Footprint over Teaching Mathematica Quantum Mechanics

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Contents

01. Introduction

In a linear medium, the alignment of atomic dipoles is maintained by a magnetic field imposed from the outside. Ferromagnets-which are emphatically not linear require no external fields to sustain the magnetization; the alignment is "frozen in."

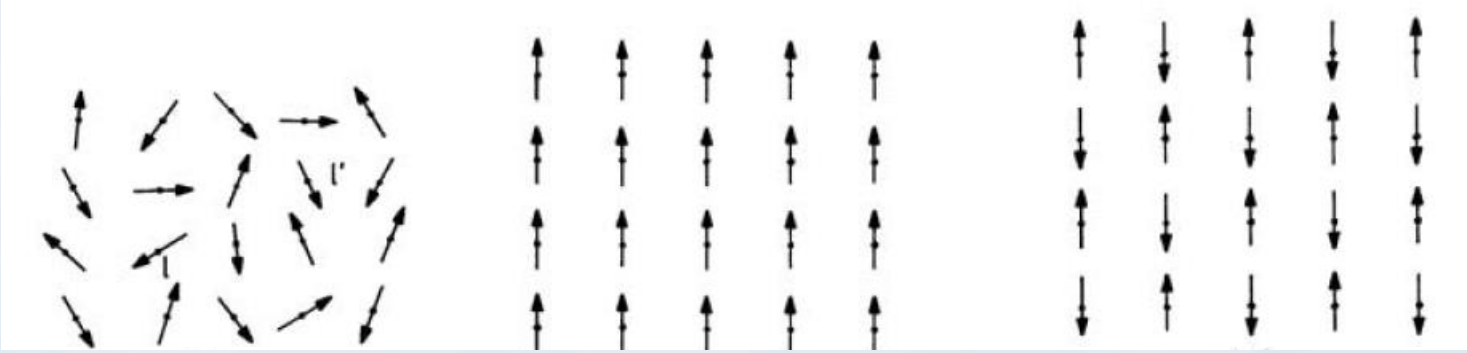
- David J. Griffiths -

Topic

- Heisenberg Spin Chain
  - Ferromagnetic
  - Spin Interaction(Fermions)
- Block Diagonal Hamiltonian
  - Wigner-Eckart Theorem

Ferromagnetic Hamiltonian

- Magnetism
  - Paramagnetic(상자성)
  - Ferromagnetic(강자성)
  - AntiFerromagnetic(반강자성)



- $\hat{\mathcal{H}} = -J\sum \hat{S}_i\,\hat{S}_j - B\sum \hat{S}_i$

  $\hat{\mathcal{H}}_{XY} = -J\sum \cos(\theta_i - \theta_j) - B\sum \cos\theta_i$

  $\hat{\mathcal{H}}_{Ising} = -J\sum S_i^z S_j^z - B\sum S_i^z$

Where are Spin Interaction from?

- $\widehat{\mathcal{H}} = -J \sum \hat{S}_i \hat{S}_j - B \sum \hat{S}_i$
- Dipole moment?

Problem 7.32 Two tiny wire loops, with areas $\mathbf{a}_1$ and $\mathbf{a}_2$, are situated a displacement $\boldsymbol{\imath}$ apart (Fig. 7.42).

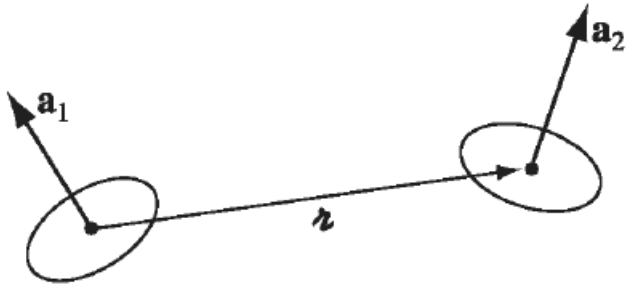


FIGURE 7.42

(a) Find their mutual inductance. [*Hint:* Treat them as magnetic dipoles, and use Eq. 5.88.] Is your formula consistent with Eq. 7.24?

(b) Suppose a current I_1 is flowing in loop 1, and we propose to turn on a current I_2 in loop 2. How much work must be done, against the mutually induced emf, to keep the current I_1 flowing in loop 1? In light of this result, comment on Eq. 6.35.

