Advanced Quantum Mechanics: Assignment #6

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Problem 1

The wave equation can be written as,

$$\begin{aligned}\frac{\partial^2 f}{\partial t^2} &= c^2 \nabla^2 f \\ \implies \frac{\partial^2 f}{\partial t^2} &= c^2 \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2}\right]\end{aligned}$$

We write $f(r, \theta, t) = R(r)\Theta(\theta)T(t)$. We then have,

$$\frac{1}{T}\frac{\mathrm{d}^2 T}{\mathrm{d}t^2} = c^2\left[\frac{1}{Rr}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{1}{r^2\Theta}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2}\right] = constant = -\lambda^2$$

where $-\lambda^2$ comes from the fact that LHS is only dependent on t, and the RHS does not depend on t. Let's look at the RHS.

$$\begin{aligned}c^2\left[\frac{1}{Rr}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{1}{r^2\Theta}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2}\right] &= -\lambda^2 \\ \implies \frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{1}{\Theta}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2} &= -\frac{\lambda^2 r^2}{c^2} \\ \implies \frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2} = -\mu^2\Theta \quad \text{and} \quad \frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) &= -\frac{\lambda^2 r^2}{c^2} + \mu^2 \\ \implies \Theta = Ae^{i\mu\theta} + Be^{-i\mu\theta} \quad \text{and} \quad rR''(r) + R'(r) + &\left(\frac{\lambda^2 r^2}{c^2} - \mu^2\right)R(r) = 0 \\ \implies \Theta = Ae^{i\mu\theta} + Be^{-i\mu\theta} \quad \text{and} \quad R &= CJ_\mu\left(\frac{\lambda R}{c}\right)\end{aligned}$$

So μ, λ are the required quantum numbers.

Part (b)

We have to find $G(\mathbf{x}, \mathbf{x}')$. We know that the Green's function in momentum space is $\tilde{G}(\mathbf{p}) = \dfrac{1}{E - p^2/2m}$

$$\begin{aligned}\therefore G(\mathbf{x}, \mathbf{x}') &= \langle \mathbf{x}|\tilde{G}(\mathbf{p})|\mathbf{x}'\rangle \\ &= \int \frac{d^2\mathbf{p}'}{(2\pi)^2}\frac{d^2\mathbf{p}}{(2\pi)^2}\langle \mathbf{x}|\mathbf{p}\rangle \langle \mathbf{p}|\tilde{G}(\mathbf{p})|\mathbf{p}'\rangle \langle \mathbf{p}'|\mathbf{x}'\rangle \\ &= \int \frac{d^2\mathbf{p}'}{(2\pi)^2}\frac{d^2\mathbf{p}}{(2\pi)^2}\langle \mathbf{x}|\mathbf{p}\rangle \frac{1}{E - p^2/2m}\delta_{\mathbf{p},\mathbf{p}'}\langle \mathbf{p}'|\mathbf{x}'\rangle\end{aligned}$$

$$
\begin{aligned}
G(\mathbf{x},\mathbf{x}') &= \int \frac{d^2\mathbf{p}}{(2\pi)^2} \langle \mathbf{x}|\mathbf{p}\rangle \frac{1}{E-p^2/2m} \langle \mathbf{p}|\mathbf{x}'\rangle \\
&= \int \frac{d^2\mathbf{p}}{(2\pi)^2} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \frac{1}{E-p^2/2m} \\
&= \frac{1}{4\pi^2}\int_0^\infty pdp \int_{-1}^{1} d(\cos\theta) e^{ip|\mathbf{x}-\mathbf{x}'|} \frac{1}{E-p^2/2m} \\
&= \frac{2m}{4\pi^2}\int_0^\infty pdp \int_{-1}^{1} d(\cos\theta) e^{ip|\mathbf{x}-\mathbf{x}'|\cos\theta} \frac{1}{2mE-p^2} \\
&= \frac{2m}{4\pi^2}\int_0^\infty pdp \frac{e^{ip|\mathbf{x}-\mathbf{x}'|}-e^{-ip|\mathbf{x}-\mathbf{x}'|}}{i|\mathbf{x}-\mathbf{x}'|} \frac{1}{2mE-p^2} \\
&= \frac{2mi}{4\pi^2|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^\infty pdpe^{ip|\mathbf{x}-\mathbf{x}'|} \frac{1}{p^2-2mE-i\epsilon} \\
&= \frac{2mi}{4\pi^2|\mathbf{x}-\mathbf{x}'|}(\pi i) e^{ik|\mathbf{x}-\mathbf{x}'|} \\
G(\mathbf{x},\mathbf{x}') &= -\frac{me^{ik|\mathbf{x}-\mathbf{x}'|}}{2\pi|\mathbf{x}-\mathbf{x}'|}
\end{aligned}
$$

The integration is exactly the same as the contour integral which was described in class, and so is the Green's function.

