Introduction to mathematical physics: Quantum dynamics — Homework set 12, 28.4.2017

Exercise 1

Choose a project topic for your "final exam" from the list given on the course webpage, and inform the lecturer about your choice by e-mail. Please also mention in the e-mail whether you plan to give a talk about your project (2.5. or 4.5.) or, instead, take an oral exam later in May. If you have no particular preference, choose a few most promising topics, and I will make the selection for you. You can also suggest a topic outside the list.

Exercise 2

Consider some $d, d' \geq 1$ and denote $N := d+d'$. Suppose $\psi \in \mathcal{S}_N$ and assume $A \in \mathbb{R}^{N\times N}$ is an invertible matrix and $y \in \mathbb{R}^{d'}$. For every $z \in \mathbb{R}^d$ we can then identify $(z, y) \in \mathbb{R}^d \times \mathbb{R}^{d'} \cong \mathbb{R}^N$, and thus define

$$g(z) := \psi(A(z,y))\,, \quad z \in \mathbb{R}^d.$$

Show that $g \in \mathcal{S}_d$. Is it also true in general if you do not assume A to be invertible? (This result was used in the proof of Theorem 11.4.1. *Hint*: Induction.)

Exercise 3

Suppose $N, M \in \mathbb{N}_+$ and assume that $\mathbf{R}_j \in \mathbb{R}^3$, $Z_j \in \mathbb{Z}$ are given for $j = 1, 2, \ldots, M$. Show that the operator $H := H_0 + \alpha V_{\rm c}$ is self-adjoint with $D(H) = D(H_0)$ for every $\alpha \in \mathbb{R}$ on the Hilbert space $L^2((\mathbb{R}^3)^N)$, and that it is essentially self-adjoint on the test-functions spaces $\mathcal{S}_{3N}$ and $\mathcal{D}_{3N}$.

Here $V_{\rm c}$ is defined as in the lecture notes: for $x = (\mathbf{x}_i)_{i=1}^N \in (\mathbb{R}^3)^N$ set

$$V_{\rm c}(x) := -\sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z_j}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i=1}^{N}\sum_{i'=1}^{i-1} \frac{1}{|\mathbf{x}_{i'} - \mathbf{x}_i|} + \sum_{j=1}^{M}\sum_{j'=1}^{j-1} \frac{Z_{j'} Z_j}{|\mathbf{R}_{j'} - \mathbf{R}_j|}\,.$$

(This provides the mathematical definition for the "Molecular Hamiltonian" given in Section 11.4. *Hint*: Theorem 11.4.1.)

(Please turn over. . .)

Exercise 4

Translation semigroups

Consider $N \geq 2$ spinless particles of mass $m_i > 0$, $i = 1, 2, \ldots, N$, and let $\mathcal{H} := L^2((\mathbb{R}^3)^N)$ denote the corresponding Hilbert space. A *translation* by $\mathbf{y} \in \mathbb{R}^3$ on $\mathcal{H}$ is defined via the formula

$$(\tau_{\mathbf{y}}\psi)(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \psi(\mathbf{x}_1 - \mathbf{y}, \ldots, \mathbf{x}_N - \mathbf{y}), \quad x \in (\mathbb{R}^3)^N, \, \psi \in \mathcal{H}. \tag{1}$$

(a) Explain why (1) defines an operator on $\mathcal{H}$. Prove that every $\tau_{\mathbf{y}}$ is unitary.

(b) Show that $\tau_{\mathbf{y}}\tau_{\mathbf{y}'} = \tau_{\mathbf{y}+\mathbf{y}'}$ for all $\mathbf{y}, \mathbf{y}' \in \mathbb{R}^3$. When do the operators $\tau_{\mathbf{y}}$ and $\tau_{\mathbf{y}'}$ commute?

(c) Consider some fixed $\mathbf{y} \in \mathbb{R}^3$, and prove that $t \mapsto \tau_{t\mathbf{y}}$ defines a strongly continuous unitary semigroup.

Exercises 5

Translation invariant pair potentials

Consider N, m_i, $\mathcal{H}$ and $\tau_{\mathbf{y}}$, defined as in the previous Exercise. Assume that each pair (i', i), $i' \neq i$, of particles interacts via a potential which depends only their separation, as determined by the function $V_{i'i} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.

(a) Prove that the resulting Hamiltonian

$$H := -\sum_{i=1}^{N} \frac{1}{2m_i}\nabla^2_{\mathbf{x}_i} + \sum_{i=1}^{N} \sum_{\substack{i'=1, \\ i' \neq i}}^{N} V_{i'i}(\mathbf{x}_{i'} - \mathbf{x}_i) \tag{2}$$

is self-adjoint on $\mathcal{H} := L^2((\mathbb{R}^3)^N)$ with $D(H) = D(H_0)$.

(b) Show that H is translation invariant: $\tau_{\mathbf{y}} H \subset H\tau_{\mathbf{y}}$, for every $\mathbf{y} \in \mathbb{R}^3$. (*Hint*: It suffices to check the translation invariance for test-functions. Explain why.)

(c) Suppose $\psi_0 \in \mathcal{H}$ is given and denote $\psi_t := \mathrm{e}^{-\mathrm{i}tH}\psi_0$ for $t > 0$. Consider some fixed $\mathbf{y} \in \mathbb{R}^3$, denote $\phi_0 := \tau_{\mathbf{y}}\psi_0$, and set then $\phi_t := \mathrm{e}^{-\mathrm{i}tH}\phi_0$ for $t > 0$. Show that $\phi_t = \tau_{\mathbf{y}}\psi_t$ for all $t \geq 0$. (Hint: spectral theory, in particular, the new material on page 63b.)