

Today's outline - October 23, 2024





- Writing a General User Proposal

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- Writing a General User Proposal
- Dynamical theory and the Darwin curve

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- Writing a General User Proposal
- Dynamical theory and the Darwin curve
- Extinction and absorption

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- Writing a General User Proposal
- Dynamical theory and the Darwin curve
- Extinction and absorption
- Perfect crystal integrated intensity



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Reading Assignment: Chapter 6.5; Chapter 7.1



- Writing a General User Proposal
- Dynamical theory and the Darwin curve
- Extinction and absorption
- Perfect crystal integrated intensity

Reading Assignment: Chapter 6.5; Chapter 7.1

Homework Assignment #05:

Chapter 5: 1,2,7,9,10

due Monday, October 28, 2024



- Writing a General User Proposal
- Dynamical theory and the Darwin curve
- Extinction and absorption
- Perfect crystal integrated intensity

Reading Assignment: Chapter 6.5; Chapter 7.1

Homework Assignment #05:

Chapter 5: 1,2,7,9,10

due Monday, October 28, 2024

Homework Assignment #06:

Chapter 6: 1,6,7,8,9

due Monday, November 11, 2024

Writing a General User Proposal



1. Log into the UPS site
2. Start an APS general user proposal
3. Add an Abstract
4. Choose a beam line
5. Answer the 6 important questions

A tutorial can be found on the course home page

http://csrri.iit.edu/~segre/phys570/24F/gu_proposal.html

Register & log into the UPS Portal



Knowledge Base | Contacts | Feedback

Welcome to the Universal Proposal System

A common platform for the management of user scientific proposals at APS, LCLS & NSLS-II

Log in
LOG IN WITH ORCID

World class

- State-of-the-art synchrotron radiation light sources at APS and NSLS-II offer continuous spectrum, high flux and brightness allowing scientists to probe the fundamental properties of matter.
- The free electron laser at LCLS generates ultra-bright, ultrafast, high coherence pulses, with the MV-LUED offering a powerful "electron camera" to study ultrafast atomic & molecular dynamics.

Learn more

- User facilities provide open access to specialized instrumentation to scientists from universities, national laboratories, and industry.
- For approved, peer-reviewed projects, instrument time is available without charge to researchers who intend to publish their results in the open literature.
- Thousands of scientists conduct experiments at BES user facilities every year.

Get started

- Create a free ORCID profile or use your existing ORCID ID to register to use the proposal system.
- Submit a proposal to request experimental time or submit a request against a proposal that has already been awarded time.
- Contact User Program staff with any questions – they are there to help!

U.S. DEPARTMENT OF ENERGY OFFICE OF SCIENCE X-RAY LIGHT SOURCES

Participating Facilities

This tool is currently being used to support the proposal submission and review processes for the following facilities

Advanced Photon Source

APS

The APS, at Argonne National Laboratory, is one of only four third-generation, hard x-ray synchrotron radiation light sources in the world. The 1,104-meter circumference facility—large enough to house a baseball park in its center—includes 34 bending magnets and 34 insertion devices, which has a capacity of at least 60 beamlines for experimental research.

Linac Coherent Light Source

LCLS

The LCLS, at the SLAC National Accelerator Laboratory, is the world's first hard x-ray free electron laser facility and became operational in June 2010. This is a milestone for x-ray user facilities that advances the state-of-the-art from storage-ring-based third generation synchrotron light sources to a Linac-based light source.

National Synchrotron Light Source II

NSLS-II

NSLS-II is a state-of-the-art, medium-energy electron storage ring (3 GeV) that generates ultrabright, highly stable beams of synchrotron light, ranging from infrared to hard x-rays. It came online in 2014 and currently operates 25 beamlines with a capacity for about 60 beamlines when fully built out.

U.S. DEPARTMENT OF ENERGY Privacy and Security Notice

Facility websites: [APS](#) | [LCLS](#) | [NSLS-II](#)

Select the APS



My Dashboard | Proposal Calls | Knowledge Base | Contacts | User Profile | Facility Console | Feedback | Tours | Carlo Segre

Carlo Segre
Email: segre@iit.edu
Employer Institution: Illinois Institute of Technology

Announcements
User Acknowledgement

MY PROPOSALS

- SLAC @ LCLS** Linac Coherent Light Source
Draft 0 | Archive 0 | Active 0
- LaserNetUS**
Draft 0 | Archive 0 | Active 0
- Argonne** Advanced Photon Source
Draft 1 | Archive 0 | Active 4
- Brookhaven** National Synchrotron Light Source II
Draft 0 | Archive 0 | Active 0
- Brookhaven** Laboratory for BioMolecular Structure
Draft 0 | Archive 0 | Active 0
- SLAC** Megaelectronvolt Ultrafast Electron Diffraction
Draft 0 | Archive 0 | Active 0

Advanced Photon Source



Feature Beamlines | Contact Info | Beamlines

Active | Draft | Archived

Number	Title	Type	Principal Investigator	Submitted	Status	Score	Rec'd Shifts	Used	View Experiment Time Requests
1008727	Transition Metal Phosphides as catalysts in the electrochemical reduction of Carbon Dioxide	CAT Member	Carlo Segre	10/01/2024 12:24:12	Proposal Active				▼
1008803	XAS investigation into the local atomic environment of Zr K-edge in Zr ₆ O ₄ (OH) ₆ (BTC) ₂ (HCOO) ₆ (MOF-808) for CO ₂ capture and conversion.	CAT Member	Bernard Palawah	10/04/2024 23:15:41	Proposal Active				▼
1009226	Probing lanthanide solvation structure in imidazolium ionic liquid-water mixture using extended X-ray absorption fine structure spectroscopy	General User - Rapid Access	Venkateshkumar Prabhakaran	10/21/2024 12:23:02	Submitted in Review				▼
1009286	Understanding potential-driven lanthanide complexation with ionic liquid using operando extended X-ray absorption fine structure spectroscopy	General User - Regular	Venkateshkumar Prabhakaran	10/21/2024 12:23:13	Submitted in Review				▼

