Los Alamos Computational Condensed Matter Summer School 2026

Many-Body Primer Lecture Notes

Christopher Lane

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Recommended Books and Resources

Gianluca Stefanucci and Robert van Leeuwen, *Nonequilibrium Many-Body Theory of Quantum Systems: A Modern Introduction*

Alexander Fetter and John Dirk Walecka, *Quantum Theory of Many-particle Systems*

Gordon Baym, *Lectures on Quantum Mechanics*

Jørgen Rammer, *Quantum Field Theory of Non-equilibrium States*

G. Rickayzen, *Green's Functions and Condensed Matter*

Richard M. Martin, Lucia Reining, and David M. Ceperley, *Interacting Electrons: Theory and Computational Approaches*

A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*

Eleftherios N. Economou, *Green's Functions in Quantum Physics*

Richard D. Mattuck, *A Guide to Feynman Diagrams in the Many-body Problem*

Acknowledgments

These lecture notes are not particularly original. My primary contribution has been to borrow and assimilate the best discussions and explanations I could find from the vast literature on the subject. I have relied heavily on the sources listed at the beginning.

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Introduction

> "There are no real one-particle systems in nature, not even few-particle systems. The existence of virtual pairs and of pair fluctuations shows that the days of fixed particle numbers are over." —-Viki Weisskopf

When studying solids, or more generally condensed phases of matter, we cannot follow the reductionist route by analyzing the constituent pieces alone, because the properties of solids emerge from the mutual interaction of $\sim 10^{23}$ particles[1]. There are indeed regimes where excitation in this soup of degrees of freedom behave as *independent* bodies, albeit with *renormalized* properties, e.g. mass, charge, and so on, however some of the most fascinating and open challenges in condensed matter arise from regimes where the characteristic of the individual is lost, and it is the motion of the collective that dominates. Here, we find magnetism, superconductivity, and Kondo physics to name a few intrinsically non-perturbative emergent phases. In these notes, we introduce the tools needed to begin to inspect these systems and characterize their properties. This text does not presume to be exhaustive, but to give an initial introduction and hopefully instill curiosity and propel the reader forward to more specialized topics.

[1]

Second Quantization

Similar to the painter who needs brushes and pigments to articulate ideas about the world around them, we need a language to be able to describe the phenomena of many-particle systems. Second quantization is such a tool. Here, we will introduce and apply the method of second quantization, a technique that sets the foundation for quantum many-particle theories. We will see that this formulation provides a compact representation of the many-body space and the algebra of the field operators encode the symmetry via simple commutation relations rather than explicitly constructing some Hilbert space representation. Additionally, this approach provides a convenient flexible vehicle to respect the quantum statistics of identical particles. We will rely on this tool in subsequent sections to build models and formulate approximate solutions to the many-body problem.

Why Second Quantization?

To motivate our discussion, we start by inspecting the many-body Schrödinger equation. If we consider a system of particles its Hamiltonian in almost all cases of

interest takes the form:

$$H = \sum_{i=1}^{N} T(x_i) + \frac{1}{2} \sum_{i \neq j=1}^{N} V(x_i, x_j), \tag{1}$$

where T is the kinetic energy and V is the potential energy of interaction between particles. The quantity x_i denotes the coordinates of the ith particle, that is, it includes both the spatial coordinate $\mathbf{r}_i$ and any discrete label such as spin, orbital, and so on. The potential-energy term represents the interaction between every pair of particles, *counted once*, which accounts for the factor of $\frac{1}{2}$ and the double sum running over i and j indices separately, except when the value of i and j are equal. With this Hamiltonian, the time dependent many-particle Schrödinger equation is given by

$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, \ldots, x_n, t) = H\Psi(x_1, \ldots, x_n, t) \tag{2}$$

together with an appropriate set of boundary conditions for the wavefunction Ψ. To obtain physically relevant solutions Ψ must also obey the statistics of the particles, e.g., indistinguishable fermions/bosons dictate that $\Psi(x_1, x_2) = \mp\Psi(x_2, x_1)$. If one is able to solve this equation with these conditions, Ψ contains all the information of the system.

Unfortunately, applying this approach to real systems has a number of drawbacks:

- Cumbersome for systems of 10^{23} particles
- The particle number is fixed
- Particles are accessed one or two at a time, but the full information of the system must be carried along
- Approximations yield independent particle solutions, e.g. Hartree-Fock.

Therefore, in order to tackle systems with a large number of particles we need to reformulate our approach and move away from the first quantization. We will see that by elevating to the second quantization framework the description of response functions simplifies and we avoids dealing with the totality of $\Psi(x_1, \ldots, x_n, t)$.[2]

[2] Though we are mainly concerned with non-relativistic many-particle systems here, second quantization is also essential for formulating relativistic quantum mechanics.

Creation and Annihilation Operators

The central quantity under investigation in quantum mechanics is the wavefunction since it contains the full information and evolution of the system. The wavefunction belongs to a Hilbert space–a vector space endowed with the inner product–, with a dimension typically dictated by the physical problem at hand. A fundamental property of the vector nature of the Hilbert space is that any linear superposition of physical states in the Hilbert space results in another physical state within the Hilbert space. These states may be described using Dirac bra-ket notation, where a physical quantum mechanical state is given in terms of a *ket* $|\Psi\rangle$. [3] The advantage of this notation is two-fold: (i) it provides a geometric interpretation of the physical state in the Hilbert space as abstract kets independent of basis in which they are

[3] It does not matter whether we expand $|\Psi\rangle$ in terms of the position-spin kets or momentum-spin kets; $|\Psi\rangle$ remains the same although the expansion coefficients in the two basis are different.

expanded, and (ii) the abstract kets can be systematically constructed by repeated applications of a creation operator on the empty or zero-particle state. This approach forms the basis of the formalism know as second quantization.

To deal with the arbitrary number of identical particles we first define a collection of $\mathcal{F}$ of Hilbert spaces, otherwise known as Fock space, as

$$\mathcal{F} = \{\mathcal{H}_0, \mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_N, \ldots\} \tag{3}$$

where $\mathcal{H}_N$ is a Hilbert space for N identical particles. An arbitrary state vector in Fock space may be written as

$$|\Psi\rangle = \sum_{N=0}^{\infty} c_N |\Psi_N\rangle \tag{4}$$

where $|\Psi_N\rangle$ is a state belonging to $\mathcal{H}_N$. Similar to the Hilbert space for a fixed number of particles[4], the inner product between $|\Psi\rangle$ and another element $|\phi\rangle$ in $\mathcal{F}$

$$|\phi\rangle = \sum_{N=0}^{\infty} a_N |\phi_N\rangle \tag{6}$$

is defined as

$$\langle\phi|\Psi\rangle \equiv \sum_{N=0}^{\infty} a_N^* c_N \langle\phi_N|\Psi_N\rangle\,, \tag{7}$$

where $\langle\phi_N|\Psi_N\rangle$ is the inner product in $\mathcal{H}_N$. Inherent in this definition is the common sense notion that states of different particle numbers ($N \neq M$) are orthogonal, i.e. have zero overlap. It is important to point out, that the zero-particle space ($\mathcal{H}_0$) is a one dimensional space that describes the *empty system* denoted as $|0\rangle$ with normalization $\langle 0|0\rangle = 1$. According to the expansion (Eq. 4) the empty state has all $c_N = 0$ except for c_0. This state should not be confused with the null state $|\varnothing\rangle$ which is defined with $c_N = 0 \;\forall\; N$ and is not a physical state.

To construct a basis for each Hilbert space we will follow a process in direct analogy to the algebraic solution of the simple harmonic oscillator, where so-called ladder operators *annihilate* and *create* one quantum excitation.[5] Here, our task is to extend this idea to particles, where operators add and remove particle from the system. To accomplish this we define *field operators* that generate position-spin kets (i.e. eigenstates of the position operator and the z-compent of the spin operator, e.g., $\hat{r}\,|x\rangle = r\,|x\rangle$ and $\hat{S}_z\,|x\rangle = \sigma\,|x\rangle$) by repeated action on the empty state, i.e.,

$$\begin{aligned} |x_1\rangle &= \hat{\psi}^\dagger(x_1)\,|0\rangle \\ |x_1, x_2\rangle &= \hat{\psi}^\dagger(x_2)\,|x_1\rangle = \hat{\psi}^\dagger(x_2)\hat{\psi}^\dagger(x_1)\,|0\rangle \\ |x_1, x_2, \ldots, x_N\rangle &= \hat{\psi}^\dagger(x_N)\,|x_1, x_2, \ldots, x_{N-1}\rangle = \hat{\psi}^\dagger(x_N)\ldots\hat{\psi}^\dagger(x_2)\hat{\psi}^\dagger(x_1)\,|0\rangle\,. \end{aligned} \tag{8}$$

Since an operator is defined from its action on a complete set of states in the Hilbert space (Fock space in our case) the above relation defines the field operator $\hat{\psi}^\dagger(x)$ for all x. The field operator transforms a state in $\mathcal{H}_N$ into a state of $\mathcal{H}_{N+1}$ for all N, as

[4] This is a generalization of the basic principles of single-particle quantum mechanics, where we can assign a state $|\lambda\rangle$ to the particle just after measurement. Since these states are orthonormal and form a basis of the single-particle Hilbert space, any particle wavefunction $|\Psi\rangle$ can be expanded in terms of them

$$|\Psi\rangle = \sum_{\lambda} \Psi_\lambda\,|\lambda\rangle \tag{5}$$

where the coefficient $\Psi_\lambda = \langle\lambda|\Psi\rangle$ and its square modulus is the probability of finding the particle in state $|\lambda\rangle$. For a many-particle system the expansion is the result of a coincidence experiment where the expansion coefficients $\Psi_{\lambda\kappa}$ describes a the probability of finding one particle with λ and the other with κ properties.

[5] Recall $H_{SHO} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$, where the creation and annihilation operators obey $[\hat{a}, \hat{a}^\dagger] = 1$, and the $n$the eigenstate $|n\rangle$ may be constructed from the ground state as $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\,|0\rangle$.

illustrated in Fig. 1. In this way, we say $\hat{\psi}^\dagger(x)$ creates a particle at x, and therefore it is called a *creation operator*.

For systems of identical particles[6], if we interchange two particles the state is the same up to a phase $(\pm)$. This implies

$$\begin{aligned}\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\left|x_1,\ldots,x_N\right\rangle &= \left|x_1,\ldots,x_N,y,x\right\rangle = \pm\left|x_1,\ldots,x_N,x,y\right\rangle \\ &= \pm\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)\left|x_1,\ldots,x_N\right\rangle \end{aligned} \tag{10}$$

where the upper sign in $\pm$ refers to bosons and the lower to fermions. This is true for all states in $\mathcal{F}$ and hence

$$\left[\hat{\psi}^\dagger(x),\hat{\psi}^\dagger(y)\right]_\mp = 0, \tag{11}$$

where we have used the (anti)commutator between two generic operators $\hat{A}$ and $\hat{B}$:

$$\left[\hat{A},\hat{B}\right]_\mp = \hat{A}\hat{B} \mp \hat{B}\hat{A}. \tag{12}$$

In analogy to the simple harmonic oscillator, there is an adjoint operator of $\hat{\psi}^\dagger(x)$, namely $\hat{\psi}(x)$. The field operator $\hat{\psi}(x)$ maps a state in $\mathcal{H}_N$ into a state in $\mathcal{H}_{N-1}$. Thus where $\hat{\psi}^\dagger(x)$ adds a particle to the system, $\hat{\psi}(x)$ removes a particle from the system, i.e. $\hat{\psi}(x)$ is known as the *annihilation operator*. By taking the adjoint of Eq. 11 we immediately obtain the (anti)commutator

$$\left[\hat{\psi}(x),\hat{\psi}(y)\right]_\mp = 0. \tag{13}$$

We can get a third and final (anti)commutation relation from the inner product of two single particle states. Since,

$$\delta(x,y) = \langle x|y\rangle = \langle 0|\hat{\psi}(x)\hat{\psi}^\dagger(y)|0\rangle = \langle 0|\left[\hat{\psi}(x),\hat{\psi}^\dagger(y)\right]_\mp|0\rangle \tag{14}$$

we must have

$$\left[\hat{\psi}(x),\hat{\psi}^\dagger(y)\right]_\mp = \delta(x,y) \tag{15}$$

for all $\langle x|y\rangle$. Now, if we wish to remove a particle from the many-particle system, we inspect the action of $\hat{\psi}(x)$ on a N-particle state

$$\begin{aligned}\hat{\psi}(x)\left|x_1,\ldots,x_N\right\rangle &= \hat{\psi}(x)\hat{\psi}^\dagger(x_N)\ldots\hat{\psi}^\dagger(x_1)\left|0\right\rangle \\ &= \left(\left[\hat{\psi}(x),\hat{\psi}^\dagger(x_N)\right]_\mp \pm \hat{\psi}^\dagger(x_N)\hat{\psi}(x)\right)\hat{\psi}^\dagger(x_{N-1})\ldots\hat{\psi}^\dagger(x_1)\left|0\right\rangle \\ &= \left(\delta(x-x_N) \pm \hat{\psi}^\dagger(x_N)\hat{\psi}(x)\right)\hat{\psi}^\dagger(x_{N-1})\ldots\hat{\psi}^\dagger(x_1)\left|0\right\rangle \\ &= \delta(x-x_N)\left|x_1,\ldots,x_{N-1}\right\rangle \pm \hat{\psi}^\dagger(x_N)\hat{\psi}(x)\left|x_1,\ldots,x_{N-1}\right\rangle \\ &= \sum_{k=1}^{N}(\pm)^{N+k}\delta(x-x_k)\left|x_1,\ldots,x_{k-1},x_{k+1},\ldots,x_N\right\rangle. \end{aligned} \tag{16}$$

Where the key is to 'pull' $\hat{\psi}(x)$ to the right to annihilate the vacuum. By doing so the annihilation operator systematically removes a particle from every position-spin

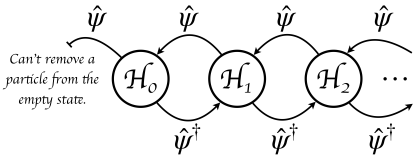


Figure 1

Action of the creation $\hat{\psi}^\dagger$ and annihilation $\hat{\psi}$ operators on the collection of Hilbert spaces $\mathcal{F}$.

