# Variational Monte Carlo method for Bragg reflectors

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**Abstract.** Perturbed Hamiltonian's expectation value minimization and it corresponding parameter optimization can be done via Variational method. To adopt the variational method, a computational tool Variational Monte Carlo (VMC) can be utilized. In this case the perturbation is introduced in the Hamiltonian via dielectric tensor. To compare with a real system, Bragg reflectors are chosen as their results are known and be good example to perform the method. The perturbation of dielectric tensor is already in the structure of the Bragg reflectors, which solves the problem of choosing the perturbation. As the computational power required for this to work was very high to get some accurate results. However essential observations were made such as minimization of the expectation value of Hamiltonian (For both one and two unit cells), parameter ($\beta$)'s dependence on the wavelength. The graph between $\beta$ vs $\lambda$ satisfies the theoretical predictions.

*Keywords*: VMC (Variational Monte Carlo), Bragg reflectors, Hamiltonian

## 1. Theory

### *1.1.* ***Variational Monte Carlo***

Evolution of any system can be described via operating Hamiltonian on the eigenstates of the system. For the systems whose Hamiltonian's solution requires a lot of resources and approximation to solve, we use variational monte carlo. The variational principle in proposes to make an educated guess of the wave function, the trial wave function $\psi_T(r,\alpha)$, and calculate the expectation value of $\hat{H}$ with respect to $\psi_T$,

$$< \hat{H} >= \frac{\int dr \psi_T^*(r,\alpha)\hat{H}\psi_T(r,\alpha)}{\int dr \psi_T^*(r,\alpha)\psi_T(r,\alpha)} \geq E_o \tag{1}$$

Therefore, $< \hat{H} >$ is the upper bound of $E_o$ which can be imporved by tuning the paramere set $\alpha$

$$\frac{\partial < \hat{H} >}{\partial \alpha_i} = 0 \text{ where } i = 1, 2, 3, ..., N \tag{2}$$

by using some minimization algorithm. In most cases a wavefunction has only small values in large parts of configuration space, therefore scanning the space uniformly will slow down the calculation to a grinding halt. This suggests the need for importance sampling i.e. the regions of configuration space where the wavefunction takes appreciable values are sampled more efficiently. The importance sampling can be implemented by defining appropriate probability distribution function,

$$p(r) = \frac{\psi_T^*(r,\alpha)\psi_T(r,\alpha)}{\int dr \psi_T^*(r,\alpha)\psi_T(r,\alpha)} \tag{3}$$

which when plugged in the expression (2), we get

$$< \hat{H} >= \int dr p(r)\hat{\xi}, \text{ where } \hat{\xi}(r) = \frac{1}{\phi_T(r,\alpha)\hat{H}\phi_T(r,\alpha)} \tag{4}$$

where the new operator $\hat{\xi}$ is called local energy density. This equation expresses the variational Monte Carlo approach. Therefore,

$$< \hat{H} >=< \hat{\xi}(r) >= \int dr p(r)\hat{\xi}(r) = \frac{1}{N_s}\sum_i \xi(r_i) \tag{5}$$

where $r_i$ are to be distributed according to the p.d.f. $p(r)$ and $N_s$ are the number of sample points. The points to sum over in $r$-space are selected by importance sampling.

After a large number of iterations, the local energy $\xi$ should fluctuate around an average which gives the estimate for $E_o$. The trial wavefunction has to be chosen with some care to reduce the variance of the local energy $\xi$ as small as possible. [1]

### *1.2.* ***Perturbed periodic media***

To obtain the solution for the propagation of electromagnetic radiation in a periodic layered medium, generally Bloch-wave formalism and coupled mode theory methods are used. But there can be another approach via variational method. Here the periodic variation of the dielectric tensor as a function of space can be written as:

$$\epsilon(x,y,z) = \epsilon_o(x,y) + \Delta\epsilon(x,y,z) \tag{6}$$

where $\epsilon_o(x,y)$ is the unperturbed part of the dielectric tensor, and $\Delta\epsilon(x,y,z)$ is periodic in the z direction and is the only periodically varying part of the dielectric tensor.

