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The Dance of Atoms

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A primer on some fundamental concepts in Condensed Matter Physics

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"Nunc scio nihil."

– perhaps some disillusioned Roman philosopher in his 20's

Preface

Semiconductor-based devices have become the lifeblood of modern civilisation, powering the tiniest microprocessor to the largest of the ICBMs. In our quest for smaller and still smaller transistors, we have now hit a fundamental barrier beyond which deterministic Newtonian mechanics is helpless and quantum mechanics reigns with all its glory of probabilistic chaos. This calls immediately for a fundamental understanding of the quantum mechanical nature of such beyond-Moore devices, viz., *quantum devices*. This article is devoted to a brief exploration of such concepts, starting from simple toy models of quantum condensed matter systems—reviewing the tight-binding ansatz, physics of quantum bands, second quantization—and touching upon the state-of-the-art in modern condensed matter—quantum topology and topological electronics.

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Chapter 1

Second Quantisation

Before we begin our incursion into the so-called 'second quantisation', we need to appreciate the reason why the need for second quantization arose. The properties of quantum condensed matter systems and, by extension, that of real materials are controlled by the *collective behaviour* of electrons in the presence of some background potential due to an underlying crystal lattice. This statement, in fact, is a simpler rendition of the Bohr-Oppenheimer approximation. So, what factors do we need to consider during the analysis of a condensed matter system?

- Focus on electrons and their collective dynamics
- Electrons are free to move from one orbital to another (tunnelling/hopping)
- They are subject to a background potential from the lattice
- They can interact with each other due to Coulomb repulsion

The question remains, how do we formulate the Hamiltonian for many-body systems? How do we encode anti-symmetry of fermions into this many-particle wavefunction? And most importantly, how do we find out the eigenstates/eigenvalues of momentum and/or energy of the system?

So, how do we encode fermionic anti-symmetry in many-particle wavefunctions? Consider a single-particle quantum state $\phi_\nu(\vec{r})$, where ν refers to labels for the quantum state. The basis for a two-particle system is then given by

$$\psi(\vec{r_1}, \vec{r_2}) = \frac{1}{\sqrt{2}}[\phi_{\nu_1}(\vec{r_1})\phi_{\nu_2}(\vec{r_2}) - \phi_{\nu_1}(\vec{r_2})\phi_{\nu_2}(\vec{r_1})]$$

This basis satisfies the anti-symmetry property, and also, there happens to be a less verbose manner through which we can express such wavefunctions - Slater's determinants. For a generalized N-particle system such that the basis states are perfectly anti-symmetric under exchanging the labels of any two particles, the wavefunction can be expressed as

$$\psi(\vec{r_1},\vec{r_2},...,\vec{r_N}) = \frac{1}{\sqrt{N!}}\begin{bmatrix} \phi_{\nu_1}(\vec{r_1}) & \phi_{\nu_2}(\vec{r_1}) & ... & \phi_{\nu_N}(\vec{r_1}) \\ \phi_{\nu_1}(\vec{r_2}) & \phi_{\nu_2}(\vec{r_2}) & ... & \phi_{\nu_N}(\vec{r_2}) \\ . & . & & . \\ . & . & & . \\ . & . & & . \\ \phi_{\nu_1}(\vec{r_N}) & \phi_{\nu_2}(\vec{r_N}) & ... & \phi_{\nu_N}(\vec{r_N}) \end{bmatrix}$$

The 'first quantisation' principle cannot be used to satisfactorily explain condensed matter systems since calculations become cumbersome and expensive as the number of particles in the system increases, and the representation requires the number of particles, N, to be fixed. As N approaches the limit associated with statistical physics, N is allowed to fluctuate as per the grand canonical ensemble. Second quantisation or occupation number formalism is the standard way in which many-particle QM is formulated. It is based on the algebra of ladder operators.

- Second quantisation provides a compact way of representing the many-body space of excitations.
- Properties of operators are now encoded in a single set of commutation/anti-commutation relations rather than in some explicit Hilbert space representation.

In essence, second quantisation formalism offers us significant computational advantage and a more compact and efficient representation of the Hamiltonian when dealing with many-particle quantum systems. For example, consider a *symmetrised* N-particle wwavefunction of fermions ($\zeta = -1$) or bosons ($\zeta = +1$) expressed in the form

$$|\lambda_1, \lambda_2, \dots \lambda_N\rangle = \frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} n_\lambda!}} \sum_{\mathcal{P}} \zeta^{\mathcal{P}} |\psi_{\lambda_{\mathcal{P}1}}\rangle \otimes |\psi_{\lambda_{\mathcal{P}2}}\rangle \dots \otimes |\psi_{\lambda_{\mathcal{P}N}}\rangle \tag{1.1}$$

where n_λ is the total number of particles in state λ (for fermions, Pauli exclusion principle dictates that $n_\lambda = 0, 1$, i.e. $n_\lambda! = 1$). The summation runs over all $N!$ permutations of the quantum numbers λ_i, and $\mathcal{P}$ denotes the parity.
[1]

