Theory of solar cell light trapping through a nonequilibrium Green’s function formulation of Maxwell’s equations

Siddharth Buddhiraju and Shanhui Fan
Ginzton Laboratory, Department of Electrical Engineering, Stanford University, Stanford, California 94305, USA
(Received 27 April 2017; revised manuscript received 18 June 2017; published 14 July 2017)

We develop a theory of solar cell light trapping based on directly solving Maxwell’s equations through a nonequilibrium Green’s function formalism. This theory rigorously connects the maximum power absorbed by the solar cell to the density of states of the cell. With this theory we are able to reproduce all standard results in solar cell light trapping previously derived using approximate formalisms. Therefore our development places solar cell light trapping theory on a much firmer theoretical foundation. Moreover, here the maximum power formula is derived without the assumption of reciprocity, unlike previous theories on solar cell light trapping. Therefore, we prove that the upper bound of light trapping enhancement cannot be overcome with the use of nonreciprocal structures. As a numerical test, we simulate an absorber structure that consists of a nonreciprocal material, and show that the absorption enhancement factor is largely independent of nonreciprocity, in consistency with the theory.

DOI: 10.1103/PhysRevB.96.035304

I. INTRODUCTION

For practical solar cell design, various techniques of light trapping have been widely applied in order to achieve near-complete absorption of sunlight using a cell with a thickness that is smaller than the absorption depth of the material [1–23]. The use of light trapping can reduce the amount of material used in a solar cell and hence reduce the cost of solar energy. In addition, the use of a thinner cell without sacrificing absorption capability enhances carrier ejection and therefore the efficiency of the solar cell [24].

The practical importance of light trapping in solar cells, in turn, has motivated a significant body of theoretical works aiming to understand the fundamental limits of absorption enhancement that can be achieved with light trapping techniques. Reference [1] considered the theoretical limits for light trapping in standard crystalline silicon cells. Using an argument combining ray optics with thermodynamics, it was shown that compared to a single-pass absorption coefficient, light trapping previously derived using approximate formalisms. For these structures, ray optics theory is no longer applicable. Therefore, in parallel there have been substantial developments seeking to formulate light trapping theory instead from an electromagnetic point of view [26–30]. In particular, in Refs. [28–30] a statistical coupled mode theory formalism for light trapping in solar cells was developed. Using this formalism, the standard results of light trapping in crystalline silicon solar cells, as previously derived with ray optics, could be reproduced. Moreover, it was predicted that in the nanophotonic regime the 4 limit could be significantly overcome through nanoscale modal confinement over broad bandwidths. Related to these works, it was discussed in Ref. [31] that the light trapping enhancement factor can be related to the local density of electromagnetic modes.

The coupled mode theory formalism that underlies the work of Refs. [28–30], however, is an approximate formalism. While it is very well justified especially when considering the coupling of external light with a structure containing only a few modes [32–34], in a solar cell system one needs to consider a large number of optical modes. In order to place the theory of light trapping in nanophotonic structures on a firmer theoretical foundation, it is therefore of fundamental importance to formulate the problem of light trapping directly from Maxwell’s equations.

In this paper, we develop a theory of light trapping directly from Maxwell’s equations. For this purpose, we adapt the nonequilibrium Green’s function (NEGF) formalism [35,36], which has been widely used in studying transport in nanoscale electronic systems, for Maxwell’s equations. Our theory provides a rigorous proof of the connection of light trapping enhancement factor to the density of states (DOS) of the device. This connection can then be used to reproduce the standard predictions of light trapping theory. Moreover, as a key theoretical component, the proof here does not use reciprocity or detailed balance. This is in contrast to Ref. [28] where the underlying temporal coupled mode theory formalism is derived using the assumption of reciprocity. It is also in contrast with Ref. [1] which uses a detailed balance of nanophotonic solar cells, where both the thickness of the cell and the size of features used for light trapping purposes are on a single-wavelength or even deep subwavelength scale [7–12,14–16,18,20]. For these structures, ray optics theory is no longer applicable. Therefore, in parallel there have been substantial developments seeking to formulate light trapping theory instead from an electromagnetic point of view [26–30]. In particular, in Refs. [28–30] a statistical coupled mode theory formalism for light trapping in solar cells was developed. Using this formalism, the standard results of light trapping in crystalline silicon solar cells, as previously derived with ray optics, could be reproduced. Moreover, it was predicted that in the nanophotonic regime the 4 limit could be significantly overcome through nanoscale modal confinement over broad bandwidths. Related to these works, it was discussed in Ref. [31] that the light trapping enhancement factor can be related to the local density of electromagnetic modes.

The coupled mode theory formalism that underlies the work of Refs. [28–30], however, is an approximate formalism. While it is very well justified especially when considering the coupling of external light with a structure containing only a few modes [32–34], in a solar cell system one needs to consider a large number of optical modes. In order to place the theory of light trapping in nanophotonic structures on a firmer theoretical foundation, it is therefore of fundamental importance to formulate the problem of light trapping directly from Maxwell’s equations.

In this paper, we develop a theory of light trapping directly from Maxwell’s equations. For this purpose, we adapt the nonequilibrium Green’s function (NEGF) formalism [35,36], which has been widely used in studying transport in nanoscale electronic systems, for Maxwell’s equations. Our theory provides a rigorous proof of the connection of light trapping enhancement factor to the density of states (DOS) of the device. This connection can then be used to reproduce the standard predictions of light trapping theory. Moreover, as a key theoretical component, the proof here does not use reciprocity or detailed balance. This is in contrast to Ref. [28] where the underlying temporal coupled mode theory formalism is derived using the assumption of reciprocity. It is also in contrast with Ref. [1] which uses a detailed balance of nanophotonic solar cells, where both the thickness of the cell and the size of features used for light trapping purposes are on a single-wavelength or even deep subwavelength scale [7–12,14–16,18,20]. For these structures, ray optics theory is no longer applicable. Therefore, in parallel there have been substantial developments seeking to formulate light trapping theory instead from an electromagnetic point of view [26–30]. In particular, in Refs. [28–30] a statistical coupled mode theory formalism for light trapping in solar cells was developed. Using this formalism, the standard results of light trapping in crystalline silicon solar cells, as previously derived with ray optics, could be reproduced. Moreover, it was predicted that in the nanophotonic regime the 4 limit could be significantly overcome through nanoscale modal confinement over broad bandwidths. Related to these works, it was discussed in Ref. [31] that the light trapping enhancement factor can be related to the local density of electromagnetic modes.