The normal modes of propagation in the unperturbed dielectric medium described by the dielectric tensor $\epsilon_o(x,y)$ are can be given by

$$E_m(x,y)e^{\iota(\omega t - \beta_m z)} \tag{7}$$

where the m is the mode subscript. The propagation of any arbitrary field in the unperturbed medium can always be expressed in terms of a linear combination of normal modes,

$$E = \sum_m A_m E_m(x,y)e^{\iota(\omega t - \beta_m z)} \tag{8}$$

where the $A_m$'s are constants. Substituting above equation into wave equation

$$[\nabla^2 + \omega^2\mu[\epsilon_o(x,y) + \Delta\epsilon(x,y,z)]]E = 0 \tag{9}$$

solving above equation via assuming the weak dielectric perturbation, applying orthogonal property and expanding dielectric perturbation $\Delta\epsilon(x,y,z)$ as a Fourier series

The solution of wave equation after substituting above values and equations is

$$\frac{d}{dz}A_k = -\iota\frac{\beta_k}{|\beta_k|}\sum_l\sum_m C_{kl}^{(m)}A_l e^{\iota(\beta_k-\beta_l-m2\pi/\Lambda)z} \tag{10}$$

This equation is known as the coupled mode equation which gives the coupling between $k^{th}$ and $l^{th}$ mode of the $m^{th}$ Fourier component of the dielectric perturbation. Here the coupling coefficient $C_{kl}^m$ is defined as

$$C_{kl}^{(m)} = \omega/4\int E_k^*(x,y).\epsilon_m(x,y)E_l(x,y)dxdy \tag{11}$$

This coefficient reflects the magnitude of coupling between the $k^{th}$ and $l^{th}$ mode of the $m^{th}$ Fourier component of the dielectric perturbation.

*1.2.1.* ***Bragg reflectors*** The Bragg reflectors can be described as one dimensional photonic crystals, which can be represented as:

$$\epsilon(z) = \begin{cases}\epsilon_o n_2^2, & 0 < z < d_1\\ \epsilon_o n_1^2, & d_1 < z < d_2\end{cases} \tag{12}$$

where $d_1$ is the thickness of the layer with $n_2$ refractive index and $d_2$ is the thickness of the layer with $n_1$ refractive index. And we can also define the periodicity of the material as $\epsilon(z) = \epsilon(z+\Lambda)$, where $\Lambda = d_1 + d_2$. This dielectric constant can be decomposed accordingly

$$\epsilon(z) = \frac{1}{2}\epsilon_o(n_1^2+n_2^2) + \frac{1}{2}\epsilon_o(n_2^2-n_1^2)f(z) \tag{13}$$

where $f(z)$ is periodic square-wave function and defined as

$$f(z) = \begin{cases}1, & 0 < z < d_1\\ -1, & d_1 < z < d_2\end{cases} \tag{14}$$

Here we assumed the dielectric distribution only along z direction.

The normal modes of the unperturbed medium are plane waves $e^{-\iota k.r}$ with wave number given by

$$k^2 = (\frac{\omega}{c})^2\frac{n_1^2+n_2^2}{2} \tag{15}$$

These plane waves are divided into TE and TM waves according to their polarization states. Here we will move forward with TM waves.

Let $\theta$ be the angle between the wave vector and the axis z. The coupling constants according are given as

$$\kappa = \frac{\iota(1-\cos(m\pi))}{2m\lambda\cos(\theta)} \frac{\sqrt{2}(n_2^2 - n_1^2)}{\sqrt{n_2^2 + n_1^2}} \cos(2\theta) \tag{16}$$

And the phase missmatch condition is given by

$$\Delta\beta = 2K\cos(\theta) - m(\frac{2\pi}{\Lambda}) \tag{17}$$

To obtain an expression for the reflectivity, we assume that the light is incident at z=0, so that the boundary condition is

$$A_1(0) = 1$$

$$A_2(L) = 0$$

where $A_1$ is the amplitude of the incident wave and $A_2$ is the amplitude of the reflected wave. The solution of the coupled equation is given by

$$A_1(z) = e^{\iota(\Delta\beta/2)z} \frac{s\,\cosh(s(L-z)) + \iota(\Delta\beta/2)\sinh(s(L-z))}{s\,\cosh(sL) + \iota(\Delta\beta/2)\sinh(sL)} \tag{18}$$

$$A_2(z) = e^{-\iota(\Delta\beta/2)z} \frac{-\iota\kappa^*\sinh(s(L-z))}{s\,\cosh(sL) + \iota(\Delta\beta/2)\sinh(sL)} \tag{19}$$

where s is given by $s^2 = \kappa^*\kappa - (\Delta\beta/2)^2$ [2]

