Advanced Quantum Mechanics: Assignment #6

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Aditya Vijaykumar

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Problem 1

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,

$$\begin{aligned}
\phi_{n+1}(\mathbf{r}) &= \left(\frac{-m}{2\pi}\right)\int d^3\mathbf{r}' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')\phi_n(\mathbf{r}) \\
\text{in particular} \quad \phi_1(\mathbf{r}) &= \left(\frac{-m}{2\pi}\right)\frac{e^{ikr}}{r}\int d^3\mathbf{r}' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'} = \left(\frac{-m}{2\pi}\right)\frac{e^{ikr}}{r}\int d^3\mathbf{r}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'}V(\mathbf{r}') \\
\text{and} \quad \phi_2(\mathbf{r}) &= \left(\frac{-m}{2\pi}\right)^2\frac{e^{ikr}}{r}\frac{e^{ikr}}{r}\int d^3\mathbf{r}' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')\int d^3\mathbf{r}'' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}''}V(\mathbf{r}'')
\end{aligned}$$

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.

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

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

By considering terms upto second order in the potential and writing $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \phi_1(\mathbf{r}) + \phi_2(\mathbf{r})$, we get,

$$
\begin{aligned}
f^{(2)}(\mathbf{k},\mathbf{k}') &= \left(\frac{-m}{2\pi}\right)\int d^3\mathbf{r}'e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'}V(\mathbf{r}') + \left(\frac{-m}{2\pi}\right)^2\frac{e^{ikr}}{r}\int d^3\mathbf{r}'e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')\int d^3\mathbf{r}''e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}''}V(\mathbf{r}'')\\
f^{(2)}(\mathbf{k},\mathbf{k}) &= \left(\frac{-m}{2\pi}\right)\int d^3\mathbf{r}'V(\mathbf{r}') + \left(\frac{-m}{2\pi}\right)^2\frac{e^{ikr}}{r}\int d^3\mathbf{r}'e^{-i\mathbf{k}\cdot\mathbf{r}'}V(\mathbf{r}')\int d^3\mathbf{r}''V(\mathbf{r}'')\\
\operatorname{Im} f^{(2)}(\mathbf{k},\mathbf{k}) &= \left(\frac{m^2}{4\pi^2}\right)\frac{e^{ikr}}{r}\int d^3\mathbf{r}'d^3\mathbf{r}''V(\mathbf{r}')V(\mathbf{r}'')\frac{e^{-i\mathbf{k}\cdot\mathbf{r}'}-e^{i\mathbf{k}\cdot\mathbf{r}'}}{2i}
\end{aligned}
$$

Problem 2

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Problem 3

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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

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

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

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 $\log d$.

Problem 5

Given,

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

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,

$$S = -\,\mathrm{Tr}\, \rho_1 \log \rho_1 = \sum_E \kappa^2 e^{-\beta E} (-\beta E + \log \kappa^2)$$