Exercise 4

PHYS4000 Advanced Computational Quantum Mechanics

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1 Q1:

We are given:

$$Im(T_{fi}^{SN}) = -\pi \sum_{n=1}^{N_o} k_n T_{fn}^* T_{ni} \tag{1}$$

$$\sigma_{fi}^{SN} = \frac{k_f}{k_i} |T_{fi}^{SN}|^2 \tag{2}$$

$$\sigma_i^{SN} = \sum_{f=1}^{N_o} \sigma_{fi}^{SN} \tag{3}$$

We write:

$$|T_{fi}|^2 = Re(T_{fi})^2 + Im(T_{fi})^2 \tag{4}$$

The imaginary part can be develop under the assumption $i = f$ and that T is symmetric to produce:

$$Im(T_{fi}^{SN}) = -\pi \sum_{n=1}^{N_o} k_n T_{in}^* T_{ni} \tag{5}$$

$$Im(T_{fi}^{SN}) = -\pi \sum_{n=1}^{N_o} k_n |T_{ni}|^2 \tag{6}$$

At this point if we let $n = f$ for equation 6, as they are essentially interchangeable:

$$Im(T_{fi}^{SN}) = -\pi \sum_{f=1}^{N_o} k_f |T_{fi}|^2 \tag{7}$$

we can see a relation between σ_{fi}^{SN} and $Im(T_{fi}^{SN})$;

$$-\frac{1}{\pi k_i} Im(T_{fi}^{SN}) = \sigma_{fi}^{SN} = \frac{k_f}{k_i} |T_{fi}^{SN}|^2 \tag{8}$$

Which then reveals that:

$$\sigma_i^{SN} = \sum_{f=1}^{N_o} \sigma_{fi}^{SN} = \sum_{f=1}^{N_o} \frac{k_f}{k_i} |T_{fi}^{SN}|^2 = -\frac{1}{\pi k_i} Im(T_{fi}^{SN}) \tag{9}$$

2 Q2

2.1 Q2, a)

We start with

$$(\frac{k^2}{2} - K - U) |k^+\rangle = 0 \tag{10}$$

Re-arrange and apply greens theorem

$$(\frac{k^2}{2} - K) |k^+\rangle = U |k^+\rangle \tag{11}$$

$$|k^+\rangle = |k\rangle + \frac{U}{k^2/2 - K} |k^+\rangle \tag{12}$$

$$|k^+\rangle = |k\rangle + \int_0^\infty dk' k'^2 \frac{|k'\rangle \langle k'| U |k^+\rangle}{k^2/2 - k'^2/2} \tag{13}$$

We now substitute with the definition $\langle k'| U |k^+\rangle = \langle k'| t |k\rangle$:

$$|k^+\rangle = |k\rangle + \int_0^\infty dk' k'^2 \frac{|k'\rangle \langle k'| t |k\rangle}{k^2/2 - k'^2/2} \tag{14}$$

2.2 Q2,b)

premultiply my $\langle k| U$

$$\langle k| U |k^+\rangle = \langle k| U |k\rangle + \int_0^\infty dk' k'^2 \frac{\langle k| U |k'\rangle \langle k'| t |k\rangle}{k^2/2 - k'^2/2} \tag{15}$$

$$\langle k| t |k\rangle = \langle k| U |k\rangle + \int_0^\infty dk' k'^2 \frac{\langle k| U |k'\rangle \langle k'| t |k\rangle}{k^2/2 - k'^2/2} \tag{16}$$

$$\tag{17}$$

This gives the Lippmann Schwinger equation.

2.3 Q2,c)

The value of $\langle k| U |k\rangle$ can be given in coordinate space by the following:

$$\langle k|U|k\rangle = \int_0^\infty dr r^2 \langle k|r\rangle \langle r|U|k\rangle \tag{18}$$

When $\langle r|k\rangle$ is defined as $\sin(kr)$, and is fully real, the conjugate returns the same function, thus:

$$\langle k|U|k\rangle = \int_0^\infty dr r^2 \langle r|k\rangle \langle r|U|k\rangle \tag{19}$$

$$\langle k|U|k\rangle = \int_0^\infty dr r^2 U(r) \langle r|k\rangle^2 \tag{20}$$

$$\langle k|U|k\rangle = \int_0^\infty dr U(r)[r\sin(kr)]^2 \tag{21}$$

The part of the integrand, $[r\sin(kr)]^2$ results in an infinite size integral over infinity, thus we know that $U(r)$ must be short ranged to allow the integrand to asymptotically go to zero, forcing this integral to be finite.