## 2. Applying Variational Monte Carlo on Bragg reflectors

Now we would apply the monte carlo formalism on the Bragg reflectors to optimize the propagating mode. Lets have a trail function for MC (Monte Carlo)

$$\psi_T(z,\beta) = A(z)e^{\iota\beta z} \tag{20}$$

where A(z) will be given via equation(18) and required values inside the A(z) can be obtained via section 1.2.1. As we have a perturbed dielectric function along z-direction that will be responsible for z dependence of the amplitude. As discussed above that to be more precise with the results, we choose our trail function with a little bias towards original function.

Now coming towards the Hamiltonian of the system which will have perturbation of dielectric constant, will be given as

$$[\nabla^2 + \omega^2\mu\epsilon(z)] = 0 \tag{21}$$

where $\epsilon(z)$ is given by equation(13). Following the procedure for the VMC described in section 1.1, minimized momentum of the system and wave-vector is determined. Detailed results are discussed below.

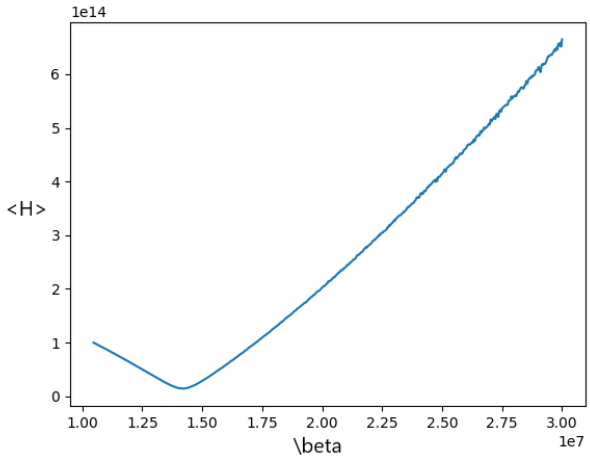


**Figure 1:** $< \hat{H} >$ vs $\beta$

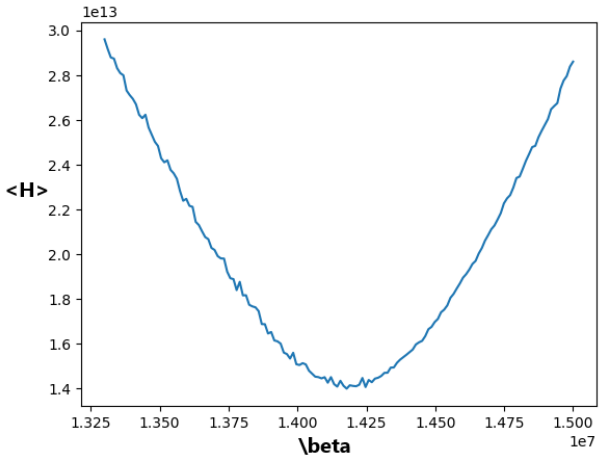


**Figure 2:** Zoomed in at minima ($< \hat{H} >$ vs $\beta$)

Figure 1: Optimization of $\beta$ for two layer (one unit cell) system using VMC

### *2.1. Design-1*

First design contains 2-layer system. First layer have thickness ($d_1$) $70nm$ and refractive index ($n_1$) of 2.5. Second later have thickness ($d_2$) $150nm$ and refractive index of 1.5. Algorithm parameters are defined below.

- Initial incident angle $\theta = 0$
- Wavelength ($\lambda$) $= 600nm$
- Initial range for $\beta = [2\pi/\lambda, 6\pi/\lambda]$ and 500 points
- Step size $= 0.1 \times 10^{-9}$
- Number of Monte Carlo steps = 1500

### *2.2. Design-2*

Second design contains 4-layer (two unit cell) system. First layer have thickness ($d_1$) $70nm$ and refractive index ($n_1$) of 2.5. Second later have thickness ($d_2$) $150nm$ and refractive index of 1.5.