02. Exchange Interaction

In spite of the fact that the interactions between electrons in a solid, as well as the forces exerted by the ions on the electrons, are essentially of Coulomb origin, the necessity of an interaction between the magnetic moments of the electrons had been recognized long ago.

- Edouard Brezin -

Exchange Interaction

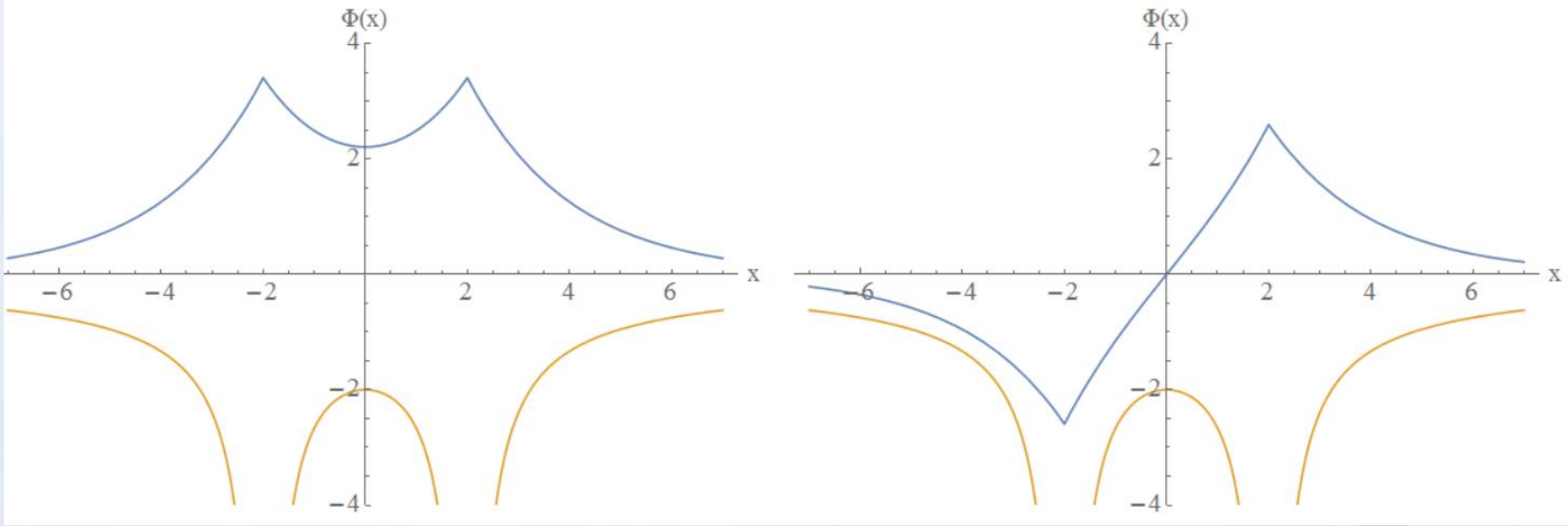
- Interactions are essentially of Coulomb origin.
- Electron characteristics From Fermions

  → Antisymmetric!

Coulomb and Fermi

Exchange Interaction

- Wave function have Spatial Part and Spin Part
- $\Psi = |\Phi(r_1, r_2)\rangle \otimes |S\rangle$
- Spatial antisymmetric energy lower
  → Spin symmetric energy lower(triplet)