The coupled mode theory formalism that underlies the work of Refs. [28–30], however, is an approximate formalism. While it is very well justified especially when considering the coupling of external light with a structure containing only a few modes [32–34], in a solar cell system one needs to consider a large number of optical modes. In order to place the theory of light trapping in nanophotonic structures on a firmer theoretical foundation, it is therefore of fundamental importance to formulate the problem of light trapping directly from Maxwell’s equations.

In this paper, we develop a theory of light trapping directly from Maxwell’s equations. For this purpose, we adapt the nonequilibrium Green’s function (NEGF) formalism [35,36], which has been widely used in studying transport in nanoscale electronic systems, for Maxwell’s equations. Our theory provides a rigorous proof of the connection of light trapping enhancement factor to the density of states (DOS) of the device. This connection can then be used to reproduce the standard predictions of light trapping theory. Moreover, as a key theoretical component, the proof here does not use reciprocity or detailed balance. This is in contrast to Ref. [28] where the underlying temporal coupled mode theory formalism is derived using the assumption of reciprocity. It is also in contrast with Ref. [1] which uses a detailed balance of nanophotonic solar cells, where both the thickness of the cell and the size of features used for light trapping purposes are on a single-wavelength or even deep subwavelength scale [7–12,14–16,18,20]. For these structures, ray optics theory is no longer applicable. Therefore, in parallel there have been substantial developments seeking to formulate light trapping theory instead from an electromagnetic point of view [26–30]. In particular, in Refs. [28–30] a statistical coupled mode theory formalism for light trapping in solar cells was developed. Using this formalism, the standard results of light trapping in crystalline silicon solar cells, as previously derived with ray optics, could be reproduced. Moreover, it was predicted that in the nanophotonic regime the 4 limit could be significantly overcome through nanoscale modal confinement over broad bandwidths. Related to these works, it was discussed in Ref. [31] that the light trapping enhancement factor can be related to the local density of electromagnetic modes.

The coupled mode theory formalism that underlies the work of Refs. [28–30], however, is an approximate formalism. While it is very well justified especially when considering the coupling of external light with a structure containing only a few modes [32–34], in a solar cell system one needs to consider a large number of optical modes. In order to place the theory of light trapping in nanophotonic structures on a firmer theoretical foundation, it is therefore of fundamental importance to formulate the problem of light trapping directly from Maxwell’s equations.

In this paper, we develop a theory of light trapping directly from Maxwell’s equations. For this purpose, we adapt the nonequilibrium Green’s function (NEGF) formalism [35,36], which has been widely used in studying transport in nanoscale electronic systems, for Maxwell’s equations. Our theory provides a rigorous proof of the connection of light trapping enhancement factor to the density of states (DOS) of the device. This connection can then be used to reproduce the standard predictions of light trapping theory. Moreover, as a key theoretical component, the proof here does not use reciprocity or detailed balance. This is in contrast to Ref. [28] where the underlying temporal coupled mode theory formalism is derived using the assumption of reciprocity. It is also in contrast with Ref. [1] which uses a detailed balance of nanophotonic solar cells, where both the thickness of the cell and the size of features used for light trapping purposes are on a single-wavelength or even deep subwavelength scale [7–12,14–16,18,20]. For these structures, ray optics theory is no longer applicable. Therefore, in parallel there have been substantial developments seeking to formulate light trapping theory instead from an electromagnetic point of view [26–30]. In particular, in Refs. [28–30] a statistical coupled mode theory formalism for light trapping in solar cells was developed. Using this formalism, the standard results of light trapping in crystalline silicon solar cells, as previously derived with ray optics, could be reproduced. Moreover, it was predicted that in the nanophotonic regime the 4 limit could be significantly overcome through nanoscale modal confinement over broad bandwidths. Related to these works, it was discussed in Ref. [31] that the light trapping enhancement factor can be related to the local density of electromagnetic modes.

The coupled mode theory formalism that underlies the work of Refs. [28–30], however, is an approximate formalism. While it is very well justified especially when considering the coupling of external light with a structure containing only a few modes [32–34], in a solar cell system one needs to consider a large number of optical modes. In order to place the theory of light trapping in nanophotonic structures on a firmer theoretical foundation, it is therefore of fundamental importance to formulate the problem of light trapping directly from Maxwell’s equations.
The device under consideration in this work is a solar cell with an arbitrary geometry. The cell surface may be patterned with gratings \[8,28\] or textured \[4,37\] to enhance coupling with incident radiation. Figure 1(a) depicts a typical cell operating under solar radiation that covers a narrow angular range (orange). The cell surfaces may be patterned to enhance coupling with incident radiation. The emission from the cell has a broad angular (green) response. A rear reflector is usually placed underneath such a cell to enhance absorption. (b) The same cell under concentrated, near-isotropic incident radiation from the upper half-space. (c) A setup theoretically related to (b), with a near-isotropic incident radiation as well as emission from the cell.

FIG. 1. (a) A typical cell operating under solar radiation that covers a narrow angular range (orange). The cell surfaces may be patterned to enhance coupling with incident radiation. The emission from the cell has a broad angular (green) response. A rear reflector is usually placed underneath such a cell to enhance absorption. (b) The same cell under concentrated, near-isotropic incident radiation from the upper half-space. (c) A setup theoretically related to (b), with a near-isotropic incident radiation as well as emission from the cell.

The solar radiation incident on the cell can be described by a stationary random process, such that the ensemble average of the incident electric and magnetic fields are time independent. Therefore, the field-field correlation for the incident electric field \(E_i\) is given by \(\langle E_i(r,\omega)E_i^*(r',\omega')\rangle = 2\pi\delta(\omega - \omega')\langle E_i(r)E_i^*(r')\rangle\), where the \(\delta(\omega - \omega')\) term appears because of stationarity. In this paper, the superscript refers to a conjugate transpose, while the \(T\) superscript refers to only a transpose.

