PhD Course 2023: Mathematical Methods for Many-Body Quantum Systems

Exam Preparation

For all of the following problems let $\mathfrak{h}$, $\mathfrak{h}_1$, $\mathfrak{h}_2$ be Hilbert spaces.

Problem 1: Slater Determinants

Let $\mathfrak{h} = L^2(\mathbb{R}^d)$. Let $(f_j)_{j=1}^N$ an orthonormal system in $\mathfrak{h}$. Consider the fermionic case.

a. Show that $\psi := a^*(f_1)a^*(f_2)\cdots a^*(f_N)\Omega \in \mathcal{F}_-(\mathfrak{h})$ can be identified with the function

$$\psi(x_1,\ldots,x_N) = (N!)^{-1/2} \det\Big((f_i(x_j))_{i,j=1}^N \Big) \;, \qquad x_1,\ldots,x_N \in \mathbb{R}^d \;.$$

b. Show that the one-particle density matrix γ_ψ of a Slater determinant $\psi = \bigwedge_{j=1}^N f_j$ is a rank-N projection on the Hilbert space $\mathfrak{h}$, specifically in Dirac notation

$$\gamma = \sum_{j=1}^N |f_j\rangle\langle f_j| \;.$$

Problem 2: Unitary Groups and their Generator

Let $A = A^*$ a self-adjoint operator on $\mathfrak{h}$. Show that $U(t) := \Gamma(e^{-itA})$, on fermionic as on bosonic Fock space $\mathcal{F}_\pm(\mathfrak{h})$, satisfies

$$U(t)U(s) = U(t+s)$$

and that, for vectors $\varphi \in \mathcal{F}_\pm(\mathfrak{h})$ such that the limit exists, we have

$$i\frac{\mathrm{d}}{\mathrm{d}t}U(t)\varphi\Big|_{t=0} := \lim_{\varepsilon\to 0} i\frac{U(\varepsilon)-1}{\varepsilon}\varphi = \mathrm{d}\Gamma(A)\varphi \;.$$

Problem 3: Canonical Commutation and Anticommutation Relations CCR/CAR

In the following consider ψ, φ as sequences in bosonic/fermionic Fock space with only a finite number of non-vanishing elements. Let $f, g \in \mathfrak{h}$.

a. Show that, in bosonic as in fermionic Fock space, we have

$$\langle \psi, a(f)\varphi\rangle_{\mathcal{F}_\pm} = \langle a^*(f)\psi, \varphi\rangle_{\mathcal{F}_\pm} \;.$$

b. Let $[A, B] := AB - BA$ be the commutator of two operators A, B. Show that for $\psi \in \mathcal{F}_+$ we have

$$[a(f), a(g)]\psi = 0 , \quad [a^*(f), a^*(g)]\psi = 0 , \quad [a(f), a^*(g)]\psi = \langle f, g\rangle_{\mathfrak{h}}\psi .$$

Show that on fermionic Fock space $\mathcal{F}_-$ the analogous relations hold with the commutator replaced by the anticommutator $\{A, B\} := AB + BA$.

Problem 4: Pair Interaction

Let $\mathbb{T}^d$ be the d-dimensional torus of side lengths 2π.

a. Show that on $L^2(\mathbb{T}^{dN})$, understood as a subspace of $\mathcal{F}_\pm(L^2(\mathbb{T}^d))$, in terms of the operator valued distributions, we have

$$\langle\psi, \sum_{i<j} V(x_i - x_j)\psi\rangle = \langle\psi, \frac{1}{2}\int V(x-y)a_x^* a_y^* a_y a_x \mathrm{d}x\mathrm{d}y\ \psi\rangle . \tag{1}$$

b. The plane waves

$$e_k(x) := (2\pi)^{-d/2}e^{ik\cdot x} , \quad k \in \mathbb{Z}^d ,$$

form an orthonormal basis of $L^2(\mathbb{T}^d)$. (Verify this claim if you are unsure!)

The identity operator can then be written as the infinite-rank projection

$$\mathrm{id} = \sum_{k\in\mathbb{Z}^d} |e_k\rangle\langle e_k| .$$

(Don't worry about convergence of the sums over $\mathbb{Z}^d$.) The Fourier transform of the operator-valued distributions can then be obtained as

$$\begin{aligned} a_x^* = a^*(\delta(\cdot - x)) = a^*(\sum_{k\in\mathbb{Z}^d} e_k\overline{e_k(x)}) &= \sum_{k\in\mathbb{Z}^d}(2\pi)^{-d/2}e^{-ik\cdot x}a^*(e_k) \\ &=: \sum_{k\in\mathbb{Z}^d}(2\pi)^{-d/2}e^{-ik\cdot x}a_k^* . \end{aligned} \tag{2}$$

(In the last step we wrote $a_k^* := a^*(e_k)$. Despite the abuse of notation, usually no confusion of a_k^* with the operator-valued distributions a_x^* should arise.) One says that a_k^* creates a particle in momentum-mode k.

Use (2) to express the second-quantized interaction (i. e., the operator on the right hand side of (1)) in terms of the momentum-mode operators a_k^*, a_k and the Fourier transform $\hat{V}$ of the interaction potential V. Your final result should contain three sums over momenta.

Problem 5: Example of Wick's Theorem

Let ψ be a quasifree state in bosonic or fermionic Fock space $\mathcal{F}_\pm(\mathfrak{h})$. Let $f_1, f_2, f_3, f_4 \in \mathfrak{h}$ be pairwise orthonormal. By explicit computation, check that the expectation value

$$\langle \psi, a^*(f_1)a^*(f_2)a(f_3)a(f_4)\psi \rangle$$

is given by the sum over pairings as claimed in Wick's theorem.