[1] Parity is defined as the number of transpositions of two elements which brings the permutation $(\mathcal{P}_1, \mathcal{P}_2, \dots \mathcal{P}_N)$) back to the ordered sequaence (1,2,... N)

Second quantisation formalism provides for a much more condensed and intuitive representation for the generalised wavefunction via the **vacuum state** $|\Omega\rangle$, and a set of creation (annihilation) **field operators** c_λ ($c^\dagger_\lambda$), as follows:

$$c_\lambda |\Omega\rangle = 0, \quad \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} c^\dagger_{\lambda_N} \dots c^\dagger_{\lambda_1} |\Omega\rangle = |\lambda_1, \lambda_2, \dots \lambda_N\rangle \tag{1.2}$$

In terms of physical interpretation, the operator $c^\dagger_\lambda$ creates a particle in state λ while the operator c_λ annihilates it. The commutation relations between these operators are captured via Clifford algebra [2]:

$$[c_\lambda, c^\dagger_\mu]_{-\zeta} = \delta_{\lambda,\mu}, \quad [c_\lambda, c_\mu]_{-\zeta} = [c^\dagger_\lambda, c^\dagger_\mu]_{-\zeta} = 0 \tag{1.3}$$

The physical interpretation of 1.2 and the commutation relations of the field operators is no trivial matter – these equations imply that for *any* N, the N-body wavefunction can be generated by an application of a set of N-independent operators to a vacuum state. Similarly, the formal definition of the general many-body or **Fock space** can be given as the direct sum $\oplus_{N=0}^{\infty} \mathcal{F}_N$, where $\mathcal{F}_N$ is defined as the linear span of all N-particle states $|\lambda_1, \lambda_2, \dots \lambda_N\rangle = \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} c^\dagger_{\lambda_N} \dots c^\dagger_{\lambda_1} |\Omega\rangle$. Intuitively, the Fock-subspaces $\mathcal{F}_N$ are generated by repeated action of creation operators on the vacuum space $\mathcal{F}_0$, and application of creation/annihilation field operator on a wavefunction takes it from one Fock-subspace to another.

Before proceeding further, we need to determine the basis transformation for the field operators, and the Fourier transform of the operators from the real space to k-space (otherwise known as the momentum space). These results will prove incredibly useful while analysing the Hamiltonians for interacting fermionic systems.

[2] $[\hat{A}, \hat{B}]_{-\zeta} = \hat{A}\hat{B} - \zeta \hat{B}\hat{A}$ is the commutator $\zeta = 1$ (anticommutator $\zeta = -1$) for bosons (fermions). As per convention, the notation [.,.] denotes the commutator while {.,.} the anticommutator.

1.0.1 Change of basis

The identity operator, $\mathcal{I}$ can be resolved as $\mathcal{I} = \sum_{\lambda=0}^{\infty} |\lambda\rangle \langle\lambda|$. Using the relations $\left|\tilde{\lambda}\right\rangle = \sum_\lambda |\lambda\rangle \left\langle\lambda|\tilde{\lambda}\right|\lambda|\tilde{\lambda}\right\rangle$, $|\lambda\rangle = a_\lambda^\dagger |\Omega\rangle$, and $\left|\tilde{\lambda}\right\rangle = a_{\tilde{\lambda}}^\dagger |\Omega\rangle$, the transformation law is given by:

$$a_{\tilde{\lambda}}^\dagger = \sum_\lambda \left\langle\lambda|\tilde{\lambda}\right|\lambda|\tilde{\lambda}\right\rangle a_\lambda^\dagger, \quad a_{\tilde{\lambda}} = \sum_\lambda \left\langle\tilde{\lambda}|\lambda\right|\tilde{\lambda}|\lambda\right\rangle a_\lambda \tag{1.4}$$

1.0.2 Fourier transform of field operators

The physical interpretation provided for the creation (annihilation) operators states that they can be thought of as creating (annihilating) a particle in a state λ. In particular, this can be thought of as creating (annihilating) a particle at a dimensional site r, or equivalently, with a momentum k. This distinction is important since it is subtly related to the Heisenberg Uncertainty Principle – the first scenario implies that the position of the particle is known with a very high certainty, and therefore is delocalised in momentum space and vice-versa. The transformation from real space to k-space is captured via Fourier transform of the field operators.

$$\hat{c}_r^{(\dagger)} = \frac{1}{\sqrt{N}} \sum_k e^{-(+)ikr} \hat{c}_k^{(\dagger)}, \quad \hat{c}_k^{(\dagger)} = \frac{1}{\sqrt{N}} \int_r e^{-(+)ikr} \hat{c}_r^{(\dagger)} \tag{1.5}$$

If we are dealing with discrete lattice sites, the Fourier transform has to be modified accordingly

$$\hat{c}_r^{(\dagger)} = \frac{1}{\sqrt{N}} \sum_k e^{-(+)ikar} c_k^{(\dagger)} \tag{1.6}$$

and k lies inside the first Brillouin zone, i.e. $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ and a is the lattice constant.