[6] Identical particles have the same internal properties such as mass, charge, spin and so on. Lets suppose we measure the position of two electrons in coincidence (at the same time) with the same detector and perform the experiment $N >> 1$ times. If we use $|x_1,x_2\rangle$ to denote the physical state, it is material to ask if $|x_1,x_2\rangle$ and $|x_2,x_1\rangle$ are different states. Since we have identical particles we cannot tell the difference, thus $|x_1,x_2\rangle$ is the same physical state as $|x_2,x_1\rangle$. Consequently, $|x_1,x_2\rangle$ is $|x_2,x_1\rangle$ up to a phase: $|x_1,x_2\rangle = \pm|x_2,x_1\rangle$, either symmetric or antisymmetric under exchange of electron positions. All particles can then be grouped into two main classes: bosons and fermions described by symmetric and antisymmetric states, respectively. A peculiarity of fermions is that $|x_1,x_2\rangle$ must be the null state (i.e., $|x_1,x_1\rangle = -|x_1,x_1\rangle$), meaning it is not possible to create two fermions in the same state. This is known as the Pauli exclusion principle. Generalizing to a system of N identical particles, the orthonormal fully (anti)symmetric basis states are

$$\begin{aligned}&|x_1,x_2,\ldots,x_N\rangle = \\ &\frac{1}{\sqrt{N!}}\sum_P(\pm)^{\zeta_P}\left|x_1\right\rangle\left|x_2\right\rangle\cdots\left|x_N\right\rangle \end{aligned} \tag{9}$$

where the summation is over all permutations P of particles and ζ_P counts the number of transpositions are needed to build a permutation P. The phase $+$ $(-)$ is for Bosons (Fermions). Finally, $|x_1\rangle|x_2\rangle\cdots|x_N\rangle$ is shorthand for the tensor product of states $|x_1\rangle\otimes|x_2\rangle\otimes\cdots\otimes|x_N\rangle$.

Example 1. For a two particle state $|x,y\rangle$, if we apply $\hat{\psi}(z)$,

$$\begin{aligned}&\hat{\psi}(z)\left|x,y\right\rangle = \hat{\psi}(z)\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)\left|0\right\rangle \\ &= \left(\delta(z,y) \pm \hat{\psi}^\dagger(y)\hat{\psi}(z)\right)\hat{\psi}^\dagger(x)\left|0\right\rangle \\ &= \delta(z,y)\left|x\right\rangle \pm \hat{\psi}^\dagger(y)\left(\delta(z,x) \pm \hat{\psi}^\dagger(x)\hat{\psi}(z)\right)\left|0\right\rangle \\ &= \delta(z,y)\left|x\right\rangle \pm \delta(z,x)\left|y\right\rangle (\pm)^2\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)\cancelto{0}{\hat{\psi}(z)\left|0\right\rangle} \\ &= \delta(z,y)\left|x\right\rangle \pm \delta(z,x)\left|y\right\rangle \end{aligned}$$

coordinate while respecting the symmetry of the particles. We can further ask: what happens if we follow up the removal of a particle at x by creating a particle at x? This is explicitly given by,

$$\begin{aligned}
\hat{\psi}^\dagger(x)\hat{\psi}(x)\,|x_1,\ldots,x_N\rangle &= \sum_{k=1}^{N}(\pm)^{N+k}\delta(x-x_k)\hat{\psi}^\dagger(x)\,|x_1,\ldots,x_{k-1},x_{k+1},\ldots,x_N\rangle \\
&= \sum_{k=1}^{N}(\pm)^{N+k}\delta(x-x_k)\,|x_1,\ldots,x_{k-1},x_{k+1},\ldots,x_N,x\rangle \\
&= \sum_{k=1}^{N}(\pm)^{N+k}\delta(x-x_k)(\pm)^{N-k}\,|x_1,\ldots,x_{k-1},x,x_{k+1},\ldots,x_N\rangle \\
&= \sum_{k=1}^{N}\delta(x-x_k)\,|x_1,\ldots,x_{k-1},x_k,x_{k+1},\ldots,x_N\rangle \\
&= \sum_{k=1}^{N}\delta(x-x_k)\,|x_1,\ldots,x_N\rangle\,, \qquad (17)
\end{aligned}$$

where we recognize $\sum_{k=1}^{N}\delta(x-x_k)$ is the first-quantized particle density operator. Thus, $\hat{\psi}^\dagger(x)\hat{\psi}(x)$ is typically refereed to as the *density operator* $\hat{n}(x)$. So, the action of $\hat{\psi}^\dagger(x)\hat{\psi}(x)$ yields the particle density at $\mathbf{r}$.

Using the fact that

$$|x\rangle = \hat{\psi}^\dagger(x)\,|0\rangle = \left[\langle 0|\,\hat{\psi}(x)\right]^\dagger = [\langle x|]^\dagger \qquad (18)$$

we can determine the overlap of two N-particle states

$$\begin{aligned}
\langle x_1,\ldots,x_N|y_1,\ldots,y_N\rangle &= \langle 0|\,\hat{\psi}(x_1)\cdots\hat{\psi}(x_N)\,|y_1,\ldots,y_N\rangle \\
&= \langle 0|\,\hat{\psi}(x_1)\cdots\hat{\psi}(x_{N-1})\times \\
&\times\left(\sum_{k=1}^{N}(\pm)^{N+k}\delta(x_N-y_k)\,|y_1,\ldots,y_{k-1},y_{k+1},\ldots,y_N\rangle\right) \\
&= \sum_{P}(\pm)^P\Pi_{j=1}^{N}\delta(x_j-y_{P_j}), \qquad (19)
\end{aligned}$$

where the sum is over all permutations of $y_1, y_2\ldots, y_N$ orderings with even and odd permutations yielding the sign $(\pm)^P$. This is the expression for a permanent/determinant

$$|A|_\pm = \sum_P(\pm)^P A_{1P_1}A_{2P_2}\cdots A_{NP_N}$$

where $A_{jP_j} = \delta(x_j - y_{P_j})$ in the case of Eq. 19. In other words, we can also write the overlap of position-spin basis elements as

$$\langle x_1,\ldots,x_N|y_1,\ldots,y_N\rangle = \begin{vmatrix}\delta(x_1-y_1) & \cdots & \delta(x_1-y_N)\\ \vdots & \ddots & \vdots \\ \delta(x_N-y_1) & \cdots & \delta(x_N-y_N)\end{vmatrix}. \qquad (20)$$

To be complete the completeness relation is given by

$$\frac{1}{N!}\int dx_1 \cdots dx_N \ |x_1, \ldots, x_N\rangle \langle x_1, \ldots, x_N| = \hat{\mathbb{1}}. \tag{21}$$

We have seen how to construct states of many identical particles with a given position and spin, however, this is just one choice of quantum numbers out of an infinite set of possibilities to characterize a every particle in the system. We will now see how to convert between various bases of many identical particles in which each particle is labeled by general quantum numbers, such as orbital, momentum, energy, and so on. In general the single particle state $|n\rangle$ can be expanded into the position-spin states via the completeness relation

$$|n\rangle = \int dx \, |x\rangle\langle x|n\rangle = \int dx \ \varphi_n(x) \, |x\rangle = \int dx \ \varphi_n(x)\hat{\psi}^\dagger(x) \, |0\rangle \tag{22}$$

with the overlap matrix elements $\langle x|n\rangle$ equal to the basis functions $\varphi_n(x)$ and the normalization of $\langle n|n\rangle = 1$ directly follows from the normalization of $\varphi_n(x)$, $\int dx|\varphi_n(x)|^2 = 1$. Additionally, $|n\rangle$ is obtained by applying

Exercise 2. Prove that the normalization of $\langle n|n\rangle = 1$ directly follows from $\int dx|\varphi_n(x)|^2 = 1$.

$$\hat{c}_n^\dagger = \int dx \ \varphi_n(x)\hat{\psi}^\dagger(x) \tag{23}$$

to the empty state $|0\rangle$, i.e. $\hat{c}_n^\dagger = |n\rangle$. In this way we may say $\hat{c}_n^\dagger$ creates a particle with quantum number n. Similarly, by applying the adjoint we get

$$\hat{c}_n = \int dx \ \varphi_n^*(x)\hat{\psi}(x), \tag{24}$$

the operator that annihilates a particle with quantum number n since

$$\begin{aligned}
\hat{c}_n \, |n\rangle &= \int dy \int dx \ \varphi_n^*(y)\varphi_n(x)\hat{\psi}(y)\hat{\psi}^\dagger(x) \, |0\rangle = \int dy \int dx \ \varphi_n^*(y)\varphi_n(x)\hat{\psi}(y) \, |x\rangle \\
&= \int dy \int dx \ \varphi_n^*(y)\varphi_n(x)\delta(x,y) \, |0\rangle = \int dx \ |\varphi_n(x)|^2 \, |0\rangle \\
&= |0\rangle \, .
\end{aligned} \tag{25}$$

Lets take a moment to reflect on the meaning of these operators. Given a set of quantum numbers, $\hat{c}_n^\dagger$ ($\hat{c}_n$) create (annihilate) a particle with a quantum number n. In the case of Bosons $\hat{c}_n^\dagger$ may create multiple particles with the same state, whereas only one particle can occupy a single fermion state. So, the basis states provide a means to keep track of how many particles are in the system and how many particles occupy each state. This is typically referred to as the *occupation basis*. Since the operators $\hat{c}_n^\dagger, \hat{c}_n$ are linear combinations of field operators the (anti)commutation relations between $\hat{c}_n^\dagger$ and $\hat{c}_n$

$$\left[\hat{c}_n, \hat{c}_m^\dagger\right]_\mp = \delta_{nm}, \quad [\hat{c}_n, \hat{c}_m]_\mp = \left[\hat{c}_n^\dagger, \hat{c}_m^\dagger\right]_\mp = 0 \tag{26}$$

directly follow from those of the field operators. Specifically, the $\hat{c}$-operators obey the same (anti)commutation relations as the field operators with the index n playing the role of x and the Kronecker delta in place of the Dirac delta function for discrete

Exercise 3. Prove the (anti)commutation relations between $c_n^\dagger$ and c_n.

quantum numbers n. Hence the results for field operators carry over and remain valid for a more general basis. We define the N-particle state

$$|n_1, n_2, \ldots, n_N\rangle \equiv \hat{c}^\dagger_{n_N} \cdots \hat{c}^\dagger_{n_1} |0\rangle = \hat{c}^\dagger_{n_N} |n_1, n_2, \ldots, n_{N-1}\rangle \tag{27}$$

and has the symmetry property

$$|n_{P_1}, n_{P_2}, \ldots, n_{P_N}\rangle = (\pm)^P |n_1, n_2, \ldots, n_N\rangle \tag{28}$$

which follow directly from the (anti)commutation relations in Eq. 26. Like the position-spin states, the states $|n_1, n_2, \ldots, n_N\rangle$ span the N-particle Hilbert space $\mathcal{H}_N$. The action of $\hat{c}_n$ on $|n_1, n_2, \ldots, n_N\rangle$ is also found by moving $\hat{c}_n$ through the string of $\hat{c}^\dagger_n$-operators towards the empty state

Exercise 4. Prove Eq. 29, Eq. 30, and Eq. 34.

$$\hat{c}_n |n_1, n_2, \ldots, n_N\rangle = \sum_{k=1}^{N} (\pm)^{N+k} \delta_{n n_k} |n_1, \ldots, n_{k-1}, n_{k+1}, \ldots, n_N\rangle . \tag{29}$$

Moreover, the overlap between N-particle states in a general basis is expressed as

$$\langle n'_1, n'_2, \ldots, n'_N | n_1, n_2, \ldots, n_N\rangle = \sum_P (\pm)^P \Pi_j^N \delta_{n', n_{P_j}} \tag{30}$$

which is analogous to $\langle x_1, \ldots, x_N | y_1, \ldots, y_N\rangle$ in Eq. 19. The completeness relation is

$$\frac{1}{N!} \sum_{n_1, n_2, \ldots, n_N} |n_1, n_2, \ldots, n_N\rangle\langle n_1, n_2, \ldots, n_N| = \hat{\mathbb{1}} \tag{31}$$

and hance may be used to expand $|\Psi\rangle$ belonging to $\mathcal{H}_N$ as

$$\begin{aligned} |\Psi\rangle = \hat{\mathbb{1}} |\Psi\rangle &= \frac{1}{N!} \sum_{n_1, n_2, \ldots, n_N} |n_1, n_2, \ldots, n_N\rangle\langle n_1, n_2, \ldots, n_N|\Psi\rangle \\ &= \frac{1}{N!} \sum_{n_1, n_2, \ldots, n_N} \Psi_{n_1, n_2, \ldots, n_N} |n_1, n_2, \ldots, n_N\rangle . \end{aligned} \tag{32}$$

The key to direct translation of expressions from field operators to a general occupation basis is provided that $|n\rangle$ is a orthonormal basis for $\mathcal{H}_1$. Therefore, any transformation that preserves the orthonormal basis will yield operators that obey the (anti)commutation relations. Consequently,

$$\hat{d}_\alpha = \sum_n U_{\alpha n} \hat{c}_n, \quad \hat{d}^\dagger_\alpha = \sum_n U^*_{\alpha n} \hat{c}^\dagger_n \tag{33}$$

obeys

$$\left[\hat{d}_\alpha, \hat{d}^\dagger_\beta\right]_\mp = \delta_{\alpha\beta}, \quad \left[\hat{d}_\alpha, \hat{d}_\beta\right]_\mp = \left[\hat{d}^\dagger_\alpha, \hat{d}^\dagger_\beta\right]_\mp = 0 \tag{34}$$

provided that $U_{\alpha n} = \langle \alpha | n\rangle$ is the inner product between elements of two orthonormal basis $|n\rangle$ and $|\alpha\rangle$, which is the case if and only if $U_{\alpha n}$ is a unitary matrix

$$\sum_n U_{\alpha n} U^\dagger_{n\beta} = \sum_n \langle \alpha | n\rangle\langle n | \beta\rangle = \langle \alpha | \beta\rangle = \delta_{\alpha\beta}. \tag{35}$$

In particular, if $\alpha = x$ we have $U_{x|n} = \langle x|n\rangle = \varphi_n(x)$, and we recover the field operators

$$\hat{\psi}(x) = \sum_n \varphi_n(x)\hat{c}_n, \quad \hat{\psi}^\dagger(x) = \sum_n \varphi_n^*(x)\hat{c}_n^\dagger. \tag{36}$$

Then by extension the expansion of the N-particle position-spin states is given by

$$|x_1, \ldots, x_N\rangle = \sum_{n_1,\ldots,n_N} \varphi_{n_1}(x_1)\cdots\varphi_{n_N}(x_N)\,|n_1, \ldots, n_N\rangle \tag{37}$$

and conversely a N-particle state in a genal basis may be expanded into the position-spin basis

$$|n_1, \ldots, n_N\rangle = \int dx_1\cdots dx_N\ \varphi_{n_1}(x_1)\cdots\varphi_{n_N}(x_N)\,|x_1, \ldots, x_N\rangle \tag{38}$$

To test out these techniques we derive the many-particle Schrödinger equation from base principles.