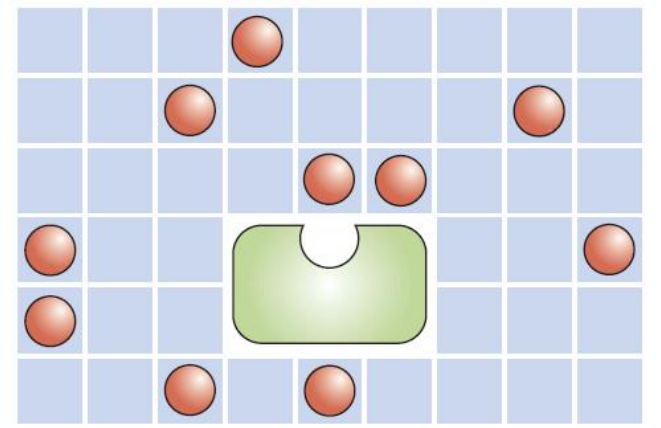


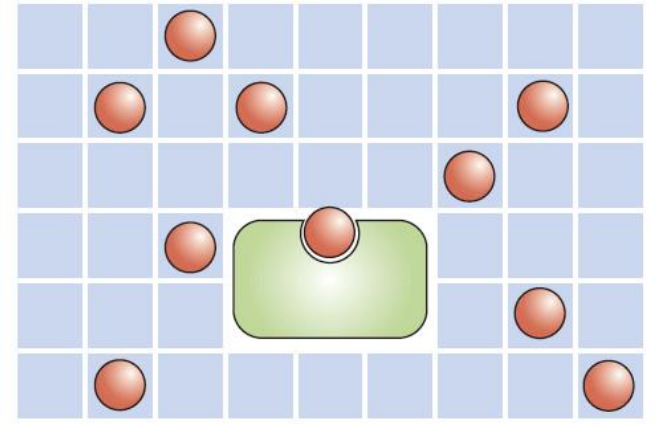
Goal of Finding Hamiltonian

- Partition Function $\mathcal{Z} = \sum e^{-\beta \hat{H}}$
- Free Energy 를 찾고 싶다!
- Energy(E) and Entropy(S, $k_B \log \Gamma(E)$)

Free Energy

- Free Energy
  - Helmholtz Free Energy $F = E - TS|_{S=S(T)}$
  - Simple Example : Water
    - Low Temperature $F \simeq E \rightarrow$ Ice
    - High Temperature $F \simeq -TS \rightarrow$ Vapor
  - Simple Example : Ligand





03. Heisenberg Spin Chain

Construct Basis and Hamiltonian in Mathematica

Since only scalar products of spin vectors occur, it has the following important property: H is invariant with respect to a common rotation of all the spin vectors. No direction is especially distinguished and therefore the ferromagnetic order which can occur may point in any arbitrary direction.

- Franz Schwabl -

Basis Used *Mathematica*

- N Spin → 2^N Basis
  - e.g.
    - N = 2, We have 4 Basis
      - S = 0, Singlet (1)
      - S = 1, Triplet (3)
    - N = 3, We have 8 Basis
      - S = $^1/_2$, M = $^1/_2$,$^{-1}/_2$ → 2?
      - S = $^3/_2$, M = $^3/_2$, $^1/_2$,$^{-1}/_2$, $^{-3}/_2$ → 4
  - We can use Clebsch-Gordan Constant(Table).

N	1	2	3	4	5
#(S)	1	2	2	3	3
S	1/2	1 0	3/2 1/2	2 1 0	5/2 3/2 1/2

$\{1, \frac{1}{2}\}$	$\left\|\frac{3}{2}, \frac{3}{2}\right\rangle$	$\left\|\frac{3}{2}, \frac{1}{2}\right\rangle$	$\left\|\frac{3}{2}, -\frac{1}{2}\right\rangle$	$\left\|\frac{3}{2}, -\frac{3}{2}\right\rangle$	$\left\|\frac{1}{2}, \frac{1}{2}\right\rangle$	$\left\|\frac{1}{2}, -\frac{1}{2}\right\rangle$
$\left\langle 1, \frac{1}{2}\right\|$	1	0	0	0	0	0
$\left\langle 1, -\frac{1}{2}\right\|$	0	$\frac{1}{\sqrt{3}}$	0	0	$\sqrt{\frac{2}{3}}$	0
$\left\langle 0, \frac{1}{2}\right\|$	0	$\sqrt{\frac{2}{3}}$	0	0	$-\frac{1}{\sqrt{3}}$	0
$\left\langle 0, -\frac{1}{2}\right\|$	0	0	$\sqrt{\frac{2}{3}}$	0	0	$\frac{1}{\sqrt{3}}$
$\left\langle -1, \frac{1}{2}\right\|$	0	0	$\frac{1}{\sqrt{3}}$	0	0	$-\sqrt{\frac{2}{3}}$
$\left\langle -1, -\frac{1}{2}\right\|$	0	0	0	1	0	0

$\{0, \frac{1}{2}\}$	$\left\|\frac{1}{2}, \frac{1}{2}\right\rangle$	$\left\|\frac{1}{2}, -\frac{1}{2}\right\rangle$
$\left\langle 0, \frac{1}{2}\right\|$	1	0
$\left\langle 0, -\frac{1}{2}\right\|$	0	1

