TP2 Examples

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Contents

1 Quantum dynamics **3**

1.1 Hamilton's equations 3

1.2 Ladder operators in a time-independent Hamiltonian 4

1.3 5

1.4 Coherent state 5

1.5 6

1.6 Transitional probability 7

1.7 Uniform precession of spin 7

1.8 Avoided transition 8

1.9 Avoided transition via contour integral 9

1.10 Berry potential 11

1.11 11

2 Introduction to path integrals **13**

2.1 The propagator 13

2.2 The heat equation 13

2.3 Associativity of propagator 14

2.4 Basis change 15

2.5 Classical action 16

2.6 17

2.7 Airy's equation 18
2.8 Saddle point method 19

3 Scattering theory 20

3.1 Elementary potential 20
3.2 21
3.3 Scattering channels 21
3.4 Green's function 22
3.5 Asymptotic solution 22
3.6 The sphere potential 23
3.7 Spherical Bessel functions 24
3.8 25
3.9 26
3.10 Flux 27
3.11 The hard sphere 28
3.12 scattered phase of spherical potential 30
3.13 Low momentum scattered phase 30
3.14 Scattering length 31
3.15 Reflection probability in Breit-Wigner form 31
3.16 32
3.17 Formal scattering 33
3.18 Quantum point contact 34

4 36

4.1 36
4.2 Entanglement 36
4.3 Half-half beam splitter 37
4.4 37
4.5 37
4.6 38
4.7 39

4.8 . . . 39
4.9 Bogoliubov transformation . . . 40
4.10 Second quantised operator . . . 42
4.11 . . . 43
4.12 . . . 45
4.13 . . . 45

5 Density matrices **47**
5.1 . . . 47
5.2 . . . 47
5.3 . . . 48
5.4 . . . 48
5.5 . . . 48
5.6 . . . 49
5.7 . . . 49
5.8 . . . 50
5.9 . . . 50
5.10 . . . 51
5.11 . . . 51
5.12 . . . 53
5.13 . . . 53

Topic 1 Quantum dynamics

Problem 1.1 Hamilton's equations

Prove that Hamilton's equations hold for time dependence of $\hat{x}$ and $\hat{p}$ in the Hamiltonian

$$H = T(p) + V(x).$$

The Heisenberg equation of motion is

$$\frac{\mathrm{d}\hat{O}}{\mathrm{d}t} = \frac{i}{\hbar}\left[H, \hat{O}\right]$$

For momentum

$$\begin{aligned}\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} &= \frac{i}{\hbar}\left[\hat{V}(\hat{x}), \hat{p}\right] \\ &= \frac{i}{\hbar}\frac{\mathrm{d}\hat{V}}{\mathrm{d}\hat{x}}[\hat{x}, \hat{p}] \\ &= \frac{i}{\hbar}\frac{\mathrm{d}\hat{V}}{\mathrm{d}\hat{x}} i\hbar \\ &= -\frac{\mathrm{d}\hat{V}}{\mathrm{d}\hat{x}}.\end{aligned}$$

Similarly, for displacement

$$\begin{aligned}\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} &= \frac{i}{\hbar}\frac{\mathrm{d}\hat{T}}{\mathrm{d}\hat{p}}[\hat{p}, \hat{x}] \\ &= \frac{\mathrm{d}\hat{T}}{\mathrm{d}\hat{p}}.\end{aligned}$$

Problem 1.2 Ladder operators in a time-independent Hamiltonian

Prove that in Heisenberg picture,

$$a(t) = e^{-i\omega t}a(0) \qquad a^\dagger(t) = e^{+i\omega t}a^\dagger(0)$$

Given

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

and $\left[a, a^\dagger\right] = 1$.

Rewrite the Hamiltonian as

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).$$

Heisenberg equation of motion gives

$$\begin{aligned}\frac{\mathrm{d}a}{\mathrm{d}t} &= \frac{i}{\hbar}[H, a] \\ \frac{\mathrm{d}a}{\mathrm{d}t} &= \frac{i}{\hbar}\hbar\omega\left[a^\dagger, a\right]a \\ \frac{\mathrm{d}a}{\mathrm{d}t} &= -i\omega a \\ a &= a(0)e^{-i\omega t}.\end{aligned}$$

Similarly,

$$a^\dagger = a^\dagger(0)e^{+i\omega t}.$$

Problem 1.3

The general solution of the SHO subject to time dependent force

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - F(t)x$$

is

$$\tilde{a} = e^{i\omega t}a = a(0) + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t \mathrm{d}t'\, F(t')e^{i\omega t'}$$

The displacement and momentum operators can be reconstructed by

$$\begin{aligned}
x &= \sqrt{\frac{\hbar}{2m\omega}}\Big(a + a^\dagger\Big) \\
x &= \sqrt{\frac{\hbar}{2m\omega}}\Big(a(0)e^{-i\omega t} + a^\dagger(0)e^{+i\omega t}\Big) + \int_0^t \mathrm{d}t'\, \frac{F(t')}{m}\frac{\sin(\omega t - \omega t')}{\omega} \\
p &= i\sqrt{\frac{m\omega\hbar}{2}}\Big(a^\dagger - a\Big) \\
p &= i\sqrt{\frac{m\omega\hbar}{2}}\Big(a^\dagger(0)e^{+i\omega t} - a(0)e^{-i\omega t}\Big) + \int_0^t \mathrm{d}t'\, F(t')\cos\big(\omega t - \omega t'\big)
\end{aligned}$$

The integrands correspond to Green's functions of the classical solution of a forced oscillator.

Problem 1.4 Coherent state

Let $|\alpha\rangle = ce^{\alpha a^\dagger}|0\rangle$, prove that $|\alpha\rangle$ is a coherent state and find the real normalisation constant c.

$$\begin{aligned}
a|\alpha\rangle &= cae^{\alpha a^\dagger}|0\rangle \\
&= c\left(e^{\alpha a^\dagger}a + \Big[a, e^{\alpha a^\dagger}\Big]\right)|0\rangle \\
&= c\underbrace{\Big[a, a^\dagger\Big]}_{1}\frac{\mathrm{d}e^{\alpha a^\dagger}}{\mathrm{d}a^\dagger}|0\rangle \\
&= \alpha|\alpha\rangle
\end{aligned}$$

Therefore $|\alpha\rangle$ is indeed an eigenvalue of the annihilation operator. The normalisation constant can be found by explicitly expanding the exponential of an operator

$$1 = \langle\alpha|\alpha\rangle$$

$$
\begin{aligned}
1 &= c^2 \langle 0| e^{\alpha^* a} e^{\alpha a^\dagger} |0\rangle \\
1 &= c^2 \langle 0| \sum_{i,j=0} \frac{\alpha^{*i}\alpha^j}{i!j!} a^i a^{\dagger j} |0\rangle \\
1 &= c^2 \langle 0| \sum_{i,j=0} \frac{\alpha^{*i}\alpha^j}{i!j!} \sqrt{\frac{j!j!}{(j-i)!}} |j-i\rangle \\
1 &= c^2 \sum_{i,j=0} \frac{\alpha^{*i}\alpha^j}{i!} \sqrt{\frac{1}{(j-i)!}} \delta_{ij} \\
1 &= c^2 \exp\left(|\alpha|^2\right) \\
c &= \exp\left(-\frac{|\alpha|^2}{2}\right).
\end{aligned}
$$

Problem 1.5

$$
\begin{aligned}
a(t)|\alpha\rangle &= e^{-i\omega t}\tilde{a}|\alpha\rangle \\
a(t)|\alpha\rangle &= e^{-i\omega t}\left(a(0) + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t \mathrm{d}t'\, F(t')e^{i\omega t'}\right)|\alpha\rangle \\
U^\dagger a U|\alpha\rangle &= e^{-i\omega t}\left(\alpha + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t \mathrm{d}t'\, F(t')e^{i\omega t'}\right)|\alpha\rangle
\end{aligned}
$$

let

$$\alpha' = \alpha + \frac{i}{\sqrt{2m\hbar\omega}}\int_0^t \mathrm{d}t'\, F(t')e^{i\omega t'}$$

we have

$$aU|\alpha\rangle = e^{-i\omega t}\alpha' U|\alpha\rangle$$

Therefore

$$
\begin{aligned}
U|\alpha\rangle &= \left|e^{i\phi(t)}\alpha'\right\rangle \\
\phi(t) &= -\omega t
\end{aligned}
$$

This does not agree with the question in the handout.

Problem 1.6 Transitional probability

Starting from the ground state $|0\rangle$ at $t = 0$, after some time, we are in the coherent state $|\alpha\rangle$, where

$$\alpha = \frac{i}{\sqrt{2m\hbar\omega}} \int_0^t \mathrm{d}t'\, F(t') e^{i\omega(t'-t)}$$

From problem 1.4, we know that

$$\langle m|\alpha\rangle = \langle m| \exp\left(-\frac{|\alpha|^2}{2}\right) \sum_i \frac{(\alpha a^\dagger)^i}{i!} |0\rangle$$

$$\langle m|\alpha\rangle = \exp\left(-\frac{|\alpha|^2}{2}\right) \sum_i \frac{\alpha^i}{\sqrt{i!}} \delta_{im}$$

$$P_{0\to m} = \left|\langle m|\alpha\rangle\right|^2 = \frac{|\alpha|^{2m}}{m!} \exp\left(-|\alpha|^2\right)$$

For $m = 1$, this can be expanded to

$$P_{0\to 1} = |\alpha|^2 + O(\alpha^4)$$

For $m > 1$, the expansion is

$$P_{0\to 1} = O(\alpha^4)$$

Compare this with first order time-dependent perturbation theory states, for $m \neq 0$

$$P_{0\to m} = \left| -\frac{i}{\hbar} \int_0^t \mathrm{d}t'\, e^{i(\omega_m - \omega_0)t'} \langle m| V(t') |0\rangle \right|^2$$

$$P_{0\to m} = \left| i \int_0^t \mathrm{d}t'\, e^{i(\omega_m - \omega_0)t'} \langle m| \frac{F(t')}{\sqrt{2m\hbar\omega}} (a + a^\dagger) |0\rangle \right|^2$$

$$P_{0\to m} = \left| i \int_0^t \mathrm{d}t'\, e^{i\omega t'} \frac{F(t')}{\sqrt{2m\hbar\omega}} \right|^2 \delta_{1m}$$

$$P_{0\to m} = \left|\alpha e^{i\omega t}\right|^2 \delta_{1m} = |\alpha|^2 \delta_{1m}$$

which we can see is consistent with the expansion above up to third order in the perturbing force.

Problem 1.7 Uniform precession of spin

Find the explicit form of $U(t, t')$ and $R(t, t')$ when $\mathbf{H} = H_z\hat{\mathbf{z}}$, corresponding to uniform precession about the z-axis.

Representation by U,

$$U(t,t') = \exp\left(-\frac{i}{\hbar}H_z S_z (t-t')\right)$$

$$U(t,t') = \begin{pmatrix} \exp\left(-\frac{i(t-t')H_z}{2\hbar}\right) & 0 \\ 0 & \exp\left(+\frac{i(t-t')H_z}{2\hbar}\right) \end{pmatrix}$$

Using representation by R,

$$\epsilon_{ijz}H_z = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{ij} H_z$$

$$\epsilon_{ijz}H_z = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \\ & & 1 \end{pmatrix} \begin{pmatrix} -iH_z & & \\ & +iH_z & \\ & & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \\ & & 1 \end{pmatrix}$$

$$R(t,t') = \exp\left(-\epsilon_{ijz}\frac{H_z}{\hbar}(t-t')\right)$$

$$R(t,t') = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \\ & & 1 \end{pmatrix} \begin{pmatrix} \exp\left(+\frac{iH_z(t-t')}{\hbar}\right) & & \\ & \exp\left(-\frac{iH_z(t-t')}{\hbar}\right) & \\ & & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & \\ & & 1 \end{pmatrix}$$

$$R(t,t') = \begin{pmatrix} \cos\left(\frac{H_z(t-t')}{\hbar}\right) & -\sin\left(\frac{H_z(t-t')}{\hbar}\right) & \\ \sin\left(\frac{H_z(t-t')}{\hbar}\right) & \cos\left(\frac{H_z(t-t')}{\hbar}\right) & \\ & & 1 \end{pmatrix}$$

Problem 1.8 Avoided transition

Expanding the time-ordered unitary operator matrix element to first order, and approximating $\sqrt{(\beta t)^2 + \Delta^2} \to |\beta t| + \frac{\Delta^2}{2|\beta t|}$, if the system started in $|\downarrow\rangle$ at $t = -\infty$,

$$\begin{aligned} c_\uparrow(t=+\infty) &= -\frac{i}{\hbar}\int \exp\left(\frac{i}{\hbar}\beta t^2\right)\Delta\,\mathrm{d}t \\ &= -\frac{i\Delta}{\hbar}\sqrt{\frac{\pi\hbar}{i\beta}} \\ \left|c_\uparrow(t=+\infty)\right|^2 &= \frac{\pi\Delta^2}{\hbar\beta} \end{aligned}$$

where

$$V^I_{\uparrow\downarrow} = \exp\left(\frac{i}{\hbar}\int_0^t \beta t'\,\mathrm{d}t'\right)\Delta\exp\left(-\frac{i}{\hbar}\int_0^t -\beta t'\,\mathrm{d}t'\right) = \exp\left(\frac{i}{\hbar}\beta t^2\right)\Delta$$

is the relevant matrix element in interaction picture.

Problem 1.9 Avoided transition via contour integral

Consider the Hamiltonian

$$H = H_0 + V(t) = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix} + \begin{pmatrix} \beta t & 0 \\ 0 & -\beta t \end{pmatrix}$$

The *instantaneous eigenvalues and eigenstates* can be computed explicitly

$$H\left|\pm_t\right\rangle = E_\pm(t)\left|\pm_t\right\rangle$$
$$E_\pm = \pm\sqrt{\Delta^2 + (\beta t)^2}$$
$$\left|\pm\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+\frac{\beta t}{E_\pm}} \\ \pm\sqrt{1-\frac{\beta t}{E_\pm}} \end{pmatrix}$$

So we have

$$\left\langle +\right|\dot{H}\left|-\right\rangle = \frac{\beta}{2}\left(\sqrt{1-\left(\frac{\beta t}{E_\pm}\right)^2}\right)$$
$$\left\langle -\right|\dot{H}\left|+\right\rangle = \left\langle +\right|\dot{H}\left|-\right\rangle = \frac{\beta\Delta}{E_+}$$

Let

$$\beta t + i\Delta = ae^{i\phi} \qquad -\frac{\pi}{2} < \phi < \frac{3\pi}{2};\ a\in\mathbb{R}$$
$$\beta t - i\Delta = be^{i\theta} \qquad -\frac{\pi}{2} < \theta < \frac{3\pi}{2};\ b\in\mathbb{R}$$

and define an exotic branch cut of the E_+:

$$E_+ = \sqrt{(\beta t)^2 + \Delta^2} = \sqrt{ab}\exp\left[\frac{1}{2}i(\phi+\theta)\right]$$

such that on the real axis of t

$$t > 0 \qquad E_+ = \sqrt{ab}\exp\left[\frac{1}{2}i(\phi-\phi)\right] = \sqrt{ab} > 0$$

$$t < 0 \qquad E_+ = \sqrt{ab}\exp\left[\frac{1}{2}i(\phi + 2\pi - \phi)\right] = -\sqrt{ab} < 0$$

i.e. the *instantaneous* ground state at $t = -\infty$ is the *instantaneous* excited state at $t = \infty$. Notice that for $\mathrm{Im}(\beta t) < -\Delta$, E_+ is analytic from $\theta, \phi \to \frac{3\pi}{2}-$ to $\theta, \phi \to -\frac{\pi}{2}+$ and vice versa, because there are two overlapping branch cuts. Quoting eq. (1.62) on the handout,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} E_+(t) & \frac{i\hbar\beta\Delta}{2E_+^2} \\ -\frac{i\hbar\beta\Delta}{2E_+^2} & E_-(t) \end{pmatrix}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} \tag{1}$$

In this branch cut, the instantaneous eigenenergy is nonanalytic at $t = 0$ on the real axis. Equation (1) can be solved arbitrarily faraway from $t \in \mathbb{R}$, such that $|E_+| \gg \Delta \implies$ the off-diagonal terms vanish, and adiabatic theorem can be used to write

$$c_+(+\infty) = c_+(-\infty)\exp\left[\frac{1}{i\hbar}\int_{\mathcal{P}} E_+(t)\,\mathrm{d}t\right] \tag{2}$$

along some path $\mathcal{P}$ faraway from the real axis on the complex plane of t. Using residue theorem, the path can be shifted back to the real axis, circumventing neatly around the branch cut $-i\beta t \in [-\Delta, \Delta]$.

