THE UNIVERSITY OF WARWICK

FOURTH YEAR EXAMINATION: 2023

QUANTUM MECHANICS: BASIC PRINCIPLES AND PROBABILISTIC METHODS

Time Allowed: **3 hours**

Read carefully the instructions on the answer book and make sure that the particulars required are entered on each answer book.

Calculators are not needed and are not permitted in this examination.

Candidates should answer COMPULSORY QUESTION 1 and THREE QUESTIONS out of the four optional questions 2, 3, 4 and 5.

The compulsory question is worth 40% of the available marks. Each optional question is worth 20%.

If you have answered more than the compulsory Question 1 and three optional questions, you will only be given credit for your QUESTION 1 and THREE OTHER best answers.

The numbers in the margin indicate approximately how many marks are available for each part of a question.

Notation: The following notation will be used throughout the exam.

- $\mathbb{R}$ and $\mathbb{C}$ denote the fields of real and complex numbers. $\mathbb{N} = \{1, 2, 3, \ldots\}$ denotes the set of positive natural numbers.
- All the operators are assumed to be linear unless otherwise stated.
- $\mathcal{S}(\mathbb{R}^d)$ denotes the set of all Schwartz class functions on $\mathbb{R}^d$.
- Given $\varphi \in \mathcal{S}(\mathbb{R}^d)$, its Fourier transform $\widehat{f}$ is defined as

$$\widehat{\varphi}(p) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \varphi(x)\, \mathrm{e}^{-\mathrm{i}x\cdot p}\, \mathrm{d}x\,.$$

- $\mathbf{1}$ denotes the identity operator.
- $[\cdot,\cdot]$ denotes the commutator, i.e. $[A, B] = AB - BA$.

COMPULSORY QUESTION

1. (a) Define $\{\cdot,\cdot\} : C^\infty(\mathbb{R}^d) \times C^\infty(\mathbb{R}^d) \to C^\infty(\mathbb{R}^d)$ by

$$\{f,g\} := \sum_{i=1}^{d} \Big(\frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x_i} - \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial p_i} \Big) .$$

Show that for $f,g,h \in C^\infty(\mathbb{R}^d)$, one has

$$\{fg,h\} = \{f,h\}g + f\{g,h\} .$$

[3]

(b) Consider the Hilbert space $\mathcal{H} = \mathbb{C}^d$. Let $\mathcal{B}$ denote the set of all (linear) operators on $\mathcal{H}$.

(i) Define what it means for $\omega : \mathcal{B} \to \mathbb{C}$ to be a quantum state. **[3]**

(ii) Show that the space of all quantum states is convex. **[3]**

(iii) What does it mean for a quantum state to be pure? **[3]**

(iv) Give an example of a quantum state which is pure. **[3]**
(No justification is required.)

(c) (i) Define the operator norm $\|A\|$ of an operator $A : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$. **[2]**

(ii) Recall what it means for an operator $A : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ to be bounded. **[1]**

(d) (i) State what it means for an unbounded operator on $L^2(\mathbb{R}^d)$ to be densely-defined. **[2]**

(ii) Give an example of a densely-defined unbounded operator on $L^2(\mathbb{R}^d)$.
(No justification is needed). **[2]**

(iii) Given a densely-defined operator A, state the definition of its adjoint A^*. **[2]**

(e) State the Trotter product formula. **(No proofs are required).** **[5]**

(f) Given $x \in \mathbb{R}^d$, state the definition of the Wiener measure on the space $\mathcal{C}_x$ of continuous paths $\omega : [0,\infty) \to \mathbb{R}^d$. Here, one should also state the definition of the appropriate sigma algebra Σ_x. **[6]**

(g) State the Feynman-Kac formula. **(No proofs are required).** **[5]**

OPTIONAL QUESTIONS

2. In this exercise we consider the Hilbert space $\mathcal{H} = \mathbb{C}^d$. Let $\mathcal{B}$ denote the set of all (linear) operators on $\mathcal{H}$.

(a) Given $A, B \in \mathcal{B}$, define $\langle A, B\rangle := \mathrm{Tr}(A^*B)$, where Tr denotes the trace on $\mathbb{C}^d$.