Since the cell receives this stationary input field, the electric field in the device, \(E_D(r)\), is also described by a stationary random process with a field-field correlation function:

\[
\langle E_D(r,\omega)E_D^*(r',\omega')\rangle = 2\pi\delta(\omega - \omega')\langle E_D(r)E_D^*(r')\rangle\omega.
\]

The ensemble-averaged power absorbed by the cell can then be determined from Poynting’s theorem (Ref. [38], p. 259) in the absence of any currents:

\[
\int dS \cdot (E_D \times H_D) = -\int dV \left\{ E_D(r) \cdot \frac{\partial D_D(r)}{\partial t} + H_D(r) \cdot \frac{\partial B_D(r)}{\partial t} \right\}.
\]

A nonzero value of the left-hand side would indicate a net flow of power into the cell, i.e., absorption in the cell. We evaluate the first term on the right-hand side of Eq. (2) as follows:

\[
P = -\int dV \left\{ E_D(r) \cdot \frac{\partial D_D(r)}{\partial t} \right\},
\]

\[
= \int dV \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} E_D(r,\omega) \cdot i\omega' D_D^*(r,\omega') e^{i(\omega-\omega')t},
\]

\[
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega'd\omega}{(2\pi)^2} i\omega' \text{Tr}(E_D(\omega)D_D^*(\omega')) e^{i(\omega-\omega')t}.
\]
Note that in Eqs. (2) and (3) the fields are the underlying physical, time-dependent fields that are real, whereas in the rest of the paper the fields are complex plasmons.

In obtaining Eq. (5), we use $E_D(\omega)$ to represent a column vector, which, when all indices are explicitly shown, denotes $E_{D,m}(\mathbf{r}, \omega)$, where $m$ denotes the indices for the polarization. $E_D(\omega)D_0(\omega')$ therefore represents a tensorial quantity, which corresponds to $E_{D,m}(\mathbf{r}, \omega)D_{D,m}^{\dagger}(\mathbf{r}', \omega')$, where $m$ and $n$ again denote the polarization index. For any tensorial quantity $A \equiv A_{mn}(\mathbf{r}, \mathbf{r}')$, the trace operator $\text{Tr}$ is defined as

$$\text{Tr} A \equiv \sum_m \int dV A_{mn}(\mathbf{r}, \mathbf{r}).$$

That is, the operator $A$ can be considered a large matrix indexed both in polarization and position. The $\text{Tr}$ operation is then simply the sum of the diagonal elements of the matrix. For the continuous position coordinate, this sum is in fact an integral over the volume of the device. For the rest of the paper, we will be using such vector and tensor quantities whenever we do not explicitly exhibit the coordinate and polarization indices.

Next, we used Eq. (1) to obtain Eq. (7). To obtain Eq. (8) we use the fact that, because the underlying fields $E(\mathbf{r},t)$ and $D(\mathbf{r},t)$ are real, $\epsilon^*(-\omega) = \epsilon(\omega)$ and $E^*(-\omega) = E(\omega)$ (Ref. [38], p. 262).

With a similar derivation, one can show that the second term on the right-hand side of Eq. (2) is zero since we assume that permeability to be $\mu_0$ with no imaginary part.

In order to compute the absorption of the solar cell, we need to relate the fields inside the device, $E_D$, to the incident solar radiation $E_I$. This relation is obtained from the nonequilibrium Green’s function (NEGF) formalism in the next section.

III. NEGF FORMULATION FOR A LOSSLESS SYSTEM

Certainly, the materials used in solar cells are absorptive, and therefore are described by a dielectric function $\epsilon(\mathbf{r})$ with a nonzero imaginary part. However, in the understanding of light trapping theory, the computation of the enhancement factor when the material loss is infinitesimal plays a significant role [1,4,28,39]. Therefore, in this paper we will start by considering the case where the material absorption is infinitesimal. The formalism that we develop here, however, can be generalized to treat the case where the material absorption is non-negligible, which we will discuss in Sec. VII.

To compute the absorption enhancement factor where the material absorption is infinitesimal, in this section we consider the corresponding lossless system as described by the real part $\epsilon_R(\mathbf{r})$ of the dielectric function $\epsilon(\mathbf{r})$, i.e., $\epsilon_R(\mathbf{r}) = \text{Re}[\epsilon(\mathbf{r})]$, and describe the electromagnetic structure and the coupling of externally incident waves to such a system. In the next section we then relate the absorption properties of the system with infinitesimal loss to such a lossless system.

Further, for simplicity, we ignore material dispersion in the real part of the dielectric function, i.e., $\epsilon_R(\mathbf{r}, \omega) = \epsilon_R(\mathbf{r})$. This simplification is justified since, for light-trapping purposes, one typically considers a frequency range near the semiconductor band-edge where the variation in the real part of the dielectric function, i.e., in $\epsilon_R(\mathbf{r}, \omega)$, is usually small. In addition, we restrict $\epsilon_R(\mathbf{r})$ to be positive definite, which is applicable for typical semiconductors. However, we note that both the material dispersion and the negative dielectric constant cases can be treated in a fashion similar to what we consider here by an auxiliary field approach [40]. With this approach, one can formulate the modal structure of a dispersive medium as a standard eigenvalue problem where the system matrix has no explicit frequency dependence. Therefore, the formalism that we develop here can be generalized for systems such as plasmonics-enhanced solar cells [11].

Consider Maxwell’s equations in the frequency domain for a system described by $\epsilon_R$:

$$\nabla \times E(\omega) = -i\omega B(\omega),$$
$$\nabla \times H(\omega) = i\omega D(\omega),$$

with the constitutive relations

$$B(\omega) = \mu_0 H(\omega),$$
$$D(\omega) = \epsilon_0 \epsilon_R E(\omega).$$

Since $\epsilon_R$ is positive semidefinite, a positive semidefinite square root $\sqrt{\epsilon_R}$ exists, and Eqs. (11) to (14) can be combined to form a Hermitian eigenvalue problem [41]:

$$\mathbb{H} \mathbf{F} = \left[\sqrt{\epsilon_R^{-1}} \nabla \times \nabla \times \sqrt{\epsilon_R^{-1}}\right] \mathbf{F} = \frac{\omega^2}{c^2} \mathbf{F},$$

where $\mathbf{F} = \sqrt{\epsilon_R} \mathbf{E}$. To make a connection to the standard NEGF literature, we refer to the operator $\mathbb{H}$ defined above as the “Hamiltonian” of the system.

