\varepsilon \to 0$. Also, we assume that the surface of the ball is denoted by S'. As the volume bounded by surface S and S' does not contain $r = r_0$, from Eq. 2.7 we can write the following:

$$\oiint_{(S+S')} \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\overrightarrow{dS} = 0$$

$$\Rightarrow \oiint_S \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\hat{n}dS = -\oiint_{S'} \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\hat{n}dS$$

$$\Rightarrow \oiint_S \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\hat{n}dS = -\oiint_{S'} \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n}\right)dS \tag{2.8}$$

On S', the outward normal $\hat{n}$ points along the direction opposite to the radial vector $\overrightarrow{\varepsilon}$. Also, we choose the $G(\varepsilon)$ to be the free-space Green's function, i.e., $G(\varepsilon) = \frac{e^{ik\varepsilon}}{\varepsilon}$. Thus, on S', $\frac{\partial G}{\partial n} = -\frac{\partial G}{\partial \varepsilon} = -\frac{\partial}{\partial \varepsilon}\left(\frac{e^{ik\varepsilon}}{\varepsilon}\right)$.

Thus, we can rewrite Eq. 2.8 as:

$$\oiint_S \left(u\vec{\nabla}G - G\vec{\nabla}u\right).\hat{n}dS = -\underset{\varepsilon\to 0}{Lt}\, 4\pi\left[u(r_0)e^{ik\varepsilon}\left(1 - ik\varepsilon\right) + \varepsilon e^{ik\varepsilon}\frac{\partial u}{\partial r}\,|_{r=\varepsilon}\right]$$

$$\Rightarrow u(r_0) = -\frac{1}{4\pi} \oiint_S \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n} \right) dS \tag{2.9}$$

We assume the surface S, over which the integral is carried out, to be composed of the infinite screen S_1 at $z = 0$ and a hemisphere S_2 of radius R_2 $(R_2 \to \infty)$ Also, we assume that its center is situated on the screen. Since the diffracted field must satisfy Sommerfeld's radiation condition, the integral of Eq. 2.9 vanishes over S_2 [73, **?**]. So, $u(r_0)$ reduces to:

$$u(r_0) = -\frac{1}{4\pi} \iint_{S_1} \left(u\frac{\partial G}{\partial n} - G\frac{\partial u}{\partial n} \right) dS \tag{2.10}$$

At this point, we consider the choice of the Green's function by Sommerfeld. According to Sommerfeld's formulation, the Green's function (G_-) is represented as:

$$G_- = \frac{e^{ikr}}{r} - \frac{e^{ikr'}}{r'} \tag{2.11}$$

Physically, this form of G_- at any point can be interpreted as being originated from two point sources, which are mirror images of each other with respect to the screen at $z = 0$ and having 180° phase-shift between themselves (shown in Fig.). For this choice of Green's function the solution of the diffracted field $u(r_0)$ is denoted as $u_I(r_0)$. Clearly, G_- vanishes at all points on S_1 and Eq. 2.10 reduces to:

$$u_I(r_0) = -\frac{1}{4\pi} \iint_{S_1} u\frac{\partial G_-}{\partial n} dS \tag{2.12}$$

Now, we make use of the assumption made in the problem statement to simplify Eq. 2.12 further. Since, $u(x', y', 0)$ vanishes everywhere on the screen S_1 except for the points on the aperture Σ, the diffracted field at an arbitrary point $r = r_0$ can be written as:

$$u_I(r_0) = -\frac{1}{4\pi} \iint_{\Sigma} u\frac{\partial G_-}{\partial n} dS \tag{2.13}$$

Now, on the aperture the surface normal $\hat{n}$ is directed along $-\hat{z}$. As a result we can evaluate $\frac{\partial G_-}{\partial n}$ as:

$$\frac{\partial G_-}{\partial n} = -\frac{\partial G_-}{\partial z} = -\frac{\partial}{\partial z}\left(\frac{e^{ikr}}{r} - \frac{e^{ikr'}}{r'} \right) = \frac{\partial}{\partial z'}\left(\frac{e^{ikr}}{r} - \frac{e^{ikr'}}{r'} \right) \tag{2.14}$$

To simplify the above expression further, we can rewrite the above equation using Kirchoff's choice of Green's function G (which is just the free-space Green's function) as:

$$\frac{\partial G_-}{\partial n} = -\frac{\partial}{\partial z}\left(\frac{e^{ikr}}{r} - \frac{e^{ikr'}}{r'}\right) = -\frac{\partial G}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial}{\partial r'}(\frac{e^{ikr'}}{r'})\frac{\partial r'}{\partial z} = -\frac{\partial G}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial G}{\partial r}\frac{\partial r'}{\partial z}$$

$$\Rightarrow \frac{\partial G_-}{\partial n} = -2\frac{\partial G}{\partial r}\frac{\partial r}{\partial z} = -2\frac{\partial G}{\partial z} \tag{2.15}$$

Thus, we can write the solution of the diffracted field at $r = r_0$ as:

$$u_I(r_0) = -\frac{1}{2\pi}\iint_{\Sigma} u\frac{\partial G}{\partial n}dS \tag{2.16}$$

Within this theoretical framework, we now try to find out the diffracted field at a point P at distance $r = R$, where $R = \sqrt{(x-x')^2 + (y-y')^2 + z^2}$ andthe Green's function $G(R) = \frac{e^{ikR}}{R}$. From Eq. 2.16, we can evaluate $u(x,y,z)$ as:

$$u(R) = \frac{1}{2\pi}\iint_{\Sigma} dx'dy'u(x',y',0)\frac{\partial G}{\partial z}$$

$$\Rightarrow u(R) = \frac{1}{2\pi}\iint_{\Sigma} dx'dy'u(x',y',0)\frac{\partial}{\partial R}\left(\frac{e^{ikR}}{R}\right)\frac{\partial R}{\partial z}$$

$$\Rightarrow u(R) = \iint dx'dy'u(x',y',0)\left(\frac{e^{ikR}}{2\pi R}\right)\left(\frac{ik}{R} - \frac{1}{R^2}\right)\frac{z}{R} \tag{2.17}$$