Spin Chain Basis(Glue it)

- We have optimize to construct basis.
- Tensor Product 최소화 → 시간 이득

```
Glue[Basis, Q[S_], {Q[S1_], Q[S2_]}] := Module[{mm = Range[S1, -S1, -1], cg0, cg1, bs0, bs1},
  cg0 = CG[{S1, #}, {1/2, +1/2}, {S, # + 1/2}] & /@ mm;
  cg1 = CG[{S1, #}, {1/2, -1/2}, {S, # - 1/2}] & /@ mm;
  bs0 = Map[CircleTimes[#, Ket[0]] &, Core[Basis, Q[S1]], {2}];
  bs1 = Map[CircleTimes[#, Ket[1]] &, Core[Basis, Q[S1]], {2}];
  bs0 *= cg0;
  bs1 *= cg1;
   Which[
    S == S1 + S2,
    Join[{First[bs0]}, Rest[bs0] + Most[bs1], {Last[bs1]}],
    S == S1 - S2,
    Rest[bs0] + Most[bs1],
    True, Message[UpdateBasis::badq];
     {}]]

Glue[{Q[S_], {Q[S1_], Q[S2_]}}] := Module[{},
   Core[Basis, Q[S]] = Glue[Basis, Q[S], {Q[S1], Q[S2]}];];
Glue[{Q[S_], {Q[S1_], Q[S2_]}, {Q[S3_], Q[S4_]}}] := Module[{},
   Core[Basis, Q[S]] = Join[Glue[Basis, Q[S], {Q[S1], Q[S2]}], Glue[Basis, Q[S], {Q[S3], Q[S4]}], 2];];
```

Spin Chain Basis(Glue it, Result)

- e.g.

```
Glue[]

Glue[]

Sectors
```

$$\frac{3}{2}$$

```
Core[Basis, Q[3 / 2]]
KetForm @@@ Core[Basis, Q[3 / 2]]
```

$$\left\{\{\{1, 0, 0, 0, 0, 0, 0, 0\}\}, \left\{\left\{0, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, 0, \frac{1}{\sqrt{3}}, 0, 0, 0\right\}\right\},\right.$$

$$\left.\left\{\left\{0, 0, 0, \frac{1}{\sqrt{3}}, 0, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, 0\right\}\right\}, \{\{0, 0, 0, 0, 0, 0, 0, 1\}\}\right\}$$

$$\left\{|0, 0, 0\rangle, \frac{|0, 0, 1\rangle}{\sqrt{3}} + \frac{|0, 1, 0\rangle}{\sqrt{3}} + \frac{|1, 0, 0\rangle}{\sqrt{3}}, \frac{|0, 1, 1\rangle}{\sqrt{3}} + \frac{|1, 0, 1\rangle}{\sqrt{3}} + \frac{|1, 1, 0\rangle}{\sqrt{3}}, |1, 1, 1\rangle\right\}$$

Hamiltonian Used *Mathematica*

- Wigner-Eckart Thm.
- It looks like a Eigen states.

$$\left[\hat{J}_z, \hat{T}_M^{(J)}\right] = M\hat{T}_M^{(J)}$$

$$\left[\hat{J}_\pm, \hat{T}_M^{(J)}\right] = \sqrt{J(J+1) - M(M\pm 1)}\,\hat{T}_{M\pm 1}^{(J)}$$

- In spin chain
- $\hat{T}_0^{(1)} = \hat{S}^z,\ \hat{T}_1^{(1)} = -\hat{S}^+/\sqrt{2},\ \hat{T}_{-1}^{(1)} = \hat{S}^-/\sqrt{2}$
- $\hat{T}_m^{(1)}|J, M; \alpha\rangle = \sum |J', M'; \alpha'\rangle\langle J', M'; \alpha'|\hat{T}_m^{(1)}|J, M; \alpha\rangle$

Wigner Eckart Thm

- $\langle J', M'; \alpha' \left| \hat{T}_m^{(1)} \right| J, M; \alpha \rangle = \Omega \langle J', M' \, | 1, m | J, M \rangle$