- Initial incident angle $\theta = 0$
- Wavelength ($\lambda$) $= 600nm$
- Initial range for $\beta = [\pi/\lambda, 6\pi/\lambda]$ and 100 points
- Step size $= 0.1 \times 10^{-9}$
- Number of Monte Carlo steps = 1500

To further see the variation in the minima corresponding to the $\beta$ with respect to wavelength. We have taken the same parameters as described above such as number of steps and ten different wavelengths. Corresponding results are plotted in the Figure (3).

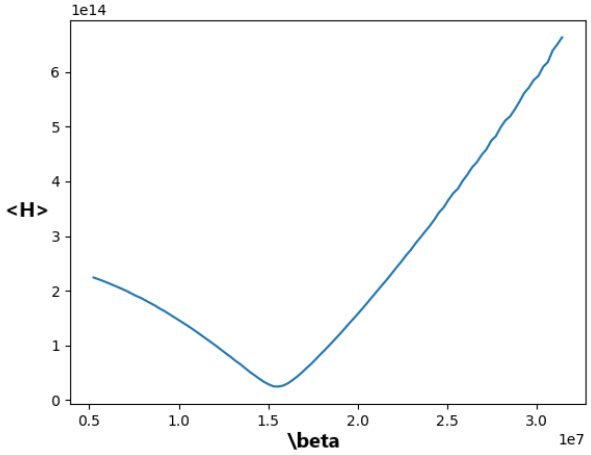


**Figure 1:** $< \hat{H} >$ vs $\beta$

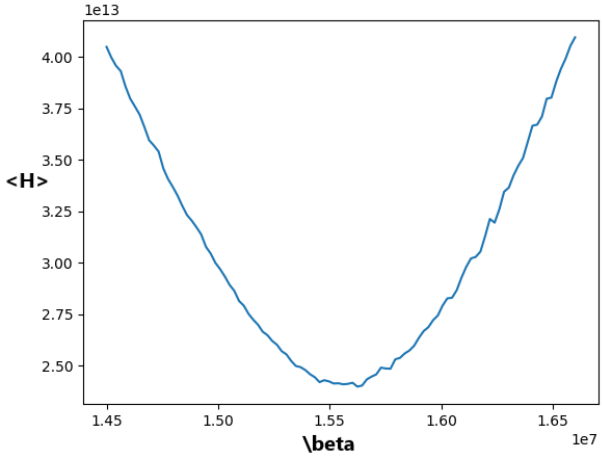


**Figure 2:** Zoomed in at minima ($< \hat{H} >$ vs $\beta$)

Figure 2: Optimization of $\beta$ for four layer (two unit cell) system using VMC