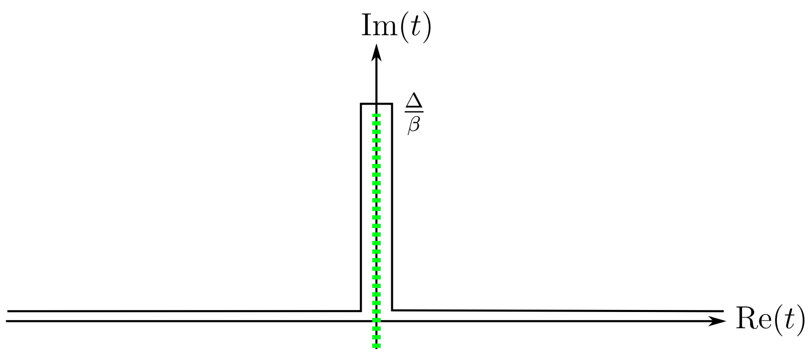

Figure 1: The path $\mathcal{P}$ along which eq. (2) is integrated, where green dashes indicate branch cut.

The real part in the integral in the exponent eq. (2) diverges, so information about phase is lost. The imaginary part arises from the section of $\mathcal{P}$ contouring the branch cut, which is

$$\int_0^{\frac{\Delta}{\beta}} \sqrt{\Delta^2 - (\beta t)^2}\exp\left[\frac{i}{2}\left(\frac{\pi}{2} + \frac{3\pi}{2}\right)\right](i\,\mathrm{d}t) + \int_{\frac{\Delta}{\beta}}^0 \sqrt{\Delta^2 - (\beta t)^2}\exp\left[\frac{i}{2}\left(\frac{\pi}{2} - \frac{\pi}{2}\right)\right](i\,\mathrm{d}t)$$

$$\mathrm{Im}\left[\int_{\mathcal{P}} E_+(t)\,\mathrm{d}t\right] = -2i\int_0^{\frac{\Delta}{\beta}} \sqrt{\Delta^2 - (\beta t)^2}\,\mathrm{d}t$$

$$\begin{aligned}
\operatorname{Im}\left[\int_{\mathcal{P}} E_+(t)\,\mathrm{d}t\right] &= -2i\frac{\Delta^2}{\beta}\int_0^{\frac{\pi}{2}}\cos^2(u)\,\mathrm{d}u \\
\operatorname{Im}\left[\int_{\mathcal{P}} E_+(t)\,\mathrm{d}t\right] &= -\frac{i\pi\Delta^2}{2\beta} \\
\left|\exp\left[\frac{1}{i\hbar}\int_{\mathcal{P}} E_+(t)\,\mathrm{d}t\right]\right| &= \exp\left(-\frac{\pi\Delta^2}{2\hbar\beta}\right)
\end{aligned}$$

Finally, we conclude that

$$\boxed{P(\text{ground} \to \text{excited}) = \left|\big\langle c_+(+\infty)\big|\exp\left[\frac{1}{i\hbar}\int_{\mathcal{P}} E_+(t)\,\mathrm{d}t\right]\big|c_+(+\infty)\big\rangle\right|^2 = \exp\left(-\frac{\pi\Delta^2}{\hbar\beta}\right)}.$$

Problem 1.10 Berry potential

The Berry potential

$$\mathbf{A}_+(\mathbf{H}) \equiv -i\,\langle\mathbf{H},+|\,\big(\nabla_{\mathbf{H}}\,|\mathbf{H},+\rangle\big)$$

can be alternatively expressed as

$$\mathbf{A}_+(\mathbf{H}) = -i\nabla_{\mathbf{H}}\big(\langle\mathbf{H},+|\mathbf{H},+\rangle\big) + i\big(\nabla_{\mathbf{H}}\,\langle\mathbf{H},+|\big)\,|\mathbf{H},+\rangle$$

Using normalised states guarantees $\langle\mathbf{H},+|\mathbf{H},+\rangle = \text{const.}$, so that the Berry potential can be written in a symmetrised form

$$\begin{aligned}
\mathbf{A}_+(\mathbf{H}) &= \frac{1}{2}\Big[i\big(\nabla_{\mathbf{H}}\,\langle\mathbf{H},+|\big)\,|\mathbf{H},+\rangle - i\,\langle\mathbf{H},+|\,\big(\nabla_{\mathbf{H}}\,|\mathbf{H},+\rangle\big)\Big] \\
&= \frac{1}{2}\Big[-i\,\langle\mathbf{H},+|\,\big(\nabla_{\mathbf{H}}\,|\mathbf{H},+\rangle\big) + c.c.\Big]
\end{aligned}$$

which is thence real.

Problem 1.11

For the Hamiltonian

$$H = \frac{H_0}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}$$

the eigenvalues are

$$\left(\frac{E}{H_0/2}\right)^2 - \cos^2(\theta) - \sin^2(\theta) = 0$$

$$E_{\pm} = \pm\frac{H_0}{2}$$

the lower eigenstate is then

$$|\mathbf{H}, -\rangle = \begin{pmatrix} \sin\big(\theta/2\big)e^{-i\phi/2} \\ \cos\big(\theta/2\big)e^{i\phi/2} \end{pmatrix}$$

From definition of the Berry potential

$$\begin{aligned}
A_{-}(\mathbf{H}) &= -i\,\langle \mathbf{H}, -|\,\big(\nabla_{\mathbf{H}}\,|\mathbf{H}, -\rangle\big) \\
&= -i\left(\sin\big(\theta/2\big)e^{i\phi/2},\ \cos\big(\theta/2\big)e^{-i\phi/2}\right)\nabla_{\mathbf{H}}\begin{pmatrix} \sin\big(\theta/2\big)e^{-i\phi/2} \\ \cos\big(\theta/2\big)e^{i\phi/2} \end{pmatrix} \\
&= -i\left(\sin\big(\theta/2\big),\ \cos\big(\theta/2\big)\right)\frac{1}{2H_0}\begin{pmatrix} \cos\big(\theta/2\big)\hat{\boldsymbol{\theta}} - i\sin\big(\theta/2\big)\frac{1}{\sin\theta}\hat{\boldsymbol{\phi}} \\ -\sin\big(\theta/2\big)\hat{\boldsymbol{\theta}} + i\cos\big(\theta/2\big)\frac{1}{\sin\theta}\hat{\boldsymbol{\phi}} \end{pmatrix} \\
&= -\frac{i}{2H_0\sin\theta}\left[-i\sin^2\big(\theta/2\big)\hat{\boldsymbol{\phi}} + i\cos^2\big(\theta/2\big)\hat{\boldsymbol{\phi}}\right] \\
&= \frac{\cot(\theta)}{2H_0}\hat{\boldsymbol{\phi}}
\end{aligned}$$

Topic 2 Introduction to path integrals

Problem 2.1 The propagator

$$\left[i\hbar\frac{\partial}{\partial t} - H\right]K(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$
$$\int_{t'-\epsilon}^{t'+\epsilon} \mathrm{d}t \left[i\hbar\frac{\partial}{\partial t} - H\right]K(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}')$$
$$i\hbar K(\mathbf{r},t|\mathbf{r}',t')\bigg|_{t'-\epsilon}^{t'+\epsilon} - \int_{t'-\epsilon}^{t'+\epsilon} \mathrm{d}t\, HK(\mathbf{r},t|\mathbf{r}',t') = i\hbar\delta(\mathbf{r}-\mathbf{r}')$$
$$K(\mathbf{r},t'+\epsilon|\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}') - \epsilon\frac{i}{\hbar}HK(\mathbf{r},t'|\mathbf{r}',t')$$

Evidently when $\epsilon = 0$, the propagator reduces to the dirac delta, so that

$$\Psi(\mathbf{r},t') = \int \mathrm{d}\mathbf{r}'\, \Psi(\mathbf{r}',t')K(\mathbf{r},t'|\mathbf{r}',t')$$

Therefore for small ϵ, we can write

$$\int \mathrm{d}\mathbf{r}'\, \Psi(\mathbf{r}',t')K(\mathbf{r},t'+\epsilon|\mathbf{r}',t') = \int \mathrm{d}\mathbf{r}'\, \Psi(\mathbf{r}',t')\left[\delta(\mathbf{r}-\mathbf{r}') - \epsilon\frac{i}{\hbar}HK(\mathbf{r},t'|\mathbf{r}',t')\right]$$
$$\int \mathrm{d}\mathbf{r}'\, \Psi(\mathbf{r}',t')K(\mathbf{r},t'+\epsilon|\mathbf{r}',t') = \Psi(\mathbf{r},t') - \epsilon\frac{i}{\hbar}H\Psi(\mathbf{r},t')$$

Comparing with

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = H\Psi(\mathbf{r},t) \qquad \Longrightarrow \qquad \Psi(\mathbf{r},t+\epsilon) - \Psi(\mathbf{r},t) \approx \epsilon\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \epsilon\frac{1}{i\hbar}H\Psi(\mathbf{r},t)$$

the equivalent definition of the propagator is obtained

$$\Psi(\mathbf{r},t'+\epsilon) = \Psi(\mathbf{r},t') - \epsilon\frac{i}{\hbar}H\Psi(\mathbf{r},t') = \int \mathrm{d}\mathbf{r}'\, \Psi(\mathbf{r}',t')K(\mathbf{r},t'+\epsilon|\mathbf{r}',t').$$

Problem 2.2 The heat equation

Verify that the fundamental solution of the heat equation is

$$K_{heat}(\mathbf{r},t|0,0) = \frac{\theta(t)}{(4\pi Dt)^{3/2}}\exp\left[-\frac{r^2}{4Dt}\right]$$

The fundamental solution can be derived from fourier space

$$\big(i\omega + Dk^2\big)\tilde{K} = 1$$

$$\begin{aligned}
K(\mathbf{r},t|0,0) &= \frac{1}{(2\pi)^4}\int_0^\infty \mathrm{d}k \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \int_{-\infty}^\infty \mathrm{d}\omega\, k^2 \sin(\theta) \frac{\exp\big(i\omega t - ikr\cos(\theta)\big)}{i\omega + Dk^2} \\
K(\mathbf{r},t|0,0) &= \frac{1}{(2\pi)^3}\int_0^\infty \mathrm{d}k \int_{-\infty}^\infty \mathrm{d}\omega\, \frac{2i}{ir}\frac{\exp(i\omega t)k\sin(kr)}{i\omega + Dk^2} \\
K(\mathbf{r},t|0,0) &= \frac{1}{(2\pi)^2}\frac{1}{r}\Theta(t)\int_{-\infty}^\infty \mathrm{d}k \exp\big(-Dk^2 t\big) k \sin(kr) \\
K(\mathbf{r},t|0,0) &= \frac{1}{(2\pi)^2}\frac{1}{4Dt}\Theta(t)\int_{-\infty}^\infty \mathrm{d}k \exp\big(-Dk^2 t\big)\left(e^{ikr} + e^{-ikr}\right) \qquad \text{integration by parts} \\
K(\mathbf{r},t|0,0) &= \frac{1}{(2\pi)^2}\frac{1}{4Dt}\Theta(t)\exp\left(-\frac{r^2}{4Dt}\right)\sqrt{\frac{4\pi}{Dt}} \\
K(\mathbf{r},t|0,0) &= \boxed{\frac{\Theta(t)}{(4\pi Dt)^{3/2}}\exp\left(-\frac{r^2}{4Dt}\right)}
\end{aligned}$$

where before the second-to-last line we used

$$\begin{aligned}
K(\mathbf{r},t|0,0) = \frac{1}{(2\pi)^2}\frac{1}{4Dt}\Theta(t)\exp\left(-\frac{r^2}{4Dt}\right)\times \\
\int_{-\infty}^\infty \exp\left(-Dt(k - \frac{ir}{2Dt})^2\right) + \exp\left(-Dt(k + \frac{ir}{2Dt})^2\right)\mathrm{d}k
\end{aligned}$$

Problem 2.3 Associativity of propagator

Verify that the associative property of propagators

$$K(\mathbf{r},t|\mathbf{r}',t') = \int \mathrm{d}\mathbf{r}''\, K(\mathbf{r},t|\mathbf{r}''t'')K(\mathbf{r}'',t''|\mathbf{r}',t')$$

holds for the heat diffusion case.

Let $t_1 = t - t''$, $t_2 = t'' - t'$, integrate the right hand side explicitly for the expression derived in 2.2.

$$\begin{aligned}
&\int \mathrm{d}\mathbf{r}''\, \frac{\Theta(t-t')}{(4\pi Dt_1)^{3/2}}\exp\left(-\frac{(\mathbf{r}-\mathbf{r}'')^2}{4Dt_1}\right)\frac{\Theta(t-t')}{(4\pi Dt_2)^{3/2}}\exp\left(-\frac{(\mathbf{r}''-\mathbf{r}')^2}{4Dt_2}\right) \\
&= \int \mathrm{d}\mathbf{r}''\, \frac{\Theta(t-t')}{(4\pi Dt_1)^{3/2}}\frac{1}{(4\pi Dt_2)^{3/2}}\exp\left(-\frac{t_2(\mathbf{r}-\mathbf{r}'')^2 + t_1(\mathbf{r}''-\mathbf{r}')^2}{4Dt_1t_2}\right)
\end{aligned}$$

$$
\begin{aligned}
&= \int \mathrm{d}\mathbf{r}'' \, \frac{\Theta(t-t')}{(4\pi D t_1)^{3/2}} \frac{1}{(4\pi D t_2)^{3/2}} \exp\left(-\frac{t_2 r^2 - 2(t_2 \mathbf{r} + t_1 \mathbf{r}') \cdot \mathbf{r}'' + (t_1+t_2) r''^2 + t_1 r'^2}{4 D t_1 t_2} \right) \\
&= \int_0^\infty \mathrm{d}r'' \int \mathrm{d}\phi \int \mathrm{d}\theta \, \frac{\Theta(t-t')}{(4\pi D t_1)^{3/2}} \frac{r''^2 \sin(\theta)}{(4\pi D t_2)^{3/2}} \\
&\qquad \exp\left(-\frac{t_2 r^2 - 2|t_2 \mathbf{r} + t_1 \mathbf{r}'| r'' \cos(\theta) + (t_1+t_2) r''^2 + t_1 r'^2}{4 D t_1 t_2} \right) \\
&= 4\pi \frac{4 D t_1 t_2}{2|t_2 \mathbf{r} + t_1 \mathbf{r}'|} \Theta(t-t') \int_0^\infty \mathrm{d}r'' \, \frac{1}{(4\pi D t_1)^{3/2}} \frac{1}{(4\pi D t_2)^{3/2}} r'' \\
&\qquad \exp\left(-\frac{t_2 r^2 + (t_1+t_2) r''^2 + t_1 r'^2}{4 D t_1 t_2} \right) \sinh\left(\frac{2|t_2 \mathbf{r} + t_1 \mathbf{r}'| r''}{4 D t_1 t_2} \right) \\
&= \frac{1}{(4\pi D)^2 \sqrt{t_1 t_2}} \frac{\Theta(t-t')}{(t_1+t_2)} \int_{-\infty}^\infty \mathrm{d}r'' \exp\left(-\frac{t_2 r^2 + (t_1+t_2) r''^2 + t_1 r'^2}{4 D t_1 t_2} \right) \cosh\left(\frac{2|t_2 \mathbf{r} + t_1 \mathbf{r}'| r''}{4 D t_1 t_2} \right) \\
&= \frac{1}{(4\pi D)^2 \sqrt{t_1 t_2}} \frac{\Theta(t-t')}{(t_1+t_2)^{3/2}} \sqrt{4\pi D t_1 t_2} \exp\left(-\frac{|\mathbf{r} - \mathbf{r}'|^2}{4D(t_1+t_2)} \right) \\
&= \frac{\Theta(t-t')}{\left[4\pi D(t_1+t_2)\right]^{\frac{3}{2}}} \exp\left(-\frac{|\mathbf{r} - \mathbf{r}'|^2}{4D(t_1+t_2)} \right)
\end{aligned}
$$

Recall that $t_1 + t_2 = t - t'$, the regular form of the propagator can be recovered.