Start a proposal for and APS call





Website
<https://www.aps.anl.gov/>

Location
9700 S. Cass Ave.
Lemont, IL 60439

Phone
630-252-9090


Advanced Photon Source

Feature Beamlines Contact Info Beamlines

Title ▲	Types ▲	Proposal Cycles ▲	Deadline ▲	Proposal Call Status ▲
2025-1 eBERlight Macromolecular Crystallography	General User - Macromolecular Crystallography	APS: 2025-1	10/25/2024 21:59:59	SUBMIT A PROPOSAL
2025-1 Partner User Proposals (PUP)	Partner Proposals	APS: 2025-1	10/25/2024 21:59:59	SUBMIT A PROPOSAL
2025-1 eBERlight General User	General User - Regular	APS: 2025-1	10/25/2024 21:59:59	SUBMIT A PROPOSAL
2025-1 Standard General User Proposals	General User - Regular	APS: 2025-1	10/25/2024 21:59:59	SUBMIT A PROPOSAL
2025-1 Macromolecular Crystallography Proposals	General User - Macromolecular Crystallography	APS: 2025-1	10/25/2024 21:59:59	SUBMIT A PROPOSAL
2024-3 Standard General User - Rapid Access Proposals	General User - Rapid Access	APS: 2024-3	12/18/2024 21:59:59	SUBMIT A PROPOSAL
2024-3 CAT Member Proposals	CAT Member	APS: 2025-1, APS: 2024-3	12/18/2024 21:59:59	SUBMIT A PROPOSAL
2024-3 Resource Staff Proposals (Includes CAT and APS Staff)	Resource Staff	APS: 2025-1, APS: 2024-3	12/18/2024 21:59:59	SUBMIT A PROPOSAL
2024-3 Macromolecular Crystallography Proposals	General User - Macromolecular Crystallography	APS: 2025-1, APS: 2024-3	12/18/2024 21:59:59	SUBMIT A PROPOSAL
2025-1 Resource Staff Proposals (Includes CAT and APS Staff)	Resource Staff	APS: 2025-1	04/17/2025 21:59:59	SUBMIT A PROPOSAL
2025-1 CAT Member Proposals	CAT Member	APS: 2025-1	04/17/2025 21:59:59	SUBMIT A PROPOSAL

Enter basic information and an abstract





Proposal Submission Steps

- Start Proposal**
Provide basic information about your proposed research
- Funding Sources
Enter sources of funding for your research
- Experiment Time Request
Submit requests for access to resources
- Additional Questions
Answer detailed questions relating to the proposal
- Review
Review and Submit the proposal

Proposal Submission Guidance

As the APS accelerator and storage ring return to operations, beamlines around the facility will begin to resume their user programs. The timelines for bringing users back will vary beamline to beamline based on a variety of technical factors. This call for the 2025-1 cycle is soliciting proposals for possible experiments that will be considered based on each beamline's individual schedule and capabilities. Submission of a request for time is not a guarantee of allocation.

To be added to an APS proposal, a user will need to have logged into UPS and also authenticated APS as a trusted party for ORCID through an [APS user registration](#) (if you have not completed an APS user registration since before 2021, you will need to re-register).

BEFORE SUBMITTING: Please thoroughly review your proposal content prior to submission. After submission, only minor changes can be made by an administrator.

IMPORTANT TIP: Please be sure to be as thorough and detailed as possible with your abstract AND when answering all proposal form questions. Beam time for the upgraded APS will be highly competitive. To give your proposal the best chance at allocation, be in-depth with your responses, and see our [tips for writing a successful APS proposal](#).

Enter basic information and an abstract



1009536 *To attach supporting documentation with this proposal, use Paperclip Icon.

Proposal

* Proposal Title
PHYS 570 Experiments

Proposal Call
2025-1 Standard General User Proposals

* Proposal Type
General User - Regular

* Primary Area of Research
Materials science

Additional Area(s) of Research

* Keywords
x-ray absorption spectroscopy (XAS)

* Please suggest the most appropriate review panel for your proposal.
Spectroscopy-Chem/Catalysis

Abstract

* Abstract
This is the dummy experiment for PHYS 570

1959 characters remaining of 2000 characters

SAVE (CTRL + S)

Enter basic information and an abstract



My Dashboard Proposal Calls Knowledge Base Contacts User Profile Facility Console Feedback Tours Carlo Segre

Proposal Submission Steps

- Proposal Form: Provide basic information about your proposed research
- Funding Sources: Enter sources of funding for your research (100%)
- Experiment Time Request: Submit requests for access to resources
- Additional Questions: Answer detailed questions relating to the proposal
- Review: Review and Submit the proposal

Funding information is required for facility reporting purposes

Funding Source	Details	Grant	Percentage	
Other	Duchossois Leadership Program	N/A	100%	EDIT
			Total: 100%	

ADD FUNDING SOURCE

Register & log into the APS Portal



Experiment Time Request

Experiment Time Request - new record

Experiment Time Request

* Proposal
1009536

* Run Cycle
APS: 2025-1

* 1st Choice Resource
10-ID-B

* 1st Choice Instrument
10-ID-B X-ray absorption fine structure

* 1st Choice Technique
X-ray absorption spectroscopy (XAS)

* Shifts Requested This ETR
8

Minimum Useful Shifts This ETR
8

* Lifetime Shifts Requested
24

Argonne NATIONAL LABORATORY

ETR Number
1033603

2nd Choice Resource

2nd Choice Instrument

2nd Choice Technique

SAVE (CTRL + S)

Register & log into the APS Portal



My Dashboard Proposal Calls Knowledge Base Contacts User Profile Facility Console Feedback Tours Carlo Segre

Proposal Submission Steps

- Proposal Form: Provide basic information about your proposed research (Completed)
- Funding Sources: Enter sources of funding for your research (100%) (Completed)
- Experiment Time Request: Submit requests for access to resources (Completed)
- Additional Questions: Answer detailed questions relating to the proposal (Incomplete)
- Review: Review and Submit the proposal (Not Started)

There are incomplete ETR surveys which must be completed.