Example 5. The time evolution of the state vector $|\Psi\rangle$ is given by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\,|\Psi(t)\rangle = \hat{H}\,|\Psi(t)\rangle \tag{39}$$

and may be projected onto the position-spin basis for N-particles to recover the first quantized form of the many-particle Schrödinger equation (Eq. 2)

$$\frac{1}{N!}\int dx_1\cdots dx_N\ \left(i\hbar\frac{\partial}{\partial t}\,|x_1, \ldots, x_N\rangle\,\langle x_1, \ldots, x_N|\Psi(t)\rangle = \hat{H}\,\langle x_1, \ldots, x_N|\Psi(t)\rangle\right)$$
$$\frac{1}{N!}\int dx_1\cdots dx_N\ \left(i\hbar\frac{\partial}{\partial t}\Psi(x_1, \ldots, x_N, t) = H\Psi(x_1, \ldots, x_N, t)\right)|x_1, \ldots, x_N\rangle\,.$$

This explicitly shows that the many-particle Schrödinger equation appears as the time evolution of the expansion coefficients $\Psi(x_1, \ldots, x_N, t)$ and is by definition restricted to describing a fixed N-particle system. We can additionally expand $\Psi(x_1, \ldots, x_N, t)$ into a set of basis functions via

$$\begin{aligned}\Psi(x_1, \ldots, x_N, t) &= \frac{1}{N!}\sum_{n_1,\ldots,n_N}\langle x_1, \ldots, x_N|n_1, \ldots, n_N\rangle\,\langle n_1, \ldots, n_N|\Psi(t)\rangle \\ &= \frac{1}{N!}\sum_{n_1,\ldots,n_N}\Psi_{n_1,\ldots,n_N}(x_1, \ldots, x_N)\,\langle n_1, \ldots, n_N|\Psi(t)\rangle\end{aligned} \tag{40}$$

where the overlap $\Psi_{n_1,\ldots,n_N}(x_1, \ldots, x_N)$ between position-spin states and the set of quantum numbers can be straight forwardly evaluated

$$\begin{aligned}\Psi_{n_1,\ldots,n_N}(x_1, \ldots, x_N) &= \int dy_1\cdots dy_N\ \varphi_{n_1}(y_1)\cdots\varphi_{n_N}(y_N)\,\langle x_1, \ldots, x_N|y_1, \ldots, y_N\rangle \\ &= \sum_P(\pm)^P\Pi_{j=1}^N\int dy_1\cdots dy_N\ \varphi_{n_1}(y_1)\cdots\varphi_{n_N}(y_N)\delta(x_j - y_{P_j}) \\ &= \sum_P(\pm)^P\varphi_{n_1}(y_{P_1})\cdots\varphi_{n_N}(y_{P_N})\end{aligned}$$

$$= \begin{vmatrix} \varphi_{n_1}(x_1) & \cdots & \varphi_{n_1}(x_N) \\ \vdots & \ddots & \vdots \\ \varphi_{n_N}(x_1) & \cdots & \varphi_{n_N}(x_N) \end{vmatrix}. \tag{41}$$

Since for any matrix A we have $|A|_\pm = |A^T|_\pm$, where A^T is the transpose of A we can equivalently write

$$\Psi_{n_1,\ldots,n_N}(x_1,\ldots,x_N) = \begin{vmatrix} \varphi_{n_1}(x_1) & \cdots & \varphi_{n_N}(x_1) \\ \vdots & \ddots & \vdots \\ \varphi_{n_1}(x_N) & \cdots & \varphi_{n_N}(x_N) \end{vmatrix} \tag{42}$$

which for the case of fermions the determinate is known as the *Slater determinant*. This example begins to illustrate the power of the the field operator *second quantized* point of view, where we have freed ourselves from being confined to a fixed particle number system to allow an arbitrary number of particles.

Operators in Second Quantization

So far we have seen how to construct various basis representations of the N-particle states using general set of creation and annihilation operators. Now, we will connect operators written in first quantization to those in second quantization. To illustrate the process it is illustrative to consider the action of the center-of-mass operator on two identical particles $|\mathbf{r}_1\mathbf{r}_2\rangle$. The center-of-mass operator in first quantization is[7]

$$\hat{R}_{CM} = \frac{1}{N}\sum_{j=1}^{N}\hat{\mathbf{r}}_j \tag{43}$$

and if it acts on $|\mathbf{r}_1\mathbf{r}_2\rangle$

$$\hat{R}_{CM}\,|\mathbf{r}_1\mathbf{r}_2\rangle = \frac{1}{N}\sum_{j=1}^{N}\hat{\mathbf{r}}_j\,|\mathbf{r}_1\mathbf{r}_2\rangle = \frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)\,|\mathbf{r}_1\mathbf{r}_2\rangle\,. \tag{44}$$

Alternatively, we can write R_{CM} as

$$R_{CM} = \frac{1}{N}\int d\mathbf{r}\;\mathbf{r}\sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}_j). \tag{45}$$

We recognize $\sum_j^N \delta(\mathbf{r}-\mathbf{r}_j)$ as the first quantized particle density operator. This suggests we can relate the action of an arbitrary operator to one that 'counts' the number of appearances of the expectation of that operator for a given set of quantum numbers.[8] As we have seen in the previous section, the first quantized particle density operator is given by the second quantized density operator $\hat{\psi}^\dagger(x)\hat{\psi}(x)$ (Eq.17). The center-of-mass operator is then

$$\hat{R}_{CM} = \frac{1}{\hat{N}}\int d\mathbf{r}\;\mathbf{r}\;\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) = \frac{1}{\hat{N}}\int d\mathbf{r}\;\mathbf{r}\;\hat{n}(\mathbf{r}) \tag{46}$$

[7] Note, this is a short hand notation for

$$\hat{R}_{CM} = \frac{1}{N}\left(\hat{\mathbf{r}}_j\otimes\hat{\mathbb{1}}\otimes\cdots\otimes\hat{\mathbb{1}} + \hat{\mathbb{1}}\otimes\hat{\mathbf{r}}_2\otimes\cdots\otimes\hat{\mathbb{1}}+\cdots\right)$$

[8] This reflects the fundamental meaning behind the second quantization, namely to keep track of the creation/annihilation of particles and the occupation of various states.

where the total number of particles $\hat{N}$ is $\int d\mathbf{r}\ \hat{\psi}^\dagger(x)\hat{\psi}(x)$. We can readily extend this to a general first quantized 1-particle operator

$$\hat{O}\left|\alpha_1,\ldots,\alpha_N\right\rangle = \sum_{i=1}^{N} O_{\alpha_i}\left|\alpha_1,\ldots,\alpha_N\right\rangle \tag{47}$$

to

$$\hat{O} = \sum_{i=1}^{N} O_{\alpha_i}\hat{n}_{\alpha_i} \tag{48}$$

or via a basis transformation from a discrete set of quantum numbers to the position-spin basis

$$\hat{O} = \int\int d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\left\langle\mathbf{r}|\hat{O}|\mathbf{r}'\right\rangle\hat{\psi}(\mathbf{r}'). \tag{49}$$

Table 1 lists several examples of 1-particle operators in first and second quantization.

Similarly, 2-particle operators can be translated from first to second quantization. We consider a general two body operator

$$\hat{U}\left|\alpha_1,\ldots,\alpha_N\right\rangle = \frac{1}{2}\sum_{i\neq j} U_{\alpha_i\alpha_j}\left|\alpha_1,\ldots,\alpha_N\right\rangle. \tag{50}$$

We know $\hat{n}_\beta = \sum_{i=1}^{N}\delta_{\beta,\alpha_i}$, so $\hat{n}_\beta\hat{n}_\gamma = \sum_{i=1}^{N}\sum_{j=1}^{N}\delta_{\beta,\alpha_i}\delta_{\gamma,\alpha_j}$, but this runs over i,j including $i=j$, which we need to exclude, i.e., $i\neq j$. To accomplish this we remove the $i=j$ term by subtracting it out $\hat{n}_\beta\hat{n}_\gamma - \delta_{\beta\gamma}\hat{n}_\beta$. Thus, we can convert the general first quantized 2-particle operator to second quantized form

$$\hat{U} = \frac{1}{2}\sum_{i,j=1} U_{ij}(\hat{n}_i\hat{n}_j - \delta_{ij}\hat{n}_i) \tag{51}$$

or via a basis transformation to the position-spin basis

$$\begin{aligned}
\hat{U} &= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' U(\mathbf{r},\mathbf{r}')\left(\hat{n}(\mathbf{r})\hat{n}(\mathbf{r}') - \delta(\mathbf{r},\mathbf{r}')\hat{n}(\mathbf{r})\right)\\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' U(\mathbf{r},\mathbf{r}')\left(\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}') - \delta(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right)\\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' U(\mathbf{r},\mathbf{r}')\left(\hat{\psi}^\dagger(\mathbf{r})\left[\delta(\mathbf{r},\mathbf{r}') \pm \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})\right]\hat{\psi}(\mathbf{r}') - \delta(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right)\\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' U(\mathbf{r},\mathbf{r}')\left(\pm\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}')\right)\\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')U(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})
\end{aligned} \tag{52}$$

Note the order of operators in the final line, this is missed in some texts and depends on convention. In summary the Hamiltonian in Eq. 1 may be written in second quantized form as

$$H = \int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\left(\frac{-\hbar^2\nabla^2}{2m}\right)\hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}). \tag{53}$$

Before closing out this section we consider a few examples of physical importance to exercise this new technique.

Observable	1^{st} Quantized	Field Operators	Momentum Basis
Particle Density at r	$\sum_i \delta(\mathbf{r}-\mathbf{r}_i)$	$\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$	$\sum_{\mathbf{pq}\sigma} \hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}+\mathbf{q}\sigma}e^{i\mathbf{q}\cdot\mathbf{r}}$
Total Number of particles	$N=\sum_i 1$	$\int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$	$\sum_{\mathbf{p}\sigma} \hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}\sigma}$
Charge Density at r	$e\sum_i \delta(\mathbf{r}-\mathbf{r}_i)$	$e\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$	$e\sum_{\mathbf{pq}\sigma} \hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}+\mathbf{q}\sigma}e^{i\mathbf{q}\cdot\mathbf{r}}$
Current Density at r	$\frac{e}{2m}\sum_i [\mathbf{p}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i]$	$\frac{-ie}{2m}\left[\hat{\psi}^\dagger(\mathbf{r})\nabla_{\mathbf{r}}\hat{\psi}(\mathbf{r}) - \left(\nabla_{\mathbf{r}}\hat{\psi}^\dagger(\mathbf{r})\right)\hat{\psi}(\mathbf{r})\right]$	$\frac{-ie}{2m}\sum_{\mathbf{pq}\sigma}(2\mathbf{p}+\mathbf{q}) \times \hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}+\mathbf{q}\sigma}e^{i\mathbf{q}\cdot\mathbf{r}}$
Kinetic Energy	$-\sum_i \frac{\hbar^2}{2m}\nabla^2$	$-\frac{1}{2m}\int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\nabla^2\hat{\psi}(\mathbf{r})$	$\sum_{\mathbf{p}\sigma}\frac{\hbar^2\mathbf{p}^2}{2m}\hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}\sigma}$
Potential energy in an external potential	$\sum_i V(\mathbf{r}_i)$	$\int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})V(\mathbf{r})\hat{\psi}(\mathbf{r})$	$\frac{1}{\mathcal{V}}\sum_{\mathbf{pq}\sigma}\hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}+\mathbf{q}\sigma} \times \int d\mathbf{r}\ V(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}$
Magnetic moment density at r	$\frac{g}{2}\sum_i \boldsymbol{\sigma}_i\delta(\mathbf{r}_i-\mathbf{r})$	$\frac{g}{2}\sum_{\alpha\beta}\hat{\psi}^\dagger_\alpha(\mathbf{r})\sigma_{\alpha\beta}\hat{\psi}_\beta(\mathbf{r})$	$\frac{g}{2}\sum_{\mathbf{pq}\alpha\beta}\hat{a}^\dagger_{\mathbf{p}\alpha}\hat{a}_{\mathbf{p}+\mathbf{q}\beta} \times \sigma_{\alpha\beta}e^{i\mathbf{q}\cdot\mathbf{r}}$
Total magnetic moment	$\frac{g}{2}\sum_i \boldsymbol{\sigma}_i$	$\frac{g}{2}\sum_{\alpha\beta i}\int d\mathbf{r}\ \hat{\psi}^\dagger_\alpha(\mathbf{r})\sigma^i_{\alpha\beta}\hat{\psi}_\beta(\mathbf{r})$	$\frac{g}{2}\sum_{\mathbf{pq}\alpha\beta i}\hat{a}^\dagger_{\mathbf{p}\alpha}\sigma^i_{\alpha\beta}\hat{a}_{\mathbf{p}+\mathbf{q}\beta}$

Table 1: Correspondence of single-particle operators in the coordinate and occupation number representation.

Example 6. What is the amplitude for removing a particle at $\mathbf{r}'$ with spin σ from the ground state of a Fermi gas and return to the ground state by replacing a particle with spin σ at point $\mathbf{r}$?