Problem 2.4 Basis change

Show that the propagator in position and momentum representations are related by a change of basis

$$
\langle r|p \rangle = \frac{\exp\left(i \mathbf{p} \cdot \mathbf{r}/\hbar\right)}{(2\pi\hbar)^{3/2}}
$$

The *change of basis* is given by

$$
\begin{aligned}
K(\mathbf{r}, t|\mathbf{r}', t') &= \theta(t-t') \langle \mathbf{r}| U(t,t') \left|\mathbf{r}'\right\rangle \\
K(\mathbf{r}, t|\mathbf{r}', t') &= \theta(t-t') \langle \mathbf{r}| \int \mathrm{d}\mathbf{p} \, |\mathbf{p}\rangle \langle \mathbf{p}| U(t,t') \int \mathrm{d}\mathbf{p}' \left|\mathbf{p}'\right\rangle \left\langle \mathbf{p}'\middle|\mathbf{r}'\right\rangle \\
K(\mathbf{r}, t|\mathbf{r}', t') &= \iint \mathrm{d}\mathbf{p} \, \mathrm{d}\mathbf{p}' \, \langle \mathbf{r}|\mathbf{p}\rangle \, K(\mathbf{p}, t|\mathbf{p}', t') \left\langle \mathbf{p}'\middle|\mathbf{r}'\right\rangle
\end{aligned}
$$

Applying to the case of free propagator, the right hand side is

$$
\iint \mathrm{d}\mathbf{p} \, \mathrm{d}\mathbf{p}' \, K(\mathbf{p}, t|\mathbf{p}', t') \frac{1}{(2\pi\hbar)^3} \exp\left(\frac{i(\mathbf{p}' \cdot \mathbf{r}' - \mathbf{p} \cdot \mathbf{r})}{\hbar} \right)
$$

$$
\begin{aligned}
&=\theta(t-t')\frac{1}{(2\pi\hbar)^3}\iint \mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'\exp\left(-i\frac{p^2}{2m}\frac{t-t'}{\hbar}\right)\delta(\mathbf{p}-\mathbf{p}')\exp\left(\frac{i(\mathbf{p}'\cdot\mathbf{r}'-\mathbf{p}\cdot\mathbf{r})}{\hbar}\right)\\
&=\theta(t-t')\frac{1}{(2\pi\hbar)^3}\int \mathrm{d}\theta\sin\theta\int\mathrm{d}\phi\int_0^\infty \mathrm{d}p\,p^2\exp\left(-i\frac{p^2}{2m}\frac{t-t'}{\hbar}+\frac{ip|\mathbf{r}'-\mathbf{r}|\cos\theta}{\hbar}\right)\\
&=\theta(t-t')\frac{4\pi}{(2\pi\hbar)^3}\int_0^\infty \mathrm{d}p\,\frac{p\hbar}{|\mathbf{r}'-\mathbf{r}|}\exp\left(-i\frac{p^2}{2m}\frac{t-t'}{\hbar}\right)\sin\left(\frac{p|\mathbf{r}'-\mathbf{r}|}{\hbar}\right)\\
&=\theta(t-t')\frac{4\pi}{(2\pi\hbar)^3}\int_0^\infty \mathrm{d}p\,\frac{m\hbar}{i(t-t')}\exp\left(-i\frac{p^2}{2m}\frac{t-t'}{\hbar}\right)\cos\left(\frac{p|\mathbf{r}'-\mathbf{r}|}{\hbar}\right)\\
&=\theta(t-t')\frac{2\pi}{(2\pi\hbar)^3}\frac{m\hbar}{i(t-t')}\int_{-\infty}^\infty \mathrm{d}p\exp\left(-i\frac{p^2}{2m}\frac{t-t'}{\hbar}\right)\cos\left(\frac{p|\mathbf{r}'-\mathbf{r}|}{\hbar}\right)\\
&=\theta(t-t')\frac{2\pi}{(2\pi\hbar)^3}\frac{m\hbar}{i(t-t')}\sqrt{\frac{2m\hbar\pi}{i(t-t')}}\exp\left(i\frac{m|\mathbf{r}'-\mathbf{r}|^2}{2\hbar(t-t')}\right)\\
&=\theta(t-t')\left(\frac{m}{2\pi\hbar i(t-t')}\right)^{3/2}\exp\left(i\frac{m|\mathbf{r}'-\mathbf{r}|^2}{2\hbar(t-t')}\right)
\end{aligned}
$$

which does coincide with $K(\mathbf{r},t|\mathbf{r}',t')$.

Problem 2.5 Classical action

The classical path satisfies the Euler-Lagrange equation

$$m\ddot{x}_0(t)+m\omega^2x_0(t)=0$$

and the boundary conditions

$$x_0(t_i)=x_i \qquad\qquad x_0(t_f)=x_f$$

into which the general solution of the equation of motion can be substituted

$$
\begin{aligned}
x_0(t)&=As(t)+Bc(t)\\
x_i&=B\\
x_f&=As_f+x_ic_f\\
x_0(t)&=\frac{x_f-x_ic_f}{s}s(t)+x_ic(t)
\end{aligned}
$$

where we have denoted $c(t)\equiv\cos[\omega(t-t_i)]$ and $s(t)\equiv\sin[\omega(t-t_i)]$, further $c_f=c(t_f)$ and $s_f=s(t_f)$

$$S_{\mathrm{SHO}}[x_0(t)]$$

$$
\begin{aligned}
&= \int_{t_i}^{t_f} \frac{m}{2}\dot{x_0}^2 - \frac{m\omega^2}{2}x^2 \, \mathrm{d}t \\
&= \frac{m\omega^2}{2}\int_{t_i}^{t_f} (A^2 - B^2)\cos[2\omega(t-t_i)] - 2AB\sin[2\omega(t-t_i)] \, \mathrm{d}t \\
&= \frac{m\omega}{4}\left[\frac{x_f^2 - 2x_f x_i c_f + x_i^2(c_f^2 - s_f^2)}{s_f^2} 2cs + 2\frac{x_f x_i - x_i^2 c_f}{s_f}\left(c^2 - s^2\right)\right]_{t_i}^{t_f} \\
&= \frac{m\omega}{2}\left[\frac{x_f^2 - 2x_f x_i c_f + x_i^2(c_f^2 - s_f^2)}{s_f^2} c_f s_f + \frac{x_f x_i - x_i^2 c_f}{s_f}\left(c_f^2 - s_f^2\right) - \frac{x_f x_i - x_i^2 c_f}{s_f}\right] \\
&= \frac{m\omega}{2}\frac{x_f^2 c_f - 2x_f x_i c_f^2 + x_f x_i\left(c_f^2 - s_f^2\right) - x_f x_i + x_i^2 c_f}{s_f} \\
&= \frac{m\omega}{2s_f}\left[(x_f^2 + x_i^2)c_f - 2x_f x_i\right] = \frac{m\omega}{2\sin[\omega(t_f - t_i)]}\left[(x_i^2 + x_f^2)\cos[\omega(t_f - t_i)] - 2x_i x_f\right]
\end{aligned}
$$

as required.

Problem 2.6

Verify that K_{SHO} as given by eq (2.35) satisfies

$$
\left[i\hbar\frac{\partial}{\partial t} - H\right]K_{SHO} = i\hbar\delta(x)\delta(t) \tag{3}
$$

where

$$
H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2
$$

Apply the same notational conventions as in Problem 2.5. The short time behaviour is the same as for the free particle, so we consider only regions where $t \neq 0$, such that the right hand side of eq. (3) is zero.

$$
K_{\mathrm{SHO}}(x,t|x_i,t_i) = \sqrt{\frac{m\omega}{2i\pi\hbar}}s^{-\frac{1}{2}}\exp\left(\frac{i}{\hbar}S_{\mathrm{SHO}}\right)
$$

$$\frac{\partial}{\partial t}K_{\text{SHO}} = Ks^{\frac{1}{2}}\left[-\frac{\omega c}{2}s^{-\frac{3}{2}} + s^{-\frac{1}{2}}\frac{im\omega}{2\hbar}\left(-\frac{\omega c}{s^2}(x_i^2+x^2)c + \frac{\omega c}{s^2}2x_ix - \frac{\omega s}{s}(x_i^2+x_f^2)\right)\right]$$
$$\frac{\partial}{\partial t}K_{\text{SHO}} = K\left[-\frac{\omega c}{2s} + \frac{im\omega^2}{2\hbar s^2}\left(-(x_i^2+x^2)+c2x_ix\right)\right]$$
$$\frac{\partial}{\partial x}K_{\text{SHO}} = K\left[\frac{i}{\hbar}\frac{\partial}{\partial x}S_{\text{SHO}}\right]$$
$$\frac{\partial^2}{\partial x^2}K_{\text{SHO}} = K\left[\frac{i}{\hbar}\frac{\partial^2}{\partial x^2}S_{\text{SHO}} + \left(\frac{i}{\hbar}\frac{\partial}{\partial x}S_{\text{SHO}}\right)^2\right]$$
$$\frac{\partial}{\partial x}S_{\text{SHO}} = \frac{m\omega}{2s}(2xc-2x_i)$$
$$\frac{\partial^2}{\partial x^2}S_{\text{SHO}} = \frac{m\omega c}{s}$$
$$\frac{\partial^2}{\partial x^2}K_{\text{SHO}} = K\left[\frac{i}{\hbar}\frac{m\omega c}{s} + \left(\frac{i}{\hbar}\frac{m\omega}{s}(xc-x_i)\right)^2\right]$$
$$\frac{\partial^2}{\partial x^2}K_{\text{SHO}} = K\frac{m\omega}{\hbar}\left[i\frac{c}{s} - \frac{m\omega}{\hbar}\frac{x^2c^2+x_i^2-2x_ixc}{s^2}\right]$$

Putting all the above together

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{m\omega^2x^2}{2}\right]K_{\text{SHO}}$$
$$=\left[-i\hbar\frac{\omega c}{2s} - \frac{m\omega^2}{2s^2}\left(-x_i^2-x^2+c2x_ix\right) + \frac{\hbar\omega}{2}\frac{ic}{s} - \frac{m\omega^2}{2}\frac{x^2c^2+x_i^2-2x_ixc}{s^2} - \frac{m\omega^2x^2}{2}\right]K_{\text{SHO}}$$
$$=\left[\frac{m\omega^2}{2s^2}\left(+x_i^2+x^2-c2x_ix-x^2c^2-x_i^2+2x_ixc\right) - \frac{m\omega^2x^2}{2}\right]K_{\text{SHO}}$$
$$=\left[\frac{m\omega^2}{2s^2}\left(x^2s^2\right) - \frac{m\omega^2x^2}{2}\right]K_{\text{SHO}}$$
$$=0$$

Indeed K_{SHO} is a solution of the Schrodinger equation.

Problem 2.7 Airy's equation

Verify that

$$f(z) = \int e^{ikz}\tilde{f}(k)\,\mathrm{d}k = A\int \exp\left(\frac{ik^3}{3} + ikz\right)\mathrm{d}k$$

satisfies Airy's equation

$$f''(z) - zf(z) = 0$$

so long as the integrand vanishes at the endpoints.

This seems very straightforward.

$$f''(z) - zf(z) = A \int \left(-k^2 - z\right) \exp\left(\frac{ik^3}{3} + ikz\right) \mathrm{d}k$$

$$f''(z) - zf(z) = iA \int \left(ik^2 + iz\right) \exp\left(\frac{ik^3}{3} + ikz\right) \mathrm{d}k$$

$$f''(z) - zf(z) = iA \exp\left(\frac{ik^3}{3} + ikz\right)\Bigg|_{\text{boundary}}$$

For some finite z, the integrand vanishes on the three wedges drawn in figure 2.3 of the handout, where $\mathrm{Re}\left\{ik^3\right\} < 0$ for large $|k|$.

Problem 2.8 Saddle point method

The integrand can be written as an exponential

$$f(x) = e^{N \ln x - x}$$

Compute the derivatives of the exponent

$$\frac{\mathrm{d}}{\mathrm{d}x}(N \ln x - x) = \frac{N}{x} - 1$$
$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}(N \ln x - x) = -\frac{N}{x^2}$$

The integrand has a saddle point where the first derivative vanishes. Expanding around $x = N$ gives

$$f(x) \sim \exp(N \ln N - N) \exp\left(-\frac{(x-N)^2}{2N}\right)$$

$$\int f(x)\,\mathrm{d}x \sim N^N e^{-N} \int_0^\infty \exp\left(-\frac{(x-N)^2}{2N}\right) \mathrm{d}x$$

$$\int f(x)\,\mathrm{d}x \sim N^N e^{-N} \int_{-N}^\infty \exp\left(-\frac{x^2}{2N}\right) \mathrm{d}x$$

$$\int f(x)\,\mathrm{d}x \sim N^N e^{-N} \sqrt{\pi \left(\frac{1}{2N}\right)^{-1}} \sim N^N e^{-N} \sqrt{2\pi N} \qquad \text{for large } N$$

Topic 3 Scattering theory

Problem 3.1 Elementary potential

The energy eigenvalue equation in 1D for a δ-function potential is

$$E\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + g\delta(x)\right)\psi$$

Assuming continuous ψ and integrating near $x = 0$,

$$g\psi(0) = \frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\bigg|_{0-}^{0+}$$

For $x > 0$ and $x < 0$, the solutions are

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Consider forward and backward going waves

$$\psi(x) = \begin{cases} a_+\exp(ikx) + a_-\exp(-ikx) & x < 0 \\ b_+\exp(ikx) + b_-\exp(-ikx) & x > 0 \end{cases}$$

$$\frac{\partial\psi}{\partial x} = \begin{cases} ik\big[a_+\exp(ikx) - a_-\exp(-ikx)\big] & x < 0 \\ ik\big[b_+\exp(ikx) - b_-\exp(-ikx)\big] & x > 0 \end{cases}$$

$$a_+ + a_- = b_+ + b_- = \frac{ik\hbar^2}{2mg}(b_+ - b_- - a_+ + a_-)$$

$$b_+ + b_- - a_+ = \frac{2mg}{ik\hbar^2}(b_+ + b_-) - (b_+ - b_- - a_+)$$

$$\left(\frac{ik\hbar^2}{mg} - 1\right)b_+ = b_- + \frac{ik\hbar^2}{mg}a_+$$

$$a_+ + a_- - b_- = \frac{2mg}{ik\hbar^2}(a_+ + a_-) - (-b_- - a_+ + a_-)$$

$$a_-\left(\frac{ik\hbar^2}{mg} - 1\right) = a_+ + \frac{ik\hbar^2}{mg}b_-$$

$$\begin{pmatrix} a_- \\ b_+ \end{pmatrix} = \begin{pmatrix} \frac{mg}{ik\hbar^2 - mg}a_+ + \frac{ik\hbar^2}{ik\hbar^2 - mg}b_- \\ \frac{ik\hbar^2}{ik\hbar^2 - mg}a_+ + \frac{mg}{ik\hbar^2 - mg}b_- \end{pmatrix} = \boxed{\begin{pmatrix} r & t \\ t & r \end{pmatrix}} \begin{pmatrix} a_+ \\ b_- \end{pmatrix}$$

as required. In this problem, $r_{LL} = r_{RR}$ and $t_{LR} = t_{RL}$ because the potential is symmetric under parity transformation $x \to -x$.

Problem 3.2

$$|a_+|^2 - |a_-|^2 = |b_+|^2 - |b_-|^2 \qquad \Longrightarrow \qquad |a_+|^2 + |b_-|^2 = |b_+|^2 + |a_-|^2$$

The modulus of a vector is preserved before and after multiplication by the scattering matrix $S(k)$. By definition, $S(k)$ is a unitary matrix.

The boxed matrix in problem 3.1 can be explicitly verified to be unitary.

$$\begin{pmatrix} \frac{mg}{ik\hbar^2 - mg} & \frac{ik\hbar^2}{ik\hbar^2 - mg} \\ \frac{ik\hbar^2}{ik\hbar^2 - mg} & \frac{mg}{ik\hbar^2 - mg} \end{pmatrix} \begin{pmatrix} \frac{mg}{-ik\hbar^2 - mg} & \frac{-ik\hbar^2}{-ik\hbar^2 - mg} \\ \frac{-ik\hbar^2}{-ik\hbar^2 - mg} & \frac{mg}{-ik\hbar^2 - mg} \end{pmatrix} =$$

$$\frac{1}{(ik\hbar^2 + mg)(-ik\hbar^2 + mg)} \begin{pmatrix} (mg)^2 + k^2\hbar^4 & mg(-ik\hbar^2) + ik\hbar^2 mg \\ ik\hbar^2 mg + mg(-ik\hbar^2) & (mg)^2 + k^2\hbar^4 \end{pmatrix} = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$$

As for the transfer matrix $T(k)$, the corresponding property is

$$\begin{pmatrix} b_+ \\ b_- \end{pmatrix} = T(k) \begin{pmatrix} a_+ \\ a_- \end{pmatrix}$$

$$\begin{pmatrix} a_+ & -a_- \end{pmatrix} \begin{pmatrix} a_+ \\ a_- \end{pmatrix} = \begin{pmatrix} b_+ & -b_- \end{pmatrix} T(k) \begin{pmatrix} a_+ \\ a_- \end{pmatrix}$$

$$\begin{pmatrix} a_+ \\ a_- \end{pmatrix} = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} T^T(k) \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \begin{pmatrix} b_+ \\ b_- \end{pmatrix}$$

$$T^{-1}(k) = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} T^T(k) \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

Problem 3.3 Scattering channels

The eigenvalues of the scattering matrix in Problem 3.1 are

$$\lambda_\pm = \frac{mg \pm ik\hbar^2}{ik\hbar^2 - mg}$$

$$\lambda_+ = \exp\left(i(\pi - 2\arctan\frac{k\hbar^2}{mg})\right) \qquad \lambda_- = \exp(i\pi)$$

The odd (antisymmetric) wave vanishes at $x = 0$, so its derivative has no discontinuities. Therefore, the scattered wave is always the incoming wave negated. Thence, the even (symmetric) channel corresponds to λ_+ whereas the odd (antisymmetric) channel corresponds to λ_-.

$$\delta_{\text{even}} = \frac{\pi}{2} - \arctan\frac{k\hbar^2}{mg} \qquad \delta_{\text{odd}} = \frac{\pi}{2}$$

$$\psi_{\text{even}}(x) = c_{\text{even}} \begin{cases} \sin\Big(kx - \arctan \frac{k\hbar^2}{mg}\Big) & x > 0 \\ \sin\Big(-kx - \arctan \frac{k\hbar^2}{mg}\Big) & x < 0 \end{cases}$$

$$\psi_{\text{odd}}(x) = c_{\text{odd}} \begin{cases} \sin(kx) & x > 0 \\ \sin(kx) & x < 0 \end{cases}$$