Number	1st Choice Resource	2nd Choice Resource	Run Cycle	Shifts Requested	Lifetime Shifts Requested	Submitted	Status	
1033603	10-ID-B		APS: 2025-1	8	24		Draft	VIEW EDIT

[ADD NEW REQUEST](#)

Register & log into the APS Portal



The screenshot displays the APS Portal dashboard with a green header bar containing navigation links: My Dashboard, Proposal Calls, Knowledge Base, Contacts, User Profile, Facility Console, Feedback, Tours, and a user profile for Carlo Segre. The main content area is divided into three sections:

- Proposal Submission Steps**: A horizontal progress bar with five steps: Proposal Form (green checkmark), Funding Sources (green checkmark), Experiment Time Request (green checkmark), Additional Questions (yellow circle), and Review (grey circle). Below each step is a brief description of the task.
- Proposal Questions**: Two progress bars for question sets: "APS General User Proposal Questions" and "Export Control/S&T Matrix Research Screening Questions". Both are marked "Not Started" with a green progress bar at 0%.
- ETR Questions**: One progress bar for "APS Experiment Time Request (ETR) Questions (GU/RA/MX)" with ID 1033603:APS, also marked "Not Started" with a green progress bar at 0%.

Register & log into the APS Portal



1009536 APS General User Proposal Questions

General ▼

***What mode(s) of access would you consider for this work? (Note: not all beamlines support all modes of access, choose all that apply.)**

Remote

Mail-in

On-site

***Will the data collected be considered proprietary (e.g., work that will not be made available in the open literature)?**

yes

no

***Have you spoken to a beamline staff member?**

yes

no

***Is this research required for a student's thesis?**

yes

no

***Is this proposal related to another proposal?**

yes

no

Register & log into the APS Portal



• Did you previously receive experiment time at APS for this research?

yes
 no

• Will you be requesting beam time at APS sector 35, the Dynamic Compression Sector (DCS)?

yes
 no

Technical ▼

• What is the scientific or technical purpose and importance of the proposed research?
2000 character limit

• Why do you need the APS for this research?
2000 character limit

Register & log into the APS Portal



***Describe why you are choosing your requested beamline(s).**

2000 character limit

***How many visits during the proposal lifespan do you expect to need? How many shifts will you need per visit (approximately)? At APS, one shift = 8 hours, one day = 3 shifts.**

2000 character limit

***Describe/provide a list of samples.**

2000 character limit

***Provide an overview of the experimental plan and procedures, including sample usage.**

2000 character limit

Register & log into the APS Portal



*** Literature references (DOIs or citations)**
2000 character limit

Team ▼

*** Describe the team's previous experimental experience with synchrotron radiation.**
2000 character limit

*** List publications (DOIs or citations) resulting from work done at the APS. Please identify the beamline(s) where the work was done.**
2000 character limit

Register & log into the APS Portal



Safety ▼

▪ Does this research involve the use of radioactive samples/materials, sealed sources, or x-ray generating devices?

yes

no

▪ Does this research involve the use of any of the following (pick all that apply):

explosives or energetic materials

a new class 3 or class 4 laser that has not been approved by the Argonne Laser Safety Officer

nanoparticles (one or more dimensions is 100 nm or less), including thin films, powder, and solutions

samples/materials that require a BSL-2 (biosafety level) facility

human subjects or human tissues, body fluids, or cells in culture

plant pathogens, soil microbes, animals, insects, or insect/animal tissues, body fluids, matter, cells in culture

none

Register & log into the APS Portal



1009536 Export Control/S&T Matrix Research Screening Questions

* Are there any restrictions, contractually or otherwise, on public dissemination of the work (e.g., research, experiment) described in this proposal? Public dissemination includes presenting at conferences or open meetings, publications, or web source information.

-- Choose --

* Are you bringing any items (including specimens/samples), technical data, software, or services owned or funded by a nuclear, defense, military, space, intelligence agency, or a defense contractor of the United States or of another country?

-- Choose --

* For work (e.g., research, experiment) conducted at the user facility, are any items, technical data, software or services designed, developed, or modified exclusively for military applications, military training, spacecraft, launch vehicles, or national security or intelligence collection and analysis?

-- Choose --

* Would the research results be directly useful for- or would the research involve- a nuclear reactor application (e.g., commercial nuclear fuel, molten salts or other nuclear reactors, nuclear grade graphite, uranium enrichment)?

-- Choose --

* Are you bringing any items (including specimens/samples), technical data, or software to the user facility that require restricted access?

-- Choose --

* For DOE National Lab PIs or employees, please affirm that your research has been screened by your National Lab against the DOE "Science and Technology Risk Matrix" critical and emerging research areas and technologies. Note: If no or unsure, you should contact your home institution's office responsible for screening research for the DOE S&T Risk Matrix. The User Facility must be consulted to determine if research restrictions can be accommodated.

-- Choose --

CANCEL SAVE

Register & log into the APS Portal



1033603:APS Experiment Time Request (ETR) Details

If you will require use of laboratory space during the requested scheduling period, provide details here.
2000 character limit

• Will you be bringing any electrical or hazardous equipment to the facility during this scheduling period?