The ground state of a Fermi gas $|\Phi_0\rangle$ is characterized by all the momentum states being filled up to some momentum p_F, the Fermi momentum. In second quantized notation this is given by

$$|\Phi_0\rangle = \Pi_{|\mathbf{p}|\leq p_F,\sigma}\ \hat{a}^\dagger_{\mathbf{p}\sigma}\,|0\rangle\,. \tag{54}$$

Now the amplitude $G_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')$ we wish to evaluate may be written as:

$$G_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') \equiv \langle\Phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r}')|\Phi_0\rangle \tag{55}$$

where the annihilation operator first acts on the ground state at $\mathbf{r}'$ with spin σ followed by a creation operator at $\mathbf{r}$ with spin σ. To move forward we must convert from field operators in position-spin space to those in momentum-spin space in

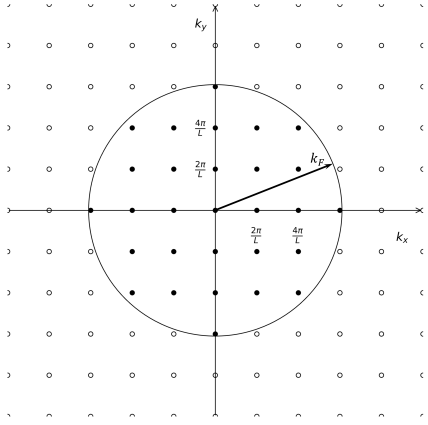


Figure 2
Fermi sphere with radius k_F in momentum space. Each volume element of size $(2\pi)^3/V$ contains two states which, inside the Fermi sphere at T=0, are occupied by electrons with opposite spin.

order to act on $|\Phi_0\rangle$. We define

$$\hat{\psi}_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}\hat{a}_{\mathbf{p}\sigma}, \quad \hat{\psi}^\dagger_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{r}}\hat{a}^\dagger_{\mathbf{p}\sigma}. \tag{56}$$

where we recognized $\langle\mathbf{r}|\mathbf{p}\rangle$ as the Fourier elements $e^{i\mathbf{p}\cdot\mathbf{r}}$. Here we have chosen to normalize the Fourier elements following box, or cavity, normalization. For this we assume the gas occupies a fixed volume V, a cube with sides L_x, L_y, and L_z. We then employ the Born-von Karman periodic boundary conditions, i.e., $\hat{\psi}_\sigma(\mathbf{r}+L_i) = \hat{\psi}_\sigma(\mathbf{r})$, which yields discreet momentum states $p_i = 2\pi n_i/L_i$ for $n_i \in \mathbb{Z}$, analogous to the solutions of the Schrödinger equation for a particle in a box. From this we see that we can represent the momentum vectors by a point lattice in a momentum space. Every momentum point in such a lattice has two one-particle states with opposite spins associated with it, see Fig. 2. [9] The creation (annihilation) operations $\hat{a}^\dagger_{\mathbf{p}\sigma}(\hat{a}_{\mathbf{p}\sigma})$ satisfying the (anti)commutation relation

$$\left[\hat{a}_{\mathbf{p}'\sigma'}, \hat{a}^\dagger_{\mathbf{p}\sigma}\right]_\mp = \delta_{\mathbf{p}'\mathbf{p}}\delta_{\sigma'\sigma}, \quad \left[\hat{a}_{\mathbf{p}'\sigma'}, \hat{a}_{\mathbf{p}\sigma}\right]_\mp = \left[\hat{a}^\dagger_{\mathbf{p}'\sigma'}, \hat{a}^\dagger_{\mathbf{p}\sigma}\right]_\mp = 0. \tag{63}$$

Upon substituting Eq. 56 into Eq. 55 we find

$$\frac{1}{\sqrt{V}}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{r}}\frac{1}{\sqrt{V}}\sum_{\mathbf{p}'} e^{i\mathbf{p}'\cdot\mathbf{r}'}\,\langle\Phi_0|\hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}'\sigma'}|\Phi_0\rangle\,. \tag{64}$$

Intuitively, $\hat{a}_{\mathbf{p}'}$ removes a particle with momentum $\mathbf{p}'$ from the Fermi sea, which is only possible if $|\mathbf{p}'| \leq p_F$, and $\hat{a}^\dagger_{\mathbf{p}}$ needs to replace this particle otherwise the resulting state is orthogonal to $\langle\Phi_0|$. We now demonstrate that our intuition is indeed correct by calculating the overlap explicitly,

$$\begin{aligned}
&\langle\Phi_0|\hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}'\sigma'}|\Phi_0\rangle \\
&= \langle\Phi_0|\,\hat{a}^\dagger_{\mathbf{p}\sigma}\left(\theta(p_F-|\mathbf{p}'|)\sum_k^N(-1)^{N+k}\delta_{\mathbf{p}'\mathbf{p}_k}\delta_{\sigma'\sigma_k}\,|\mathbf{p}_1,\ldots,\mathbf{p}_{k-1},\mathbf{p}_{k+1},\ldots,\mathbf{p}_N\rangle\right) \\
&= \theta(p_F-|\mathbf{p}'|)\sum_k^N(-1)^{N+k}\delta_{\mathbf{p}'\mathbf{p}_k}\delta_{\sigma'\sigma_k}\,\langle\Phi_0|\mathbf{p}_1,\ldots,\mathbf{p}_{k-1},\mathbf{p}_{k+1},\ldots,\mathbf{p}_N,\mathbf{p}\rangle \\
&= \theta(p_F-|\mathbf{p}'|)\sum_k^N(-1)^{N+k}\delta_{\mathbf{p}'\mathbf{p}_k}\delta_{\sigma'\sigma_k}\sum_P(-1)^P\delta_{\mathbf{p}_i\mathbf{p}_{P_i}}\cdots\delta_{\mathbf{p}_N\mathbf{p}_{P_i}}
\end{aligned}$$

where P take permutations of the ordering $\mathbf{p}_1,\ldots,\mathbf{p}_{k-1},\mathbf{p}_{k+1},\ldots,\mathbf{p}_N,\mathbf{p}$. The only permutation that survives is where $\mathbf{p}_1,\ldots,\mathbf{p}_{k-1},\mathbf{p},\mathbf{p}_{k+1},\ldots,\mathbf{p}_N$ on the condition that $\delta_{\mathbf{p}\mathbf{p}_k}$, giving

$$\begin{aligned}
\langle\Phi_0|\hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}'\sigma'}|\Phi_0\rangle &= \theta(p_F-|\mathbf{p}'|)\sum_k^N(-1)^{N+k}\delta_{\mathbf{p}'\mathbf{p}_k}\delta_{\sigma\sigma_k}(-1)^{N-k}\delta_{\mathbf{p}\mathbf{p}_k} \\
&= \theta(p_F-|\mathbf{p}'|)\sum_k^N\delta_{\mathbf{p}'\mathbf{p}_k}\delta_{\sigma'\sigma_k}\delta_{\mathbf{p}\mathbf{p}_k}\delta_{\sigma\sigma_k} \\
&= \theta(p_F-|\mathbf{p}'|)\delta_{\mathbf{p}'\mathbf{p}}\delta_{\sigma'\sigma}
\end{aligned} \tag{65}$$

[9] When considering momentum space there are two conventions used depending on the physical situation at hand. The first is box normalization (Eq. 56) and the second is continuum normalization. Here, the volume of the box $V \to \infty$ resulting in continuum momentum states, e.g., free particle solutions of the Schrödinger equation. This means, $\langle\mathbf{p}|\mathbf{p}'\rangle = (2\pi)^3\delta(\mathbf{p}-\mathbf{p}')$ and $\langle\mathbf{p}|\mathbf{r}\rangle = e^{-i\mathbf{p}\cdot\mathbf{r}}$ with

$$\hat{\psi}_\sigma(\mathbf{r}) = \int\frac{d\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot\mathbf{r}}\hat{a}_{\mathbf{p}\sigma}, \tag{57}$$

$$\hat{\psi}^\dagger_\sigma(\mathbf{r}) = \int\frac{d\mathbf{p}}{(2\pi)^3}e^{-i\mathbf{p}\cdot\mathbf{r}}\hat{a}^\dagger_{\mathbf{p}\sigma}. \tag{58}$$

and the creation (annihilation) operations $\hat{a}^\dagger_{\mathbf{p}\sigma}(\hat{a}_{\mathbf{p}\sigma})$ satisfying the (anti)commutation relation

$$\left[\hat{a}_{\mathbf{p}'\sigma'}, \hat{a}^\dagger_{\mathbf{p}\sigma}\right] = (2\pi)^3\delta(\mathbf{p}'-\mathbf{p})\delta_{\sigma'\sigma}, \tag{59}$$

$$\left[\hat{a}_{\mathbf{p}'\sigma'}, \hat{a}_{\mathbf{p}\sigma}\right]_\mp = \left[\hat{a}^\dagger_{\mathbf{p}'\sigma'}, \hat{a}^\dagger_{\mathbf{p}\sigma}\right]_\mp = 0. \tag{60}$$

One can directly convert between box normalized form –a sum over discrete momentum states– and continuum normalization –an integral over a continuum of momentum states– through the Riemann sum. That is, if we let L be the dimension of the box, with L^3 being the volume of the box, then we can rewrite the sum over states of a function $f(\mathbf{p})$ as:

$$\begin{aligned}
\sum_{\mathbf{p}} f(\mathbf{p}) &= \frac{L^3}{(2\pi)^3}\sum_{\mathbf{p}} f(\mathbf{p})\frac{(2\pi)^3}{L^3} \\
&= \frac{V}{(2\pi)^3}\sum_{\mathbf{p}} f(\mathbf{p})\Delta\mathbf{p}.
\end{aligned} \tag{61}$$

Now, if we take $V \to \infty$ then $\Delta\mathbf{p} \to 0$, which yields the definition of the Riemann integral:

$$\lim_{V\to\infty}\frac{1}{V}\sum_{\mathbf{p}} f(\mathbf{p}) = \frac{1}{(2\pi)^3}\int d\mathbf{p}\, f(\mathbf{p}). \tag{62}$$

Therefore, one can swap an integral for a sum over states and vise versa, with the appropriate normalization factors, to go between the two conventions. Depending on the problem, one convention maybe more convenient then the other.

In summary,

$$\langle\Phi_0|\hat{a}^\dagger_{\mathbf{p}\sigma}\hat{a}_{\mathbf{p}'\sigma'}|\Phi_0\rangle \begin{cases} \delta_{\mathbf{p}'\mathbf{p}}\delta_{\sigma'\sigma}, & \text{if } |\mathbf{p}'| \leq p_F \\ 0, & \text{otherwise} \end{cases} \tag{66}$$

in agreement with our intuition. The amplitude $G_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')$ now amounts to the Fourier transform of the radial box function

$$\begin{aligned}
&\delta_{\sigma'\sigma}\frac{1}{V}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\theta(p_F-|\mathbf{p}|) \\
&= \frac{\delta_{\sigma'\sigma}}{(2\pi)^3}\int d\mathbf{p} e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\theta(p_F-|\mathbf{p}|) \\
&= \frac{\delta_{\sigma'\sigma}}{(2\pi)^3}\int_0^\infty dp\ p^2\theta(p_F-|\mathbf{p}|)\int_0^{2\pi}d\varphi\int_{-1}^{+1} d\cos(\theta)\ e^{-ip|\mathbf{r}-\mathbf{r}'|\cos(\theta)} \\
&= \frac{\delta_{\sigma'\sigma}}{(2\pi)^2}\int_0^{p_F} dp\ p^2\left[\frac{e^{-ip|\mathbf{r}-\mathbf{r}'|\cos(\theta)}}{-ip|\mathbf{r}-\mathbf{r}'|}\right]\Bigg|_{-1}^{+1} \\
&= \frac{\delta_{\sigma'\sigma}}{(2\pi)^2}\int_0^{p_F} dp\ p^2\frac{-2i\sin(p|\mathbf{r}-\mathbf{r}'|)}{-ip|\mathbf{r}-\mathbf{r}'|} \\
&= \frac{2\delta_{\sigma'\sigma}}{(2\pi)^2}\int_0^{p_F} dp\ p^2\frac{\sin(p|\mathbf{r}-\mathbf{r}'|)}{p|\mathbf{r}-\mathbf{r}'|} \\
&= \frac{2\delta_{\sigma'\sigma}}{(2\pi)^2}\int_0^{x_F}\frac{dx}{|\mathbf{r}-\mathbf{r}'|}\left(\frac{x}{|\mathbf{r}-\mathbf{r}'|}\right)^2\frac{\sin(x)}{x} \\
&= \frac{2\delta_{\sigma'\sigma}}{(2\pi)^2|\mathbf{r}-\mathbf{r}'|^3}\int_0^{x_F} dx\ x\sin(x) \\
&= \frac{2\delta_{\sigma'\sigma}}{(2\pi)^2|\mathbf{r}-\mathbf{r}'|^3}\left[(-x\cos(x))|_0^{x_F}\int_0^{x_F} dx\ \cos(x)\right] \\
&= \delta_{\sigma'\sigma}\frac{p_F^3}{2\pi^2}\frac{\sin(x_F)-x_F\cos(x_F)}{x_F^3} \\
&= \delta_{\sigma'\sigma}\frac{p_F^3}{2\pi^2}\frac{j_1(x_F)}{x_F}
\end{aligned} \tag{67}$$

where j_1 is the spherical Bessel function of the first kind. The results yield a sinc-like oscillations that decay as $1/p_F^{3/2}$ and where the width of the transform is inversely proportional to the separation $|\mathbf{r}-\mathbf{r}'|$.[10] Notably, the existence of a Fermi surface (finite p_F) implies the integration over momentum states is truncated, forming an incomplete set of plane-waves. So, only in the limit of $p_F \to \infty$, $G_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')$ becomes localized at $\mathbf{r}=\mathbf{r}'$. Since,

$$N = 2\sum_{|\mathbf{p}|<p_F} 1 = \frac{2V}{(2\pi)^3}\int_0^{p_F} d\mathbf{p} = \frac{2V}{(2\pi)^3}\left(\frac{4}{3}\pi p_F^3\right) \tag{68}$$

the Fermi momentum is $p_F^3 = 3\pi^2\frac{N}{V} = 3\pi^2 n$ we can write

$$G_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') = \delta_{\sigma'\sigma}\frac{3n}{2}\frac{\sin(x_F)-x_F\cos(x_F)}{x_F^3} \equiv \delta_{\sigma'\sigma}\frac{3n}{2}\frac{j_1(x_F)}{x_F}. \tag{69}$$

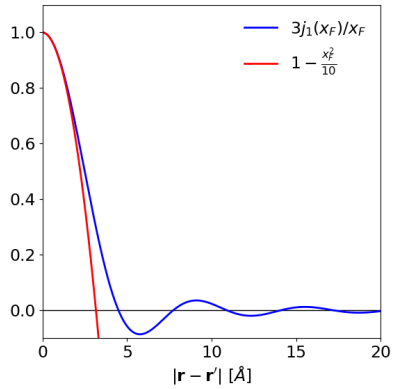


Figure 3
Plot of $\frac{3j_1(x_F)}{x_F}$ (red) and $\left(1-\frac{x_F^2}{10}\right)$ (blue) for free electron number density of copper $n = 8.47\times10^{-2}$ Å^{-3}.

[10] In 1D, the Fourier transform of the box function gives $\mathrm{sinc}(x) = \frac{sin(x)}{x}$, which is equivalent to the zeroth-order spherical Bessel function of the first kind $j_0(x)$.

Clearly for $\mathbf{r} = \mathbf{r}'$, $G_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') = \delta_{\sigma'\sigma}\frac{n}{2}$ and more generally for small separations

$$G_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') \approx \delta_{\sigma'\sigma}\frac{n}{2}\left(1 - \frac{x_F^2}{10}\right). \tag{70}$$

Exercise 7. What is the amplitude for removing a particle at $\mathbf{r}$ with spin σ and from $\mathbf{r}'$ with spin σ' from the ground state of a Fermi gas and return to the ground state by replacing a particle with spin σ' at point $\mathbf{r}'$ and another spin σ at point $\mathbf{r}$?