1.1 Representation of operators

Appendix A

Fourier Transforming the Interacting Fermion Gas Hamiltonian

Appendix B

Bloch's Theorem

Periodic potentials are important in condensed matter physics, and we will be using the Bloch wavefunctions generously during the analysis of toy models. Secondly, periodic potentials will give us our first examples of Hamiltonian systems with symmetry, and they will serve to illustrate certain general principles of such systems.

We wish to solve the one-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi$$

where the potential is assumed to be spatially periodic,

$$V(x+a) = V(x) \tag{B.1}$$

Here a is the lattice spacing or spatial period of the 1-D lattice. No further assumptions need be made about the behaviour of $V(x)$ within any period apart from its periodicity.

Next, we shall make a strong assumption that there is a super-symmetry that rides over the good ole periodicity of the lattice points such that the lattice repeats itself after N lattice spacings. This is equivalent to imposing a periodic/circular boundary condition on the solutions to the Hamiltonian.

We introduce the translation operator, $T(a)$, which has the effect of displacing the wave function by the lattice spacing a along the x-axis.

$$T(a)\psi(x) = \psi(x-a) \tag{B.2}$$

Functionally, the translation operator is given by,

$$T(a) = e^{-\frac{iap}{\hbar}} \tag{B.3}$$

An easy check will ascertain that this operator commutes with both kinetic energy, as well as potential energy operators. This means that *T(a)* commutes with the entire Hamiltonian,

$$[T(a), H] = 0 \tag{B.4}$$

Put more generally, H commutes with any power of $T(a)$, $T(a)^n = T(na)$, which is to say that it commutes with the entire group of symmetry operations generated by $T(a)$.

The fact that H and $T(a)$ commute provides us a powerful tool to determine the eigenfunctions of H. More often than not, it is hard to find the eigenfunctions of H, but much easier to find those for the translation operator. Since we now know the eigenfunctions of the translation operator, it makes the search for the eigenfunctions of H easier since they are a subset of the eigenspace of $T(a)$.

Since $T(a)$ is unitary, its eigenvalue τ must be a phase factor, $\tau = e^{-i\theta}$. The angle θ characterizes the eigenvalues of $T(a)$ and may be restricted to the range $-\pi < \theta \leq \pi$. It is conventional to write this angle in the form $\theta = ka$, where k is a quantity with dimensions of wave number, which characterizes the eigenvalue. We now have,

$$T(a)\psi_k(x) = \psi_k(x-a) = e^{-ika}\psi_k(x) \tag{B.5}$$

Equivalently, we can write this as,

$$\psi_k(x+a) = e^{ika}\psi_k(x) \tag{B.6}$$

Now we are faced with a dilemma - for any given value of k, there are functions ψ_k which satisfy B.6, so the spectrum of $T(a)$ is the entire unit circle in the complex plane.

Furthermore, the number of such functions for any value of e^{-ika} is infinite, so the eigenvalues are infinite-fold degenerate and the eigenspaces of $T(a)$ are infinite-dimensional. This would render the entire analysis using translation operators inconsequential since it was asserted that this approach would help limit the space in which we have to search for the eigenfunctions of H. This is exactly where the initial boundary condition assuming a super-symmetry comes into play. In case the lattice repeats itself after N lattice spacings, the single-valuedness of the wavefunction requires

$$\psi(x + Na) = \psi(x)$$

so the eigenvalues of $T(a)$ are phase factors of the form $e^{-\frac{2n\pi i}{N}}$, for $n = 0, ..., N-1$. In this case, the spectrum of $T(a)$ is discrete, although each eigenvalue is still infinite-fold degenerate. Rather than $\psi_k(x)$, it is often easier to work with a function $u_k(x)$, defined by

$$\psi_k(x) = e^{ikx} u_k(x) \tag{B.7}$$

where u_k is periodic, $u_k(x + a) = u_k(x)$. *Bloch's theorem* states that since H commutes with $T(a)$, H possesses eigenfunctions which are of the form of $\psi_k(x)$, that is, e^{ikx} times a periodic function $u_k(x)$. [1]

[1] An interesting offshoot of the Bloch wavefunction is the concept of 'crystal momentum', which does not represent the momentum of the electron in real space but rather encapsulates the effect of the net external potential acting on it without having to worry about the internal forces.

Bibliography