Problem 2

We first lay out our notation. From the Lippmann-Schwinger equation, we know,

$$
\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} \underbrace{\left[\left(\frac{-m}{2\pi}\right)\int d^3\mathbf{r}' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(\mathbf{r}')\psi(\mathbf{r}')\right]}_{f(\mathbf{k},\mathbf{k}')}
$$

To solve this order by order, we use the ansatz $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{n=1}^{\infty}\phi_n(\mathbf{r})$. Substituting in the above equation, we get the recurrence relation,

$$
\begin{aligned}
\phi_{n+1}(\mathbf{r}) &= \int d^3\mathbf{r}' G_0^+(k,\mathbf{r}-\mathbf{r}') V(\mathbf{r}')\phi_n(\mathbf{r}) \\
\text{in particular} \quad \phi_1(\mathbf{r}) &= \left(\frac{-m}{2\pi}\right)\frac{e^{ikr}}{r}\int d^3\mathbf{r}' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} = \left(\frac{-m}{2\pi}\right)\frac{e^{ikr}}{r}\int d^3\mathbf{r}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} V(\mathbf{r}')
\end{aligned}
$$

In the Born approximation, one sets $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \phi_1(\mathbf{r}) \implies f^{(1)}(\mathbf{k},\mathbf{k}') = \left(\frac{-m}{2\pi}\right)\int d^3\mathbf{r}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} V(\mathbf{r}')$

$$
\begin{aligned}
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \left|f^{(1)}(\mathbf{k},\mathbf{k}')\right|^2 \\
&= \frac{m^2}{4\pi^2}\int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x})V(\mathbf{x}') e^{-i\mathbf{k}'\cdot\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}'} e^{i\mathbf{k}'\cdot\mathbf{x}} \\
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{m^2}{4\pi^2}\int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x})V(\mathbf{x}') e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{x}-\mathbf{x}')}
\end{aligned}
$$

The total cross-section σ_T can be obtained by integrating over outgoing momenta and averaging over ingoing momenta.

Problem 2 continued on next page. . .

$$\begin{aligned}\implies \sigma_T &= \frac{m^2}{4\pi^2}\int d^3\mathbf{x}d^3\mathbf{x}'\frac{d\Omega_{\mathbf{k}}}{4\pi}d\Omega_{\mathbf{k}'}V(\mathbf{x})V(\mathbf{x}')e^{i(\mathbf{k})\cdot(\mathbf{x}-\mathbf{x}')}e^{i(-\mathbf{k}')\cdot(\mathbf{x}-\mathbf{x}')}\\ &= \frac{m^2}{4\pi^2}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')\int_0^{2\pi}\frac{d\phi_{\mathbf{k}}}{4\pi}\int_{-1}^{1}d(\cos\theta_{\mathbf{k}})e^{i|\mathbf{k}||\mathbf{x}-\mathbf{x}'|\cos\theta_{\mathbf{k}}}\int_0^{2\pi}d\phi_{\mathbf{k}'}\int_{-1}^{1}d(\cos\theta_{\mathbf{k}'})e^{-i|\mathbf{k}'||\mathbf{x}-\mathbf{x}'|\cos\theta_{\mathbf{k}'}}\end{aligned}$$

$$\begin{aligned}\sigma_T &= \frac{m^2}{4\pi}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}-e^{-ik|\mathbf{x}-\mathbf{x}'|}}{ik|\mathbf{x}-\mathbf{x}'|}\times\frac{e^{-ik|\mathbf{x}-\mathbf{x}'|}-e^{ik|\mathbf{x}-\mathbf{x}'|}}{-ik|\mathbf{x}-\mathbf{x}'|} \impliedby (|\mathbf{k}|=|\mathbf{k}'|=k)\\ &= \frac{m^2}{4\pi}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')\frac{2\sin k|\mathbf{x}-\mathbf{x}'|}{k|\mathbf{x}-\mathbf{x}'|}\times\frac{2\sin k|\mathbf{x}-\mathbf{x}'|}{k|\mathbf{x}-\mathbf{x}'|}\\ \sigma_T &= \frac{m^2}{\pi}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')\frac{\sin^2 k|\mathbf{x}-\mathbf{x}'|}{k^2|\mathbf{x}-\mathbf{x}'|^2}\end{aligned}$$