Yes
 No

• Would the work associated with this request for time involve any of the following (choose all that apply):

Pure gases (or single gas component) greater than 1.3 ft³, 36 L or 1 lb. (inert gasses excluded)
 Liquids greater than 5 gal. or 19 L
 Solids greater than 18.1 kg or 40 lbs.
 None of these apply

Answer this question only for second or later ETRs: List any new publications resulting from work at APS (DOIs or citations). Please identify the beamline(s) where the work was done.
2000 character limit

Register & log into the APS Portal



Preferred experiment dates for this request, enter date span(s) in format MM/DD/YYYY.

Unacceptable experiment dates for this request, enter date span(s) in format MM/DD/YYYY.

CANCEL SAVE

Register & log into the APS Portal



The screenshot displays the APS Portal dashboard with a green navigation bar at the top. The navigation bar includes a logo on the left and several menu items: My Dashboard, Proposal Calls, Knowledge Base, Contacts, User Profile, Facility Console, Feedback, Tours, and a user profile for Carlo Segre. Below the navigation bar, the 'Proposal Submission Steps' section shows a progress bar with five steps: Proposal Form (completed), Funding Sources (completed), Experiment Time Request (completed), Additional Questions (completed), and Review (in progress). The 'Proposal Questions' section shows two completed question sets: 'APS General User Proposal Questions' and 'Export Control/S&T Matrix Research Screening Questions'. The 'ETR Questions' section shows one completed question set: 'APS Experiment Time Request (ETR) Questions (GU/RA/MX)'. Each question set is represented by a green box with a progress bar and the word 'Completed'.

Proposal Submission Steps

- Proposal Form: Provide basic information about your proposed research (Completed)
- Funding Sources: Enter sources of funding for your research (100%) (Completed)
- Experiment Time Request: Submit requests for access to resources (Completed)
- Additional Questions: Answer detailed questions relating to the proposal (Completed)
- Review: Review and Submit the proposal (In Progress)

Proposal Questions

- APS General User Proposal Questions (Completed)
- Export Control/S&T Matrix Research Screening Questions (Completed)

ETR Questions

- APS Experiment Time Request (ETR) Questions (GU/RA/MX) (Completed)

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

Why do you need the APS for this research?

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

Why do you need the APS for this research?

Describe why you are choosing your requested beamline(s).

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

Why do you need the APS for this research?

Describe why you are choosing your requested beamline(s).

How many visits during the proposal lifespan do you expect to need? How many shifts will you need per visit (approximately)?

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

Why do you need the APS for this research?

Describe why you are choosing your requested beamline(s).

How many visits during the proposal lifespan do you expect to need? How many shifts will you need per visit (approximately)?

Describe/provide a list of samples.

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

Why do you need the APS for this research?

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How many visits during the proposal lifespan do you expect to need? How many shifts will you need per visit (approximately)?

Describe/provide a list of samples.

Provide an overview of the experimental plan and procedures, including sample usage.

Answer the 7 important questions (2000 characters each)



What is the scientific or technical purpose and importance of the proposed research?

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How many visits during the proposal lifespan do you expect to need? How many shifts will you need per visit (approximately)?

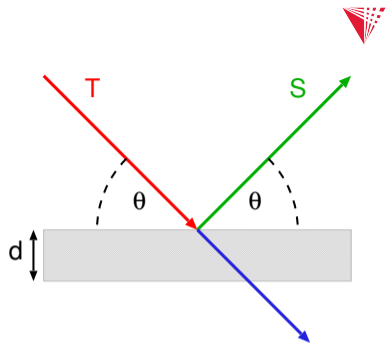
Describe/provide a list of samples.

Provide an overview of the experimental plan and procedures, including sample usage.

Describe the team's previous experimental experience with synchrotron radiation.

Darwin approach review

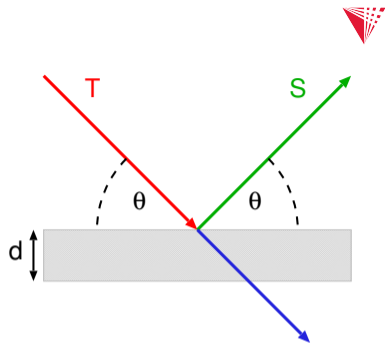
$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$



Darwin approach review

$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$

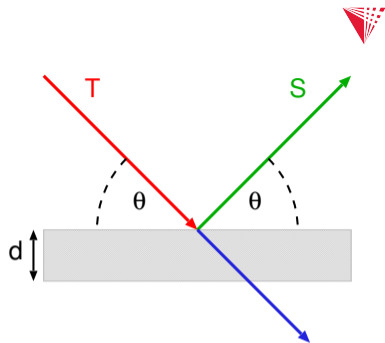
since $v_c \sim d^3$ then $g \sim r_0/d \approx 10^{-5}$



Darwin approach review

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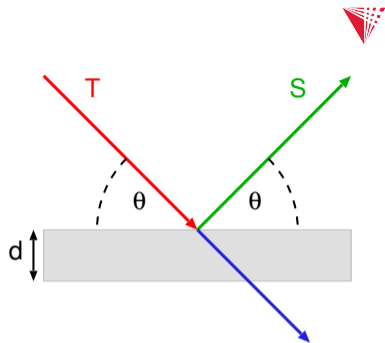


the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

Darwin approach review

$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$

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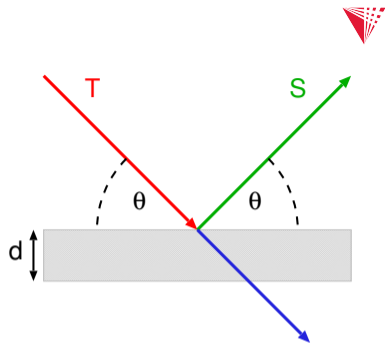
the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

$$T' = (1 - ig_0) T$$

Darwin approach review

$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$

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the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