Namely, show that the pair correlation function is related to the one-particle density matrix according to:

$$\langle\Phi_0|\hat{\psi}_\sigma^\dagger(\mathbf{r})\hat{\psi}_{\sigma'}^\dagger(\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r})|\Phi_0\rangle = \begin{cases} \left(\frac{n}{2}\right)^2 & \sigma' \neq \sigma \\ \left(\frac{n}{2}\right)^2 - G_\sigma^2(\mathbf{r} - \mathbf{r}') & \sigma' = \sigma \end{cases} \tag{71}$$

and interpret the result.

Quantum Dynamical Pictures

In the previous section we have seen how we can transform the Hamiltonian and various one- and two-particle operators from first to second quantization representations along with rotating between varying bases, e.g., energy, momentum, position, and so on. However all of this has been applied for a given instance in time t. To be able to go beyond simple perturbation theory techniques and describe the interacting many-particle system, we need to address how the system evolves in time. We will find in the following there are three 'pictures' to address this issue.

Schrödinger Picture

The time evolution of the state vector $|\Psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle. \tag{72}$$

with the state vector $|\Psi(t)\rangle$ of the system at time t. The Schrödinger equation is a first-order differential equation in time, and therefore, $|\Psi(t)\rangle$ is uniquely determined once the initial state $|\Psi(t_0)\rangle$ is given. We note that the Hamiltonian can depend on time, as shown, or be time independent so that $\hat{H}(t) = \hat{H}(t_0)$ for all t. Since $|\Psi(t)\rangle$ is normalized $\langle\Psi(t)|\Psi(t)\rangle = 1$ and conserves probability, i.e. preseveres the norm of the states $\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(t_0)|\Psi(t_0)\rangle$, $|\Psi(t)\rangle$ must evolve via an unitary transformation. We can introduce the time evolution operator

$$|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi(t_0)\rangle. \tag{73}$$

that connects state vectors at different times and provides a complete description of the evolution system from t_0 to t. This object amazingly encapsulates the quantum dynamics of the system in a compact manner.

Substituting Eq. 73 into the Schrödinger equation gives the equation of motion for the evolution operator

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0), \quad \hat{U}(t,t_0) = \mathbb{1}. \tag{74}$$

with $\mathbb{1}$ the identity operator. This differential equation together with the initial condition at t_0 uniquely determines $\hat{U}(t,t_0)$. Integrating both sides on the interval t and t_0

$$\hat{U}(t,t_0) = \hat{U}(t_0,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\ \hat{H}(t_1)\hat{U}(t_1,t_0). \tag{75}$$

This integral equation contains the same information as Eq. 74, and is automatically endowed with the boundary information. If $\hat{U}$ was a c-number this would be a Voltera integral equation. With this spirit, we solve using Picard iteration:

$$\begin{aligned}
\hat{U}(t,t_0) &= \hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\ \hat{H}(t_1)\left(\hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t_1} dt_2\ \hat{H}(t_2)\hat{U}(t_2,t_0)\right) \\
&= \hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\ \hat{H}(t_1) + \left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\ \hat{H}(t_1)\hat{H}(t_2)\hat{U}(t_2,t_0) \\
&\ \ \vdots \\
&= \sum_k^{\infty}\left(-\frac{i}{\hbar}\right)^k\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\cdots\int_{t_0}^{t_{k-1}} dt_k\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_k)
\end{aligned} \tag{76}$$

We seemingly just made our life more complicated.

To gain insight into the behavior of this expression let us examine the 2nd order term

$$\left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\hat{H}(t_1)\hat{H}(t_2). \tag{77}$$

The domain of the double integral is $\{(t_1,t_2)|\ t_0 < t_1 < t\ ,\ t_0 < t_2 < t_1\ \}$, in other words the domain of t_2 is bounded by t_1 covering the lower triangle in the t_1-t_2 plane. Equivalently, we can switch the order of integration and associated bounds such that the integration domain is $\{(t_1,t_2)|\ t_2 < t_1 < t\ ,\ t_0 < t_2 < t\ \}$, yielding

$$\left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt_2\int_{t_2}^{t} dt_1\hat{H}(t_1)\hat{H}(t_2). \tag{78}$$

Now, we relabel dummy indices swapping $t_1 \leftrightarrow t_2$

$$\left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt_1\int_{t_1}^{t} dt_2\hat{H}(t_2)\hat{H}(t_1) \tag{79}$$

with an integration domain of $\{(t_1,t_2)|\ t_0 < t_1 < t\ ,\ t_1 < t_2 < t\ \}$ covering the upper triangle in the t_1-t_2 plane. Finally, the second order term (Eq. 77) may be written as

$$\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\hat{H}(t_1)\hat{H}(t_2) = \frac{1}{2}\left(\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\hat{H}(t_1)\hat{H}(t_2) + \int_{t_0}^{t} dt_1\int_{t_1}^{t} dt_2\hat{H}(t_2)\hat{H}(t_1)\right)$$

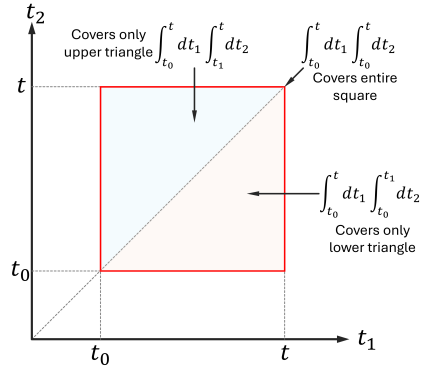


Figure 4
Integration domains of the various terms in Eq. 80.

$$= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \left(\hat{H}(t_1)\hat{H}(t_2)\theta(t_1-t_2) + \hat{H}(t_2)\hat{H}(t_1)\theta(t_2-t_1)\right) \tag{80}$$

where the step function is essential because the operators $\hat{H}(t_k)$ do not necessarily commute at different times. Figure 4 illustrates the integration domain. This expression has the characteristic feature that the operator containing the latest time stands farthest to the left. We call this the *time-ordered product of operators*, denoted by $\mathcal{T}$. In light of this, we rewrite this repression as

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \hat{H}(t_1)\hat{H}(t_2) = \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \mathcal{T}\left[\hat{H}(t_1)\hat{H}(t_2)\right]. \tag{81}$$

This result readily generalizes, and the resulting expression for the time evolution operator becomes

$$\begin{aligned}\hat{U}(t,t_0) &= \sum_{k}^{\infty}\left(-\frac{i}{\hbar}\right)^k \frac{1}{k!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_k \, \mathcal{T}\left[\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_k)\right] \\ &= \mathcal{T}\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\bar{t}\ \hat{H}(\bar{t})}\right].\end{aligned} \tag{82}$$

With the last line being a formal expression of the infinite sum. If the Hamiltonian is independent of time Eq. 82 reduces to

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t_0)(t-t_0)}. \tag{83}$$

A defining feature of this picture is that the state vector carries the time dependence of the state while the operators are time independent.[11]

[11] This is more of a statement about the time dependence of the state vector and does not preclude operators that contain time dependence intrinsically.

Heisenberg Picture

We will now go from the Schrödinger to Heisenberg pictures. This picture greatly simplifies the analysis of correlation functions and is used throughput the literature and textbooks. In this picture the entire dynamics is contained in the operators, with static state vectors and equivalent to those in the Schrödinger picture at some time t_a.

To make this concrete, we start with the expectation value of a generic operator $\hat{O}$

$$\langle\Psi(t)|\hat{O}|\Psi(t)\rangle = \langle\Psi(t)|U(t,t_a)U(t_a,t)\hat{O}U(t,t_a)U(t_a,t)|\Psi(t)\rangle \tag{84}$$

where we have inserted pairs of time-evolution operators that propagate the system from t to t_a and back to t, which leaves the state unchanged, or equivalently $U(t,t_a)U(t_a,t) = \hat{\mathbb{1}}$. In general $\hat{U}$ and $\hat{O}$ do not commute and are a very complicated objects. We now define the Heisenberg state vector

$$|\Psi_H\rangle \equiv U(t_a,t)\,|\Psi(t)\rangle \tag{85}$$

and the operator in the Heisenberg representation

$$\hat{O}_H(t) \equiv U(t_a,t)\hat{O}U(t,t_a). \tag{86}$$

We note that the operator has now picked up an effective time dependence via the time-evolution operators and the state vector is evaluated at time t_a for all t.

We now ask how the state vector and the operators in the Heisenberg representation evolve with time. Firstly, the state vector follows

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left|\Psi_H(t_a)\right\rangle &= i\hbar\frac{\partial}{\partial t}\left(U(t_a,t)\left|\Psi(t)\right\rangle\right) \\ &= i\hbar\left(\frac{\partial}{\partial t}U(t_a,t)\right)\left|\Psi(t)\right\rangle + i\hbar U(t_a,t)\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle \\ &= \left(-U(t_a,t)\hat{H}(t) + U(t_a,t)\hat{H}(t)\right)\left|\Psi(t)\right\rangle \\ &= 0 \end{aligned} \tag{87}$$

where we used the adjoint of the schrödinger equation

$$-i\hbar\frac{\partial}{\partial t}\hat{U}^\dagger(t_a,t) = \hat{U}^\dagger(t_a,t)\hat{H}(t_a) \tag{88}$$

and the property $\hat{U}^\dagger(t_a,t) = \hat{U}(t,t_a)$ to get second to last line. The state vector is a constant for all t. Now, the operator obeys

Exercise 8. Prove $\hat{U}^\dagger(t_a,t) = \hat{U}(t,t_a)$.

$$\begin{aligned} &i\hbar\frac{\partial}{\partial t}\hat{O}_H(t) = i\hbar\frac{\partial}{\partial t}\left(U(t_a,t)\hat{O}U(t,t_a)\right) \\ &= i\hbar\left(\frac{\partial}{\partial t}U(t_a,t)\right)\hat{O}U(t,t_a) + i\hbar U^\dagger(t_a,t)\left(\frac{\partial}{\partial t}\hat{O}\right)U(t,t_a) + i\hbar U^\dagger(t_a,t)\hat{O}\frac{\partial}{\partial t}U(t,t_a) \\ &= \left(-U(t_a,t)\hat{H}(t)\right)\hat{O}U(t,t_a) + i\hbar U(t_a,t)\left(\frac{\partial}{\partial t}\hat{O}\right)U(t,t_a) + U(t_a,t)\hat{O}\hat{H}(t)U(t,t_a) \\ &= -U(t_a,t)\hat{H}(t)U(t,t_a)U(t_a,t)\hat{O}U(t,t_a) + i\hbar U(t_a,t)\frac{\partial}{\partial t}\hat{O}U(t,t_a) \\ &\quad + U(t_a,t)\hat{O}U(t,t_a)U(t_a,t)\hat{H}(t)U(t,t_a) \\ &= \hat{O}_H(t)\hat{H}_H(t) - \hat{H}_H(t)\hat{O}_H(t) + i\hbar U(t_a,t)\frac{\partial}{\partial t}\hat{O}U(t,t_a) \\ &= \left[\hat{O}_H(t),\hat{H}_H(t)\right]_- + i\hbar\left(\frac{\partial}{\partial t}\hat{O}\right)_H \end{aligned} \tag{89}$$

the Heisenberg equation of motion which resembles the classical equation of motion with the Poisson bracket. Operators in the Heisenberg representation contain the full time evolution of the problem.

Dirac (Interaction) Picture

The Schrödinger and Heisenberg representations are excellent if the problem at hand is solvable. However, for cases where we can't outright solve the Hamiltonian we must resort to the Dirac representation. The Dirac representation is suitable for problems where the Hamiltonian $\hat{H}$ may be partitioned into a solvable part $\hat{H}_0$ and unsolvable terms $\hat{V}$,

$$\hat{H} = \hat{H}_0 + \hat{V}. \tag{90}$$

Typically, $\hat{H}_0$ is time-independent and/or non-interacting, where as $\hat{V}$ carries the time-dependence and/or the interactions between particles in the system.

We define the Dirac picture via the same expectation value of a generic operator $\hat{O}$, as with the previous pictures,

$$\langle \Psi(t)|\hat{O}|\Psi(t)\rangle = \langle \Psi(t)|e^{-\frac{i}{\hbar}\hat{H}_0 t}e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t}e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle \tag{91}$$

however, instead of inserting pairs of time-evolution operators with respect to $\hat{H}$ that propagate the system from t to t_a and back to t, we have inserted unitary transformations of the Schrödinger state vector at time t allowing us to define the Dirac state vector

$$|\Psi_I(t)\rangle \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle \tag{92}$$

and the operator in the Dirac representation

$$\hat{O}_I(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t}. \tag{93}$$

Furthermore, the time evolution operator can be identified in the Dirac picture via

$$\begin{aligned}|\Psi_I(t)\rangle &= e^{\frac{i}{\hbar}\hat{H}_0 t}U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}e^{\frac{i}{\hbar}\hat{H}_0 t_0}|\Psi(t_0)\rangle \\ &= U_I(t,t_0)|\Psi_I(t_0)\rangle\end{aligned} \tag{94}$$

and defined as

$$U_I(t,t_0) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}. \tag{95}$$

The equation of motion of the state vector obeys a Schröding-like equation

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle &= i\hbar\frac{\partial}{\partial t}\left(e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle\right) \\ &= i\hbar\left(\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\right)|\Psi(t)\rangle + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\frac{\partial}{\partial t}|\Psi(t)\rangle \\ &= -e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0|\Psi(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}|\Psi(t)\rangle \\ &= e^{\frac{i}{\hbar}\hat{H}_0 t}\left(\hat{H}-\hat{H}_0\right)|\Psi(t)\rangle \\ &= \hat{V}_I|\Psi_I(t)\rangle\end{aligned} \tag{96}$$

and operator takes the form of the Heisenberg equation of motion

$$\begin{aligned}&i\hbar\frac{\partial}{\partial t}\hat{O}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t} \\ &= i\hbar\left(\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\right)\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t} + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\left(\frac{\partial}{\partial t}\hat{O}\right)e^{-\frac{i}{\hbar}\hat{H}_0 t} + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}\frac{\partial}{\partial t}e^{-\frac{i}{\hbar}\hat{H}_0 t} \\ &= -e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t} + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\left(\frac{\partial}{\partial t}\hat{O}\right)e^{-\frac{i}{\hbar}\hat{H}_0 t} + e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0 \\ &= \hat{O}_I(t)\hat{H}_{0I}(t) - \hat{H}_{0I}(t)\hat{O}_I(t) + i\hbar\left(\frac{\partial}{\partial t}\hat{O}\right)_I \\ &= \left[\hat{O}_I(t),\hat{H}_{0I}(t)\right]_- + i\hbar\left(\frac{\partial}{\partial t}\hat{O}\right)_I\end{aligned} \tag{97}$$

in the Dirac picture. A complete description of the problem can be obtained from knowledge of the time evolution operator $U_I(t, t_0)$, which follows