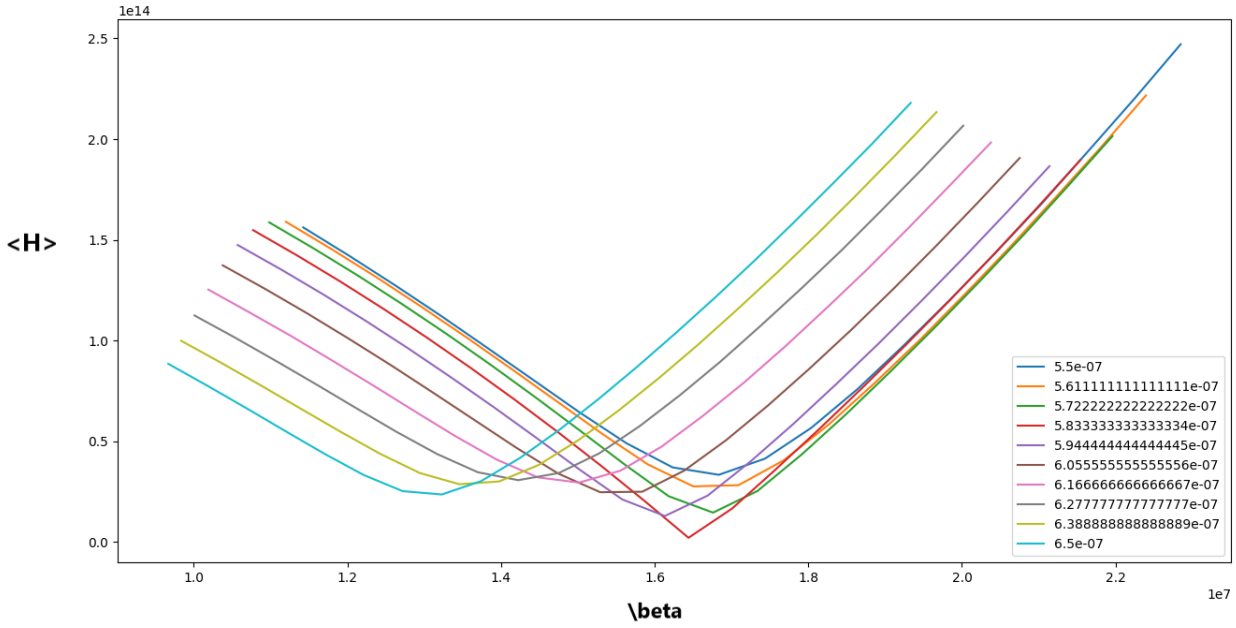


Figure 3: $< \hat{H} >$ vs $\beta$ for different wavelengths

Then further the graph was plotted between $\lambda$ vs $\beta$ and fitted with linear fit (Figure (4)). Fit gives us negative slop of $\frac{d\beta}{d\lambda}$ which satisfies the theoretical predictions. However the error in the fitting ("Pearson's r": 0.9767071360229749) shows the effect of taking less number of Monte Carlo steps. But the constraints being computational time and complexity which was around 6 hours for 5000 Monte Carlo steps. Hence to save the computational load some errors in the data was allowed.

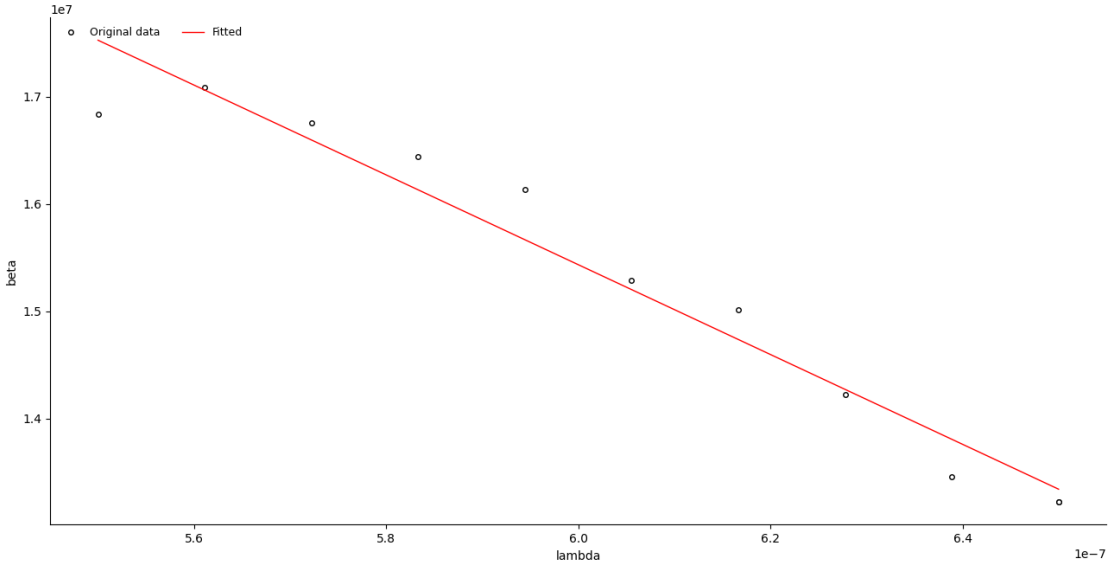


Figure 4: $\lambda$ vs $\beta$ ('Coefficients': [40550630.57184601, -41857974692198.0] "Pearson's r": 0.9767071360229749)

## 3. Conclusion

Here to solve the wave equation for an Bragg reflector we have used the variational Monte Carlo method. In which a trail function was optimized and corresponding parameter $\beta$. System's Hamiltonian had perturbation in the form of dielectric constant. As the computational power required for this to work was very high to get some accurate results, some aspects of the study was dropped. However essential observations were made such as minimization of the expectation value of Hamiltonian (For both one and two unit cells), parameter ($\beta$)'s dependence on the wavelength. The graph between $\beta$ vs $\lambda$ satisfies the theoretical predictions.

## References

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