$$T' = (1 - ig_0) T \approx e^{-ig_0} T$$

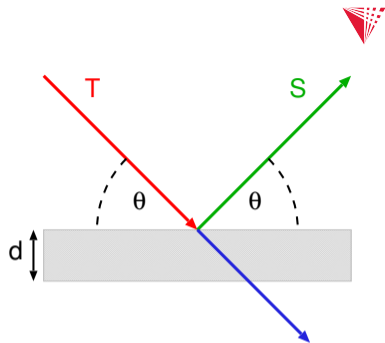
Darwin approach review

$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$

since $v_c \sim d^3$ then $g \sim r_0/d \approx 10^{-5}$

from Chapter 3

$$g_0 = \frac{\lambda \rho_{at} f^0(0) r_0 d}{\sin \theta}$$



the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

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Darwin approach review

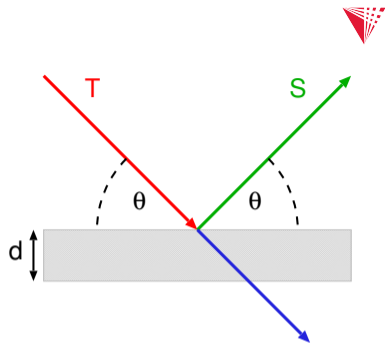
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since $v_c \sim d^3$ then $g \sim r_0/d \approx 10^{-5}$

from Chapter 3

$$g_0 = \frac{\lambda \rho_{at} f^0(0) r_0 d}{\sin \theta} = \frac{\lambda |F_0| r_0 d}{v_c \sin \theta}$$

where $|F_0| = \rho_{at} f^0(0) v_c$ is the unit cell structure factor in the forward direction at $Q = \theta = 0$



the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

$$T' = (1 - ig_0) T \approx e^{-ig_0} T$$

Darwin approach review

$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$

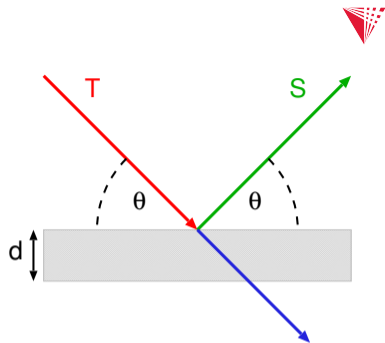
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where $|F_0| = \rho_{at} f^0(0) v_c$ is the unit cell structure factor in the forward direction at $Q = \theta = 0$

this can be rewritten in terms of g as



the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

$$T' = (1 - ig_0) T \approx e^{-ig_0} T$$

Darwin approach review



$$g = \frac{1}{m} \frac{2d^2 r_0}{v_c} |F| = \frac{\lambda r_0 d}{v_c \sin \theta} |F|$$

since $v_c \sim d^3$ then $g \sim r_0/d \approx 10^{-5}$

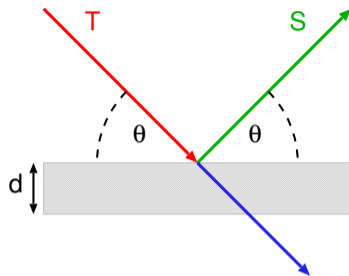
from Chapter 3

$$g_0 = \frac{\lambda \rho_{at} f^0(0) r_0 d}{\sin \theta} = \frac{\lambda |F_0| r_0 d}{v_c \sin \theta}$$

where $|F_0| = \rho_{at} f^0(0) v_c$ is the unit cell structure factor in the forward direction at $Q = \theta = 0$

this can be rewritten in terms of g as

$$g_0 = g \frac{|F_0|}{|F|}$$



the **transmitted** wave is equal in amplitude to the **incident** wave but gains a phase shift as it passes through the layer

$$T' = (1 - ig_0) T \approx e^{-ig_0} T$$

Kinematical reflection



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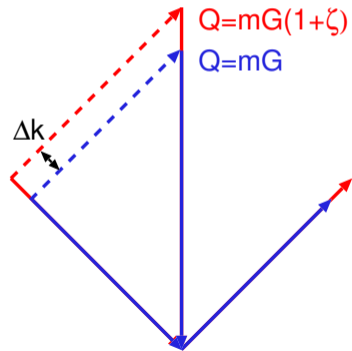
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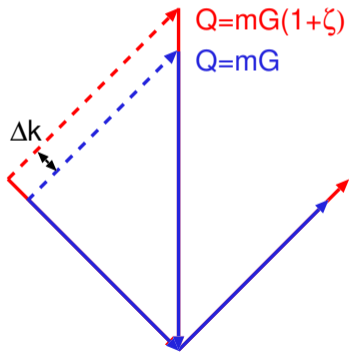
these N unit cell layers will give a reciprocal lattice with points at multiples of $G = 2\pi/d$ we are interested in small deviations from the Bragg condition:

$$\zeta = \frac{\Delta Q}{Q} = \frac{\Delta k}{k} = \frac{\Delta \mathcal{E}}{\mathcal{E}} = \frac{\Delta \lambda}{\lambda}$$

Multiple layer reflection



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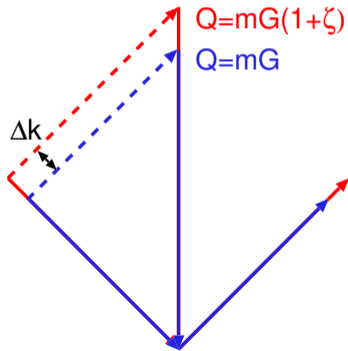


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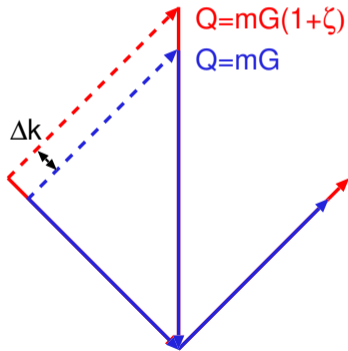