(i) Show carefully that $\langle \cdot, \cdot \rangle$ defines an inner product on $\mathcal{B}$. **[3]**

(ii) Does the norm arising from this inner product coincide with the operator norm for all values of d? **[2]**

(iii) Write down explicitly the Cauchy-Schwarz inequality for the inner product given in (i). **[2]**

(b) State what it means for an operator ρ on $\mathbb{C}^d$ to be a density operator. **[2]**

(c) Let $\omega : \mathcal{B} \to \mathbb{C}$ denote a quantum state.

(i) Show that there exists a unique linear operator ρ on $\mathbb{C}^d$ such that for all $A \in \mathcal{B}$ we have $\omega(A) = \mathrm{Tr}(\rho^* A)$.
Here, you can use the Riesz representation theorem in Hilbert spaces without proof. **[2]**

(ii) Show that the operator ρ in part (i) is positive.
HINT: Show that for $\varphi \in \mathbb{C}^d$ with $\|\varphi\| = 1$, we have $\langle \varphi, \rho^* \varphi\rangle_{\mathbb{C}^d} = \omega(P_\varphi)$, where $P_\varphi(\psi) := \langle \varphi, \psi\rangle_{\mathbb{C}^d}\, \varphi$.
You may use without proof the fact that positive operators are self-adjoint.
[5]

(iii) Show that $\mathrm{Tr}(\rho) = 1$. **[3]**

(iv) Deduce that there exists a unique density operator ρ such that for all $A \in \mathcal{B}$ we have $\omega(A) = \mathrm{Tr}(\rho A)$. **[1]**

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3. (a) (i) Let $A : \mathcal{D}(A) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ be a linear operator. Define its graph $\Gamma(A)$. **[2]**

(ii) Given an operator $A : \mathcal{D}(A) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, define what it means for A to be closed. **[2]**

(iii) Given a densely-defined closed operator A, define its resolvent set $\rho(A)$ and its resolvent R_A. **[2]**

(b) Answer the following questions as TRUE/FALSE. **No justification is needed.**

(i) If A is a self-adjoint operator on $L^2(\mathbb{R}^d)$, then it is symmetric. **[2]**

(ii) The adjoint of a densely-defined operator is densely-defined. **[2]**

(iii) If A is a bounded operator $L^2(\mathbb{R}^d)$, then its resolvent set $\rho(A)$ is nonempty. **[2]**

(c) Let (φ_n) be an orthonormal basis of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d)$. Let $e_\infty \in \mathcal{H}$ be a vector that is not a finite linear combination of the basis vectors (φ_n). Given $n \in \mathbb{N}$ and $b, c_1, \ldots, c_n$, we define

$$A(be_\infty + \sum_{i=1}^{n} c_i \varphi_i) = be_\infty \,.$$

(i) Show that A is a densely-defined linear operator on $\mathcal{H}$. **[3]**

(ii) Show that $(e_\infty, e_\infty) \in \overline{\Gamma(A)}$ and $(e_\infty, 0) \in \overline{\Gamma(A)}$. **[3]**

(iii) Deduce that there does not exist a linear operator B on $\mathcal{H}$ such that $\overline{\Gamma(A)} = \Gamma(B)$. **[2]**

4. (a) In part (a) of the exercise, we set $d = 1$.

(i) Recall the definition of the position and momentum operator X, P respectively. Give a choice of domain with which both operators are densely defined on $L^2(\mathbb{R})$. **[2]**

(ii) With X and P given as above, recall the definition of the creation and annihilation operators

$$a^* := \frac{1}{\sqrt{2}}(X - \mathrm{i}P)\,, \qquad a = \frac{1}{\sqrt{2}}(X + \mathrm{i}P)\,.$$

Show that $[a, a^*] = \mathbf{1}$.

