Problem Set 9

1. Particle in a box

Consider a one-dimensional, infinite potential well of width a, represented as the interval $0 \leqslant x \leqslant a$. The energy of a particle therein corresponds to the Hamilton operator H on $\mathcal{H} = L^2([0,a])$:

$$H\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\,, \qquad (\psi(0) = \psi(a) = 0)\,,$$

where the boundary conditions determine the domain of definition of the operator.

Let the particle be in the state of least energy (ground state) of the well of width $a/2$. At a specific time, the right border is abruptly shifted from $x = a/2$ to $x = a$.

(i) Compute the probability of the particle being in the first excited state, and the probability of it being in the ground state of the potential well of width a respectively.

Hint: The state immediately after the shift is still the same as before the shift.

(ii) Is the expectation value of the energy of the particle conserved throughout the abrupt change? Compute also the variance of the energy.

2. Transfer matrix and scattering matrix

In one dimension, a particle with energy $E = k^2$, $(\hbar = 2m = 1)$, meets a scatterer in the interval $[a, b]$. The scatterer is given by a potential V and a vector potential A, with

$$V(x) = 0\,,\ A(x) = 0 \quad \text{for } x \leqslant a \text{ or } x \geqslant b. \tag{1}$$

The state of the particle is described by the solutions of the time-independent Schrödinger equation

$$\left(-\mathrm{i}\frac{d}{dx} - A(x)\right)^2\psi(x) + V(x)\psi(x) = E\psi(x)\,, \qquad (x \in \mathbb{R})\,. \tag{2}$$

Remark: The introduction of a vector potential does not change the problem, since in 1 dimension it can be transformed away using a gauge transformation $(A(x) = \chi'(x))$. However, it ensures the appropriate generality in the following, see part (vi).

(i) Show that the solutions of (2) satisfy the current conservation $j'(x) = 0$, where

$$j(x) = 2\mathrm{Im}\left(\overline{\psi(x)}(\psi'(x) - \mathrm{i}A(x)\psi(x))\right)\,.$$

Remark: $j'(x) = 0$ is the usual continuity equation, generalized to $A \neq 0$ and specialized to the stationary case and to dimension 1.

(ii) Show: the solutions have the form

$$\psi(x) = \begin{cases} a_+ \mathrm{e}^{\mathrm{i}kx} + a_- \mathrm{e}^{-\mathrm{i}kx}\,, & (x \le a) \\ a'_+ \mathrm{e}^{\mathrm{i}kx} + a'_- \mathrm{e}^{-\mathrm{i}kx}\,, & (x \ge b) \end{cases}$$

outside of the interval. Furthermore, motivate the following linear relation between the $a_\pm$ and the $a'_\pm$:

$$\begin{pmatrix} a_+ \\ a_- \end{pmatrix} = T(E) \begin{pmatrix} a'_+ \\ a'_- \end{pmatrix}\,, \tag{3}$$

($T = T(E)$ is called *transfer matrix*); where

$$T^* \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} T = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,. \tag{4}$$

Hint: Use (i).

(iii) A wave coming from the left has the form

$$\psi_1(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + r\mathrm{e}^{-\mathrm{i}kx}\,, & (x \le a) \\ t\mathrm{e}^{\mathrm{i}kx}\,, & (x \ge b)\,, \end{cases} \tag{5}$$

with reflection amplitude r and transmission amplitude t. Similarly for a wave coming from the right:

$$\psi_2(x) = \begin{cases} t'\mathrm{e}^{-\mathrm{i}kx}\,, & (x \le a) \\ r'\mathrm{e}^{\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx}\,, & (x \ge b)\,. \end{cases} \tag{6}$$

The *scattering matrix* is defined as

$$S(E) = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}\,.$$

Show that $S = S(E)$ is unitary, i.e. that the rows are orthonormal w.r.t. each other:

$$|r|^2 + |t|^2 = 1 = |r'|^2 + |t'|^2\,, \qquad \bar{r}t' + \bar{t}r' = 0\,. \tag{7}$$

(In particular $R + T = 1$ for $R = |r|^2$, $T = |t|^2$, cf. exercise 8.2).

Hint: Apply (4) as a quadratic form to the appropriate vectors.

(iv) Determine the relation between the entries of the matrices S and T (in both directions). *Hint:*

$$\begin{pmatrix} a_- \\ a'_+ \end{pmatrix} = S(E) \begin{pmatrix} a_+ \\ a'_- \end{pmatrix}\,. \tag{8}$$

(v) Consider two scatterers as in (1), labeled by the indices 1 and 2 respectively. Let the first one be on the left of the second: $b_1 < a_2$. Express the scattering matrix of the combined scatterer (potentials $V_1 + V_2$, $A_1 + A_2$) by those of the individual scatterers.

(vi) Let now $A(x) \equiv 0$. Show that $\det T = 1$, respectively that S is symmetric.

Hint: If $\psi(x)$ is a solution of (2), then so is $\overline{\psi(x)}$.

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