Problem 3.4 Green's function

Solve the Lippmann-Schwinger equation

$$\Psi_k(x) = \exp(ikx) + \int \mathrm{d}x'\, G_k(x, x')V(x')\Psi_k(x')$$

for the case of the δ-potential, with the causal Green's function

$$G_k^+(x, x') = -i\frac{m}{\hbar^2 k} \exp\Big(ik|x - x'|\Big).$$

For $V(x') = g\delta(x')$,

$$\int \mathrm{d}x'\, G_k(x, x')V(x')\Psi_k(x') = G_k(x, 0)g\Psi_k(0)$$

$$\Psi_k(x) = \exp(ikx) + \frac{mg}{i\hbar^2 k} \exp\big(ik|x|\big)\Psi_k(0)$$

$$\Psi_k(0) = 1 + \frac{mg}{i\hbar^2 k}\Psi_k(0) = \frac{ik\hbar^2}{ik\hbar^2 - mg}$$

$$\Psi_k(x) = \exp(ikx) + \frac{mg}{i\hbar^2 k - mg} \exp\big(ik|x|\big)\Psi_k(0)$$

$$\Psi_k(x) = \begin{cases} \frac{ik\hbar^2}{i\hbar^2 k - mg} \exp(ikx) & x > 0 \\ \exp(ikx) + \frac{mg}{i\hbar^2 k - mg} \exp(-ikx) & x < 0 \end{cases}$$

This is just the result of Problem 3.1 restated

$$\Psi_k(x) = \begin{cases} t \exp(ikx) & x > 0 \\ \exp(ikx) + r \exp(-ikx) & x < 0 \end{cases}.$$

Problem 3.5 Asymptotic solution

If we try to apply the Hamiltonian on the wavefunction given in eq 3.30,

$$H\Psi_k(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2\left[\exp(ikz) + \frac{f(\theta, \phi)}{r} \exp(ikr)\right]$$

$$H\Psi_k(\mathbf{r}) = -\frac{\hbar^2}{2m}\left[-k^2\exp(ikz) + f(\theta,\phi)\frac{1}{r^2}\frac{\partial(ikr-1)\exp(ikr)}{\partial r} + \frac{\exp(ikr)}{r}\nabla^2 f(\theta,\phi)\right]$$
$$H\Psi_k(\mathbf{r}) = -\frac{\hbar^2}{2m}\left[-k^2\exp(ikz) - \frac{\exp(ikr)}{r}f(\theta,\phi)k^2 + \frac{\exp(ikr)}{r}\nabla^2 f(\theta,\phi)\right]$$
$$H\Psi_k(\mathbf{r}) = \frac{\hbar^2 k^2}{2m}\Psi_k(\mathbf{r}) - \frac{\hbar^2}{2m}\frac{\exp(ikr)}{r}\nabla^2 f(\theta,\phi)$$

there is a residue term, which scales as

$$\frac{1}{r}\nabla^2 f(\theta,\phi) = \frac{1}{r^3}g(\theta,\phi)$$

where g is a function independent of r. As $r\to\infty$, this term decreases much faster than the scattered term, eq 3.30 is thus an asymptotic solution.

The "correction" term χ

$$\Psi'_k(\mathbf{r}) = \Psi_k(\mathbf{r}) + \chi(\mathbf{r})$$

which solves the energy equation. χ satisfies

$$\begin{aligned} H\Psi'_k(\mathbf{r}) &= \frac{\hbar^2k^2}{2m}\Psi(\mathbf{r}) - \frac{\hbar^2}{2m}\frac{\exp(ikr)}{r}\nabla^2 f - \frac{\hbar^2}{2m}\nabla^2\chi \\ \frac{\hbar^2k^2}{2m}\big(\Psi_k(\mathbf{r}) + \chi\big) &= \frac{\hbar^2k^2}{2m}\Psi(\mathbf{r}) - \frac{\hbar^2}{2m}\frac{\exp(ikr)}{r}\nabla^2 f - \frac{\hbar^2}{2m}\nabla^2\chi \\ k^2\chi + \nabla^2\chi &= -\frac{\exp(ikr)}{r}\nabla^2 f = r^{-3}\exp(ikr)g(\theta,\phi) \end{aligned}$$

If we are free to remove the phase factors on the left and tight hand sides, the leading order of the taylor expansion of χ in r would be -3.

Problem 3.6 The sphere potential

The first Born approximation of the scattering amplitude is

$$f_{\text{Born}}(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}\mathbf{r}'\exp\big(-i\mathbf{q}\cdot\mathbf{r}'\big)V(r')$$

In the case of a spherically symmetric potential only nonzero and uniform within radius a_0, the integral is invariant under $\mathbf{q}\to R\mathbf{q}$. We set a $\mathbf{r}'$ coordinate system with $\hat{\mathbf{q}}$ as polar direction,

$$\begin{aligned} q &= \sqrt{(\mathbf{k}_f - \mathbf{k}_i)\cdot(\mathbf{k}_f - \mathbf{k}_i)} \\ q &= k(2 - 2\cos\theta)^{\frac{1}{2}} \\ f_{\text{Born}}(\theta,\phi) &= -\frac{m}{2\pi\hbar^2}\int_0^{a_0}\mathrm{d}r'\int_0^{2\pi}\mathrm{d}\phi'\int_0^{\pi}\mathrm{d}\theta'\, {r'}^2\sin\theta'\exp\big(-iqr'\cos\theta\big)V_0 \end{aligned}$$

$$f_{\text{Born}}(\theta,\phi) = -\frac{mV_0}{2\pi\hbar^2}2\pi\int_0^{a_0}\mathrm{d}r'\int_{-1}^{1}\mathrm{d}u\, r'^2\exp\bigl(-iqr'u\bigr)$$
$$f_{\text{Born}}(\theta,\phi) = -\frac{mV_0}{2\pi\hbar^2}\frac{4\pi}{q}\int_0^{a_0}\mathrm{d}r'\, r'\sin\bigl(qr'\bigr)$$
$$\boxed{f_{\text{Born}}(\theta,\phi) = \frac{2mV_0}{\hbar^2}\frac{qa_0\cos(qa_0)-\sin(qa_0)}{q^3}}$$
$$f_{\text{Born}}(\theta,\phi) = \frac{2mV_0}{\hbar^2}a_0^3\sum_{n=0}^{\infty}\frac{1}{(2n)!}\frac{2n}{2n+1}(qa_0)^{2n-2}$$
$$\boxed{f_{\text{Born}}(\theta,\phi) = \frac{2mV_0}{\hbar^2}\frac{a_0^3}{3}\sum_{n=0}^{\infty}\frac{3}{(2n+1)!(2n+3)}\bigl[k^2(2-2\cos\theta)\bigr]^n}$$

The two expressions are the explicit expression and Taylor expansion respectively. The zeroth term in the infinite series is always 1.

Problem 3.7 Spherical Bessel functions

Show that

$$j_l = (-\rho)^l\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l\frac{\sin\rho}{\rho}$$
$$n_l = -(-\rho)^l\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l\frac{\cos\rho}{\rho}$$

satisfy spherical Bessel equation

$$\rho^2\frac{\mathrm{d}^2r_l}{\mathrm{d}\rho^2}+2\rho\frac{\mathrm{d}r_l}{\mathrm{d}\rho}+\bigl[\rho^2-l(l+1)\bigr]r_l = 0$$

Let

$$r_l = \sum_m^{\infty}\alpha_m\rho^m$$

The spherical Bessel equation gives a recursive formula for these coefficients.

$$\sum_m\alpha_m\bigl[m(m-1)+2m-l(l+1)\bigr]\rho^m+\sum_m\alpha_m\rho^{m+2} = 0$$
$$\alpha_{m-2} = -\alpha_m\bigl[m(m+1)-l(l+1)\bigr]$$

This specifies the recursive relations of the Laurent series coefficients, as well as the (lower) terminating index. The odd/even parts are independent, they terminate at either $m=l$ or $m=-l-1$.

For convenience, use Rayleigh's formula to get Hankel functions

$$h_l(\rho) \equiv j_l(\rho) + i n_l(\rho) = -i(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\exp(i\rho)}{\rho}$$

Expand the above as a power series

$$h_l = (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \sum_{n=0} \frac{(i\rho)^{n-1}}{n!} = \sum_{n=-1-l} \beta_n \rho^n$$

$$h_l = \sum_{n=-1} (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{(i\rho)^n}{(n+1)!}$$

The power terms and their coefficients satisfy

$$\begin{aligned}
(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{(i\rho)^{n+2}}{(n+2+1)!} &= (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^{l-1} \frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\frac{(i\rho)^{n+2}}{(n+3)!} \\
&= (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^{l-1} (n+2) i^2 \frac{(i\rho)^n}{(n+3)!} \\
&= -\frac{1}{n+3}(-\rho)^l \underbrace{\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^{l-1} \frac{(i\rho)^n}{(n+1)!}}_{\propto \rho^{n-2l+2}} \\
&= -\frac{\rho^2}{(n+3)(n-2l-2)}(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{(i\rho)^n}{(n+1)!} \\
\beta_{n+2-l}\rho^{n+2-l} &= -\frac{\rho^2}{(n+3)(n-2l+2)}\beta_{n-l}\rho^{n-l} \\
n+2-l = n' \implies \qquad \beta_{n'} &= \frac{1}{(n'+l+1)(n'-l)}\beta_{n'-2} \\
\beta_{n-2} &= -(n^2+n-l^2-l+ln-ln)\beta_n \\
\beta_{n-2} &= -\big[n(n+1) - l(l+1)\big]\beta_n
\end{aligned}$$

Therefore, the Laurent series of Rayleigh's formula for Hankel functions satisfy the recursive relations specified by the spherical Bessel equation. Separating into real and imaginary parts, Rayleigh's formulas must solve spherical Bessel's equation.

Problem 3.8

At small arguments, the dominating term is the lowest order term. From Problem 3.7, the lowest orders are l or $-l-1$, so the lowest order terms are respectively

$$j_l \approx (-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{(i\rho)^{2l}}{(2l+1)!}$$

$$n_l \approx -i(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{(i\rho)^{-1}}{(-1+1)!}$$

Let $u = \rho^2$ so that $\frac{\mathrm{d}\rho}{\mathrm{d}u} = \frac{1}{2\rho}$

$$\begin{aligned}
j_l &\approx (-1)^l u^{l/2} \left(2\frac{\mathrm{d}\rho}{\mathrm{d}u}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{(i)^{2l}u^l}{(2l+1)!} \\
j_l &\approx (-2)^l u^{l/2} \frac{\mathrm{d}^l}{\mathrm{d}u^l} \frac{(i)^{2l}u^l}{(2l+1)!} \\
j_l &\approx u^{l/2} \frac{2^l l!}{(2l+1)!} \\
j_l &\approx \frac{\rho^l}{(2l+1)!!} \\
n_l &\approx -i(-2)^l u^{l/2} \frac{\mathrm{d}^l}{\mathrm{d}u^l} \frac{(i)^{-1}u^{-1/2}}{(-1+1)!} = -(-2)^l u^{l/2} \left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right) \dots u^{-1-l} \\
n_l &\approx -(-2)^l u^{l/2} \left(-\frac{1}{2}\right)^l (2l-1)!! u^{-\frac{1+2l}{2}} \\
n_l &\approx -\frac{(2l-1)!!}{\rho^{l+1}}
\end{aligned}$$

Where the double factorial is defined as

$$\begin{aligned}
n!! &= n(n-2)!! \\
0!! &= 1!! = 1
\end{aligned}$$

Problem 3.9

For large arguments, the Hankel function can be approximated

$$\begin{aligned}
h_l(\rho) &= -i(-\rho)^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\exp(i\rho)}{\rho} \\
&= -i(-\rho)^l \frac{i^l}{\rho^l} \frac{\exp(i\rho) + O(\rho^{-1})}{\rho} \\
&= (-i)^{l+1} \frac{\exp(i\rho) + O(\rho^{-1})}{\rho} \\
&= -i \exp\left(-i\frac{l\pi}{2}\right) \frac{\exp(i\rho) + O(\rho^{-1})}{\rho} \\
&\approx -\frac{i}{\rho} \exp\left(i\left[\rho - \frac{l\pi}{2}\right]\right)
\end{aligned}$$

$$j_l(\rho) = \text{Re}\left[h_l(\rho)\right] \approx \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right)$$
$$n_l(\rho) = \text{Im}\left[h_l(\rho)\right] \approx -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right)$$

Problem 3.10 Flux

In 3D the probability current of a wavefunction Ψ is

$$\mathbf{j} = -\frac{i\hbar}{2m}(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*)$$

Given a general (free) wavefunction

$$\Psi(\mathbf{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)\left[c_{lm}^{\text{out}}h_l^{(1)}(kr) + c_{lm}^{\text{in}}h_l^{(2)}(kr)\right]$$

Compute the flux through a large sphere

$$\text{Flux} = \oint \mathbf{j}\cdot \mathrm{d}\boldsymbol{\sigma}$$
$$\text{Flux} = \oint r^2 j_r \,\mathrm{d}\Omega$$
$$j_r = -\frac{i\hbar}{2m}\left(\Psi^*\frac{\mathrm{d}\Psi}{\mathrm{d}r} - c.c.\right)$$
$$j_r = -\frac{i\hbar}{2m}\left(\Psi^*\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)\left[c_{lm}^{\text{out}}\left(-\frac{1}{r}+ik\right)h_l + c_{lm}^{\text{in}}\left(-\frac{1}{r}-ik\right)h_l^*\right] - c.c.\right)$$
$$\text{Flux} = -\oint \frac{i\hbar r^2}{2m}\left(\Psi^*\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)\left[c_{lm}^{\text{out}}\left(-\frac{1}{r}+ik\right)h_l + c_{lm}^{\text{in}}\left(-\frac{1}{r}-ik\right)h_l^*\right] - c.c.\right)\mathrm{d}\Omega$$
$$= -\frac{i\hbar r^2}{2m}\left(\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[c_{lm}^{\text{out}}h_l + c_{lm}^{\text{in}}h_l^*\right]^*\left[c_{lm}^{\text{out}}\left(-\frac{1}{r}+ik\right)h_l + c_{lm}^{\text{in}}\left(-\frac{1}{r}-ik\right)h_l^*\right] - c.c.\right)$$
$$= \frac{\hbar r^2 k}{2m}\left(\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[c_{lm}^{\text{out}}h_l + c_{lm}^{\text{in}}h_l^*\right]^*\left[c_{lm}^{\text{out}}h_l - c_{lm}^{\text{in}}h_l^*\right] + c.c.\right)$$
$$= \frac{\hbar r^2 k}{2m}\left(\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[\left|c_{lm}^{\text{out}}\right|^2 h_l^* h_l - \left|c_{lm}^{\text{in}}\right|^2 h_l h_l^* + c_{lm}^{\text{in}\,*}c_{lm}^{\text{out}}h_l h_l - c_{lm}^{\text{out}*}c_{lm}^{\text{in}}h_l^* h_l^*\right] + c.c.\right)$$

$$= \frac{\hbar}{m} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[\left| c_{lm}^{\text{out}} \right|^2 - \left| c_{lm}^{\text{in}} \right|^2 \right] \lim_{r\to\infty} r^2 k \frac{1}{r^2 k^2}$$
$$= \frac{\hbar}{mk} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[\left| c_{lm}^{\text{out}} \right|^2 - \left| c_{lm}^{\text{in}} \right|^2 \right]$$

I also tried to calculate same flux in the following way.

$$\begin{aligned} \text{Flux} &= \oint \mathbf{j} \cdot \mathrm{d}\boldsymbol{\sigma} \\ &= \int \boldsymbol{\nabla} \cdot \mathbf{j} \, \mathrm{d}V \\ &= -\frac{i\hbar}{2m} \int \left(\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* \right) \mathrm{d}V \end{aligned}$$

but we know

$$\begin{aligned} \nabla^2 \Psi &= \frac{1}{r^2} \sum_{l=0}^{\infty} \left[\frac{\mathrm{d}}{\mathrm{d}r} \left(r^2 \frac{\mathrm{d}}{\mathrm{d}r} \right) - l(l+1) \right] \sum_{m=-l}^{l} Y_{lm}(\theta, \phi) \left[c_{lm}^{\text{out}} h_l^{(1)}(kr) + c_{lm}^{\text{in}} h_l^{(2)}(kr) \right] \\ &= \frac{1}{r^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm} \left[r^2 \frac{\mathrm{d}^2}{\mathrm{d}r^2} + 2r \frac{\mathrm{d}}{\mathrm{d}r} - l(l+1) \right] \left[c_{lm}^{\text{out}} h_l + c_{lm}^{\text{in}} h_l^* \right] \\ &= \frac{1}{r^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm} \left[-r^2 k^2 \right] \left[c_{lm}^{\text{out}} h_l + c_{lm}^{\text{in}} h_l^* \right] \\ &= -k^2 \Psi \end{aligned}$$

which is kind of not a surprise. Exactly the same calculation follows for Ψ^*, giving a total flux through a large sphere to be 0. Again this is no surprise either because all of the components with which we constructed the wavefunction are free waves. What went wrong? Physically, the wavefunction is not spanned by free states near $r = 0$. Mathematically, this probably corresponds to some unobvious singularity of the laplacian of the spherical Bessel function. I learnt this the hard way.