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}U_I(t,t_0) &= i\hbar\frac{\partial}{\partial t}\left(e^{\frac{i}{\hbar}\hat{H}_0 t}U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}\right)\\
&= i\hbar\frac{\partial}{\partial t}\left(e^{\frac{i}{\hbar}\hat{H}_0 t}U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}\right)\\
&= i\hbar\left(\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\right)U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0} + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\left(\frac{\partial}{\partial t}U(t,t_0)\right)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}\\
&= -e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0 U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0} + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}(t)U(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}\\
&= \left(\hat{H}_I(t) - \hat{H}_{0I}\right)U_I(t,t_0)\\
&= V_I(t)U_I(t,t_0).
\end{aligned} \tag{98}$$

Following the procedure for the Schröding time evolution operator the solution can be written formally as

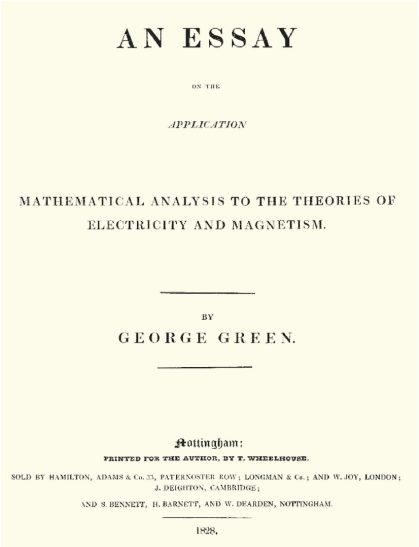
$$\hat{U}_I(t,t_0) = \mathcal{T}\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\bar{t}\ \hat{V}_I(\bar{t})}\right]. \tag{99}$$

This picture lies somewhere in between the Schrödinger and the Heisenberg pictures with both the state vector and the operators carrying time-dependence. The power of this picture lies in the fact the it isolates $\hat{V}$ and allows us to treat it via perturbation expansions.

Green's Functions

Whether a system has a few or very many degrees of freedom the wave function, or density matrix, becomes a complex unwieldy object. For many years the wave function and density matrix were discussed as if these detailed infinity complicated functions of infinitely many variables really mattered. However, it was clear to those who measured or calculated physical properties of large interacting systems that it is futile to measure complicated correlations between many physical observables. Since the 1950s, Green's function methods of quantum field theory have become generally recognized as a powerful mathematical technique for studying complex interacting systems of condensed matter physics. Like wave functions these Green's functions, or field correlation functions more generally, contain the information necessary to explain observations, but in contrast to wave functions they carry very little surplus information then is needed. Although the description is economical it can be both sophisticated and complicated. When correlation functions were introduced to describe the properties of interacting systems they were viewed as formal devices and treated with some suspicion due to difficult calculation techniques and poorly understood experiential physical content. By now, correlation function have been universally adopted and are a natural tool and indispensable for discussing problems in condensed matter physics.[12,13]

In this section, we will develop the Green's function for large interacting systems by first reminding ourselves of its origin in classical physics, then move to the quantum world. By examining the Green's function for the Schrödinger equation we


AN ESSAY

ON THE

APPLICATION

MATHEMATICAL ANALYSIS TO THE THEORIES OF ELECTRICITY AND MAGNETISM.

BY

GEORGE GREEN.

Nottingham:
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AND S. BENNETT, H. BARNETT, AND W. DEARDEN, NOTTINGHAM.
1828.

Figure 5
The title page to Green's original treaties: *An Essay on the Application of Mathematical Analysis to the Theories of Electricity and Magnetism*, notably including what is now universally called Green's Theorem.

[12] Paul C. Martin. *Measurements and correlation functions*. CRC Press, 1968

[13] Gerald Rickayzen. *Green's functions and condensed matter*. Courier Corporation, 2013

will gain intuition to firmly define the many-particle Green's functions. Their equations of motion will suggest methods of approximation which are not solely based on a small interaction parameter and describe the properties of particle excitations in many-body systems as renormalized version of their bare independent particle counterparts yielding *quasi-particles* of finite lifetimes. Finally, we will derive and explore the set of self-consistent equations introduced by Lars Hedin[14,15] to treat the many-body electron system, along with a few typical approximations.

[14] Lars Hedin. New method for calculating the one-particle green's function with application to the electron-gas problem. *Physical Review*, 139(3A):A796, 1965

[15] JJ Rehr. Lars hedin and the quest for a theory of excited states. *Physica Scripta*, 2005(T115):19–23, 2005

George Green—Mathematician, Physicist, and Miller

George Green (14 July 1793-31 May 1841) was a British mathematician, physicist, and miller from Nottingham England–the home of Robin Hood– who made contributions to optics, acoustics, and hydrodynamics, and most famously wrote *An Essay on the Applications of Mathematical Analysis to the Theories of Electricity and Magnetism*[16,17]. This essay introduced several important concepts and techniques, among them the idea of potential functions currently used in physics, a theorem similar to the modern *Green's theorem*, and the concept of what are now called *Green's functions*.

Importantly Green's life stands as a testament to the fact that scientific contributions can come from from anyone at anytime and anywhere. As Julian Schwinger said during his lecture at University of Nottingham in 1993:

> The young theoretical physicists of a generation or two earlier subscribed to the belief that: If you haven't done something important by age 30, you never will. Obviously, they were unfamiliar with the history of George Green, the miller of Nottingham.[18]

[16] George Green. *An essay on the application of mathematical analysis to the theories of electricity and magnetism*. Printed for the author, by T. Wheelhouse., Nottingham, 1828

[17] Lawrie Challis. The Green of Green functions. *Physics Today*, 56(12):41–46, 2003

[18] Julian Schwinger. The greening of quantum field theory: George and I. In *Julian Schwinger: The Physicist, the Teacher, and the Man*, pages 13–27. World Scientific, 1996

The remarkable feats of Green originate from humble beginnings. As the son of a baker he only received $\sim$ 18 months of formal education, much of which was before the age of 9. He was then sent by his father to the local mill to learn to be a miller. While at the mill, he fell in love with Jane Smith, the miller's daughter, whom Green's father forbid him to marry. Although Green and Jane never married, the couple had seven children together. The youngest child was born 13 months before Green's death. In the meantime, he self-studied in mathematics and physics–it is unclear to historians exactly where Green obtained information on current developments in mathematics as Nottingham had little intellectual resources–, when in 1828, at age 35 he published his now famous Essay. At the age of 40 Green matriculated at Cambridge in 1833 and graduated with a BA in 1838 as a 4th Wrangler in the Mathematical Tripos. After just two and a half years academic life and activities, Green fell ill with influenza and returned to Nottingham where he died on 31 May of 1841. George Green and Jane were buried in St Stephen's Church, a few hundred yards from the Mill. In 1986, Green's mill was restored to working order. It now serves both as a working example of a 19th century mill and as a museum and science center dedicated to George Green. [19]

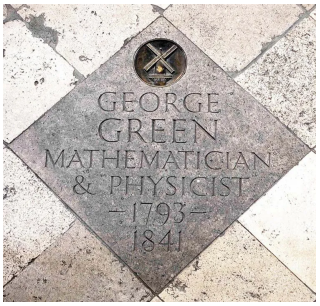

Figure 6
George Green memorial in the nave of Westminster Abbey with the inscription: George Green Mathematician & Physicist 1793-1841. Note the inlay in bronze showing the windmill in Nottingham.

[19] Lawrie Challis. The Green of Green functions. *Physics Today*, 56(12):41–46, 2003

During his lifetime Green's work was not well-known in the mathematical community. In 1846, Green's work was rediscovered by Lord Kelvin (William Thomson), who popularized it for future mathematicians and physicists. His work has gone on to inspire Lord Kelvin, George Stokes, Lord Rayleigh, James Clerk Maxwell, Horace

Lamb, J. J. Thomson, Larmor and Augustus Love, to name very few. Today, George Green's analysis has found applications in areas ranging from classical electrostatics to modern quantum field theory. In recognition of his work a memorial stone was unveiled in the nave of Westminster Abbey in July 1993, adjoining the graves of Sir Isaac Newton and Lord Kelvin.[20]

[20] Westminster Abbey Memorial of George Green. https://www.westminster-abbey.org/abbey-commemorations/commemorations/george-green

Why Green's Functions?

Any differential equation establishes a relation between the increments of certain quantities and these quantities themselves. This property of a differential equation makes it a natural expression of the principle of causality which is the foundation of exact natural science. Differential equations come in two flavors: (i) ordinary if there is only one independent variable, and (ii) partial if there are several independent variables. Thought this difference appears merely cosmetic, their manifestation in understanding physical processes reveals their deeper significance. Our classical atomistic description of matter takes the point of view that the motion of elementary particles is the sole basis for all physical processes. Here, the position of each particle is determined as a function of time–the only independent variable. On the other hand, all physical processes in the domains of electromagnetism and optics are determined by field quantities which have a well defined value at each point in space and time. Thus, there are four independent variables– three space coordinates and one time. Intriguingly, ordinary and partial differential equations are mathematical expressions of two fundamental points of view, the synthesis of which in quantum theory is a major problem in cotemporary physics.[21]

[21] L. Hopf and W. Nef. *Introduction to the Differential Equations of Physics*. Dover books on intermediate and advanced mathematics.120. Dover Publications, 1948

Central to the spatial and dynamical description of matter and fields is the introduction of sources and force terms. Since these terms do not involve the dynamical variables or fields themselves they give way to inhomogeneous differential equations. In general, a linear inhomogeneous differential equation can be expressed as

$$\hat{\mathcal{L}}_{\mathbf{r}t}\varphi(\mathbf{r}t) = f(\mathbf{r}t), \tag{100}$$

where $\hat{\mathcal{L}}_{\mathbf{r}t}$ is a general linear differential operator and $\varphi(\mathbf{r}t)$ is the desired solution. If we squint, this expression resembles a system of linear equations of the form $\mathbf{A}\mathbf{x} = \mathbf{b}$. From linear algebra, we know that if the matrix $\mathbf{A}$ is invertible ($\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$), then the system has a unique solution given by $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$. So in essence, if we can find the inverse of $\hat{\mathcal{L}}_{\mathbf{r}t}$ the problem is solved. Drawing on this analogy, we search for solutions of

$$\hat{\mathcal{L}}_{\mathbf{r}t}G(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t'), \tag{101}$$

where G is effectively the inverse of the linear operator $\hat{\mathcal{L}}_{\mathbf{r}t}$ and is called the Green's function. G may then be used to yield $\varphi(\mathbf{r}t)$ for a general f:

$$\varphi(\mathbf{r}t) = \varphi_0(\mathbf{r}t) + \int d\mathbf{r}dt\; G(\mathbf{r}t, \mathbf{r}'t')f(\mathbf{r}'t'), \tag{102}$$

with φ_0 being a solution of the homogeneous equation. Physically, the Green's function can be thought of as follows. To obtain the field φ at position $\mathbf{r}$ and time

t caused by a distributed source $f(\mathbf{r}'t')$ (e.g., charge or heat generator or whatever it is that causes the field) we calculate the effects of each elementary portion of source and add them all. If $G(\mathbf{r}t, \mathbf{r}'t')$ is the field at the *observer's point* $\mathbf{r}t$ caused by a unit point source at the *source point* $\mathbf{r}'t'$, then the field at $\mathbf{r}t$ caused by the source distribution $f(\mathbf{r}'t')$ is the integral of $G(\mathbf{r}t, \mathbf{r}'t')f(\mathbf{r}'t')$ over the whole range of $\mathbf{r}'t'$ occupied by the source. Boundary conditions can be satisfied in the same manner.[22,23]

[23] In fact, there is a dualism between between sources and boundary conditions since the Green's function is a solution for a case which homogeneous every where except at one point. Therefore, when a point is on the boundary, the Green's function may be used to satisfy inhomogeneous boundary conditions while when it is in space it may be used to satisfy the inhomogeneous equation.

[22] Philip McCord Morse and Herman Feshbach. *Methods of theoretical physics*. Technology Press, 1946

Classical Green's Functions

To illustrate the character and power of Green's functions we consider an illustrative example from classical electrodynamics. Maxwell's equations consist of a set of coupled first-order partial differential equations relating the various components of electric and magnetic fields. They can be solved as they stand in simple situations, but it is often convenient to introduce potentials that yield a smaller number of second-order equations while satisfying Maxwell's equations identically. Specifically, the scalar potential Φ and the vector potential $\mathbf{A}$ are found to satisfy[24]

[24] J.D. Jackson. *Classical electrodynamics*. Wiley, New York, 1. edition, 1962

$$\nabla^2\Phi - \frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = -4\pi\rho(\mathbf{r}, t) \tag{103}$$

$$\nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} = -\frac{4\pi}{c}\mathbf{j}(\mathbf{r}, t). \tag{104}$$

These wave equations have the same basic structure:

$$\nabla^2\varphi - \frac{1}{c^2}\frac{\partial^2\varphi}{\partial t^2} = -4\pi f(\mathbf{r}, t) \tag{105}$$

where $f(\mathbf{r}, t)$ is a known source distribution and the factor c is the velocity of propagation in the medium. In order to handle problems involving source distributions as well as the boundary values and initial conditions for the potential it is necessary to determine the Green's function $G(\mathbf{r}t, \mathbf{r}'t')$ which satisfies the appropriate boundary and initial conditions. The Green's function satisfies the same equation albeit for a 'delta' distribution or kick,

$$\left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] G(\mathbf{r}t, \mathbf{r}'t') = -4\pi\delta(\mathbf{r} - \mathbf{r}')\delta(t - t'), \tag{106}$$

and the field for an arbitrary distribution is given by

$$\varphi(\mathbf{r}, t) = \varphi_h(\mathbf{r}, t) + \int d\mathbf{r}'dt'\ G(\mathbf{r}t, \mathbf{r}'t')f(\mathbf{r}'t') \tag{107}$$

where φ_h is a solution of the homogeneous equation. Then the Green's function can be readily found and is given by

Exercise 9. Prove Eq. 108.

$$G(\mathbf{r} - \mathbf{r}', t - t') = \frac{c\delta(|\mathbf{r} - \mathbf{r}'| - c(t - t'))}{4\pi|\mathbf{r} - \mathbf{r}'|} \tag{108}$$

and describes a pulse at $\mathbf{r}'t'$ generating a field at a distance $|\mathbf{r} - \mathbf{r}'|$ away at a later time $|\mathbf{r} - \mathbf{r}'|/c$. The solution G therefore, describes a *causal* retarded interaction. The

field is then given by

$$\varphi(\mathbf{r},t) = \int d\mathbf{r}'dt' \; \frac{c\delta(|\mathbf{r}-\mathbf{r}'| - c(t-t'))}{4\pi|\mathbf{r}-\mathbf{r}'|} f(\mathbf{r}'t') = \int d\mathbf{r}' \; \frac{cf(\mathbf{r}'(t-|\mathbf{r}-\mathbf{r}'|/c))}{4\pi|\mathbf{r}-\mathbf{r}'|}, \tag{109}$$

similar to Fig. 7, where we assumed there is no field without $f(\mathbf{r}'t')$.