We now apply Eq. (15) to the system containing both the cell itself and the surrounding air regions that have a uniform $\epsilon = 1$. The following derivation is based largely on Ref. [35], starting on p. 188, and its results are summarized in Ref. [35], p. 223. The readers are referred to Ref. [35] for a detailed discussion of the concepts in this section, and to Ref. [42] for a more formal treatment of NEGF.

The Hamiltonian of the system, $\mathbb{H}$, can be decomposed as

$$\mathbb{H} = \left(\begin{array}{cc} \mathbb{H}_S & \tau^\dagger \\ \tau & \mathbb{H}_D \end{array}\right),$$

where $\mathbb{H}_S$ and $\mathbb{H}_D$ are the Hamiltonians of the surroundings and the cell, respectively. The off-diagonal terms $\tau$ and $\tau^\dagger$ can be numerically obtained, for example, by explicitly constructing $\mathbb{H}$ in Eq. (15) by discretizing the spatial coordinates $\mathbf{r}$. We note that $\tau$ is in general not equal to $\tau^\dagger$. In other words, $\mathbb{H}$ might not be a symmetric matrix, and therefore we do not
assume reciprocity in this derivation. Using Eq. (16), Eq. (15)
can be rewritten as

\[
\begin{pmatrix}
\left( \frac{\omega}{c} \right)^2 - \mathbb{H}_S & -\tau \\
\tau & \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_D
\end{pmatrix}
\begin{pmatrix}
F_I \\
F_{S\text{c}} + F_D
\end{pmatrix} = 0,
\]
(17)

where \( F = (F_I + F_{S\text{c}}, F_D)^T \) is an eigenvector of \( \mathbb{H} \). The
subscripts of \( F \) are used to distinguish components of \( F \). \( F_I \) is
the field incident from the surroundings onto the device (solar
cell), \( F_{S\text{c}} \) is the scattered field from the device back into the
surroundings, and \( F_D \) is the field in the device. Figure 2 depicts
the incident, scattered, and device fields as described here.

An expression for the field in the device \( F_D \) can be obtained
by solving Eq. (17). To do this, we first note that the incident
field \( F_I \) satisfies \( \left( \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_S \right) F_I = 0 \). Therefore from the first
row of Eq. (17), \( \left( \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_S \right) F_{S\text{c}} - \tau F_D = 0 \), so that

\[ F_{S\text{c}} = G_{S\text{c}} \tau F_D, \]
(18)

where \( G_{S\text{c}} = \left( \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_S - i\eta \right)^{-1} \), with \( \eta \) being an infinitesimal
positive number, is the retarded Green’s function for the free
space surrounding the device. Note that the retarded
Green’s function contains a \( -\eta \) here, in contrast with \( +\eta \) in Ref. [35], due to
the \( +i\omega t \) convention used here as opposed to the
\(-i\omega t \) convention used in quantum mechanics. From the second
row of Eq. (17), \( \left( \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_D \right) F_D - \tau (F_I + F_{S\text{c}}) = 0 \),
which gives

\[
\left[ \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_D - \Sigma \right] F_D = \tau F_I,
\]
(19)

where \( \Sigma = \tau G_{S\text{c}} \tau^\dagger \) is the self-energy. Equation (19) can
be succinctly written as

\[ F_D = G_D \tau F_I, \]
(20)

where we identify

\[ G_D = \left[ \left( \frac{\omega}{c} \right)^2 - \mathbb{H}_D - \Sigma \right]^{-1}, \]
(21)

as the effective Green’s function for the device coupled to its
environment.

Before we provide a discussion of the density of states of
the device under consideration, we consider the density of
states of a closed system. Consider the Green’s function for a
general system with Hamiltonian \( \mathbb{H}, G = \left( \left( \frac{\omega}{c} \right)^2 - \mathbb{H} - i\eta \right)^{-1} \).

From the equation \( \mathbb{H} G^{(m)} = (\omega^2_m/c^2) G^{(m)} \), we have the retarded
Green’s function

\[ G = c^2 \sum_m \frac{G^{(m)} F^{(m)}(\omega^2_m)}{\omega^2 - \omega^2_m - i\eta}. \]
(22)

The density of states is related to \( \text{Im} \ G \), which from Eq. (22)
is given by

\[ \frac{1}{\pi} \text{Im} G = c^2 \sum_m \delta(\omega - \omega_m) G^{(m)} \to G^{(m)} \]

\[ = c^2 \sum_m \frac{1}{2\omega_m} \delta(\omega - \omega_m) F^{(m)} \to F^{(m)}, \]
(23)

which gives us the relation

\[ A \equiv \sum_m \delta(\omega - \omega_m) F^{(m)} \to F^{(m)} = \frac{2\omega}{\pi^2 c^2} \text{Im} G, \]
(24)

where, following the nomenclature of NEGF [35], \( A \) is called
the spectral function. Note that we dropped the negative
frequency solutions \( -\omega_m \) in the summation since we are
interested only in an integration over positive frequencies
in Eq. (9). The local density of states (LDOS) \( \rho(r) \) is given by [43]

\[ \rho(r) \equiv \sum_{i=1}^3 A_{i\text{c}}(r, r) \]

\[ = \sum_m \delta(\omega - \omega_m) F^{(m)} \to F^{(m)} \to F^{(m)} \]
(25)