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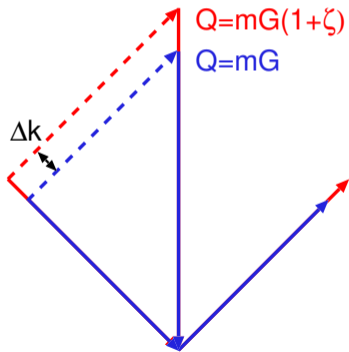
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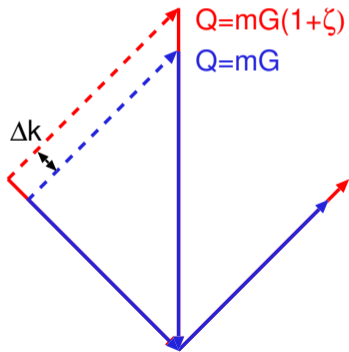
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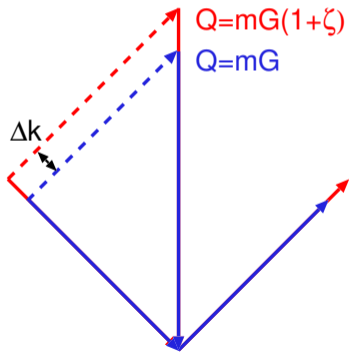
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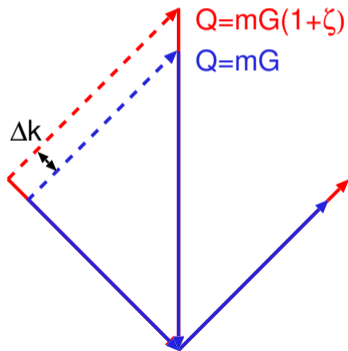
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As the crystal becomes infinite ($N \rightarrow \infty$) this kinematical approximation breaks down because $gN \sim 1$

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It is useful to look at how the intensity of the reflection varies in the kinematical limit

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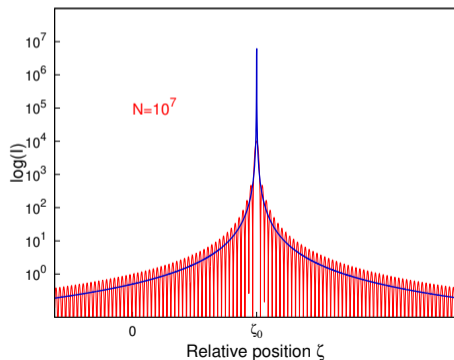
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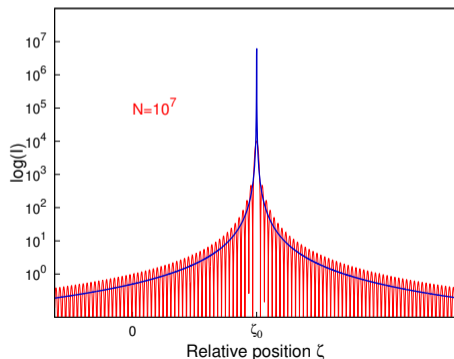
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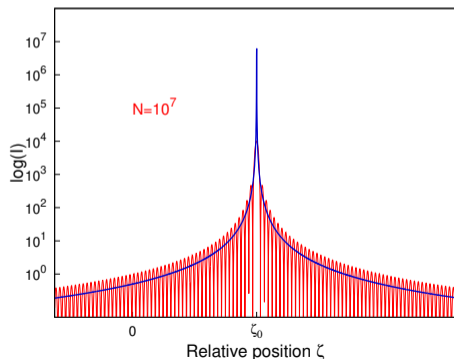
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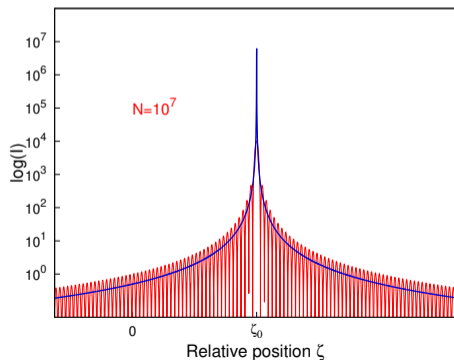
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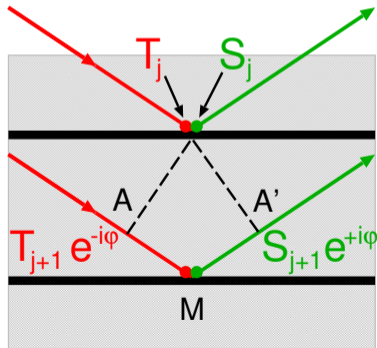
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The kinematical limit clearly breaks down near ζ_0 so we need a dynamical diffraction theory

Reflectivity of a perfect crystal



In a perfect crystal, there are always two wavefields, the T wave which propagates in the direction of the incident beam and the S wave in the direction of the reflected wave

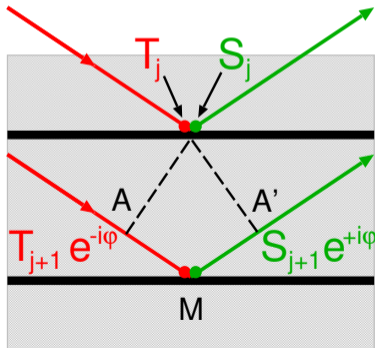




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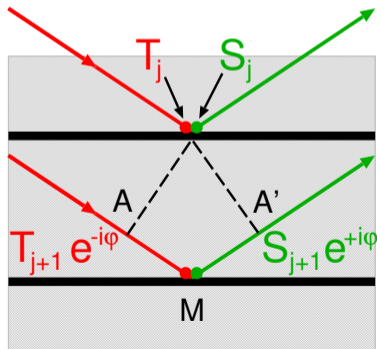