Figure 7
Water ripples spreading on a pond surface following a causal retarded propagation.

Green's Functions in Quantum Mechanics

Propagators, Green's functions, and the closely associated Green's operators are central to any reasonably sophisticated and comprehensive treatment of scattering and decay processes in quantum mechanics, and are principle components of quantum field theory and applications in high-energy and Condensed Matter physics. We begin by presenting the Green's function within quantum mechanics to gain intuition, and then we will generalize to the many-particle case.

Let us consider the inhomogeneous Schrödinger equation

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{H}\right]|\psi(t)\rangle = |S(t)\rangle \tag{110}$$

where $\hat{H}$ is the Hamiltonian and $|S\rangle$ is a 'source' term. To solve this equation we determine a time-dependent Green's function operator $\hat{G}$ that satisfies

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{H}\right]\hat{G}(t,t') = \delta(t-t'), \tag{111}$$

with $\hat{H}$ being independent of time for simplicity. The Green's function operator depends on a pair of time points, t being the *field* point and t' the *source*.[25] To obtain a closed form solution for $\hat{G}$, we first assume there is no special point in time, so that $\hat{G}$ only depends on the difference in times, i.e., $\hat{G}(t,t') \to \hat{G}(t-t')$, and then the Fourier transform of $\hat{G}$ is given by

$$\hat{G}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \; e^{-i\omega(t-t')}\hat{G}(\omega). \tag{112}$$

Inserting this into Eq. 111 along with the Fourier representation of the delta function, $\delta(t-t') = \frac{1}{2\pi}\int d\omega \; e^{-i\omega(t-t')}$, we obtain

$$\left[\hbar\omega - \hat{H}\right]\hat{G}(\omega) = \hat{\mathbb{1}}. \tag{113}$$

Solving for $\hat{G}$, we arrive at the solution for Eq. 113,

$$\hat{G}(\omega) = \frac{1}{\hbar\omega - \hat{H}} = \sum_n \frac{|\varphi_n\rangle\langle\varphi_n|}{\hbar\omega - \varepsilon_n}, \tag{114}$$

where the last equality comes from expanding $\hat{H}$ into its eigen spectrum. Since $\hat{H}$ is a Hermitian operator, all of its eigenvalues $\{\varepsilon_n\}$ are real and n is either continuous or discrete. Here, without loss of generality, we will assume the latter for simplicity.

[25] Note: some books reverse these interpretations, be careful when reading the literature.

By inspection, $\hat{G}(\omega)$ exhibits simple poles at the position of the eigenvalues of $\hat{H}$; the inverse is also true: the poles of $\hat{G}(\omega)$ give the discrete eigenvalues of H. Clearly, if we try to Fourier transform back to time, we will run into problems since by integrating along ω will have instances where $\hat{G}(\omega)$ is not well defined, i.e. at each pole $\omega = \varepsilon_n/\hbar$. To mitigate this, we can shift the eigenvalue spectrum off of the real line, into the complex plane and get back to the real line by a limiting procedure. Specifically, we can add a small imaginary part to ω, either $+i\delta$ or $-i\delta$. These two choices imply we have two solutions for $\hat{G}$! Namely, we define two Green's functions as follows

$$\hat{G}^R(\omega) = \lim_{\delta \to 0^+} \hat{G}(\omega + i\delta), \tag{115}$$

$$\hat{G}^A(\omega) = \lim_{\delta \to 0^+} \hat{G}(\omega - i\delta), \tag{116}$$

the *retarded* and *advanced* Green's functions, respectively. The physical meaning of these functions will become clear below. From this definition, we can glean a few properties of these Green's functions:

1. $\hat{G}$ is an analytic function in the complex plane except at those points or portions of the real axis which correspond to the eigenvalues of H.

2. $\hat{G}^R$ and $\hat{G}^A$ are related via the conjugate transpose

$$\left[\hat{G}^R(\omega)\right]^\dagger = \hat{G}^A(\omega), \tag{117}$$

   which implies the diagonal elements of the Green's functions are related

$$\operatorname{Re} \hat{G}^R(\omega) = \operatorname{Re} \hat{G}^A(\omega), \tag{118}$$

$$\operatorname{Im} \hat{G}^R(\omega) = -\operatorname{Im} \hat{G}^A(\omega). \tag{119}$$

3. There is a discontinuity as we cross the real ω-line, indicated by the imaginary part changing sign in Eq. 119. Explicitly, the discontinuity is given by

$$\begin{aligned}
\hat{\tilde{G}}(\omega) &= \hat{G}^R(\omega) - \hat{G}^A(\omega) \\
&= \lim_{\delta \to 0^+} \hat{G}(\omega + i\delta) - \hat{G}(\omega - i\delta) \\
&= \lim_{\delta \to 0^+} \frac{1}{\hbar} \sum_n |\varphi_n\rangle \langle\varphi_n| \left(\frac{1}{\omega - \varepsilon_n/\hbar + i\delta} - \frac{1}{\omega - \varepsilon_n/\hbar - i\delta} \right) \\
&= \frac{2i}{\hbar} \sum_n |\varphi_n\rangle \langle\varphi_n| \lim_{\delta \to 0^+} \frac{\delta}{(\omega - \varepsilon_n/\hbar)^2 + \delta^2} \\
&= \frac{2\pi i}{\hbar} \sum_n |\varphi_n\rangle \langle\varphi_n| \, \delta(\omega - \varepsilon_n/\hbar),
\end{aligned} \tag{120}$$

   which takes the form of a generalized density of states. We define the so-called spectral function as

$$\hat{A}(\omega) = \sum_n |\varphi_n\rangle \langle\varphi_n| \, \delta(\hbar\omega - \varepsilon_n) = \frac{\hbar}{2\pi i} \hat{\tilde{G}}(\omega) = \mp \frac{\hbar}{\pi} \operatorname{Im} \hat{G}^{R/A}(\omega) \tag{121}$$

which yields the total density of states under the trace,

$$N(\omega) = \mathrm{Tr}[\hat{A}(\omega)] = \frac{\hbar}{2\pi i}\,\mathrm{Tr}[\hat{\tilde{G}}(\omega)] = \mp\frac{\hbar}{\pi}\,\mathrm{Tr}[\mathrm{Im}\,\hat{G}^{R/A}(\omega)]. \tag{122}$$

4. $\hat{G}$ can be written in terms of $\hat{A}$,

$$\begin{aligned}\hat{G}(\omega) &= \sum_n \frac{|\varphi_n\rangle\langle\varphi_n|}{\hbar\omega - \varepsilon_n},\\ &= \frac{1}{\hbar}\int_{-\infty}^{\infty} d\omega' \frac{\sum_n |\varphi_n\rangle\langle\varphi_n|\,\delta(\hbar\omega' - \varepsilon_n)}{\omega - \omega'}\\ &= \frac{1}{\hbar}\int_{-\infty}^{\infty} d\omega' \frac{\hat{A}(\omega')}{\omega - \omega'}.\end{aligned} \tag{123}$$

So, if we know $\hat{A}$ then $\hat{G}$, $\hat{G}^R$, and $\hat{G}^A$ are completely determined and permits us to immediately obtain the solution of Eq. 113.

To obtain $\hat{G}(t-t')$, we now Fourier transform $\hat{G}(\omega)$ back to real time,

$$\hat{G}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\; \hat{G}(\omega) e^{-i\omega(t-t')}. \tag{124}$$

However, as we found above $\hat{G}(\omega)$ has singularities (poles and/or branch cuts) on the real ω-axis. Because of this property Eq. 124 is not well defined as it stands. So, one must use a limiting procedure to define $\hat{G}(t-t')$. In general,

$$\hat{G}^{\mathcal{C}}(t-t') = \lim_{\mathcal{C}\to\mathcal{C}_0} \frac{1}{2\pi\hbar}\sum_n |\varphi_n\rangle\langle\varphi_n| \int_{\mathcal{C}} dz\; \frac{e^{-iz(t-t')}}{z - \varepsilon_n/\hbar}, \tag{125}$$

where we integrate along a contour $\mathcal{C}$ in the complex ω-plane and take the limit as this contour $\mathcal{C}$ goes to the real ω-axis $\mathcal{C}_0$. Using this procedure, one can obtain infinitely many Green's functions depending on how $\mathcal{C}$ approaches $\mathcal{C}_0$. However, there are only two choices of physical interest shown in Fig. 8(a) and they give

$$\hat{G}^{R/A}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\; \hat{G}^{R/A}(\omega) e^{-i\omega(t-t')}. \tag{126}$$

To explicitly perform the integration over ω, we close the paths for $\hat{G}^{R/A}$ by an infinite semicircle in the lower ($\mathcal{C}_\gamma^-$) or upper ($\mathcal{C}_\gamma^+$) ω-half plane. If the semicircle closes the contour in the upper (lower) half-plane then we must have $t - t' < 0$ ($t - t' > 0$) so that $e^{-iz(t-t')} \to 0$ on the semicircle as the radius goes to infinity, otherwise the contour integral does not converge. With this, we can use Cauchy's integral theorem to evaluate Eq. 126.

For $\hat{G}^R(t-t')$, if $t - t' < 0$ then we close the contour in the upper-half ω-plane. This closed contour encloses no poles, so by Cauchy's integral theorem yields 0. However, if $t - t' > 0$ then we close the contour in the lower-half ω-plane, enclosing all the singularities along the real ω-axis [Fig. 8(b)],

$$\frac{1}{2\pi\hbar}\sum_n |\varphi_n\rangle\langle\varphi_n| \oint_{\mathcal{C}_R + \mathcal{C}_\gamma^-} dz\; \frac{e^{-iz(t-t')}}{z - \varepsilon_n/\hbar}. \tag{127}$$

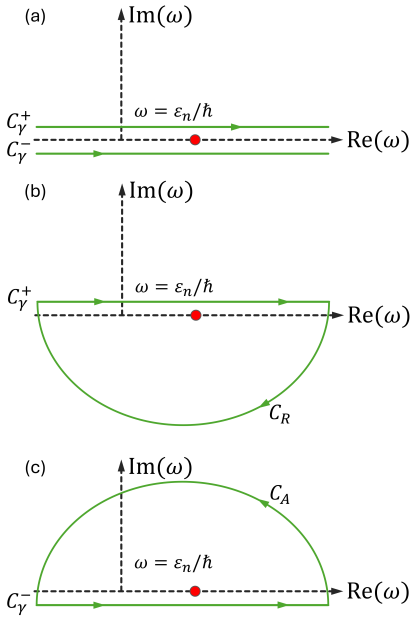

Figure 8
(a) Integration paths (solid lines) in the ω-plane for obtaining various physically relevant Green's functions for the Schrödinger equation. (b) Integration path for G^R. (c) Integration path for G^A.

This is Cauchy's integral for a simple pole and yields:

$$\hat{G}^R(t-t') = \begin{cases} \frac{i}{\hbar}\sum_n |\varphi_n\rangle \langle\varphi_n| e^{-i\varepsilon_n(t-t')/\hbar} & t-t' > 0 \\ 0 & t-t' < 0 \end{cases} \tag{128}$$

We call this the *retarded* Green's function since the observer's time is after the source, implying forward causal propagation.

For $\hat{G}^A$, if $t-t' > 0$ then we close the contour in the lower half-plane, enclosing no poles. But if $t-t' < 0$ we close the contour in the upper half-plane, enclosing all the singularities along the real ω-axis [Fig. 8(c)],

$$\frac{1}{2\pi\hbar}\sum_n |\varphi_n\rangle \langle\varphi_n| \oint_{\mathcal{C}_A+\mathcal{C}_\gamma^+} dz\, \frac{e^{-iz(t-t')}}{z-\varepsilon_n/\hbar}. \tag{129}$$

Again, this is Cauchy's integral for a simple pole and yields:

$$\hat{G}^A(t-t') = \begin{cases} 0 & t-t' > 0 \\ -\frac{i}{\hbar}\sum_n |\varphi_n\rangle \langle\varphi_n| e^{-i\varepsilon_n(t-t')/\hbar} & t-t' < 0 \end{cases} \tag{130}$$

We call this the *advanced* Green's function since the observer's time comes before that of the source, implying anticausal backward propagation.