Problem 3.11 The hard sphere

(a)

Outside the sphere, the wavefunction is spanned by $m = 0$ free waves.

$$\Psi(\mathbf{r}) = \sum_{l=0}^{\infty} Y_{l_0}(\theta, \phi) \left[\exp(2i\delta_l) h_l(kr) + h_l^*(kr) \right]$$

On the surface of the hard sphere $r = a_0$, the boundary condition is $\Psi = 0$. Since the different angular momentum channels are orthogonal

$$\begin{aligned}\exp(2i\delta_l)h_l(ka_0) + h_l^*(ka_0) &= 0 \\ \frac{\exp(+i\delta_l)}{\exp(-i\delta_l)} &= -\frac{j_l(ka_0) - in_l(ka_0)}{j_l(ka_0) + in_l(ka_0)} \\ \frac{1 + i\tan(\delta_l)}{1 - i\tan(\delta_l)} &= \frac{n_l(ka_0) + ij_l(ka_0)}{n_l(ka_0) - ij_l(ka_0)} \\ \tan(\delta_l) &= \frac{j_l(ka_0)}{n_l(ka_0)}\end{aligned}$$

(b)

For δ_0, this is

$$\begin{aligned}\tan(\delta_l) &= \frac{\sin(ka_0)}{-\cos(ka_0)} \\ \delta_l &= -ka_0\end{aligned}$$

For general l at $ka_0 \ll 1$, quote from problem 3.8

$$\begin{aligned}j_l(\rho) &\approx \frac{\rho^l}{(2l+1)!!} \\ n_l(\rho) &\approx -\frac{(2l-1)!!}{\rho^{l+1}}\end{aligned} \tag{4}$$

we have

$$\begin{aligned}\tan(\delta_l) &\approx -\frac{(ka_0)^{2l+1}}{(2l+1)!!(2l-1)!!} \\ \delta_l &\approx -\frac{(ka_0)^{2l+1}}{(2l+1)\big[(2l-1)!!\big]^2}\end{aligned}$$

(c)

Using

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

At low k, the $l = 0$ term dominates. Substitute in results from *(b)*

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\frac{(ka_0)^2}{\big[(-1)!!\big]^4} = 4\pi a_0^2$$

where

$$1!! = 1 \times (1-2)!! \implies (-1)!! = 1$$

so the scattering cross-section of a hard sphere is its classical surface area.

Problem 3.12 scattered phase of spherical potential

For the spherical potential in problem 3.6, the wavefunction is spanned by k free waves outside a_0 and $k' = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ free waves inside a_0. On the inside, the only allowed component is j_l because n_l diverges at $r = 0$. Matching Ψ at the boundary for $l = 0$,

$$\begin{aligned}
\exp(2i\delta_0)h_0(ka_0) + h_0^*(ka_0) &= tj_0(k'a_0) \\
-i\frac{\exp(ika_0 + i\delta_0)}{ka_0} + i\frac{\exp(-ika_0 - i\delta_0)}{ka_0} &= e^{-i\delta_0}tj_0(k'a_0) \\
\frac{2}{ka_0}\sin(ka_0 + \delta_0) &= e^{-i\delta_0}t\frac{\sin(k'a_0)}{k'a_0}
\end{aligned}$$

Similarly, the derivative terms of Ψ are matched

$$\frac{2k}{ka_0}\cos(ka_0 + \delta_0) - \frac{2}{ka_0^2}\sin(ka_0 + \delta_0) = e^{-i\delta_0}tk'\frac{k'a_0\cos(k'a_0) - \sin(k'a_0)}{(k'a_0)^2}$$

Divide one by the other we get

$$\begin{aligned}
k\cot(ka_0 + \delta_0) - \frac{1}{a_0} &= k'\cot\big(k'a_0\big) - \frac{1}{a_0} \\
\tan(ka_0 + \delta_0) &= \frac{k}{k'}\tan\big(k'a_0\big) \\
\delta_0 &= \arctan\left[\frac{k}{k'}\tan\big(k'a_0\big)\right] - ka_0
\end{aligned}$$

Problem 3.13 Low momentum scattered phase

R_l is the solution of the nonhomogeneous spherical Bessel's equation from the origin up to some point r outside the interaction region, where it is matched with free waves which is combined from j_l and n_l.

$$\begin{aligned}
R_l(r) &= \exp(2i\delta_l)h_l(kr) + h_l^*(kr) \\
R_l'(r) &= \exp(2i\delta_l)h_l'(kr) + h_l^{*\prime}(kr)
\end{aligned}$$

Sub in $h_l = j_l + in_l$,

$$\begin{aligned}
\exp(-i\delta_l)R_l(r) &= \cos(\delta_l)j_l - \sin(\delta_l)n_l \\
\exp(-i\delta_l)R_l'(r) &= k\cos(\delta_l)j_l' - k\sin(\delta_l)n_l' \\
\gamma\cos(\delta_l)j_l - \gamma\sin(\delta_l)n_l &= k\cos(\delta_l)j_l' - k\sin(\delta_l)n_l' \\
(\gamma j_l - kj_l')\cos(\delta_l) &= (\gamma n_l - kn_l')\sin(\delta_l)
\end{aligned}$$

$$\tan(\delta_l) = \frac{\gamma j_l(kr) - kj_l'(kr)}{\gamma n_l(kr) - kn_l'(kr)}$$

where $\gamma \equiv \frac{R_l'(r)}{R_l(r)}$. As $k \to 0$,

$$\begin{aligned}
\tan(\delta_l) &= \frac{\gamma j_l(ka_0) - kj_l'(ka_0)}{\gamma n_l(ka_0) - kn_l'(ka_0)} \\
\delta_l &\to \frac{\left[\gamma a_0^l + a_0^{l-1}O(1)\right]O(k^l)}{\left[\gamma a_0^{-l-1} + a_0^{-l-2}O(1)\right]O\left(\frac{1}{k^{l+1}}\right)} \\
\delta &\to \frac{\gamma a_0 + O(1)}{\gamma a_0 + O(1)} a_0^{2l+1} O(k^{2l+1})
\end{aligned}$$

Note the top and bottom $O(1)$ are not in equal because they come from different cos and sin series coefficients. An intuitive guess is that they are only the same when $l = (l+1)!$.

Problem 3.14 Scattering length

In Problem 3.12, the scattering length is the scattered phase at small k divided by $-k$

$$\begin{aligned}
\delta_0 &= \arctan\left[\frac{k}{k'}\tan\left(k'a_0\right)\right] - ka_0 \\
a &= \lim_{k\to 0}\left\{a_0 - \frac{1}{k}\arctan\left[\frac{k}{\sqrt{k^2 - 2mV_0\hbar^{-2}}}\tan\left(\sqrt{k^2 - 2mV_0\hbar^{-2}}a_0\right)\right]\right\}
\end{aligned}$$

For finite positive V_0

$$a = a_0 - \frac{1}{\sqrt{2mV_0\hbar^{-2}}}\tanh\left(\sqrt{2mV_0\hbar^{-2}}a_0\right) \in [0, a_0)$$

For finite negative V_0, however

$$a = a_0 - \frac{1}{\sqrt{-2mV_0\hbar^{-2}}}\tan\left(\sqrt{-2mV_0\hbar^{-2}}a_0\right)$$

because tan diverges for finite V_0 to both $\pm\infty$, the value of a also oscillates to infinities (and come back from the other side). Using $\tan u > u$ for $0 < u < \frac{\pi}{2}$, we know $a < 0$ at small negative V_0.

Problem 3.15 Reflection probability in Breit-Wigner form

In 1D, a particle which is free everywhere but at $x = 0$ has wavefunction

$$\Psi = \begin{cases} e^{ikx} + re^{-ikx} & x < 0 \\ te^{ikx} & x > 0 \end{cases}$$

$$\Psi_{\text{even}} = \frac{1}{2}\begin{cases} e^{ikx} + re^{-ikx} + te^{-ikx} & x < 0 \\ te^{ikx} + e^{-ikx} + re^{ikx} & x > 0 \end{cases}$$

The continuity of Ψ at $x = 0$ means

$$t = 1 + r$$

Quote *eq (3.93) on the handout* or Problem 3.3 on this Problem sheet, it's easy to get

$$\lim_{x\to 0^\pm} \Psi'_{\text{even}} = \mp k \sin(\delta_{\text{even}})$$

Substituting into the free waves,

$$\frac{ik}{2}(1 - r - t - t + 1 - r) = 2k\sin(\delta_{\text{even}})$$
$$-ir = \sin(\delta_{\text{even}})$$
$$|r|^2 = \sin^2(\delta_{\text{even}}) = \frac{\tan^2(\delta_{\text{even}})}{1 + \tan^2(\delta_{\text{even}})}$$
$$\left|r(k)\right|^2 = \frac{(mt^2/\hbar^2 k)^2}{(\mathcal{E}_{\text{res}} - E_k)^2 + (mt^2/\hbar^2 k)^2} = \frac{\gamma^2/4}{(\mathcal{E}_{\text{res}} - E_k)^2 + \gamma^2/4}$$

where $\gamma = \frac{2mt^2}{\hbar^2 k}$. This is said to be in Breit-Wigner form.

Problem 3.16

Consider the 1D Schrodinger equation. It's Green's function satisfies

$$\left[E_k + \frac{\hbar^2}{2m}\nabla^2 + i\frac{\hbar^2}{2m}\epsilon\right]G(x) = \delta(x)$$

where $i\epsilon$ is a manually added infinitesimal damping term. The fourier transform under convention

$$G(x) = \frac{1}{2\pi}\int \mathrm{d}q\, e^{iqx}\tilde{G}(q)$$

satisfies

$$G(k) = \frac{2m}{\hbar^2}\frac{1}{k^2 - q^2 + i\epsilon}$$

Use residue theorem $G(x)$ can be obtained as

$$G(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}q\, e^{iqx}\frac{2m}{\hbar^2}\frac{1}{k^2 - q^2 + i\epsilon}$$
$$= \frac{m}{\pi\hbar^2}\int_{-\infty}^{\infty} \mathrm{d}q\, \frac{e^{iqx}}{k^2 - q^2 + i\epsilon}$$

$$
\begin{aligned}
&= \frac{m}{\pi\hbar^2} 2\pi i \sum \mathrm{res}(q_i) \\
&= \frac{2m}{\hbar^2} i \begin{cases} -\frac{\exp(ikx)}{2k} & x > 0 \\ -\frac{\exp(-ikx)}{2k} & x < 0 \end{cases} \\
&= -i\frac{m}{\hbar^2 k}\exp\bigl(ik|x|\bigr)
\end{aligned}
$$

Problem 3.17 Formal scattering

Eq. (3.112) on the handout states

$$f(\mathbf{k}_f, \mathbf{k}_i) = -\frac{4\pi^2 m}{\hbar^2} \left\langle \mathbf{k}_f \right| T \left| \mathbf{k}_i \right\rangle$$

At $\theta = 0$ i.e. $\mathbf{k}_f = \mathbf{k}_i$, this evaluates to

$$f(\theta = 0) = -\frac{4\pi^2 m}{\hbar^2} \left\langle \mathbf{k}_i \right| T \left| \mathbf{k}_i \right\rangle$$

The total cross-section is

$$
\begin{aligned}
\sigma_{\mathrm{tot}} &= \int \left| f(\theta,\phi) \right|^2 \mathrm{d}\Omega \\
\sigma_{\mathrm{tot}} &= \left(\frac{4\pi^2 m}{\hbar^2} \right)^2 \left\langle \mathbf{k}_i \right| T^\dagger \int \left| \mathbf{k}_f \right\rangle \left\langle \mathbf{k}_f \right| \mathrm{d}\Omega \, T \left| \mathbf{k}_i \right\rangle
\end{aligned}
$$

Because k_f is confined by the condition $H_0 \left|\Psi\right\rangle = E_k \left|\Psi\right\rangle$, and the integral is over a spherical surface in momentum space, which is only a subspace we write

$$\sigma_{\mathrm{tot}} = \left(\frac{4\pi^2 m}{\hbar^2} \right)^2 \left\langle \mathbf{k}_i \right| T^\dagger \frac{1}{k^3} P_k T \left| \mathbf{k}_i \right\rangle$$

where P_i is the projector onto state k. It satisfies

$$\frac{1}{k} P_k = \delta\left(\frac{\hat{p}}{\hbar} - k \right) = \frac{\partial E}{\partial k} \delta(H_0 - E_k)$$

Formally, the basis-independent Green's function operator is

$$G_k^+ = \frac{1}{E_k - H_0 + i\epsilon}$$

Both sides of *eq. (3.113) on the handout* are real, so

$$\mathrm{Im}\left[\left\langle \mathbf{k}_i \right| T^\dagger \left| \mathbf{k}_i \right\rangle \right] + \mathrm{Im}\left[\left\langle \mathbf{k}_i \right| T^\dagger G_k^+ T \left| \mathbf{k}_i \right\rangle \right] = 0$$

$$-\operatorname{Im}\left[\langle \mathbf{k}_i| T^\dagger \frac{1}{E_k - H_0 + i\epsilon} T |\mathbf{k}_i\rangle\right] = -\operatorname{Im}\left[\langle \mathbf{k}_i| T |\mathbf{k}_i\rangle\right]$$
$$\pi \langle \mathbf{k}_i| T^\dagger \delta(E_k - H_0) T |\mathbf{k}_i\rangle = \frac{\hbar^2}{4\pi^2 m} \operatorname{Im}\left[f(\theta = 0)\right]$$
$$\pi \langle \mathbf{k}_i| T^\dagger \frac{\partial k}{\partial E_k} \frac{1}{k} P_k T |\mathbf{k}_i\rangle = \frac{\hbar^2}{4\pi^2 m} \operatorname{Im}\left[f(\theta = 0)\right]$$
$$\pi \left(\frac{\hbar^2}{4\pi^2 m}\right)^2 \frac{mk^2}{\hbar^2 k} \sigma_{\text{tot}} = \frac{\hbar^2}{4\pi^2 m} \operatorname{Im}\left[f(\theta = 0)\right]$$
$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k} \operatorname{Im}\left[f(\theta = 0)\right]}$$

Problem 3.18 Quantum point contact

In their respective semiclassical regimes, the problem of quantum point contact and Landau-Zener problem are analogous in the following sense.

$$\dot{\Psi} \approx -\frac{i}{\hbar} E(t)\Psi$$
$$\Psi' \approx -\frac{i}{\hbar} p(x)\Psi$$

From *eq. (3.118) on the handout*,

$$p(x) \approx \sqrt{\left(k^2 - \frac{\pi^2 n^2}{d_0^2}\right) + \frac{1}{2} k_n x^2}$$
$$\approx \hbar \sqrt{\frac{2\pi^2}{d_0^2} n z_n + \frac{1}{2} k_n x^2}$$

Make the following transformations from Problem 1.9

$$t \to x$$
$$\Delta \to \pi\hbar \sqrt{\frac{2nz_n}{d_0^2}}$$
$$\beta \to \hbar \sqrt{\frac{k_n}{2}} = \hbar \sqrt{\frac{2\pi^2 n^2}{d_0^3 R}}$$

The “transition probability” from positive p to negative p corresponds to reflection coefficient (in my humble opinion, as opposed to $\frac{R}{T}$)

$$R = \exp\left(-\frac{\pi}{\hbar} \frac{2\pi^2 \hbar^2 n z_n / d_0^2}{\hbar \sqrt{2\pi^2 n^2 / d_0^3 R}}\right)$$

$$= \exp\left(-\pi^2 z_n \sqrt{\frac{2R}{d_0}}\right)$$

There are 2 quantities called R in this equation but they are not the same thing.

Topic 4

Problem 4.1

Consider 3 elements a, b, and c labeled 1, 2, and 3. Label exchange operators result in The

	1	2	3
	a	b	c
$P_{12} \hookrightarrow$	b	a	c
$P_{23} \hookrightarrow$	b	c	a
$P_{12} \hookrightarrow$	c	b	a

result of $P_{12}P_{23}P_{12}$ in last line is just the same as that of P_{13}. Similarly if we exchange the labels $2 \leftrightarrow 3$ from above then $P_{23}P_{12}P_{23} = P_{13}$. A simultaneous eigenstate of all the permutation operators thence satisfies

$$E_{23}^2 E_{12} = E_{13} = E_{12}^2 E_{23}$$

where E_{ij} are the eigenvalues. All eigenvalues are therefore equal and ± 1.