Here, you may use without proof (and without analysing the domains of the operators) the identity $[X, P] = \mathrm{i}\mathbf{1}$. **[3]**

(iii) Let $\mathcal{N} := a^* a$. Show that one has $\mathcal{N} a = a(\mathcal{N} - \mathbf{1})$. **[3]**

(b) (i) Given $s \geq 0$, recall the definition of the Sobolev space $H^s(\mathbb{R}^d)$. **[2]**

(ii) Let $s > \frac{d}{2}$ be given. Show that there exists $C > 0$ depending on s and d such that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\|\varphi\|_{L^\infty(\mathbb{R}^d)} \leq C \|\varphi\|_{H^s(\mathbb{R}^d)}\,.$$

HINT: Use the Fourier inversion formula to write

$$\varphi(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \widehat{\varphi}(p)\, \mathrm{e}^{\mathrm{i}x \cdot p}\, \mathrm{d}p\,.$$

Then multiply and divide the integrand by $(1 + |p|^2)^{s/2}$. **[3]**

(iii) Show that for $s > \frac{d}{2}$, one has $H^s(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$.

Here, you may use without proof the fact that $\mathcal{S}(\mathbb{R}^d)$ is a dense subset of $H^s(\mathbb{R}^d)$. **[2]**

(c) Let $d \leq 3$ be given. Suppose that $V : \mathbb{R}^d \to \mathbb{R}$ is a measurable function such that

$$\int_{|V(x)| > m} V^2(x)\, \mathrm{d}x < \infty$$

for some fixed value of $m \geq 0$. (Above, we are integrating over the set of all $x \in \mathbb{R}^d$ with $|V(x)| > m$).

(i) Show that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\|V\varphi\|^2_{L^2(\mathbb{R}^d)} \leq m^2 \|\varphi\|^2_{L^2(\mathbb{R}^d)} + \|\varphi\|^2_{L^\infty(\mathbb{R}^d)} \int_{|V(x)| > m} V^2(x)\, \mathrm{d}x\,.$$

[3]

(ii) Show that there exists $C > 0$ depending on V, m, d such that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\|V\varphi\|_{L^2(\mathbb{R}^d)} \leq C \|\varphi\|_{H^2(\mathbb{R}^d)}\,.$$

[2]

5. (a) Given a measurable function $a : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ define the operator A by

$$(A\varphi)(x) := \int_{\mathbb{R}^d} a(x,y)\,\varphi(y)\,\mathrm{d}y\,.$$

Suppose that

$$M := \sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |a(x,y)|\,\mathrm{d}y < \infty\,, \qquad N := \sup_{y\in\mathbb{R}^d} \int_{\mathbb{R}^d} |a(x,y)|\,\mathrm{d}x < \infty\,.$$

Show that the operator A is then bounded on $L^2(\mathbb{R}^d)$ and that it satisfies the operator norm bound

$$\|A\| \le \sqrt{MN}\,.$$

[9]

(b) Given $t > 0$, we recall that the **heat kernel** $g_t : \mathbb{R}^d \to \mathbb{R}$ is defined as

$$g_t(x) := \frac{1}{(2\pi t)^{d/2}}\,\mathrm{e}^{-\frac{|x|^2}{2t}}\,.$$

We define the operator T_t by $T_t\varphi := g_t * \varphi$.

(i) Show that $T_t : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is bounded and that its operator norm satisfies $\|T_t\| \le 1$. **[4]**

(ii) Given $\varphi \in \mathcal{S}(\mathbb{R}^d)$, let

$$u(x,t) := T_t\varphi(x) = \int_{\mathbb{R}^d} g_t(x-y)\,\varphi(y)\,\mathrm{d}y\,.$$

Compute

$$\widehat{u}(p,t) = \frac{1}{(2\pi)^{d/2}} \int u(x,t)\,\mathrm{e}^{-\mathrm{i}p\cdot x}\,\mathrm{d}x\,,$$

i.e. the Fourier transform with respect to x of the function u.
Here, you can use without proof the formula $\widehat{g_t}(p) = \mathrm{e}^{-\frac{t|p|^2}{2}}$. **[3]**

(iii) Using part (ii), show that u solves the heat equation

$$\Big(\frac{\partial}{\partial t} - \frac{\Delta}{2}\Big)u(x,t) = 0\,.$$

Here, you may interchange the order of differentiation in time and the Fourier transform without justification. **[4]**

END