Express the result in terms of the one-particle reduced density operator γ and the pairing density operator α.

Problem 6: Bogoliubov Transformation

Consider a Bogoliubov map, given in the notation of Solovej's notes as

$$\mathcal{V} = \begin{pmatrix} U & J^*VJ^* \\ V & JUJ^* \end{pmatrix} .$$

a. Show that, for $\mathbb{U}_\mathcal{V}$ being the implementation of the Bogoliubov map $\mathcal{V}$ as a unitary on Fock space, we have

$$\mathbb{U}_\mathcal{V} a(f) \mathbb{U}_\mathcal{V}^* = a(Uf) + a^*(J^*Vf) .$$

b. Show that the inverse transformation $\mathcal{V}^{-1}$ is given by

$$\begin{pmatrix} U^* & -V^* \\ -JV^*J & JU^*J^* \end{pmatrix} \text{ for bosons;} \qquad \begin{pmatrix} U^* & V^* \\ JV^*J & JU^*J^* \end{pmatrix} \text{ for fermions.}$$

c. Show that the number of particles in the "quasiparticle vacuum" $\Omega' := \mathbb{U}_\mathcal{V}\Omega$ is

$$\langle \Omega', \mathcal{N}\Omega' \rangle = \operatorname{tr} V^*V .$$

Compare this to the Shale–Stinespring condition.

Problem 7: Perturbation Theory

Consider

$$\mathcal{H} := \mathcal{F}_-(L^2(\mathbb{T}^d)) \otimes \mathcal{F}_+(L^2(\mathbb{T}^d)) .$$

We denote the creation and annihilation operators on the fermionic Fock space $\mathcal{F}_-(L^2(\mathbb{T}^d))$ by a_k^*, a_k for momentum $k \in \mathbb{Z}^d$ (compare to (2)) and the creation and annihilation operators for momentum $q \in \mathbb{Z}^d$ on the bosonic Fock space $\mathcal{F}_+(L^2(\mathbb{T}^d))$ by b_q^*, b_q. On $\mathcal{H}$, we write a_k^* as an abbreviation for $a_k^* \otimes \mathrm{id}$, i. e., acting on the other tensor factor as the identity (and analogously for the b^*- and b-operators on the second tensor factor).

The Fröhlich Hamiltonian for the electron–phonon system acts on $\mathcal{H}$ by

$$H := \underbrace{\sum_{k\in\mathbb{Z}^d} \varepsilon(k) a_k^* a_k}_{=:H_{\mathrm{el}}} + \underbrace{\sum_{q\in\mathbb{Z}^d} \omega(q)(b_q^* b_q + \frac{1}{2})}_{=:H_{\mathrm{ph}}} + \underbrace{\sum_{k,q\in\mathbb{Z}^d} g(k,q) a_{k+q}^* a_k (b_q + b_{-q}^*)}_{=:H_{\text{el-ph}}} .$$

Here $\varepsilon, \omega : \mathbb{Z}^d \to [0,\infty)$ are even functions, and $g(k,q) = \overline{g(-k,-q)}$ for all $k, p \in \mathbb{Z}^d$. Moreover we write

$$H_0 := H_{\mathrm{el}} + H_{\mathrm{ph}} \quad \text{and} \quad H_1 := H_{\text{e-ph}} .$$

a. Let A, B, C arbitary operators. Show that

$$[AB, C] = A[B, C] + [A, C]B .$$

Then find a similar formula which has a commutator on the left hand side but only anticommutators on the right hand side.

b. Complete the details of the first-order perturbation theory prescription sketched in the lecture to obtain the effective, purely fermionic, interaction

$$H_{\mathrm{eff}} = \sum_{k,k',q\in\mathbb{Z}^d} V_{\mathrm{eff}}(k,k',q) a_{k+q}^* a_k a_{k'-q}^* c_{k'}$$

where

$$V_{\mathrm{eff}}(k,k',q) = g_{k,q} g_{k',-q} \frac{\omega(q)}{(\varepsilon(k') - \varepsilon(k'-q)^2 - \omega(q)^2)} .$$

(You need nothing but the CCR and CAR to complete this computation; this is the convenient property of the Fock space method.)

Problem 8: Harmonic Oscillator

Show that the bosonic Fock space $\mathcal{F}_+(\mathbb{C})$ over $\mathfrak{h} = \mathbb{C}$ can be identified with $L^2(\mathbb{R})$ such that the vacuum vector Ω is the function $x \mapsto (\pi)^{-1/4} e^{-x^2/2}$ and

$$a(1) = \frac{1}{\sqrt{2}} \left(x + \frac{\mathrm{d}}{\mathrm{d}x} \right) , \quad a^*(1) = \frac{1}{\sqrt{2}} \left(x - \frac{\mathrm{d}}{\mathrm{d}x} \right) . \tag{3}$$

Hint: If $(f_j)_j \in \mathbb{N}$ is an orthonormal basis of $\mathfrak{h}$, then vectors obtained by applying finitely many creation operators to the vacuum, $\prod_j a^*(f_j)\Omega$, form a basis of Fock space.

It is moreover useful to known that the space of functions $p(x)e^{-x^2/2}$, where p is a polynomial, is a dense subspace in $L^2(\mathbb{R})$.

Comment: Eq. (3) are the creation/annihilation operators of the harmonic oscillator.

"First quantization is a mystery, but second quantization is a functor."
Edward Nelson
https://math.ucr.edu/home/baez/nth_quantization.html