The optical theorem tells us,

$$\sigma_T = \frac{4\pi}{k}\,\mathrm{Im}\, f(\mathbf{k},\mathbf{k}) = -\frac{2mL^3}{k}\,\mathrm{Im}\,\langle\mathbf{k}|T|\mathbf{k}\rangle$$

Upto first order the imaginary part is zero. Hence,

$$\begin{aligned}\sigma_T &= -\frac{2mL^3}{k}\,\mathrm{Im}\,\langle\mathbf{k}|V\frac{1}{E-H_0+i\epsilon}V|\mathbf{k}\rangle\\ &= -\frac{2mL^3}{k}\,\mathrm{Im}\int d^3\mathbf{x}d^3\mathbf{x}'\,\langle\mathbf{k}|V|\mathbf{x}\rangle\,\langle\mathbf{x}|\frac{1}{E-H_0+i\epsilon}|\mathbf{x}'\rangle\,\langle\mathbf{x}'|V|\mathbf{k}\rangle\\ &= -\frac{2m}{k}\,\mathrm{Im}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\left(\frac{-m}{2\pi}\right)\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\\ &= -\frac{2m}{k}\,\mathrm{Im}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\left(\frac{-m}{2\pi}\right)\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\\ &= \frac{m^2}{\pi}\int d^3\mathbf{x}d^3\mathbf{x}'V(\mathbf{x})V(\mathbf{x}')\frac{\sin^2 k|\mathbf{x}-\mathbf{x}'|}{k^2|\mathbf{x}-\mathbf{x}'|^2}\end{aligned}$$

Problem 3

From equation (6.4.54) of Sakurai, we have,

$$\tan\delta_l = \frac{kRj_l'(kR)-\beta_l j_l(kR)}{kRn_l'(kR)-\beta_l n_l(kR)} \quad \text{where} \quad \beta_l = \left(\frac{r}{A_l}\frac{\mathrm{d}A_l}{\mathrm{d}r}\right)\Bigg|_{r=R}$$

Here, j_l and n_l are the spherical Bessel function, and A_l is the solution to the wave equation in the region $r > R$.
From Sakurai (6.4.55), we have, for $r < R$ and $u_l(r) = rA_l(r)$

$$\frac{\mathrm{d}^2u_l}{\mathrm{d}r^2}+\left(k^2-2mV_0-\frac{l(l+1)}{r^2}\right)u_l = 0$$

Solving the above differential equation in Mathematica, we get,

$$u_l(r) = c_1\sqrt{r}j_{\frac{1}{2}(2l+1)}\left(-ir\sqrt{2\mathrm{mV}_0-k^2}\right)+c_2\sqrt{r}n_{\frac{1}{2}(2l+1)}\left(-ir\sqrt{2\mathrm{mV}_0-k^2}\right)$$

The above solution is subject to boundary condition $u_l(0) = 0$. From the properties of Bessel functions, we know that this can only be possible when $l = 0$. Then, using $l = 0$ and applying $u_0(0) = 0$,

$$A_0(r) = \frac{i\sqrt{\frac{2}{\pi}}c_1 \sinh\left(x\sqrt{2\mathrm{mV}_0 - k^2}\right)}{x\sqrt{-i\sqrt{2\mathrm{mV}_0 - k^2}}} \implies \beta_0(r) = \frac{r}{A_0}\frac{\mathrm{d}A_0}{\mathrm{d}r} = r\sqrt{2\mathrm{mV}_0 - k^2}\coth\left(r\sqrt{2\mathrm{mV}_0 - k^2}\right) - 1$$

Problem 4

Part (a)

If ρ is the density matrix of a pure state, we know that $\rho^2 = \rho \implies \log\rho^2 = \log\rho \implies 2\log\rho - \log\rho = 0 \implies \log\rho = 0 \implies \rho\log\rho = 0 \implies S = -\operatorname{Tr}(\rho\log\rho) = 0$

Part (b)