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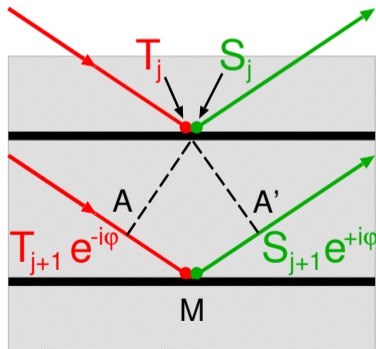




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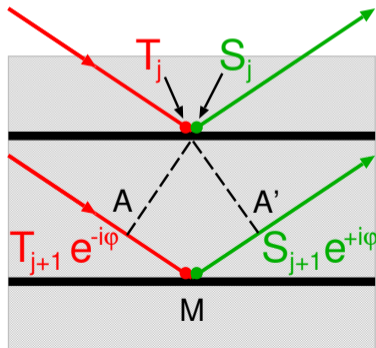
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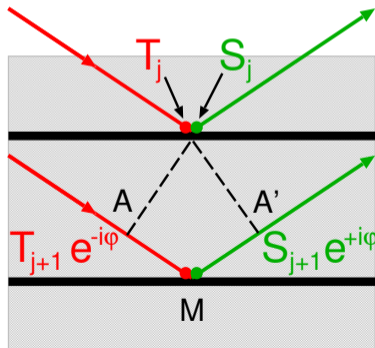
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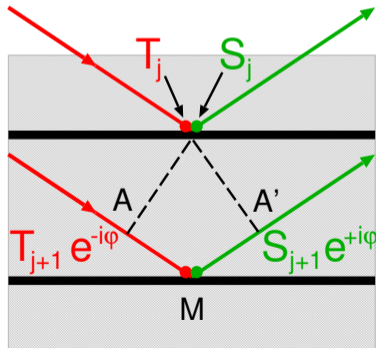
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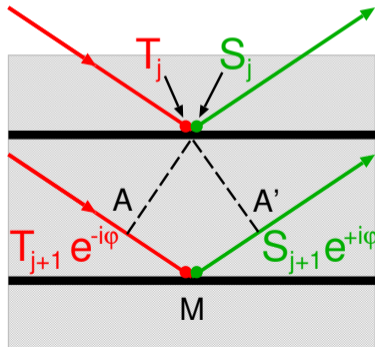
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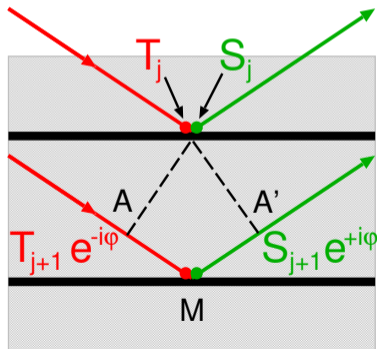
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Difference equation

Let T_j and S_j be the fields just above layer j .

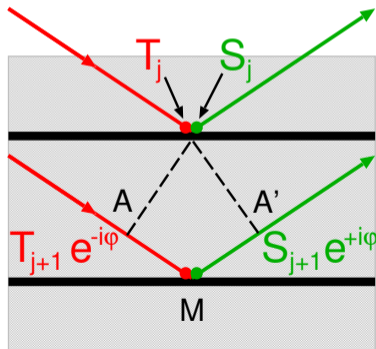




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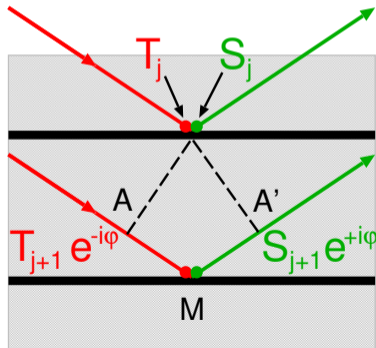


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but this must be equal to the field S_j just after passing up through the j^{th} layer which applies a phase shift



$$S_j = (1 - ig_0)S_{j+1}e^{i\phi}$$

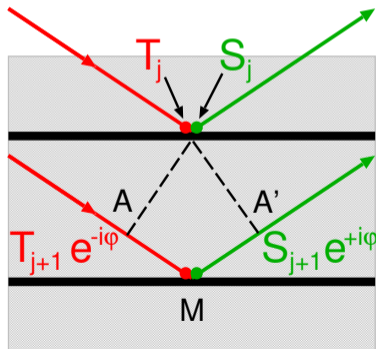


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at point M , just above the $j + 1^{\text{th}}$ layer, we have the scattered field S_{j+1} and at point A' it is $S_{j+1}e^{i\phi}$

but this must be equal to the field S_j just after passing up through the j^{th} layer which applies a phase shift plus the small part of the T_j field reflected from the top of the j^{th} layer



$$S_j = -igT_{j+1} + (1 - ig_0)S_{j+1}e^{i\phi}$$

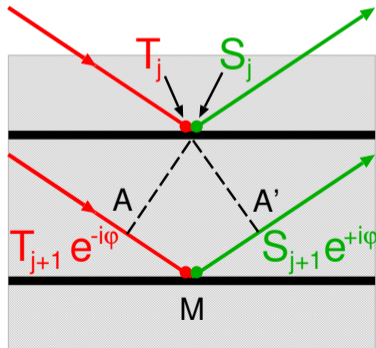


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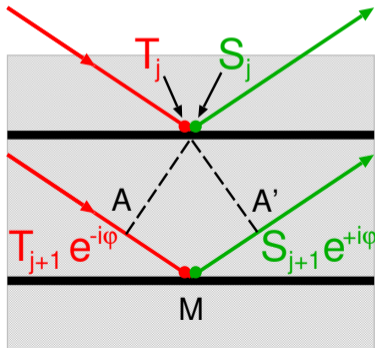