- Calculate and find Omega

→ Construct Hamiltonian strategically

Wigner Eckart Thm

- $\hat{T}_m^{(1)} = \alpha \langle J', M' \,|1, m|J, M\rangle$

	$\|1, 1, 1\rangle$	$\|1, 0, 1\rangle$	$\|1, -1, 1\rangle$	$\|0, 0, 1\rangle$
$\langle 1, 1, 1\|$	$\sqrt{2}$	0	0	0
$\langle 1, 0, 1\|$	0	0	0	1
$\langle 1, -1, 1\|$	0	0	$\sqrt{2}$	0
$\langle 0, 0, 1\|$	0	$-\sqrt{3}$	0	0

	$\|1, 1, 1\rangle$	$\|1, 0, 1\rangle$	$\|1, -1, 1\rangle$	$\|0, 0, 1\rangle$
$\langle 1, 1, 1\|$	0	$\sqrt{2}$	0	1
$\langle 1, 0, 1\|$	0	0	$\sqrt{2}$	0
$\langle 1, -1, 1\|$	0	0	0	0
$\langle 0, 0, 1\|$	0	0	$-\sqrt{3}$	0

	$\|1, 1, 1\rangle$	$\|1, 0, 1\rangle$	$\|1, -1, 1\rangle$	$\|0, 0, 1\rangle$
$\langle 1, 1, 1\|$	0	0	0	0
$\langle 1, 0, 1\|$	$\sqrt{2}$	0	0	0
$\langle 1, -1, 1\|$	0	$\sqrt{2}$	0	1
$\langle 0, 0, 1\|$	$-\sqrt{3}$	0	0	0

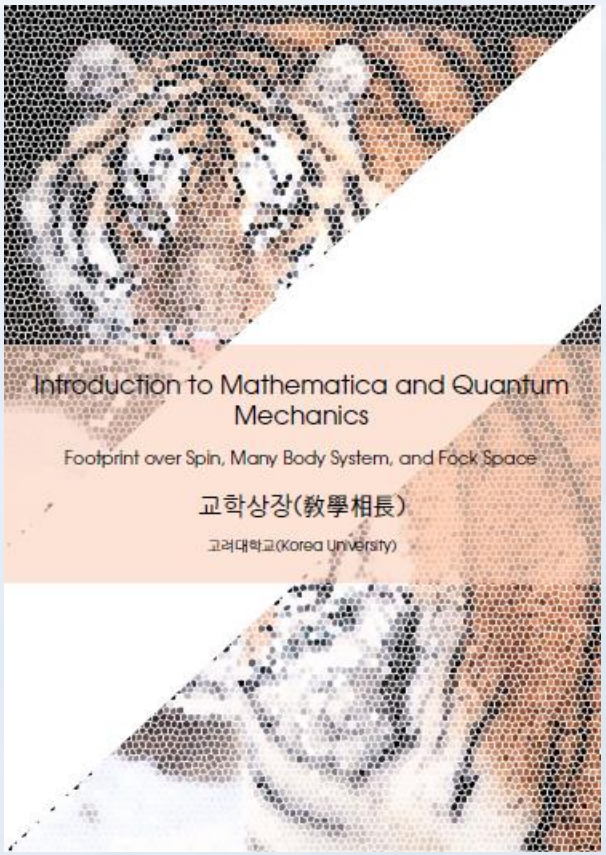
04. *Mathematica* Manual

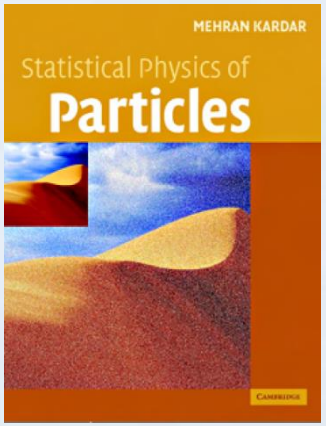
Statistical physics has its origins in attempts to describe the thermal properties of matter in terms of its constituent particles, and has played a fundamental role in the development of quantum mechanics. It describes how new behavior emerges from interactions of many degrees of freedom, and as such has found applications outside physics in engineering, social sciences, and, increasingly, in biological sciences.