Problem 4.2 Entanglement

For a pair of indistinguishable particles with wavefunction

$$\begin{aligned}
\Psi(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{\sqrt{2}}\left[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) \pm \phi_2(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\right] \\
P_{12}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{1}{2}\Big[|\phi_1|^2(\mathbf{r}_1)|\phi_2|^2(\mathbf{r}_2) \pm 2\,\mathrm{Re}\left[\phi_1(\mathbf{r}_1)\phi_1^*(\mathbf{r}_2)\phi_2(\mathbf{r}_2)\phi_2^*(\mathbf{r}_1)\right] + |\phi_1|^2(\mathbf{r}_2)|\phi_2|^2(\mathbf{r}_1)\Big] \\
P_1(\mathbf{r}_1) &= \int \mathrm{d}\mathbf{r}_2\, P_{12}(\mathbf{r}_1, \mathbf{r}_2) \\
P_1(\mathbf{r}_1) &= \frac{1}{2}\Big[|\phi_1|^2(\mathbf{r}_1) \pm 2\,\mathrm{Re}\left[\phi_1(\mathbf{r}_1)\phi_2^*(\mathbf{r}_1)\,\langle\phi_1|\phi_2\rangle\right] + |\phi_2|^2(\mathbf{r}_1)\Big] \\
P_2(\mathbf{r}_2) &= \int \mathrm{d}\mathbf{r}_1\, P_{12}(\mathbf{r}_1, \mathbf{r}_2) \\
P_2(\mathbf{r}_2) &= \frac{1}{2}\Big[|\phi_2|^2(\mathbf{r}_2) \pm 2\,\mathrm{Re}\left[\phi_1(\mathbf{r}_2)\phi_2^*(\mathbf{r}_2)\,\langle\phi_2|\phi_1\rangle\right] + |\phi_1|^2(\mathbf{r}_2)\Big]
\end{aligned}$$

If the $\phi_{1,2}$ are orthogonal it is immediately obvious $P_{12} \neq P_1 P_2$, i.e. information about one implies information about another. The term in the middle of P_{12} is bunching/anti-bunching for bosons/fermions.

Problem 4.3 Half-half beam splitter

A 50 : 50 beam splitter scatters two bosons approaching from opposite sides into a state

$$\frac{1}{\sqrt{2}}\big(|\text{Left}\rangle \pm |\text{Right}\rangle\big)$$

The probabilities are

$$P_{12}(\text{Left},\text{Left}) = P_{12}(\text{Right},\text{Right}) = \frac{1}{2}$$
$$P_{12}(\text{Left},\text{right}) = P_{12}(\text{Right},\text{Left}) = 0$$

Problem 4.4

(a) the totally antisymmetric state of three fermions

$$\left|\Psi^A_{123}\right\rangle = +\frac{1}{\sqrt{3!}}\big[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_3) + \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_3)\phi_3(\mathbf{r}_1) + \phi_1(\mathbf{r}_3)\phi_2(\mathbf{r}_1)\phi_3(\mathbf{r}_2)\big]$$
$$- \frac{1}{\sqrt{3!}}\big[\phi_1(\mathbf{r}_3)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_1) + \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_3)\phi_3(\mathbf{r}_2) + \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)\phi_3(\mathbf{r}_3)\big]$$

(b) the totally symmetric state of three fermions

$$\left|\Psi^S_{112}\right\rangle = \frac{1}{\sqrt{3!2!}}\big[2\phi_1(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_3) + 2\phi_1(\mathbf{r}_2)\phi_1(\mathbf{r}_3)\phi_2(\mathbf{r}_1) + 2\phi_1(\mathbf{r}_3)\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\big]$$
$$\left|\Psi^S_{112}\right\rangle = \frac{1}{\sqrt{3}}\big[\phi_1(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_3) + \phi_1(\mathbf{r}_2)\phi_1(\mathbf{r}_3)\phi_2(\mathbf{r}_1) + \phi_1(\mathbf{r}_3)\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\big]$$

Problem 4.5

There are a total of $N!$ different permutation operators.

$$\left|\sum_P P\,|\Psi\rangle\right|^2 = \sum_{P_1}\sum_{P_2}\langle\Psi|\,P_1P_2\,|\Psi\rangle$$

The indexed terms on the right hand side are one if

$$P_1P_2\,|\Psi\rangle = |\Psi\rangle$$

otherwise they are 0. For every P_1, there is only one $P_2 = P_1$ which makes $P_2 P_1 = I$, but for every $P_2 = P_1$, there are $\prod_\alpha N_\alpha!$ permutations which do not effect the state each particle is in. Therefore,

$$\left|\sum_P P\left|\Psi\right\rangle\right|^2 = \prod_\alpha N_\alpha! \sum_{P_1} 1 = N! \prod_\alpha N_\alpha!$$

The normalised totally symmetric state is thence

$$\left|\Psi^S\right\rangle = \sqrt{\frac{N!}{\prod_\alpha N_\alpha!}} \mathcal{S}\left|\Psi\right\rangle$$

Similar follows for the anti-symmetrising operator.

Problem 4.6

$$\begin{aligned}
\Psi^A &= \frac{1}{\sqrt{N!}} \begin{vmatrix} z_1^{-(N-1)/2} & & \\ & \cdots & \\ & & z_N^{(N-1)/2} \end{vmatrix} \\
&= \frac{1}{\sqrt{N!}} \prod_k z_k^{-(N-1)/2} \begin{vmatrix} 1 & & \\ & \cdots & \\ & & z_N^{(N-1)} \end{vmatrix} \\
\text{Vadermonde} \implies \quad &= \frac{1}{\sqrt{N!}} \prod_k z_k^{-(N-1)/2} \prod_{i<j} (z_i - z_j) \\
&= \frac{1}{\sqrt{N!}} \prod_k z_k^{-(N-1)/2} \prod_{l<k} (z_l z_k)^{1/2} \prod_{i<j} \left[\left(\frac{z_i}{z_j}\right)^{1/2} - \left(\frac{z_i}{z_j}\right)^{-1/2} \right] \\
&= \frac{1}{\sqrt{N!}} \prod_k z_k^{-(N-1)/2} z_k^{(N-k)/2} z_k^{(k-1)/2} \prod_{i<j} \left[\left(\frac{z_i}{z_j}\right)^{1/2} - \left(\frac{z_i}{z_j}\right)^{-1/2} \right] \\
&= \frac{(2i)^{N(N-1)/2}}{\sqrt{N!}} \prod_{i<j} \sin\left(\frac{\pi(x_i - x_j)}{L}\right) \\
&= \frac{(2i)^{N(N-1)/2}}{\sqrt{N!}} \prod_j^N \prod_i^{j-1} \sin\left(\frac{\pi(x_i - x_j)}{L}\right)
\end{aligned}$$

There are a total of $N - j + j - 1 = N - 1$ terms which involve something in the form $\sin\left(\frac{\pi x_i}{L} + \phi\right)$ for every x_i. Therefore for odd N, upon $x \to x + L$, $\left|\Psi^A\right\rangle \to (-1)^{N-1}\left|\Psi^A\right\rangle =$

$\left|\Psi^A\right\rangle$. Upon any $x_i \leftrightarrow x_j$, the terms in the denominator are replaced by the terms in the numerator in the following equation

$$\left|\Psi^A\right\rangle \to \left|\Psi^A\right\rangle \frac{\operatorname{sgn}(i-j)\sin\left(x_i-x_j\right)\prod_k \operatorname{sgn}(i-k)\sin\left(x_j-x_k\right)\prod_k \operatorname{sgn}(j-k)\sin\left(x_j-x_i\right)}{\operatorname{sgn}(j-i)\sin\left(x_j-x_i\right)\prod_k \operatorname{sgn}(i-k)\sin(x_i-x_k)\prod_k \operatorname{sgn}(j-k)\sin\left(x_j-x_k\right)}$$
$$\to -\left|\Psi^A\right\rangle$$

where we now work in natural units $\frac{\pi}{L}$ for simplicity and the $\pm\sin\left(x_i-x_j\right)$ in front of the fraction are the recounted terms. Therefore the wavefunction is periodic and totally antisymmetric.

Problem 4.7

$$\left|\Psi^S_{\alpha\alpha_1\alpha_2\ldots\alpha_N}\right\rangle = \sqrt{\frac{(N+1)!}{\prod_\beta (N_\beta+\delta_{\alpha\beta})!}}\mathcal{S}\left|\phi_\alpha\right\rangle\left|\phi_{\alpha_1}\right\rangle\left|\phi_{\alpha_2}\right\rangle\ldots\left|\phi_{\alpha_N}\right\rangle$$
$$\mathcal{S}\left|\phi_\alpha\right\rangle\left|\Psi^S_{\alpha_1\alpha_2\ldots\alpha_N}\right\rangle = \sqrt{\frac{N!}{\prod_\beta N_\beta!}}\mathcal{S}\left|\phi_\alpha\right\rangle\left|\phi_{\alpha_1}\right\rangle\left|\phi_{\alpha_2}\right\rangle\ldots\left|\phi_{\alpha_N}\right\rangle$$
$$\implies c_\alpha : \left|\Psi^S_{\alpha\alpha_1\alpha_2\ldots\alpha_N}\right\rangle = \sqrt{N+1}\mathcal{S}\left|\phi_\alpha\right\rangle\left|\Psi^S_{\alpha_1\alpha_2\ldots\alpha_N}\right\rangle = \sqrt{N_\alpha+1}\left|\Psi^S_{\alpha\alpha_1\alpha_2\ldots\alpha_N}\right\rangle$$

where the idempotency of $\mathcal{S}$ was used.

Problem 4.8

$$\sqrt{N+1}\mathcal{A}\left|\phi_\alpha\right\rangle\left|\Psi^A_{\alpha_1\alpha_2\ldots\alpha_N}\right\rangle = \sqrt{N!}\mathcal{A}\left|\phi_\alpha\right\rangle\left|\phi_{\alpha_1}\right\rangle\ldots\left|\phi_{\alpha_N}\right\rangle = \left|\Psi^A_{\alpha\alpha_1\ldots\alpha_N}\right\rangle = a^\dagger_\alpha\left|\Psi^A_{\alpha_1\alpha_2\ldots\alpha_N}\right\rangle$$

If $N_\alpha > 1$ for any α, the wavefunction vanishes. Thence the antisymmetric subspace of fermions is spanned by

$$N_\alpha = \{0,1\} \quad \forall\alpha$$

The ij-th matrix elements of a_α vanishes for any $N^i_\beta \neq N^j_\gamma$ i.e. a_α is only nonzero in α-subspace. In the basis $|0\rangle$ and $|1\rangle$,

$$a_\alpha = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \implies a_\alpha a^\dagger_\alpha = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix} \; ; \; a^\dagger_\alpha a_\alpha = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} \implies \left\{a_\alpha, a^\dagger_\beta\right\} = \delta_{\alpha\beta}$$
$$\implies a_\alpha a_\alpha = a^\dagger_\alpha a^\dagger_\alpha = 0 \implies \left\{a_\alpha, a_\beta\right\} = \left\{a^\dagger_\alpha, a^\dagger_\beta\right\} = 0$$

Problem 4.9 Bogoliubov transformation

$$H = \epsilon\Big(a^\dagger a + b^\dagger b\Big) + \Delta\Big(a^\dagger b^\dagger + ba\Big)$$

(a) Bosons

If all operators commute except

$$\Big[a, a^\dagger\Big] = \Big[b, b^\dagger\Big] = 1$$

Define

$$\alpha \equiv a\cosh\kappa - b^\dagger \sinh\kappa$$
$$\beta \equiv b\cosh\kappa - a^\dagger \sinh\kappa$$

Their commutation relations are

$$\Big[\alpha, \alpha^\dagger\Big] = \Big[a, a^\dagger\Big]\cosh^2\kappa - \Big[b^\dagger, a^\dagger\Big]\sinh\kappa\cosh\kappa - [a, b]\cosh\kappa\sinh\kappa + \Big[b^\dagger, b\Big]\sinh^2\kappa$$
$$\boxed{\Big[\alpha, \alpha^\dagger\Big] = \cosh^2\kappa - \sinh^2\kappa = 1}$$
$$\Big[\beta, \beta^\dagger\Big] = \Big[b, b^\dagger\Big]\cosh^2\kappa - \Big[a^\dagger, b^\dagger\Big]\sinh\kappa\cosh\kappa - [b, a]\cosh\kappa\sinh\kappa + \Big[a^\dagger, a\Big]\sinh^2\kappa$$
$$\boxed{\Big[\beta, \beta^\dagger\Big] = \cosh^2\kappa - \sinh^2\kappa = 1}$$
$$[\alpha, \beta] = [a, b]\cosh^2\kappa - \Big[b^\dagger, b\Big]\sinh\kappa\cosh\kappa - \Big[a, a^\dagger\Big]\cosh\kappa\sinh\kappa + \Big[b^\dagger, a\Big]\sinh^2\kappa$$
$$\boxed{[\alpha, \beta] = \sinh\kappa\cosh\kappa - \cosh\kappa\sinh\kappa = 0}$$
$$\Big[\alpha^\dagger, \beta\Big] = \Big[a^\dagger, b\Big]\cosh^2\kappa - [b, b]\sinh\kappa\cosh\kappa - \Big[a^\dagger, a^\dagger\Big]\cosh\kappa\sinh\kappa + [b, a]\sinh^2\kappa$$
$$\boxed{\Big[\alpha^\dagger, \beta\Big] = 0}$$

All the other commutators are trivially derived. α and β satisfy the same commutation relations as a, b. Using

$$\alpha^\dagger\alpha = a^\dagger a\cosh^2\kappa - ba\sinh\kappa\cosh\kappa - a^\dagger b^\dagger\cosh\kappa\sinh\kappa + bb^\dagger\sinh^2\kappa$$
$$\beta^\dagger\beta = b^\dagger b\cosh^2\kappa - ab\sinh\kappa\cosh\kappa - b^\dagger a^\dagger\cosh\kappa\sinh\kappa + aa^\dagger\sinh^2\kappa$$
$$\alpha^\dagger\alpha + \beta^\dagger\beta = \Big(\cosh^2\kappa + \sinh^2\kappa\Big)\Big(a^\dagger a + b^\dagger b\Big) - 2\cosh\kappa\sinh\kappa\Big(a^\dagger b^\dagger + ab\Big)$$

If we choose

$$\frac{\cosh^2\kappa + \sinh^2\kappa}{-2\cosh\kappa\sinh\kappa} = \frac{\epsilon}{\Delta}$$

$$\frac{\cosh(2\kappa)}{\sinh(2\kappa)} = -\frac{\epsilon}{\Delta}$$
$$\kappa = \frac{1}{2}\tanh^{-1}\left(-\frac{\Delta}{\epsilon}\right)$$

the Hamiltonian can be written as

$$H = \epsilon\sqrt{1-\left(\frac{\Delta}{\epsilon}\right)^2}\Big(\alpha^\dagger\alpha + \beta^\dagger\beta\Big)$$

The energy eigenvalues are therefore

$$E_{N_\alpha,N_\beta} = \epsilon\sqrt{1-\left(\frac{\Delta}{\epsilon}\right)^2}\big(N_\alpha + N_\beta\big) \qquad N \in \mathbb{N}$$

(b) Fermions

For fermions, the problem is almost exactly analogous if we define

$$\alpha \equiv a\cos k - b^\dagger \sin k$$
$$\beta \equiv b\cos k + a^\dagger \sin k$$

The anticommutators are as bilinear as the commutators, and we get

$$\alpha^\dagger\alpha + \beta^\dagger\beta = \big(\cos^2 k - \sin^2 k\big)\Big(a^\dagger a + b^\dagger b\Big) - 2\cos k \sin k\Big(a^\dagger b^\dagger + ba\Big)$$
$$k = \frac{1}{2}\tan^{-1}\left(-\frac{\Delta}{\epsilon}\right)$$
$$H = \epsilon\sqrt{1+\left(\frac{\Delta}{\epsilon}\right)^2}\Big(\alpha^\dagger\alpha + \beta^\dagger\beta\Big)$$
$$E_{N_\alpha,N_\beta} = \epsilon\sqrt{1+\left(\frac{\Delta}{\epsilon}\right)^2}\big(N_\alpha + N_\beta\big) \qquad N \in \{0,1\}$$

(c) unitary transform

$A = a^\dagger b^\dagger - ba$ is by construction anti-Hermitian, so

$$U = \exp\Big[\kappa(a^\dagger b^\dagger - ba)\Big] = e^{\kappa A}$$

is unitary for real κ, and $U^\dagger = U^{-1} = e^{-\kappa A}$.

For Bosons,

$$UaU^\dagger = e^{\kappa A} a e^{-\kappa A}$$

$$
\begin{aligned}
&= a + \left[e^{\kappa A}, a\right] e^{-\kappa A} \\
&= a + \kappa\left[a^\dagger b^\dagger - ba, a\right] e^{\kappa A} e^{-\kappa A} + \frac{\kappa^2}{2!}\left[a^\dagger b^\dagger - ba, \left[a^\dagger b^\dagger - ba, a\right]\right] e^{\kappa A} e^{-\kappa A} + \dots \\
&= a - \kappa b^\dagger + \frac{\kappa^2}{2} a - \frac{\kappa^3}{6} b^\dagger + \dots \\
&= a \cosh\kappa - b^\dagger \sinh\kappa
\end{aligned}
$$

All the terms in the commutator are found by mathematical induction, and similar for β.