Generalizing from the discussion above for the LDOS of
a closed system, we define a spectral function specific to the
device, given by

\[ A_D = \frac{2\omega}{\pi^2 c^2} \text{Im} G_D, \]
(26)

where \( G_D \) is defined by Eq. (21). Equation (26) can be
manipulated to form a useful identity [35] using the following
relation:

\[ \text{Im} G_D = \frac{1}{2i} (G_D - G_D^\dagger) \]

\[ = \frac{1}{2i} G_D (G_D^{-1} - G_D^{-1}) G_D^\dagger \]

\[ = \frac{1}{2i} G_D \left( \frac{\omega^2}{c^2} - \mathbb{H} - \Sigma^{-1} - \frac{\omega^2}{c^2} + \mathbb{H} + \Sigma \right) G_D^\dagger \]

\[ = \frac{1}{2i} G_D (\Sigma - \Sigma^{-1}) G_D^\dagger \]

\[ = G_D [\text{Im} \Sigma] G_D^\dagger \]

\[ = G_D \tau [\text{Im} G_S] \tau^\dagger G_D^\dagger \]
(27)

since \( \Sigma = \tau G_S \tau^\dagger \). Therefore,

\[ A_D = \frac{2\omega}{\pi^2 c^2} G_D \tau [\text{Im} G_S] \tau^\dagger G_D^\dagger, \]
(28)
has the interpretation of the “accessible” density of states. To see this, note that if $\Sigma$ is zero then $G_D$ is Hermitian, and therefore $A_D = 0$ from Eq. (26). This notion can be generalized: if a subset of modes do not couple with the surroundings, then $\Sigma$ for those modes is zero, and $A_D$ corresponding to those modes is zero. Therefore, $\sum mA_{mm, D}(r, r, \omega)$ is the local density of device modes that can couple with the incident radiation. On the other hand, the full Green’s function will consist of the decoupled surroundings and device Green’s functions. Therefore, $G$ over the device coordinates will simply be $(\omega^2/c^2 - \epsilon_D - i\gamma)^{-1}$, and $\sum mA_{mm}(r, r, \omega)$ will then be the device local density of states, regardless of whether these states actually couple to the incident radiation. This means that $\sum mA_{mm, D}(r, r, \omega)$ is in general less than or equal to the local density of states given by $\sum mA_{mm}(r, r, \omega)$ corresponding to the isolated device, i.e.,

$$\sum mA_{mm, D}(r, r, \omega) \leq \sum mA_{mm}(r, r, \omega).$$

## IV. Absorption under Fully Concentrated Sunlight

We now have a mathematical structure to connect the device field $F_D$ to the incident field $F$ described through Eq. (20). We have also established the concept of LDOS defined through Eqs. (26) and (28) for a lossless system. As a step forward, suppose the device has a small imaginary part of $\epsilon(r)$, i.e., $\text{Im}(\epsilon)/\text{Re}(\epsilon) \ll 1$. Then the solutions $F_D$ of the corresponding lossless system are sufficiently good approximations to the solutions in the lossy device. Therefore, for small losses, we can apply the NEGF formulation in the previous section to Eq. (9) to compute the absorbed power:

$$P = \int_0^\infty \frac{d\omega}{\pi} \omega \text{Tr} \left[ I m \epsilon(\omega) G_D^\dagger G_D \right]$$

$$= \int_0^\infty \frac{d\omega}{\pi} \omega \Theta(\omega) \text{Tr} \left[ \sqrt{\epsilon_r} \sqrt{\epsilon_{D}} G_D^\dagger \frac{2\omega}{\pi c} \frac{\epsilon_r}{\epsilon_r - 1} \frac{\text{Im} G_S}{\sqrt{\epsilon_{D}}} \right]$$

$$= \int_0^\infty \frac{d\omega}{\omega} \omega \Theta(\omega) \text{Tr} \left[ \sqrt{\epsilon_r} \sqrt{\epsilon_{D}} G_D^\dagger \frac{2\omega}{\pi c} \frac{\epsilon_r}{\epsilon_r - 1} \frac{\text{Im} G_S}{\sqrt{\epsilon_{D}}} \right],$$

where we used Eq. (28) to obtain Eq. (33). This result also tells us the optimal structural character of the cell: from Eq. (29), maximum power absorption occurs when all modes in the device become “accessible” to the environment. That is,

$$P_{\text{max}} = \int_0^\infty d\omega \omega \Theta(\omega) \text{Tr} \left[ \sqrt{\epsilon_r} \epsilon_r^\dagger \right]$$

$$= \int_0^\infty d\omega \omega \Theta(\omega) \text{Tr} \left[ \sqrt{\epsilon_r} \epsilon_r^\dagger A_D(\omega) \right].$$

The derivations leading to Eqs. (33) and (34) represent the major results of this paper. The results provide a rigorous derivation of the connection between the absorption under maximum concentration to the accessible density of states inside the device. This connection was previously argued in Ref. [1] using the argument of detailed balance, assuming that the cell consists of a bulk medium. This connection was generalized in Refs. [28] and [31] for nanophotonic geometry. Neither of these papers, however, provide a rigorous derivation of this connection directly from Maxwell’s equations. Our results here therefore provide a rigorous justification of the foundation of light trapping theory. In the next two sections we will explore the consequences of Eqs. (33) and (34). In Sec. V we provide a re-derivation of the standard light trapping results, starting from these equations.

We note that, to arrive at Eq. (34), we make no assumption of the coupling between the free space and the device as described by the matrix $\tau$, other than the assumption that all modes in the cell are accessible. Thus, Eq. (34) is equally applicable to a solar cell that has a Lambertian surface and hence absorbs and emits isotropically, as well as to a solar cell that has a strong angular selectivity. We will use this observation in Sec. V when we discuss the light trapping limit for a solar cell with a strong angular selectivity.
Before we discuss absorption enhancement, we would like to make a brief comment on spatial coherence of sunlight in the context of Eq. (31). In the formalism of fluctuational electrodynamics, which we use to obtain Eq. (31), the current-current correlation of the current source in the sun has the form

\[
\langle J(r)J^*(r') \rangle_\omega = \frac{\hbar \omega}{2k_B T} \text{coth} \frac{\hbar \omega}{2k_B T} \text{Im} \epsilon(r,r) \delta(r-r').
\]

(35)

That is, the current source in the sun is spatially incoherent. On the other hand, it is known that the sunlight is partially coherent [45,46], and that coherence impacts device performance [47,48]. We would like to point out here that our formalism, which builds upon fluctuational electrodynamics, takes spatial coherence into account in a systematic fashion because the field-field correlation of Eq. (31) is proportional to \( \text{Im} \mathcal{G}_S \), which in general is not proportional to \( \delta(r-r') \).