Thus, according to Rayleigh-Sommerfeld formulation, the solution for the diffracted field $u(x,y,z)$ can be written as a convolution of two functions as:

$$u(x,y,z) = u(x,y,0) * h(x,y,z) \tag{2.18}$$

where, $h(x,y,z) = \frac{e^{ikr}}{2\pi r}\left(ik - \frac{1}{r}\right)\left(\frac{z}{r}\right)$. This convolution in the spatial domain is equivalent to a multiplication in the Fourier domain:

$$U(f_x,f_y,z) = U(f_x,f_y,0)H(f_x,f_y,z) \tag{2.19}$$

Here, $f_x = \frac{k_x}{2\pi}$ and $f_y = \frac{k_y}{2\pi}$ represent the spatial frequencies in the transform domain.

2.2 Angular spectrum representation

According to the Rayleigh-Sommerfeld theory of diffraction, we concluded from Eq. 2.18 that if the angular spectrum (or spatial frequency domain representation) of the field $U(f_x, f_y, 0)$ is specified at the aperture plane, we can calculate the angular spectrum of the diffracted field for any $z > 0$ just by multiplying a suitable function $H(f_x, f_y, z)$ with $U(f_x, f_y, 0)$. However, we do not know yet what $H(f_x, f_y, z)$ is. To find out $H(f_x, f_y, z)$ we rewrite the scalar wave equation (i.e. Eq. 2.1) in terms of the angular spectrum $U(f_x, f_y, z)$ of the spatial field $u(x, y, z)$:

$$\left(\nabla^2 + k^2\right) \iint U(f_x, f_y, z) e^{i2\pi(f_x x + f_y y)} df_x df_y = 0$$

$$\Rightarrow \iint [-4\pi^2 \left(f_x^2 + f_y^2\right) U(f_x, f_y, z) e^{i2\pi(f_x + f_y y)}$$
$$+ e^{i2\pi(f_x + f_y y)} \frac{\partial^2 U(f_x, f_y, z)}{\partial z} + k^2 U(f_x, f_y, z) e^{i2\pi(f_x + f_y y)}] \quad df_x df_y = 0$$

$$\Rightarrow \frac{\partial^2 U}{\partial z^2} + \left[k^2 - 4\pi^2 \left(f_x^2 + f_y^2\right)\right] U = 0$$

$$\Rightarrow \frac{\partial^2 U}{\partial z^2} + \alpha^2 U = 0 \tag{2.20}$$

where, $\alpha = \sqrt{k^2 - 4\pi^2 \left(f_x^2 + f_y^2\right)}$. The solution of the above differential equation can be written as:

$$U(f_x, f_y, z) = A(f_x, f_y) e^{i\alpha z} + B(f_x, f_y) e^{-i\alpha z} \tag{2.21}$$

When $\alpha^2 > 0$, i.e. $k^2 > 4\pi^2 \left(f_x^2 + f_y^2\right)$, we have the following constraint on the spatial frequencies:

$$f_x^2 + f_y^2 < \frac{1}{\lambda^2} \tag{2.22}$$

i.e. the spectral components for the propagating solution lies within a circle of radius $\frac{1}{\lambda}$.

Similarly, when $\alpha^2 < 0$, we get the solution of the field as a superposition of exponentially decaying and exponentially growing spectral components:

$$U(f_x,f_y,z) = A(f_x,f_y)e^{-\alpha z} + B(f_x,f_y)e^{\alpha z} \tag{2.23}$$

However, we are interested in calculating the diffracted field for $z > 0$. As $z \to \infty$, the first term in Eq. 2.23 vanishes and the second term grown unboundedly. Clearly, for a solution to be physical, we must have $B(f_x,f_y) = 0$. At $z = 0$, we have $A(f_x,f_y) = U(f_x,f_y,0)$. So, in angular spectrum domain the solution of the diffracted field can be written as:

$$U(f_x,f_y,z) = U(f_x,f_y,0)e^{i\alpha z} \tag{2.24}$$

where, α is real for spectral components within $\frac{1}{\lambda}$ circle (corresponding to propagating solutions) and becomes imaginary for spectral components outside $\frac{1}{\lambda}$ circle giving rise to evanescently decaying solutions. To understand the physical implications of the Eq. 2.24 better, let us consider the spectral components situated along $f_y = 0$ line (i.e. the f_x axis). In this case, the condition to have an evanescent solution reduces to $f_x > \frac{1}{\lambda}$. Now the minimum spatial frequency is roughly inverse of the maximum feature-size (Δx_{max}) of the diffracting object: $f_{xmin} = \frac{1}{\Delta x_{max}}$. Thus, the diffracted field from an object, whose minimum spatial frequency is greater than $\frac{1}{\lambda}$, will always be evanescently decaying. In other words, for such an object we must have:

$$\frac{1}{\Delta x_{max}} > \frac{1}{\lambda}$$

$$\Rightarrow \Delta x_{max} < \lambda \tag{2.25}$$

This means, an object of sub-wavelength dimension mostly gives rise to diffracted field which is evanescent in nature. In this context we note that the structures used for experiments involving SSP contain sub-wavelength periodic features. This is an indication of the fact that angular spectrum has the potential to qualitatively describe the nature of the SSP near-field. We probe this issue in more details in Ch. 3.