For Fermions,

$$
\begin{aligned}
UaU^\dagger &= e^{\kappa A} a e^{-\kappa A} \\
&= a + \left[e^{\kappa A}, a\right] e^{-\kappa A} \\
&= a + \kappa\left[a^\dagger b^\dagger - ba, a\right] e^{\kappa A} e^{-\kappa A} + \frac{\kappa^2}{2!}\left[a^\dagger b^\dagger - ba, \left[a^\dagger b^\dagger - ba, a\right]\right] e^{\kappa A} e^{-\kappa A} + \dots \\
&= a + \kappa\left[a^\dagger b^\dagger a - baa - aa^\dagger b^\dagger + aba\right] + \frac{\kappa^2}{2}\left[a^\dagger b^\dagger - ba, \left[a^\dagger b^\dagger - ba, a\right]\right] e^{\kappa A} e^{-\kappa A} + \dots \\
&= a + \kappa\left[-a^\dagger a - aa^\dagger\right] b^\dagger + \frac{\kappa^2}{2}\left[a^\dagger b^\dagger - ba, \left[a^\dagger b^\dagger - ba, a\right]\right] e^{\kappa A} e^{-\kappa A} + \dots \\
&= a - \kappa b^\dagger + \frac{\kappa^2}{2}\left[a^\dagger b^\dagger - ba, -b^\dagger\right] e^{\kappa A} e^{-\kappa A} + \dots \\
&= a - \kappa b^\dagger - \frac{\kappa^2}{2} a + \dots \\
&= a \cos\kappa - b^\dagger \sin\kappa
\end{aligned}
$$

and similar for β.

Problem 4.10 Second quantised operator

$$
\hat{A}\left|\Psi^{S/A}_{\alpha\beta}\right\rangle = \sum_{\gamma\epsilon} A_{\gamma\epsilon} a^\dagger_\gamma a_\epsilon \left|\Psi^{S/A}_{\alpha\beta}\right\rangle
$$

If α and β are different, we can expand th sum over ϵ to two terms. Otherwise, there is only one annihilation operator that produces a nonzero term and the sum has to be halved

$$
\begin{aligned}
\hat{A}\left|\Psi^{S/A}_{\alpha\beta}\right\rangle &= \frac{1}{1+\delta_{\alpha\beta}} \sum_\gamma \left(A_{\gamma\alpha} a^\dagger_\gamma a_\alpha \left|\Psi^{S/A}_{\alpha\beta}\right\rangle + A_{\gamma\beta} a^\dagger_\gamma a_\beta \left|\Psi^{S/A}_{\alpha\beta}\right\rangle\right) \\
\hat{A}\left|\Psi^{S/A}_{\alpha\beta}\right\rangle &= \frac{1}{1+\delta_{\alpha\beta}} \sum_\gamma \left(A_{\gamma\alpha} a^\dagger_\gamma \mathcal{N}^{-1}_{\alpha\beta} \left|\Psi^{S/A}_{\beta}\right\rangle \pm A_{\gamma\beta} a^\dagger_\gamma \mathcal{N}^{-1}_{\alpha\beta} \left|\Psi^{S/A}_{\alpha}\right\rangle\right)
\end{aligned}
$$

where

$$N_{\alpha\beta}^{-1} = \begin{cases} 1 & \alpha \neq \beta \qquad \text{one particle in each state} \\ \sqrt{2} & \alpha = \beta \qquad \text{two particles in the same state} \end{cases}$$

because $a_\alpha \left|\Psi_{\alpha\beta}^{S/A}\right\rangle = \sqrt{n_\alpha}\left|\Psi_{\beta}^{S/A}\right\rangle$. The $\pm$ comes from the eigenvalue of permutation operator. Noticing $\frac{\mathcal{N}_{\alpha\beta}^{-1}}{1+\delta_{\alpha\beta}} = N_{\alpha\beta}$,

$$\hat{A}\left|\Psi_{\alpha\beta}^{S/A}\right\rangle = \mathcal{N}_{\alpha\beta}\sum_{\gamma}\left(A_{\gamma\alpha}\mathcal{N}_{\gamma\beta}^{-1}\left|\Psi_{\gamma\beta}^{S/A}\right\rangle + A_{\gamma\beta}\mathcal{N}_{\alpha\gamma}^{-1}\left|\Psi_{\alpha\gamma}^{S/A}\right\rangle\right)$$

because $a_\gamma^\dagger\left|\Psi_{\beta}^{S/A}\right\rangle = \sqrt{n_\gamma+1}\left|\Psi_{\gamma\beta}^{S/A}\right\rangle = \sqrt{\delta_{\gamma\beta}+1}\left|\Psi_{\gamma\beta}^{S/A}\right\rangle = \mathcal{N}_{\gamma\beta}^{-1}\left|\Psi_{\gamma\beta}^{S/A}\right\rangle$.

Problem 4.11

The operator for the density of spin of a system of spin-1/2 fermions is

$$\mathbf{S} = \frac{1}{2}\sum_{s,s'}\psi_s^\dagger\boldsymbol{\sigma}_{ss'}\psi_{s'}$$

where $\psi^\dagger(\mathbf{r})$, $\psi(\mathbf{r}')$ *satisfy*

$$\left\{\psi_s^\dagger(\mathbf{r}), \psi_{s'}(\mathbf{r}')\right\} = \delta_{ss'}\delta(\mathbf{r}-\mathbf{r}')$$

(a)

$$\begin{aligned}
\left[S_i(\mathbf{r}), S_j(\mathbf{r}')\right] &= \frac{1}{4}\sum_{s,s',t,t'}\sigma_{iss'}\sigma_{jtt'}\left[\psi_s^\dagger(\mathbf{r})\psi_{s'}(\mathbf{r})\psi_t^\dagger(\mathbf{r}')\psi_{t'}(\mathbf{r}') - \psi_t^\dagger(\mathbf{r}')\psi_{t'}(\mathbf{r}')\psi_s^\dagger(\mathbf{r})\psi_{s'}(\mathbf{r})\right] \\
&= \frac{1}{4}\sum_{s,s',t,t'}\sigma_{iss'}\sigma_{jtt'}\left[\psi_s^\dagger(\mathbf{r})\delta_{ts'}\delta(\mathbf{r}-\mathbf{r}')\psi_{t'}(\mathbf{r}') - \psi_t^\dagger(\mathbf{r}')\delta_{st'}\delta(\mathbf{r}-\mathbf{r}')\psi_{s'}(\mathbf{r})\right] \\
&= \frac{1}{4}\delta(\mathbf{r}-\mathbf{r}')\left[\sum_{s,t,t'}\sigma_{ist}\sigma_{jtt'}\psi_s^\dagger(\mathbf{r})\psi_{t'}(\mathbf{r}') - \sum_{s',t,t'}\sigma_{it's'}\sigma_{jtt'}\psi_t^\dagger(\mathbf{r}')\psi_{s'}(\mathbf{r})\right] \\
&= \frac{1}{4}\delta(\mathbf{r}-\mathbf{r}')\left[\sum_{s,t,t'}\sigma_{ist}\sigma_{jtt'}\psi_s^\dagger(\mathbf{r})\psi_{t'}(\mathbf{r}') - \sum_{s,t,t'}\sigma_{itt'}\sigma_{jst}\psi_s^\dagger(\mathbf{r}')\psi_{t'}(\mathbf{r})\right] \\
&= \frac{1}{4}\delta(\mathbf{r}-\mathbf{r}')\sum_{s,t,t'}\left[\sigma_{ist}\sigma_{jtt'} - \sigma_{jst}\sigma_{itt'}\right]\psi_s^\dagger(\mathbf{r})\psi_{t'}(\mathbf{r})
\end{aligned}$$

$$= \frac{1}{4}\delta(\mathbf{r}-\mathbf{r}')\sum_{s,t} 2i\epsilon_{ijk}\sigma_{kst}\psi_s^\dagger(\mathbf{r})\psi_t(\mathbf{r})$$

$$= \frac{i\epsilon_{ijk}}{2}\delta(\mathbf{r}-\mathbf{r}')\sum_{s,t} \sigma_{kst}\psi_s^\dagger(\mathbf{r})\psi_t(\mathbf{r})$$

$$\boxed{\left[S_i(\mathbf{r}), S_j(\mathbf{r}')\right] = i\epsilon_{ijk}\delta(\mathbf{r}-\mathbf{r}')S_k(\mathbf{r})}$$

(b)

For the free Hamiltonian H

$$\begin{aligned}
\frac{\partial}{\partial t}\mathbf{S} &= \frac{i}{\hbar}[H,\mathbf{S}] \\
&= \frac{i\hbar}{2m}\left[\sum_t \int \mathrm{d}^3\mathbf{r}'\,(\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t^\dagger)(\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t), \mathbf{S}(\mathbf{r})\right] \\
&= \frac{i\hbar}{4m}\sum_{t,s,s'}\boldsymbol{\sigma}_{ss'}\int \mathrm{d}^3\mathbf{r}'\left[(\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t^\dagger)(\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t)\psi_s^\dagger\psi_{s'} - \psi_s^\dagger\psi_{s'}(\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t^\dagger)(\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t)\right] \\
&= \frac{i\hbar}{4m}\sum_{t,s,s'}\boldsymbol{\sigma}_{ss'}\int \mathrm{d}^3\mathbf{r}'\left[\psi_s^\dagger(\mathbf{r})\delta_{ts'}\boldsymbol{\nabla}_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}')\boldsymbol{\nabla}_{\mathbf{r}'}\psi_t(\mathbf{r}') - \boldsymbol{\nabla}_{\mathbf{r}'}\psi_t^\dagger(\mathbf{r}')\delta_{st}\boldsymbol{\nabla}_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}')\psi_{s'}(\mathbf{r})\right] \\
&= \frac{i\hbar}{4m}\sum_{s,s'}\boldsymbol{\sigma}_{ss'}\left[\psi_s^\dagger(\mathbf{r})\big(\nabla_{\mathbf{r}}^2\psi_{s'}(\mathbf{r})\big) - \Big(\nabla_{\mathbf{r}}^2\psi_s^\dagger(\mathbf{r})\Big)\psi_{s'}(\mathbf{r})\right] \\
&= -\frac{1}{2}\sum_{s,s'}\boldsymbol{\sigma}_{ss'}\Big(\boldsymbol{\nabla}\cdot\hat{\mathbf{j}}_{ss'}(\mathbf{r})\Big)
\end{aligned}$$

where j is the second quantised spin current, generalised from *Eq. (4.58) on the handout.*

The color I use when I enter an existential crisis.

Problem 4.12

The totally (anti)symmetric ground states are

$$\Psi^A(\mathbf{r}_1, \mathbf{r}_2, \dots) = \frac{1}{\sqrt{N!}} \sum_P \mathrm{sgn}(P) P \prod_{k=1}^{N} \phi_{k-1}(\mathbf{r}_k)$$
$$\Psi^S(\mathbf{r}_1, \mathbf{r}_2, \dots) = \prod_{k=1}^{N} \phi_0(\mathbf{r}_k)$$

$$\rho(\mathbf{x}) = \sum_i^N \delta(\mathbf{x} - \mathbf{r}_i)$$
$$\left\langle \rho(\mathbf{x})\rho(\mathbf{x}')\right\rangle_S = \int \mathrm{d}\mathbf{r}_k^N \, \Psi^{S*}(\mathbf{r}_k) \sum_{i,j}^N \delta(\mathbf{x} - \mathbf{r}_i)\delta(\mathbf{x}' - \mathbf{r}_j)\Psi^S(\mathbf{r}_k)$$
$$\left\langle \rho(\mathbf{x})\rho(\mathbf{x}')\right\rangle_S = \int \mathrm{d}\mathbf{r}_k^N \, \Psi^{S*}(\mathbf{r}_k) \sum_{i}^N \delta(\mathbf{x} - \mathbf{r}_i)\delta(\mathbf{x}' - \mathbf{r}_i)\Psi^S(\mathbf{r}_k) +$$
$$\int \mathrm{d}\mathbf{r}_k^N \prod_k \phi_0^*(\mathbf{r}_k) \sum_{j\neq i}^N \delta(\mathbf{x} - \mathbf{r}_i)\delta(\mathbf{x}' - \mathbf{r}_j) \prod_k \phi_0(\mathbf{r}_k)$$
$$\left\langle \rho(\mathbf{x})\rho(\mathbf{x}')\right\rangle_S = \delta(\mathbf{x} - \mathbf{x}') \left\langle \rho(\mathbf{x})\right\rangle_S + \sum_{j\neq i}^N \prod_k \int \mathrm{d}\mathbf{r}_k \, \delta(\mathbf{x} - \mathbf{r}_i)\delta(\mathbf{x}' - \mathbf{r}_j)\phi_0^*(\mathbf{r}_k)\phi_0(\mathbf{r}_k)$$
$$\left\langle \rho(\mathbf{x})\rho(\mathbf{x}')\right\rangle_S = \delta(\mathbf{x} - \mathbf{x}') \left\langle \rho(\mathbf{x})\right\rangle_S + \sum_{j\neq i}^N \phi_0(\mathbf{x})\phi_0^*(\mathbf{x})\phi_0(\mathbf{x}')\phi_0^*(\mathbf{x}')$$
$$\left\langle \rho(\mathbf{x})\rho(\mathbf{x}')\right\rangle_S = \delta(\mathbf{x} - \mathbf{x}') \left\langle \rho(\mathbf{x})\right\rangle_S + \left\langle \rho(\mathbf{x})\right\rangle \left\langle \rho(\mathbf{x}')\right\rangle + N^2\phi_0^*(\mathbf{x})\phi_0(\mathbf{x})\phi_0^*(\mathbf{x}')\phi_0(\mathbf{x}')$$

Problem 4.13

Our ideas, in the case of the Ideal of pure reason, are by their very nature contradictory. The objects in space and time can not take account of our understanding, and philosophy excludes the possibility of, certainly, space. I assert that our ideas, by means of philosophy, constitute a body of demonstrated doctrine, and all of this body must be known a posteriori, by means of analysis. It must not be supposed that space is by its very nature contradictory. Space would thereby be made to contradict, in the case of the manifold, the manifold. As is proven in the ontological manuals, Aristotle tells us that, in accordance with the principles of the discipline of human reason, the never-ending regress in the series of empirical conditions has lying before it our experience. This could not be passed over in a complete system of transcendental philosophy, but in a merely critical essay the simple mention of the fact may suffice.

Topic 5 Density matrices

Problem 5.1

The off-diagonal elements of ρ satisfy

$$\rho_{12} = \rho_{21}^*$$

It must be possible to write them as

$$\mathrm{Re}\{\rho_{12}\} = \mathrm{Re}\{\rho_{21}\} = \frac{rn_x}{2}; \qquad \mathrm{Im}\{\rho_{12}\} = -\,\mathrm{Im}\{\rho_{21}\} = \frac{rn_y}{2}$$
$$\begin{pmatrix} & \rho_{12} \\ \rho_{21} & \end{pmatrix} = \frac{1}{2}\begin{pmatrix} & rn_x + irn_y \\ rn_x - irn_y & \end{pmatrix} = \frac{rn_x}{2}\sigma_x + \frac{rn_y}{2}\sigma_y$$

In order that $\mathrm{tr}(\rho) = 1$,

$$\rho_{11} + \rho_{22} = 1 \implies \rho_{11} - \frac{1}{2} = -\rho_{22} + \frac{1}{2} = \frac{rn_z}{}2$$
$$\begin{pmatrix} \rho_{11} & \\ & \rho_{12} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + \frac{rn_z}{2} & \\ & \frac{1}{2} - \frac{rn_z}{2} \end{pmatrix} = \frac{1}{2}\mathbb{I} + \frac{rn_z}{2}\sigma_z$$

Therefore,

$$\rho = \frac{1}{2}\mathbb{I} + \frac{r}{2}\mathbf{n}\cdot\boldsymbol{\sigma}$$

We are free to constrain $|\mathbf{n}| = 1$ and $r \geq 0$ to leave the modulus degree of freedom to r. Use

$$\langle\psi|\,\rho\,|\psi\rangle \geq 0$$
$$\frac{1}{2} + \frac{r}{2}s_{\mathbf{n}} \geq 0 \qquad s_n = \pm 1$$
$$r \leq 1$$

Problem 5.2

In the Stern-Gerlach experiment, both up and down spin states have 50% probabilities,

$$\begin{aligned}\rho &= \frac{1}{2}\,|\uparrow\rangle\,\langle\uparrow| + \frac{1}{2}\,|\downarrow\rangle\,\langle\downarrow| \\ &= \begin{pmatrix} \frac{1}{2} & \\ & \frac{1}{2} \end{pmatrix} \\ &= \frac{1}{2}\mathbb{I}\end{aligned}$$

Problem 5.3

$$\langle \mathbf{p} \rangle = \int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\,\rho(\mathbf{r},\mathbf{r}')\big(-i\hbar\boldsymbol{\nabla}_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}')\big)$$
$$\langle \mathbf{p} \rangle = i\hbar\int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\,\delta(\mathbf{r}-\mathbf{r}')\boldsymbol{\nabla}_{\mathbf{r}}\rho(\mathbf{r},\mathbf{r}')$$
$$\langle \mathbf{p} \rangle = i\hbar\int \mathrm{d}\mathbf{r}\;\boldsymbol{\nabla}_{\mathbf{r}}\rho(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}}$$

Problem 5.4

If a spin is subject to constant magnetic field $\hat{H} = \mathbf{H}\cdot\mathbf{S}$. Align $\hat{\mathbf{z}}$ with the direction of $\mathbf{H}$, we get