We also note that the derivation of Eq. (33) makes no use of reciprocity. Therefore, in Sec. VI we use these results to discuss light trapping in nonreciprocal structures.

V. ABSORPTION ENHANCEMENT

Various limits on absorption enhancement have been derived previously. The \( 4n^2 \) limit in [1] was derived from a statistical thermodynamics and ray-tracing approach. This can be extended to a \( 4n^2/\sin^2 \theta \) limit [3,49] for the case of angle-selective emission from the solar cell. In addition, Ref. [8] considers the case of light trapping with a subwavelength grating, and concludes that at normal incidence that enhancement factor can significantly exceed the \( 4n^2 \) limit. In this section, we briefly re-derive these limits starting from Eq. (34).

To derive the \( 4n^2 \) limit, following Ref. [1], we consider a solar cell as described by a dielectric slab of side \( L \) and thickness \( d \) with a uniform dielectric constant \( \epsilon = n^2 + 12n''/n \) such that \( n''/n \ll 1 \), where \( n \) and \( n'' \) are the real and imaginary parts of the refractive index, respectively. The absorption coefficient \( \alpha_0 = 2 \text{Im} \epsilon \sqrt{\epsilon/c} = 2n\epsilon''/c \). To start we assume that the device is under a full concentration of solar light, as shown in Fig. (1c). To achieve light trapping in such a solar cell, one applies random roughness with a Lambertian profile on the surface of the solar cell, which allows all modes in the device to be accessible. As a result we can use Eq. (34) to compute the absorption in the cell. For such a slab \( \text{Tr} \mathcal{A} = L^2 dn'/\omega^2/\pi^2c^3 \). With \( \epsilon''/\epsilon' = 2n''/n \) and \( \Theta(\omega) = \hbar \omega/\text{exp}(\hbar \omega/k_B T) - 1 \), the absorbed power in a narrow frequency range between \( \omega \) and \( \omega + \Delta \omega \) is then

\[
P_{\text{max}} = \frac{\hbar \omega}{e^{\hbar \omega/k_B T}} \Bigg[ \frac{2n''^2 \omega^2}{n \pi^2 c^3} \Delta \omega L^2 d \Bigg] = 2n^2 \alpha_0 d \left[ \frac{\omega^2 \Delta \omega}{4 \pi^2c^2} \frac{\hbar \omega}{e^{\hbar \omega/k_B T} - 1} - L^2 \right].
\]

(36)

where the quantity in the brackets is the well-known formula for power from isotropic blackbody radiation, incident in this case on a surface of area of \( 2L^2 \). With the bracketed quantity as the input power \( P_{\text{in}} \), the maximum enhancement is

\[
f = \frac{1}{\alpha_0 d} P_{\text{max}}/P_{\text{in}} = 2n^2.
\]

(37)

The standard result of \( 4n^2 \) corresponds to the case where a perfect rear reflector is placed with the source only incident from the upper half-hemisphere. Because of the reflector, the absorbed power remains the same; but the incident power is only a half of the isotropic radiation:

\[
f = \frac{1}{\alpha_0 d} P_{\text{max}}/P_{\text{in}}/2 = 4n^2.
\]

(38)

The commonly derived limit of \( 4n^2 \) corresponds to a single incident mode on a solar cell with a Lambertian surface. However, since a Lambertian surface results in equal absorption from all incident modes, the absorbed power as well as the incident power are scaled by the same factor in going from isotropic illumination to a single incident mode. In other words, the absorption enhancement factor remains unaffected by the angular range of incident radiation on a solar cell with a Lambertian surface.

The derivation above can be generalized to describe a solar cell with strong angular selection. As an illustration, we consider a solar cell that has equal absorption for light within the absorption cone having an angle of incidence within a range \( \theta \) around the normal direction, and has zero absorption for incident light outside the absorption cone. In this case, assuming all modes within the cell are accessible, under full concentration the absorption of solar cell is described by Eq. (36). On the other hand, since the incident light outside the absorption cone does not contribute to the solar cell absorption, the absorption remains unchanged if we restrict the incident radiation to only within the absorption cone. That is, the absorption remains unchanged even when the incident light is reduced to \( P_{\text{in}} = [\omega^2 \Delta \omega/4 \pi^2c^2] \Theta(\omega) \sin^2 \theta \), which leads to the limit of \( 4n^2/\sin^2 \theta \).

Reference [8] considered the case where the light trapping is accomplished by placing a grating with a subwavelength periodicity on the surface of solar cell, and showed that in this case the enhancement factor can significantly exceed \( 4n^2 \) for normally incident light. This increased enhancement factor arises due to angle selectivity of the grating structure in the single-channel regime, and comes at the expense of lower enhancement at large angles [8] since the total enhancement integrated across all angles is constrained for any solar cell structure [29]. This is in contrast with the scheme of Refs. [28,50], where an enhancement factor exceeding \( 4n^2 \) for all angles of incidence was achieved in a thin, low-index absorber surrounded by high-index media. We re-derive the result of Ref. [8] for normal incidence using the formalism developed in Sec. IV. When the grating period is less than the free-space wavelength, normally incident light cannot scatter into any other directions aside from normal. Therefore, the surrounding medium can be described as a one-dimensional system. In using Eq. (31) to describe the incident light, one needs to use an expression for \( \text{Im} \mathcal{G}_S \) that is appropriate for the one-dimensional system. With this modification, the derivation to Eq. (36) remains unchanged. That is, assuming that all modes in the cell are accessible, the power absorbed by the cell is

\[
P_{\text{max}} = 4n^2 \alpha_0 d \left[ \frac{\omega^2 \Delta \omega}{4 \pi^2c^2} \frac{\hbar \omega}{e^{\hbar \omega/k_B T} - 1} - L^2 \right].
\]

(39)
where \( l \) is the periodicity of the patterning on the top surface. On the other hand, the incident power changes from its three-dimensional (3D) expression of \( I^2 \Theta(\omega) \omega^2 \Delta \omega / 4 \pi^2 c^2 \) to the 1D expression of \( \Theta(\omega) \Delta \omega / \pi c \), where we used the fact that the 1D density of states is \( \Delta \omega / \pi c \). Therefore, the enhancement factor in this scenario is modified from the expression in Eq. (38) to

\[
f = 4n^2 \Theta(\omega) \frac{\Delta \omega}{2 \pi c} \frac{l^2}{s^2} = 4\pi n^2 s^2,
\]

where \( s = l / \lambda \).