2.4 Q2,d)

In the ordinary complex solution of equation 17, we would end up with:

$$\langle k|t|k\rangle = \langle k|U|k\rangle + P.V. \int_0^\infty (dk' 2k'^2 \frac{\langle k| U |k'\rangle \langle k'| t |k\rangle}{k^2 - k'^2}) - i\pi \langle k|U|k\rangle \langle k|t|k\rangle \tag{22}$$

$$\tag{23}$$

Which has a complex component. If we choose $\langle k|P|k\rangle$ to be defined as $(1 + i\pi \langle k|P|k\rangle) \langle k|t|k\rangle$, and multiply equation 22 by the factor in brackets:

$$\langle k|t|k\rangle (1 + i\pi \langle k|P|k\rangle) = \langle k|U|k\rangle (1 + i\pi \langle k|P|k\rangle) + \tag{24}$$

$$P.V. \int_0^\infty (dk' 2k'^2 \frac{\langle k| U |k'\rangle \langle k'| t |k\rangle}{k^2 - k'^2})(1 + i\pi \langle k|P|k\rangle) \tag{25}$$

$$-i\pi \langle k|U|k\rangle \langle k|t|k\rangle (1 + i\pi \langle k|P|k\rangle) \tag{26}$$

$$\tag{27}$$

Which, once expanded and simplified, results in the equation:

$$\langle k|P|k\rangle = \langle k|U|k\rangle + P.V.\int_0^\infty (dk' 2k'^2 \frac{\langle k|\,U\,|k'\rangle \langle k'|P|k\rangle}{k^2 - k'^2}) \tag{28}$$

Which has eliminated the complex components of the integral.

2.5 Q2, e)

Evaluation of $\langle r|k^+\rangle$

$$\langle r|k^+\rangle = \langle r|k\rangle + \int_0^\infty dk' k'^2 \frac{\langle r|k'\rangle \langle k'|\,t\,|k\rangle}{k^2/2 - k'^2/2} \tag{29}$$

$$\tag{30}$$

We perform the complex integration similar to 7.34 of the lecture notes

$$\int_0^\infty dk' k'^2 \frac{\langle r|k'\rangle \langle k'|\,t\,|k\rangle}{k^2/2 - k'^2/2} = \tag{31}$$

$$P.V.\int_0^\infty \frac{2k'^2 \langle r|k'\rangle \langle k'|t|k\rangle}{k^2 - k'^2} dk' - i\pi k \langle r|k\rangle \langle k|t|k\rangle \tag{32}$$

Substituting this into equation 29

$$\langle r|k^+\rangle = \langle r|k\rangle + P.V.\int_0^\infty \frac{2k'^2 \langle r|k'\rangle \langle k'|t|k\rangle}{k^2 - k'^2} dk' - i\pi k \langle r|k\rangle \langle k|t|k\rangle \tag{33}$$

We want to determine that $\langle r|k^+\rangle = \psi(r,k)e^{i\delta_k}$ We will define $\langle k|K|k\rangle = (1 + i\pi k \langle k|K|k\rangle) \langle k|t|k\rangle$ And acknowledge that it essentially represents a single complex number. We post-multiply our equation 33 by this factor in brackets.

$$\langle r|k^+\rangle (1 + i\pi k \langle k|K|k\rangle) = \langle r|k\rangle (1 + i\pi k \langle k|K|k\rangle) + \tag{34}$$

$$P.V.\int_0^\infty \frac{2k' \langle r|k'\rangle \langle k'|t|k\rangle}{k^2 - k'^2} (1 + i\pi k \langle k|K|k\rangle) \tag{35}$$

$$-i\pi k \langle r|k\rangle \langle k|t|k\rangle (1 + i\pi k \langle k|K|k\rangle) \tag{36}$$

Which can be simplified to:

$$\langle r|k^+\rangle (1 + i\pi k \langle k|K|k\rangle) = \langle r|k\rangle + P.V.\int_0^\infty \frac{2k' \langle r|k'\rangle \langle k'|K|k\rangle}{k^2 - k'^2} \tag{37}$$

The Principal Value integral is fully real and $\langle r|k\rangle = \sin(kr)$, which is a real valued function. If $(1 + i\pi k \langle k|K|k\rangle)$ is simply evaluated into a complex value, then if we divide through by this quantity and allow the inverse of $(1 + i\pi k \langle k|K|k\rangle)$ equal to an arbitrary complex value z. We can represent $\langle r|k^+\rangle$ in the following form:

$$\langle r|k^+\rangle = \left(\langle r|k\rangle + P.V.\int_0^\infty \frac{2k' \langle r|k'\rangle \langle k'|K|k\rangle}{k^2 - k'^2}\right) z \tag{38}$$

$$\langle r|k^+\rangle = \psi(r,k)Re^{i\delta_k} \tag{39}$$

$$\langle r|k^+\rangle = \psi(r,k)e^{i\delta_k} \tag{40}$$

Where z is represented in an exponential form w.r.t δ_k, and the component in brackets is a real function of k, $r \to \psi(r,k)$. We absorb the R component of our exponential into the function $\psi(r,k)$ to match the representation given in the question statement. In particular, as $Re^{i\delta_k}$ represents *some* complex value, we give $\delta_k \in [0, 2\pi)$ as the minimum domain to represent all the possible complex values.