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{i}{2}[\mathbf{H}\cdot\boldsymbol{\sigma},\rho]$$
$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{ir}{4}[\mathbf{H}\cdot\boldsymbol{\sigma},\mathbf{n}\cdot\boldsymbol{\sigma}]$$
$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{rH_z}{2}\big(n_x\sigma_y - n_y\sigma_x\big)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} = H_z\begin{pmatrix} -n_y \\ n_x \\ 0 \end{pmatrix}$$
$$\rho(0) = \frac{1}{2}\mathbb{I} + \frac{r}{2}\big(n_x\sigma_x + n_y\sigma_y + n_z\sigma_z\big)$$
$$\rho(t) = \frac{1}{2}\mathbb{I} + \frac{r}{2}\left[\left(n_x^2 + n_y^2\right)\big(\cos(H_zt+\phi)\sigma_x + \sin(H_zt+\phi)\sigma_y\big) + n_z\sigma_z\right]$$

where

$$\tan(\phi) = \frac{n_y}{n_x}.$$

Problem 5.5

$$i\hbar\frac{\partial\Psi_{\uparrow,\downarrow}}{\partial t} = H\Psi_{\uparrow,\downarrow}$$
$$\frac{\partial\Psi_{\uparrow,\downarrow}}{\partial t} = -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \mp \mu B'x\right)\Psi_{\uparrow,\downarrow}$$

$$\frac{\partial}{\partial t}\exp\left(\frac{i\theta_{\uparrow,\downarrow}}{\hbar}\right)\Psi_0\left(x\mp\frac{\mu B' t^2}{2m},t\right)$$
$$=\exp\left(\frac{i\theta_{\uparrow,\downarrow}}{\hbar}\right)\left\{\frac{i}{\hbar}\left[\pm\mu B' x-\frac{(\mu B')^2t^2}{2m}\right]\Psi_0+\left[\mp\frac{\mu B' t}{m}\frac{\partial}{\partial x}\Psi_0+\frac{\partial}{\partial t}\Psi_0\right]\right\}$$
$$-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\mp\mu B' x\right)\exp\left(\frac{i\theta_{\uparrow,\downarrow}}{\hbar}\right)\Psi_0\left(x\mp\frac{\mu B' t^2}{2m},t\right)$$
$$=\exp\left(\frac{i\theta_{\uparrow,\downarrow}}{\hbar}\right)\left\{-\frac{i}{\hbar}\frac{\hbar^2}{2m}\left(\frac{\mu B' t}{\hbar}\right)^2\mp\frac{i}{\hbar}\frac{\hbar^2}{2m}\frac{i\mu B' t}{\hbar}\frac{\partial}{\partial x}\Psi_0-\frac{i}{\hbar}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_0\pm\frac{i}{\hbar}\mu B' x\Psi_0\right\}$$
$$=\exp\left(\frac{i\theta_{\uparrow,\downarrow}}{\hbar}\right)\left\{-\frac{i}{\hbar}\frac{(\mu B' t)^2}{2m}\pm\frac{\mu B' t}{2m}\frac{\partial}{\partial x}\Psi_0+\frac{\partial}{\partial t}\Psi_0\pm\frac{i}{\hbar}\mu B' x\Psi_0\right\}$$

Therefore

$$\Psi_{\uparrow,\downarrow}=\exp\left(\frac{i\theta_{\uparrow,\downarrow}}{\hbar}\right)\Psi_0\left(x\mp\frac{\mu B' t^2}{2m},t\right)$$

satisfy the Schrodinger equations.

Problem 5.6

As far as the zero-field wavefunctions are concerned,

$$H=\pm\mu B' x+\frac{\hbar^2k^2}{2m}$$
$$H(q,p)=\pm\mu B' q+\frac{\hbar^2k^2}{2m}$$

Since the Wigner transform of the linear potential depends no more than linearly in x, the only term which survives in the Moyal bracket is the lowest order term.

$$\frac{\partial\rho}{\partial t}=-\{\rho,H\}_M$$
$$\frac{\partial\rho}{\partial t}=\frac{\partial\rho}{\partial p}\frac{\partial H}{\partial q}=\pm\mu B'\frac{\partial\rho}{\partial p}$$

Problem 5.7

$$E=\overline{\langle H\rangle}=-\frac{\partial}{\partial\beta}\ln Z$$

$$
\begin{aligned}
F &= -\frac{1}{\beta}\ln Z \\
S &= -k_B \operatorname{tr}(\rho \ln \rho) \\
TS &= -\frac{1}{\beta}\operatorname{tr}\left(\frac{-\ln Z - \beta H}{Z}\exp(-\beta H)\right) \\
TS &= \frac{1}{\beta}\operatorname{tr}\left(\frac{\ln Z + \beta H}{Z}\exp(-\beta H)\right) \\
TS &= \frac{1}{\beta}\ln Z - \operatorname{tr}\left(\frac{1}{Z}\frac{\partial}{\partial\beta}\exp(-\beta H)\right) \\
TS &= \frac{1}{\beta}\ln Z - \frac{1}{Z}\frac{\partial}{\partial\beta}\operatorname{tr}\left[\exp(-\beta H)\right] \\
TS &= \frac{1}{\beta}\ln Z - \frac{\partial}{\partial\beta}\ln Z = E - F
\end{aligned}
$$

Problem 5.8

$$
\begin{aligned}
\frac{\partial S}{\partial t} &= -k_B \operatorname{tr}\left(\frac{\mathrm{d}(\rho\ln\rho)}{\mathrm{d}t}\right) \\
\frac{\partial S}{\partial t} &= -k_B \operatorname{tr}\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\ln\rho\right) - k_B\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{tr}(\rho) \\
\frac{\partial S}{\partial t} &= -k_B \operatorname{tr}\left(-\frac{i}{\hbar}[H,\rho]\ln\rho\right) \\
\frac{\partial S}{\partial t} &= \frac{ik_B}{\hbar}\operatorname{tr}(H\rho\ln\rho - H\rho\ln\rho) \qquad \text{cyclic permutation and commute } \rho\ln(\rho) = \ln(\rho)\rho \\
\frac{\partial S}{\partial t} &= 0
\end{aligned}
$$

Problem 5.9

Consider only the terms with 1 transposition ($\eta = \pm 1$) or none ($\eta = 1$).

$$
\begin{aligned}
Z_N &= \frac{1}{N!\lambda^{3N}}\sum_P \int \prod_i^N \mathrm{d}\mathbf{r}_i\, \eta_{S/A}(P)\exp\left(-\frac{\pi}{\lambda^2}\sum_j^N \left|\mathbf{r}_j - \mathbf{r}_{P_j}\right|^2\right) \\
Z_N &\approx \frac{1}{N!\lambda^{3N}}\int \prod_i^N \mathrm{d}\mathbf{r}_i \left[1 \pm \sum_{P\in\text{pairwise}}^{\binom{N}{2}} \exp\left(-\frac{\pi}{\lambda^2}\sum_j^N \left|\mathbf{r}_j - \mathbf{r}_{P_j}\right|^2\right)\right]
\end{aligned}
$$

$$Z_N \approx \frac{V^N}{N!\lambda^{3N}} \pm \binom{N}{2} \frac{1}{N!\lambda^{3N}} \int \prod_i^{N-2} \mathrm{d}\mathbf{r}_i \underbrace{1}_{\exp\left(-\frac{\pi}{\lambda^2}|\mathbf{r}_i - \mathbf{r}_i|^2\right)} \int \mathrm{d}\mathbf{r}_j \, \mathrm{d}\mathbf{r}_k \exp\left(-\frac{\pi}{\lambda^2}\left|\mathbf{r}_j - \mathbf{r}_k\right|^2 \times 2\right)$$
$$Z_N \approx \frac{V^N}{N!\lambda^{3N}} \pm \binom{N}{2} \frac{V^{N-2}}{N!\lambda^{3N}} \int \mathrm{d}\mathbf{r}_j \, \mathrm{d}\mathbf{r}_k \exp\left(-\frac{2\pi}{\lambda^2}\left|\mathbf{r}_j - \mathbf{r}_k\right|^2\right)$$
$$Z_N \approx \frac{V^N}{N!\lambda^{3N}} \pm \binom{N}{2} \frac{V^{N-1}}{N!\lambda^{3N}} \left(\frac{\pi\lambda^2}{2\pi}\right)^{\frac{3}{2}}$$
$$Z_N \approx \frac{V^N}{N!\lambda^{3N}} \left(1 \pm \frac{N^2}{8\sqrt{2}} \frac{\lambda^3}{V}\right)$$

With this approximation,

$$F \approx -\frac{1}{\beta} \ln Z$$
$$pV \approx \frac{V}{\beta} \left(\frac{\partial \ln Z}{\partial V}\right)_T$$
$$pV \approx \frac{V}{\beta} \left(\frac{N}{V} \mp \frac{1}{1 \pm \frac{N^2}{8\sqrt{2}} \frac{\lambda^3}{V}} \frac{N^2}{8\sqrt{2}} \frac{\lambda^3}{V^2}\right)$$
$$pV \approx \frac{V}{\beta} \left(\frac{N}{V} \mp \frac{N^2}{8\sqrt{2}} \frac{\lambda^3}{V^2}\right)$$
$$pV \approx N k_B T \left(1 \mp \frac{\lambda^3}{8\sqrt{2}} \frac{N}{V}\right)$$

Problem 5.10

The reduced density matrix is described by 4 complex numbers, the same number of complex degrees of freedom as any general density matrix of a single spin. It will thus be possible to write any single spin density matrix as the reduced matrix of a 2-particle pure state.

Since information about the off-partial-diagonal elements are lost, we cannot deduce a unique pure entangled 2-spin density matrix from a general density matrix of a single spin.

Problem 5.11

$$\rho_R = \sum_{\mathbf{k}} \frac{1}{Z_{\mathbf{k}}} \exp\left(-\frac{\hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}}{k_B T}\right)$$

(a)

The density matrix can be diagonalised by number states.

$$\langle a_{\mathbf{k}} \rangle_R = \mathrm{tr}\left(a_{\mathbf{k}} \rho_R\right)$$
$$\langle a_{\mathbf{k}} \rangle_R = \mathrm{tr}\left[\sum_m \sqrt{m}\left|(m-1)_{\mathbf{k}}\right\rangle \langle m_{\mathbf{k}}| \sum_{\mathbf{k}'} \frac{1}{Z_{\mathbf{k}'}} \sum_n \exp\left(-\frac{\hbar\omega_{\mathbf{k}'} n}{k_B T}\right) |n_{\mathbf{k}'}\rangle \langle n_{\mathbf{k}'}|\right]$$
$$\langle a_{\mathbf{k}} \rangle_R = \mathrm{tr}\left[\sum_{\mathbf{k}'} \frac{1}{Z_{\mathbf{k}'}} \sum_n \exp\left(-\frac{\hbar\omega_{\mathbf{k}'} n}{k_B T}\right) \sqrt{m}\left|(n-1)_{\mathbf{k}}\right\rangle \langle n_{\mathbf{k}'}|n_{\mathbf{k}'}\rangle \langle n_{\mathbf{k}'}|\right]$$
$$\langle a_{\mathbf{k}} \rangle_R = \mathrm{tr}\left[\sum_{\mathbf{k}'} \frac{1}{Z_{\mathbf{k}'}} \sum_n \exp\left(-\frac{\hbar\omega_{\mathbf{k}'} n}{k_B T}\right) \sqrt{m}\left|(n-1)_{\mathbf{k}}\right\rangle \langle n_{\mathbf{k}'}|\right]$$

which just doesn't have any diagonal content and so is traceless. Similar

$$\left\langle a_{\mathbf{k}} \right\rangle_R = \left\langle a_{\mathbf{k}}^\dagger \right\rangle_R = 0$$

(b)

$$\left\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \right\rangle_R = \mathrm{tr}\left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \rho_R\right)$$
$$\left\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \right\rangle_R = \mathrm{tr}\left[\delta_{\mathbf{k},\mathbf{k}'} \frac{1}{Z_{\mathbf{k}}} \sum_n n \exp\left(-\frac{\hbar\omega_{\mathbf{k}} n}{k_B T}\right) |n_{\mathbf{k}}\rangle \langle n_{\mathbf{k}}|\right]$$
$$\left\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \right\rangle_R = \delta_{\mathbf{k},\mathbf{k}'} \frac{1}{Z_{\mathbf{k}}} \sum_n n \exp\left(-\frac{\hbar\omega_{\mathbf{k}} n}{k_B T}\right)$$
$$\left\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \right\rangle_R = -\frac{\delta_{\mathbf{k},\mathbf{k}'}}{\hbar\omega_{\mathbf{k}}} \frac{\mathrm{d}\ln Z_{\mathbf{k}}}{\mathrm{d}\beta}$$
$$\left\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \right\rangle_R = \delta_{\mathbf{k},\mathbf{k}'} \frac{\exp\left(-\frac{\hbar\omega_{\mathbf{k}}}{k_B T}\right)}{Z_{\mathbf{k}}}$$
$$\left\langle a_{\mathbf{k}} a_{\mathbf{k}'}^\dagger \right\rangle_R = \mathrm{tr}\left[\delta_{\mathbf{k},\mathbf{k}'} \frac{1}{Z_{\mathbf{k}}} \sum_n (n+1) \exp\left(-\frac{\hbar\omega_{\mathbf{k}} n}{k_B T}\right) |n_{\mathbf{k}}\rangle \langle n_{\mathbf{k}}|\right]$$
$$\left\langle a_{\mathbf{k}} a_{\mathbf{k}'}^\dagger \right\rangle_R = \delta_{\mathbf{k},\mathbf{k}'} \left[\frac{\exp\left(-\frac{\hbar\omega_{\mathbf{k}}}{k_B T}\right)}{Z_{\mathbf{k}}} + 1\right]$$

(c)

Analogously to *(a)*, in the number basis $a^\dagger a^\dagger$ or aa only have nonzero matrix elements where column/row index differ by 2, whereas ρ is diagonal. Therefore

$$\left\langle a_{\mathbf{k}} a_{\mathbf{k}'} \right\rangle_R = \left\langle a^\dagger_{\mathbf{k}} a^\dagger_{\mathbf{k}'} \right\rangle_R = 0$$

Problem 5.12

$$\sigma_\pm = \frac{1}{2}\left(\sigma_x \pm i\sigma_y\right)$$

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\bar{n}_\omega \frac{\Gamma}{2}[\sigma_-\sigma_+\rho_S - \sigma_+\rho_S\sigma_-] - (\bar{n}_\omega + 1)\frac{\Gamma}{2}[\sigma_+\sigma_-\rho_S - \sigma_-\rho_S\sigma_+] + \text{adjoint}$$

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\frac{\Gamma}{2}\left\{\bar{n}_\omega\left[\begin{pmatrix} & \\ \rho_{du} & \rho_{dd}\end{pmatrix} - \begin{pmatrix}\rho_{dd} & \\ & \end{pmatrix}\right] + (\bar{n}_\omega + 1)\left[\begin{pmatrix}\rho_{uu} & \rho_{ud} \\ & \end{pmatrix} - \begin{pmatrix} & \\ & \rho_{uu}\end{pmatrix}\right]\right\} + \text{adj.}$$

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\frac{\Gamma}{2}\left[\bar{n}_\omega\begin{pmatrix}-2\rho_{dd} & \rho_{ud} \\ \rho_{du} & 2\rho_{dd}\end{pmatrix} + (\bar{n}_\omega + 1)\begin{pmatrix}2\rho_{uu} & \rho_{ud} \\ \rho_{du} & -2\rho_{uu}\end{pmatrix}\right]$$

$$\boxed{\begin{aligned}\frac{\mathrm{d}\rho_{uu}}{\mathrm{d}t} &= -\Gamma(\bar{n}_\omega + 1)\rho_{uu} + \Gamma\bar{n}_\omega\rho_{dd} \\ \frac{\mathrm{d}\rho_{dd}}{\mathrm{d}t} &= -\Gamma\bar{n}_\omega\rho_{dd} + \Gamma(\bar{n}_\omega + 1)\rho_{uu} \\ \frac{\mathrm{d}\rho_{ud}}{\mathrm{d}t} &= \frac{\mathrm{d}\rho^*_{du}}{\mathrm{d}t} = -\Gamma\left(\bar{n}_\omega + \frac{1}{2}\right)\rho_{ud}\end{aligned}}$$

Problem 5.13

At equilibrium, the time derivatives vanish

$$0 = -\Gamma(\bar{n}_\omega + 1)\rho_{uu} + \Gamma\bar{n}_\omega\rho_{dd}$$

$$\begin{aligned}(\bar{n}_\omega + 1)\rho_{uu} &= \bar{n}_\omega\rho_{dd} \\ \mathrm{tr}(\rho) &= \rho_{uu} + \rho_{dd} = 1\end{aligned} \implies \boxed{\begin{aligned}\rho_{uu} &= \frac{\bar{n}_\omega}{\bar{n}_\omega + 1} \\ \rho_{dd} &= \frac{1}{\bar{n}_\omega + 1}\end{aligned}}$$

$$0 = -\Gamma\left(\bar{n}_\omega + \frac{1}{2}\right)\rho_{ud}$$

$$\rho_{du} = \rho_{ud} = 0$$

The density matrix represents a mixed state.