VI. LIGHT TRAPPING IN NONRECIPROCAL SYSTEMS

In the previous section we used the NEGF formalism to reproduce the standard theoretical results for solar cell light trapping. As noted in Sec. IV, however, our result here is in fact more general as compared to previous theoretical work on solar cell light trapping in that we do not make an assumption on reciprocity. This is in contrast to previous theoretical works in this area. For example, Ref. [1] assumes detailed balance in order to reach a conclusion similar to Eq. (33). Detailed balance is a consequence of reciprocity. In Ref. [28], results similar to Eq. (33) were derived using the temporal coupled mode theory formalism, which again assumes reciprocity. In our work here, by re-deriving all these previous results in Sec. V, we have in fact shown that these results are equally applicable to a cell containing nonreciprocal materials.

The potential of using nonreciprocal materials for solar energy conversion is a subject that is of fundamental interest. It is known that the Landsberg limit, which represents the upper limit of solar energy conversion, can only be reached with the use of non-reciprocal materials [51–54]. On the other hand, it is also known that the reciprocity between emission and absorption can be broken with the use of magneto-optical media, and such a reciprocity breaking can be further enhanced with the use of nanophotonic structures [55,56]. These results raise the question as to how breaking reciprocity affects the light trapping limit. Since Eq. (34) is applicable for both reciprocal and nonreciprocal cases, our results show that as long as the accessible density of states within the solar cell is the same, the upper limit of light trapping enhancement should not be affected by reciprocity breaking.

We validate the theoretical results above using numerical simulations. For the absorber we consider a slab of a non-reciprocal material. The slab has a thickness of 3 micron. The dielectric constant of such a material is in general asymmetric, i.e., \( \epsilon^T \neq \epsilon \). As an illustration, we choose the following form [57]:

\[
\epsilon = \begin{pmatrix}
(n + i \kappa)^2 & i \delta & 0 \\
-i \delta & (n + i \kappa)^2 & 0 \\
0 & 0 & (n + i \kappa)^2
\end{pmatrix}
\]

where \( n^2 = 12.5 \). \( \delta \) characterizes the strength of the non-reciprocity, with \( \delta = 0 \) describing the reciprocal material. The loss \( \kappa \) is chosen such that the absorption length \( a_0^{-1} \) in the reciprocal case of \( \delta = 0 \) equals \( 2 \sigma_0 k(\omega) / c \) \( = 22.5 \text{ mm} \) over the wavelength range of interest. For typical magneto-optical materials, the maximum \( \delta / n^2 \) is typically \( < 10^{-2} \) (see, e.g., Refs. [58,59]). In our numerical simulation, however, to explore the effect of nonreciprocity, we consider a much wider range \( \delta \) from 0 to 4.

To achieve light trapping in such an absorbing layer, we place a perfect electric conductor mirror at the bottom of the layer (yellow layer, Fig. 3(a)]. On the top surface we place a grating layer (orange), following Ref. [8]. The grating layer consists of several rectangle-shaped dielectric regions with dielectric constant of \( n^2 \), separated by air slots. The grating layer has a thickness of 50 nm. The periodicity \( l \) of the grating is chosen to be 600 nm on both in-plane directions. We consider a wavelength \( \lambda \) ranging from 600 to 1200 nm. The pattern of the grating is such that there is not any mirror or rotational symmetry within the plane. This choice of periodicity and the use of such an asymmetric grating pattern ensure that there is not any uncoupled mode in the slab due to either translational symmetry or point-group symmetry considerations, in our wavelength range of interest.

Within our wavelength range of interest the cell operates at the single channel regime [28], where for normally incident light in this regime there is only zeroth-order diffraction in the air region outside the cell. For the reciprocal case of \( \delta = 0 \), the theoretical upper limit of absorption enhancement in this wavelength range is given by Eq. (40), where \( s = l / \lambda \) takes values between 0.5 and 1. Therefore, the spectrally averaged
absorption enhancement over this wavelength range is
\[
\tilde{f}_{\text{TH}} = \frac{1}{\omega R - \omega L} \int_{\omega L}^{\omega R} 4\pi n^2 \omega^2 d\omega = 4\pi \frac{7}{12} n^2 \approx 91.6. \quad (42)
\]

Following the same derivation that leads to Eq. (40), the light trapping enhancement factor for the nonreciprocal case can be derived as
\[
\tilde{f}_{\text{TH}}(\delta) = \frac{1}{\omega R - \omega L} \int_{\omega L}^{\omega R} \frac{P_{\text{max}}(\omega, \delta)}{\alpha_0(\delta) d(\omega) \Delta \omega / \pi} d\omega,
\]
as shown by the black solid curve in Fig. 3(b). Here \(\alpha_0(\delta)\) is the single-pass absorption length for normally propagating light in the nonreciprocal material. The theoretical results show that the light trapping enhancement factor is largely independent of \(\delta\), in spite of the large range of \(\delta\) that we have used. We note that with our choice of a fairly sizable range of \(\delta\), the density of states does depend on \(\delta\). This dependency, however, is largely canceled out by the dependency of the group velocity on \(\delta\).

As a validation of the theoretical results, we perform a numerical simulation (blue dotted curve) using S4 [60], an electromagnetic solver for layered media based on the method of rigorous coupled wave analysis (RCWA). We vary the strength of nonreciprocity by changing \(\delta\) between 0 and 4, and compute for each case the enhancement
\[
\tilde{f}(\delta) = \frac{1}{\omega R - \omega L} \int_{\omega L}^{\omega R} \frac{\alpha(\omega)}{\alpha_0(\delta) d\omega}, \quad (44)
\]
where \(\alpha(\omega)\) is the spectrum of the absorption coefficient, averaged across polarizations. Figs. 3(c)–3(d) show such spectra for the cases of \(\delta = 0\) and \(\delta = 4\) respectively. The red curve in Fig. 3(b) serves as a reference level corresponding to the 4\(n^2\) enhancement of the single-pass absorption. We note that, in consistency with the theoretical results, the simulated enhancement \(\tilde{f}\) varies only slightly for a large variation in the nonreciprocity \(\delta\). The simulation supports our claim based on Eq. (34) that the maximum possible enhancement is set by the DOS of the material, and is unaffected by the breaking of reciprocity. The simulated enhancement \(\tilde{f}\) in all cases remains below the theoretical upper limit \(\tilde{f}_{\text{TH}}\), because at the chosen absorption length some modes are not in the overcoupling regime, where the external coupling is much greater than the intrinsic loss rate [8]. In the formalism developed here, this means that the accessible density of states \(A_D\) is smaller than the density of states \(A\) of the isolated cell.