We know that $\operatorname{Tr}\rho = 1$ and that ρ is positive semi-definite $\implies \lambda_i \leq 1$, where λ_i are the eigenvalues. In the basis where the density matrix in diagonal, λ_i's are the diagonal elements.

$$\operatorname{Tr}\rho = \sum_{i=1}^{d}\lambda_i = 1 \quad \text{and} \quad -\operatorname{Tr}\rho\log\rho = \sum_{i=1}^{d}\lambda_i\log\frac{1}{\lambda_i} = \sum_{i=1}^{d}\log\frac{1}{\lambda_i^{\lambda_i}} = \log\prod_{i=1}^{d}\frac{1}{\lambda_i^{\lambda_i}}$$

The Arithmetic Mean (AM) - Geometric Mean (GM) inequality with weights [1] says that for non-negative numbers n_i and non-negative weights w_i, the following holds

$$\frac{\sum_i w_i n_i}{\sum_i w_i} \geq \left(\prod_{i=1} n_i^{w_i}\right)^{\frac{1}{\sum_i w_i}}$$

Using $n_i = \dfrac{1}{\lambda_i}$ and $w_i = \lambda_i$,

$$\begin{aligned}
\frac{\sum_{i=1}^{d}\lambda_i\frac{1}{\lambda_i}}{\sum_i^d\lambda_i} &\geq \left(\prod_{i=1}\frac{1}{\lambda_i^{\lambda_i}}\right)^{\frac{1}{\sum_i^d\lambda_i}} \\
\implies \prod_{i=1}\frac{1}{\lambda_i^{\lambda_i}} &\leq d \\
\implies \log\prod_{i=1}\frac{1}{\lambda_i^{\lambda_i}} &\leq \log d \\
\implies S &\leq \log d
\end{aligned}$$

Hence the maximum value of S is $\log d$.

[1] https://www.jstor.org/stable/24340414

Problem 5

Given,

$$
\begin{aligned}
|\psi\rangle &= \kappa \sum_E e^{-\frac{\beta E}{2}} |E\rangle \left|\tilde{E}\right\rangle \\
\implies \langle\psi|\psi\rangle &= \kappa^2 \sum_{E,E'} e^{-\frac{\beta(E+E')}{2}} \langle E|E'\rangle \left\langle \tilde{E}\middle|\tilde{E}'\right\rangle \\
\implies 1 &= \kappa^2 \sum_{E,E'} e^{-\frac{\beta(E+E')}{2}} \delta_{E,E'} \\
\implies \kappa &= \left(\frac{1}{\sum_E e^{-\beta E}}\right)^{1/2} = \frac{1}{\sqrt{Z(\beta)}}
\end{aligned}
$$

The density matrix corresponding to $|\psi\rangle$ is,

$$
\begin{aligned}
\rho &= |\psi\rangle\langle\psi| \\
&= \kappa^2 \sum_{E,E'} e^{-\frac{\beta(E+E')}{2}} |E\rangle \left|\tilde{E}\right\rangle \langle E'| \left\langle \tilde{E}'\right|
\end{aligned}
$$

We need to find $\rho_1 = \mathrm{Tr}_2\, \rho = \left\langle \tilde{E}\middle|\rho\middle|\tilde{E}\right\rangle$,

$$
\begin{aligned}
\rho_1 &= \kappa^2 \sum_{E,E'} e^{-\frac{\beta(E+E')}{2}} |E\rangle \left\langle \tilde{E}\middle|\tilde{E}\right\rangle \langle E'| \left\langle \tilde{E}'\middle|\tilde{E}\right\rangle \\
&= \kappa^2 \sum_{E,E'} e^{-\frac{\beta(E+E')}{2}} |E\rangle \langle E'| \,\delta_{E,E'} \\
\rho_1 &= \sum_E \kappa^2 e^{-\beta E} |E\rangle \langle E|
\end{aligned}
$$

We see that ρ_1 is diagonal in the energy basis. Hence, taking the trace of a function of ρ_1 is straightforward,

$$
\begin{aligned}
S = -\,\mathrm{Tr}\,\rho_1 \log \rho_1 &= \sum_E \frac{e^{-\beta E}}{Z} (\log Z + \beta E) \\
&= \sum_E \frac{e^{-\beta E}}{Z} \beta(E - F) \\
&\sim S_{th}
\end{aligned}
$$

where S_{th} is the thermal entropy of the system.