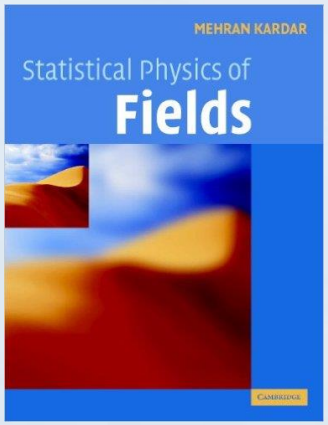
- Mehran Kardar -

Mathematica Manual

- Introduction to Mathematica and Quantum Mechanics





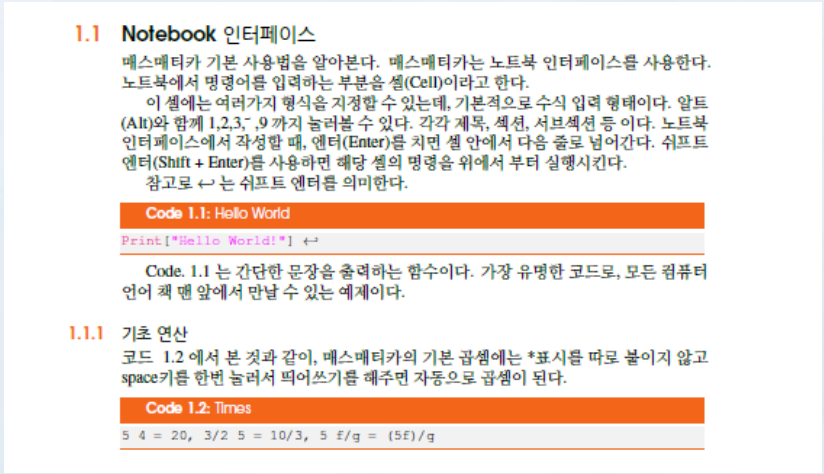


Manual's Contents

Contents

Manual Context

- 주제에 대한 설명을 적어 두고, 간단한 코드로 익힐 수 있도록 구성되었습니다.
- 간단한 예제와 문제들로 매스매티카에게 물리를 학습시킬 방법들을 제시합니다.(추후 어려운 문제 추가 예정)



1.1 **Notebook** 인터페이스

매스매티카 기본 사용법을 알아본다. 매스매티카는 노트북 인터페이스를 사용한다. 노트북에서 명령어를 입력하는 부분을 셀(Cell)이라고 한다.

이 셀에는 여러가지 형식을 지정할 수 있는데, 기본적으로 수식 입력 형태이다. 알트(Alt)와 함께 1,2,3,~,9 까지 눌러볼 수 있다. 각각 제목, 섹션, 서브섹션 등 이다. 노트북 인터페이스에서 작성할 때, 엔터(Enter)를 치면 셀 안에서 다음 줄로 넘어간다. 쉬프트 엔터(Shift + Enter)를 사용하면 해당 셀의 명령을 위에서 부터 실행시킨다.

참고로 ↩ 는 쉬프트 엔터를 의미한다.

Code 1.1: Hello World

```
Print["Hello World!"] ↩
```

Code. 1.1 는 간단한 문장을 출력하는 함수이다. 가장 유명한 코드로, 모든 컴퓨터 언어 책 맨 앞에서 만날 수 있는 예제이다.

1.1.1 기초 연산

코드 1.2 에서 본 것과 같이, 매스매티카의 기본 곱셈에는 *표시를 따로 붙이지 않고 space키를 한번 눌러서 띄어쓰기를 해주면 자동으로 곱셈이 된다.

Code 1.2: Times

```
5 4 = 20, 3/2 5 = 10/3, 5 f/g = (5f)/g
```

1.4 Exercises 7

C++, Fotran 같은 언어에서는 데이터 형식을 미리 선언하는데, 이런 점이 수치 계산을 빠르게 하는데는 도움이 될지 몰라도, 코딩하는데 시간은 더 걸리게 되는 단점이 있다. 정수, 실수, 복소수, List 등을 설정할 필요가 없다. 궁금한 경우 Head 명령어를 이용해서 확인할 수 있다.

1.4 **Exercises**

Exercise 1.1 Mathematica 를 켜보고, 사인함수를 그려본다.(Hint.Plot, Sin) ∎

1.5 **Problems**

Problem 1.1 직교좌표에서 기울기(∇) 연산자를 정의해봅니다.(Hint.D)

Reference

- David J. Griffiths, Introduction to Electrodynamics
- Edouard Brezin, Introduction to Statistical Field Theory
- Franz Schwabl, Statistical Mechanics
- Mehran kardar, Statistical Physics of Particles