**VII. NON-NEGLIGIBLE LOSS**

In this section, we extend the discussion of the NEGF formulation to solar cells whose loss is not infinitesimal. The wave equation upon combining Eqs. (11)–(14) is
\[
\nabla \times \nabla \times \mathbf{E}(\omega) = \frac{\omega^2}{c^2} \epsilon(\omega) \mathbf{E}(\omega).
\]

A non-Hermitian \(\epsilon(\mathbf{r}, \omega)\) can in principle have many square roots \(\sqrt{\epsilon(\mathbf{r}, \omega)}\); however, any choice of the square root will mathematically give the same power absorption, since Eq. (9) depends only on \(\epsilon(\mathbf{r}, \omega)\) and \(\mathbf{E}(\mathbf{r}, \omega)\). Further, we neglect material dispersion again by considering a narrow frequency range.

Choosing one such square root \(\sqrt{\epsilon(\mathbf{r})}\), we have
\[
\mathbb{H} \mathbf{F} = \{\sqrt{\epsilon^{-1}} \nabla \times \nabla \times \sqrt{\epsilon^{-1}}\} \mathbf{F} = \frac{\omega^2}{c^2} \mathbf{F},
\]
where the ‘Hamiltonian’ \(\mathbb{H}\) is no longer Hermitian. \(\mathbb{H}\) can still be decomposed in a manner similar to Eq. (16) as
\[
\mathbb{H} = \begin{pmatrix} \mathbb{H}_S & \tau_1 \\ \tau_2 & \mathbb{H}_D \end{pmatrix},
\]
where the cross-terms \(\tau_1\) and \(\tau_2\) correspond to the cell boundaries, and we make a simplifying assumption that the non-Hermiticity arising from Eq. (46) is captured purely in the bulk of the cell, i.e., \(\tau_1 = \tau_2 = \tau\) but \(\mathbb{H}_S \neq \mathbb{H}_D\). The Hamiltonian for the environment, \(\mathbb{H}_S\), remains Hermitian since it is unaffected by the dielectric function of the cell \(\epsilon(\mathbf{r})\).

The relations given by Eqs. (19)–(21) continue to hold for the non-Hermitian \(\mathbb{H}_D\). By defining the spectral function \(A_D\) as in Eq. (26), we observe a departure from Eq. (27):
\[
\text{Im} \mathbb{G}_D = \frac{\mathbb{G}_D - \mathbb{G}_D^\dagger}{2i} = \frac{\mathbb{G}_D G_D^{\dagger} - G_D^{\dagger} G_D}{2i} = \mathbb{G}_D \text{Im} \mathbb{G}_S G_D^{\dagger} + \mathbb{G}_D \text{Im} \mathbb{H}_D G_D^{\dagger} = \mathbb{G}_D \tau \text{Im} \mathbb{G}_S^\dagger G_D^{\dagger} + \mathbb{G}_D \text{Im} \mathbb{H}_D G_D^{\dagger},
\]
where the first term on the right-hand side is the same as Eq. (27). The second term corresponds to material loss. In the limit of the lossless system, we see that Eq. (48) reduces to Eq. (27) as \(\text{Im} \mathbb{H}_D \rightarrow 0\). Inserting this relation, rearranged as \(\mathbb{G}_D \tau \text{Im} \mathbb{G}_S^\dagger G_D^{\dagger} = \text{Im} \mathbb{G}_D \mathbb{G}_D - \mathbb{G}_D \text{Im} \mathbb{H}_D G_D^{\dagger}, \) in Eq. (32), we get
\[
P = \int_0^\infty d\omega \omega \Theta(\omega) \text{Tr} \left[ (\sqrt{\epsilon^{-1}})^{-1} \text{Im} \epsilon(\omega) \sqrt{\epsilon^{-1}} \frac{2\omega}{\pi c^2} \mathbb{G}_D \tau \text{Im} \mathbb{G}_S^\dagger G_D^{\dagger} \right]
= \int_0^\infty d\omega \omega \Theta(\omega) \text{Tr} \left[ (\sqrt{\epsilon^{-1}})^{-1} \text{Im} \epsilon(\omega) \sqrt{\epsilon^{-1}} \frac{2\omega}{\pi c^2} \mathbb{G}_D \text{Im} \mathbb{H}_D G_D^{\dagger} \right]
\]
where $A_D \equiv (2\omega/\pi c^2) \text{Im} G_D$ as before. The result here indicates that, due to the second term on the right, the enhancement factor decreases as the material absorption strength increases, in consistency with the derivation [30] from statistical-temporal coupled mode theory.

VIII. CONCLUSION

In this paper, we derived a theory of light trapping in solar cells based on the nonequilibrium Green’s function formalism applied to Maxwell’s equations. The theory provides a rigorous connection between light trapping and the accessible density of states of the cell, in the form of an upper bound on the absorption. Further, since the theory was derived without the assumption of reciprocity, the upper bound on absorption was applicable to nonreciprocal cells, showing that the standard light trapping enhancement cannot be overcome by breaking reciprocity alone. This result was numerically tested and verified on a slab-like cell with periodic patterning, where it was seen that the enhancement was largely independent of nonreciprocity for wide range of parameters. Our results here provide a rigorous theoretical foundation for the light trapping of solar cells. In addition, the development points to the potential significance of the nonequilibrium Green’s function (NEGF) formalism in the treatment of solar and thermal radiation problems.

ACKNOWLEDGMENTS

This work is supported by the US Department of Energy Grant No. DE-FG-07ER46426. S.B. in addition acknowledges the support of a Stanford Graduate Fellowship.