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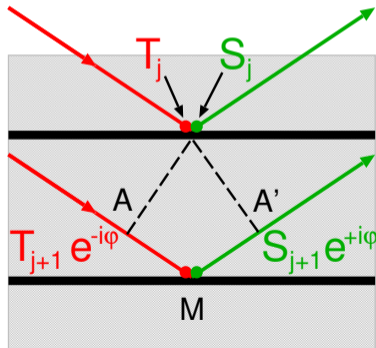


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these coupled equations must be solved for an infinite stack of atomic layers

Separation of T & S fields



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Rearranging the equation for T_j (top right)

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Separation of T & S fields



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Solving for the T field



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With the trial solution

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Solving for the T field



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Solving for the T field



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Solving for the T field



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assuming that g , g_0 , and Δ are very small quantities, we can expand

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$$\begin{aligned} (1 - ig_0) \left(1 - i\Delta - \frac{\Delta^2}{2}\right) \left[\left(1 - \eta + \frac{\eta^2}{2}\right) + \left(1 + \eta + \frac{\eta^2}{2}\right) \right] \\ \approx g^2 + (1 - 2ig_0 - g_0^2) + (1 - i2\Delta - 2\Delta^2) \end{aligned}$$

Solving for the T field



$$(1 - ig_0)(1 - i\Delta - \frac{\Delta^2}{2}) \left[(1 - \eta + \frac{\eta^2}{2}) + (1 + \eta + \frac{\eta^2}{2}) \right] \\ \approx g^2 + (1 - 2ig_0 - g_0^2) + (1 - i2\Delta - 2\Delta^2)$$

Solving for the T field



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Cancelling and expanding all products keeping only second order terms

Solving for the T field



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Cancelling and expanding all products keeping only second order terms

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Solving for the T field



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Solving for the T field



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Solving for the T field



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Cancelling and expanding all products keeping only second order terms

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The solution for the attenuation factor of the transmitted field is thus

Solving for the T field



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The solution for the attenuation factor of the transmitted field is thus

$$i\eta = \pm \sqrt{(\Delta - g_0) - g^2}$$

Solving for the T field



$$(1 - ig_0)(1 - i\Delta - \frac{\Delta^2}{2}) \left[(1 - \eta + \frac{\eta^2}{2}) + (1 + \eta + \frac{\eta^2}{2}) \right] \\ \approx g^2 + (1 - 2ig_0 - g_0^2) + (1 - i2\Delta - 2\Delta^2)$$

Cancelling and expanding all products keeping only second order terms

$$(1 - ig_0 - i\Delta - g_0\Delta - \frac{\Delta^2}{2})(2 + \eta^2) \approx g^2 + 2 - 2ig_0 - 2i\Delta - g_0^2 - 2\Delta^2 \\ \cancel{2} - \cancel{2ig_0} - \cancel{2i\Delta} - 2g_0\Delta - \Delta^2 + \eta^2 \approx g^2 + \cancel{2} - \cancel{2ig_0} - \cancel{2i\Delta} - g_0^2 - 2\Delta^2 \\ \eta^2 \approx g^2 - g_0^2 + 2g_0\Delta - \Delta^2 = g^2 - (\Delta - g_0)^2$$

The solution for the attenuation factor of the transmitted field is thus

$$i\eta = \pm \sqrt{(\Delta - g_0) - g^2}$$

with fields

Solving for the T field



$$(1 - ig_0)(1 - i\Delta - \frac{\Delta^2}{2}) \left[(1 - \eta + \frac{\eta^2}{2}) + (1 + \eta + \frac{\eta^2}{2}) \right] \\ \approx g^2 + (1 - 2ig_0 - g_0^2) + (1 - i2\Delta - 2\Delta^2)$$

Cancelling and expanding all products keeping only second order terms

$$(1 - ig_0 - i\Delta - g_0\Delta - \frac{\Delta^2}{2})(2 + \eta^2) \approx g^2 + 2 - 2ig_0 - 2i\Delta - g_0^2 - 2\Delta^2 \\ \cancel{2} - \cancel{2ig_0} - \cancel{2i\Delta} - 2g_0\Delta - \Delta^2 + \eta^2 \approx g^2 + \cancel{2} - \cancel{2ig_0} - \cancel{2i\Delta} - g_0^2 - 2\Delta^2 \\ \eta^2 \approx g^2 - g_0^2 + 2g_0\Delta - \Delta^2 = g^2 - (\Delta - g_0)^2$$

The solution for the attenuation factor of the transmitted field is thus

$$i\eta = \pm \sqrt{(\Delta - g_0) - g^2}$$

with fields

$$T_{j+1} = e^{-\eta} e^{im\pi} T_j,$$

Solving for the T field



$$(1 - ig_0)(1 - i\Delta - \frac{\Delta^2}{2}) \left[(1 - \eta + \frac{\eta^2}{2}) + (1 + \eta + \frac{\eta^2}{2}) \right] \\ \approx g^2 + (1 - 2ig_0 - g_0^2) + (1 - i2\Delta - 2\Delta^2)$$

Cancelling and expanding all products keeping only second order terms

$$(1 - ig_0 - i\Delta - g_0\Delta - \frac{\Delta^2}{2})(2 + \eta^2) \approx g^2 + 2 - 2ig_0 - 2i\Delta - g_0^2 - 2\Delta^2 \\ \cancel{2} - \cancel{2ig_0} - \cancel{2i\Delta} - 2g_0\Delta - \Delta^2 + \eta^2 \approx g^2 + \cancel{2} - \cancel{2ig_0} - \cancel{2i\Delta} - g_0^2 - 2\Delta^2 \\ \eta^2 \approx g^2 - g_0^2 + 2g_0\Delta - \Delta^2 = g^2 - (\Delta - g_0)^2$$

The solution for the attenuation factor of the transmitted field is thus

$$i\eta = \pm \sqrt{(\Delta - g_0) - g^2}$$

with fields

$$T_{j+1} = e^{-\eta} e^{im\pi} T_j, \quad S_{j+1} = e^{-\eta} e^{im\pi} S_j$$