Finally, it is useful to consider quantities defined as the difference of two Green's functions $\hat{\tilde{G}}$. Because $\hat{\tilde{G}}$ is the difference of two Green's functions, it satisfies the homogeneous Schrödinger equation and not Eq. 111. Thus, strictly speaking, $\hat{\tilde{G}}$ is not a Green's function. In the present case,

$$\hat{\tilde{G}}(t-t') = \hat{G}^R(t-t') - \hat{G}^A(t-t'). \tag{131}$$

These results can be compactly summarized by using the Heaviside step function[26] and reintroducing $\hat{H}$,

$$\hat{G}^R(t-t') = +\frac{i}{\hbar}\theta(t-t')e^{-i\hat{H}(t-t')/\hbar}, \tag{132}$$

$$\hat{G}^A(t'-t) = -\frac{i}{\hbar}\theta(t'-t)e^{-i\hat{H}(t-t')/\hbar}, \tag{133}$$

$$\hat{\tilde{G}}(t-t') = \frac{i}{\hbar}e^{-i\hat{H}(t-t')/\hbar}. \tag{134}$$

Consequently, $\hat{G}^R(t-t')$ and $\hat{G}^A(t-t')$ are related via the conjugate transpose

$$\hat{G}^A(t-t') = \left[\hat{G}^R(t'-t)\right]^\dagger. \tag{135}$$

Furthermore, we recognize $e^{-i\hat{H}(t-t')/\hbar}$ as the time-evolution operator $\hat{U}(t-t')$, that propagates a state $|\psi(t')\rangle$ at time t' to another state $|\psi(t)\rangle$ at t,

$$|\psi(t)\rangle = \hat{U}(t-t')\,|\psi(t')\rangle\,, \tag{136}$$

which satisfy the homogeneous Schrödinger equation. The retarded and advanced Green's functions, along with $\hat{\tilde{G}}(t-t')$, are related to the time evolution operator,

$$\hat{\tilde{G}}(t-t') = \frac{i}{\hbar}U(t-t'), \tag{137}$$

[26] We note that during the course of determining $\hat{G}^{R/A}$, we have implicitly derived an integral representation for the Heaviside step function:

$$\theta(\tau) = \lim_{\delta\to 0^+} -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dx \frac{e^{-i\tau x}}{x+i\delta}$$

$$\theta(-\tau) = \lim_{\delta\to 0^+} +\frac{1}{2\pi i}\int_{-\infty}^{\infty} dx \frac{e^{-i\tau x}}{x-i\delta}$$

$$\hat{G}^R(t-t') = +\frac{i}{\hbar}\theta(t-t')U(t-t'), \tag{138}$$

$$\hat{G}^A(t-t') = -\frac{i}{\hbar}\theta(t-t')U(t-t'). \tag{139}$$

Therefore,

$$|\psi(t)\rangle = \frac{\hbar}{i}\hat{\hat{G}}(t-t')\,|\psi(t')\rangle\,, \tag{140}$$

which can be expressed in terms of $\hat{G}^{R/A}(t-t')$. Similarly, both $\hat{G}^R$ and $\hat{G}^A$ satisfy Eq. 111, and solve the inhomogeneous time-dependent Schrödinger equation [Eq. 110]. The solution of the inhomogeneous equation can be expressed in terms of the general solution of the homogeneous equation and $\hat{G}^R$ as

$$|\psi(t)\rangle = |\phi(t)\rangle + \int_{-\infty}^{\infty} dt\; \hat{G}^R(t-t')\,|S(t')\rangle\,. \tag{141}$$

If we project the state vectors and Green's operators onto position states, we find

$$\psi(\mathbf{r}t) = \phi(\mathbf{r}t) + \int d\mathbf{r}\int_{-\infty}^{\infty} dt\; \hat{G}^R(\mathbf{r},\mathbf{r}';t-t')S(\mathbf{r}t'), \tag{142}$$

where

$$\hat{G}^R(\mathbf{r},\mathbf{r}';t-t') = \frac{i}{\hbar}\theta(t-t')\,\langle\mathbf{r}|\,U(t-t')\,|\mathbf{r}'\rangle\,, \tag{143}$$

is the retarded Green's function and $\langle\mathbf{r}|\,U(t-t')\,|\mathbf{r}'\rangle$ is typically called the *propagator* since it evolves the wave function from one space-time point to another,

$$\psi(\mathbf{r}t) = \langle\mathbf{r}|\,U(t-t')\,|\mathbf{r}'\rangle\,\psi(\mathbf{r}'t'). \tag{144}$$

These two functions are closely related, but the later is not a Green's function since it satisfies the *homogeneous* Schrödinger equation. $\hat{G}^R(\mathbf{r},\mathbf{r}';t-t')$ is a solution of the time-dependent Schrödinger equation for $t > t'$, since the function $\delta(t-t')$ on the right-hand side of Eq. 110 vanishes for $t > t'$. Moreover, It also satisfies the Schrödinger equation for $t < t'$, since $\hat{G}^R(\mathbf{r},\mathbf{r}';t-t') = 0$ in that case. Finally, if t approaches t' from the positive side then

$$\begin{aligned}\lim_{t\to t'}\hat{G}^R(\mathbf{r},\mathbf{r}';t-t') &= \lim_{t\to t'}\frac{i}{\hbar}\theta(t-t')\,\langle\mathbf{r}|\,U(t-t')\,|\mathbf{r}'\rangle \\ &= \langle\mathbf{r}|\,\hat{\mathbb{1}}\,|\mathbf{r}'\rangle = \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}').\end{aligned} \tag{145}$$

Thus, $\hat{G}^R(\mathbf{r},\mathbf{r}';t-t')$ for $t > t'$ can be thought of as the solution $\psi(\mathbf{r}t)$ with the singular initial conditions $\psi(\mathbf{r}t') = \delta(\mathbf{r}-\mathbf{r}')$ at $t = t'$. Analogous to the electromagnetic pulse in the previous section, for $t = -\infty$ up until $t = t'$ the wave function is zero. At that time there is a spatially and temporally localized disturbance at $\mathbf{r}'$. Then the wave field that radiates outward from the disturbance is the outgoing time-dependent Green's function. The waves for $t > t'$ are freely propagating. The analysis and visualization can equally be performed for the advanced Green's function.

Finally, we shed additional light on the Green's function for the single-particle Schrödinger equation by casting it within the second quantized notion. The retarded Green's function can be written as

$$\begin{aligned}\hat{G}^R(\mathbf{r},\mathbf{r}';t-t') &= \frac{i}{\hbar}\theta(t-t')\left\langle \mathbf{r}\right| U(t-t')\left|\mathbf{r}'\right\rangle \\ &= \frac{i}{\hbar}\theta(t-t')\left\langle 0\right|\hat{\psi}(\mathbf{r})U(t-t')\hat{\psi}^\dagger(\mathbf{r}')\left|0\right\rangle \end{aligned} \tag{146}$$

The interpretation illustrated above, now comes to into focus. For $t = -\infty$ up until $t = t'$ the vacuum is empty, then at t' a particle is created at $\mathbf{r}'$. This particle propagates to $\mathbf{r}$ where it is annihilated. Therefore, we can interpret $\hat{G}^R(\mathbf{r},\mathbf{r}';t-t')$ as the transition amplitude for a particle to propagate from $\mathbf{r}', t'$ to $\mathbf{r}, t$, and its square modulus gives the transition probability. In the next section we will generalize this concept to multi-particle systems.

Many-Particle Green's Functions

In this section we use the concepts introduced in the previous section to define and explore the properties of the Green's function for assembles of many-particles.

Definition 10. The single-particle Green's function is defined at zero temperature by

$$iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') = \frac{\left\langle \Psi_0\right|\mathcal{T}\left[\hat{\psi}_{H\alpha}(\mathbf{r}t)\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t')\right]\left|\Psi_0\right\rangle}{\left\langle \Psi_0|\Psi_0\right\rangle} \tag{147}$$

where $|\Psi_0\rangle$ is the *Heisenberg ground state* of the interacting system satisfying

$$\hat{H}\left|\Psi_0\right\rangle = E\left|\Psi_0\right\rangle \tag{148}$$

and $\hat{\psi}^\dagger_{H\beta}(\mathbf{r}t)$ is a *Heisenberg operator* with the time dependence

$$\hat{\psi}^\dagger_{H\beta}(\mathbf{r}t) = e^{i\hat{H}t/\hbar}\hat{\psi}^\dagger_\beta(\mathbf{r})e^{-i\hat{H}t/\hbar}. \tag{149}$$

Here, the indices α and β label the components of the field operators, e.g. α and β take two values for spin-1/2. The $\mathcal{T}$ here is a generalization of the *time-ordering operator* defined in Eq. 81:

$$\mathcal{T}\left[\hat{\psi}_{H\alpha}(\mathbf{r}t)\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t')\right] = \begin{cases}\hat{\psi}_{H\alpha}(\mathbf{r}t)\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t') & t > t' \\ \pm\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t')\hat{\psi}_{H\alpha}(\mathbf{r}t) & t < t'\end{cases} \tag{150}$$

where the upper (lower) sing refers to bosons (fermions). More generally, $\mathcal{T}$ of a product of several operators order from right to left in ascending time order and adds a factor of $(\pm 1)^P$ for P number of interchanges of operators from the original given order. This definition is consistent with that in Eq. 81 because $\hat{H}$ always consists of an even number of operators.

The single-particle Green's function may then be written as

$$iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') = \frac{\langle\Psi_0|\,\hat{\psi}_{H\alpha}(\mathbf{r}t)\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t')\,|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}\theta(t-t') \pm \frac{\langle\Psi_0|\,\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t')\hat{\psi}_{H\alpha}(\mathbf{r}t)\,|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}\theta(t'-t). \tag{151}$$

Relation to Observables—- Although the ground-state expectation value in the definition of G implies the loss of detailed information about the ground state, the single-particle Green's function still contains the observable properties of greatest interest:

1. The expectation value of any single-particle operator in the ground state of the system.
2. The ground state energy of the system.
3. The excitation spectrum of the system.

The first point is demonstrated below, while the third is covered in the next section.

Let us consider the general single-particle operator in second quantization,

$$\hat{O} = \int d\mathbf{r}\ \sum_{\alpha\beta}\hat{\psi}^\dagger_\beta(\mathbf{r})O_{\beta\alpha}(\mathbf{r})\hat{\psi}_\alpha(\mathbf{r}). \tag{152}$$

The ground-state expectation value of this operator is then given by

$$\langle\hat{O}\rangle = \int d\mathbf{r}\ \sum_{\alpha\beta}\langle\hat{\psi}^\dagger_\beta(\mathbf{r})O_{\beta\alpha}(\mathbf{r})\hat{\psi}_\alpha(\mathbf{r})\rangle \tag{153}$$

with

$$\begin{aligned}
\sum_{\alpha\beta}\langle\hat{\psi}^\dagger_\beta(\mathbf{r})O_{\beta\alpha}(\mathbf{r})\hat{\psi}_\alpha(\mathbf{r})\rangle\,, &= \sum_{\alpha\beta}O_{\beta\alpha}(\mathbf{r})\frac{\langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r})\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \\
&= \lim_{\mathbf{r}'\to\mathbf{r}}\sum_{\alpha\beta}O_{\beta\alpha}(\mathbf{r})\frac{\langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \\
&= \pm\lim_{t'\to t^+}\lim_{\mathbf{r}'\to\mathbf{r}}\sum_{\alpha\beta}O_{\beta\alpha}(\mathbf{r})\frac{\langle\Psi_0|\,\mathcal{T}\left[\hat{\psi}_{H\alpha}(\mathbf{r}t)\hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t')\right]\,|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \\
&= \pm i\lim_{t'\to t^+}\lim_{\mathbf{r}'\to\mathbf{r}}\sum_{\alpha\beta}O_{\beta\alpha}(\mathbf{r})G_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t'), \\
&= \pm i\lim_{t'\to t^+}\lim_{\mathbf{r}'\to\mathbf{r}}\mathrm{Tr}[O(\mathbf{r})G(\mathbf{r}t,\mathbf{r}'t')].
\end{aligned} \tag{154}$$

Here, the matrix element $O_{\beta\alpha}(\mathbf{r})$ must act before the limit $\mathbf{r}'\to\mathbf{r}$ is performed because O may contain spatial derivatives and otherwise the derivatives will act on the incorrect field operators. Also, the symbol t^+ denotes a time that is infinitesimally later than t to ensure that the field operators on the third line occur in the proper

order. Finally, the sum over spin indices is recognized as the trace of the matrix product OG.

Using this definition we may write the single-particle operators in Table 1 in terms of single-particle Green's functions. For example, the expectation value of the particle number density $\langle \hat{n}(\mathbf{r}) \rangle$, the spin density $\langle \hat{m}(\mathbf{r}) \rangle$, and the kinetic energy density $\langle \hat{T}(\mathbf{r}) \rangle$ are found to be:

$$\langle \hat{n}(\mathbf{r}) \rangle = \pm i \, \mathrm{Tr}[G(\mathbf{r}t, \mathbf{r}t^+)], \tag{155}$$

$$\langle \hat{m}(\mathbf{r}) \rangle = \pm i \, \mathrm{Tr}[\boldsymbol{\sigma} G(\mathbf{r}t, \mathbf{r}t^+)], \tag{156}$$

$$\langle \hat{T}(\mathbf{r}) \rangle = \pm i \lim_{\mathbf{r}' \to \mathbf{r}} \left[-\frac{\hbar^2 \nabla^2}{2m} \mathrm{Tr}[G(\mathbf{r}t, \mathbf{r}'t^+)] \right]. \tag{157}$$

The Lehmann and the Spectral Representations—- Here we elucidate salient features of the single-particle Green's function that stem from fundamental quantum mechanical principles and are therefore independent of the the specific form of the interaction. We note that although our final expressions are formally correct for both Bosons and Fermions, the existence of Bose condensation at $T = 0$K introduces complications and we shall consider only fermions in this section.

Despite the complicated nature of the Heisenberg field operators and state vectors in $iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t')$, it is possible to derive some general results. First, we insert a complete set of of N-particle Heisenberg states in between the field operators,

$$\begin{aligned} iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = &\sum_N \langle \Psi_0 | \, \hat{\psi}_{H\alpha}(\mathbf{r}t) \, | \Psi_N \rangle \, \langle \Psi_N | \, \hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t') \, | \Psi_0 \rangle \, \theta(t - t') \\ &- \sum_N \langle \Psi_0 | \, \hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t') \, | \Psi_N \rangle \, \langle \Psi_N | \, \hat{\psi}_{H\alpha}(\mathbf{r}t) \, | \Psi_0 \rangle \, \theta(t' - t), \end{aligned} \tag{158}$$

where we have assumed $\langle \Psi_0 | \Psi_0 \rangle = 1$, and then insert the definition of the Heisenberg field operators

$$\begin{aligned} iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = &\sum_n \langle \Psi_0 | \, e^{i\hat{H}t/\hbar} \hat{\psi}_\alpha(\mathbf{r}) e^{-i\hat{H}t/\hbar} \, | \Psi_n \rangle \, \langle \Psi_n | \, e^{i\hat{H}t'/\hbar} \hat{\psi}^\dagger_\beta(\mathbf{r}') e^{-i\hat{H}t'/\hbar} \, | \Psi_0 \rangle \, \theta(t - t') \\ &- \sum_n \langle \Psi_0 | \, e^{i\hat{H}t'/\hbar} \hat{\psi}^\dagger_\beta(\mathbf{r}') e^{-i\hat{H}t'/\hbar} \, | \Psi_n \rangle \, \langle \Psi_n | \, e^{i\hat{H}t/\hbar} \hat{\psi}_\alpha(\mathbf{r}) e^{-i\hat{H}t/\hbar} \, | \Psi_0 \rangle \, \theta(t' - t), \end{aligned} \tag{159}$$

which allows us to evaluate the time dependence of the operators

$$\begin{aligned} iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = &\sum_n e^{-i(E_n - E)(t - t')/\hbar} \, \langle \Psi_0 | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_0 \rangle \, \theta(t - t') \\ &- \sum_n e^{+i(E_n - E)(t - t')/\hbar} \, \langle \Psi_0 | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_0 \rangle \, \theta(t' - t). \end{aligned} \tag{160}$$

Assuming there is no special point in time allows us to write G as the difference in times, and we can use the integral representation of the Heaviside function $\theta(t - t')$ to further write,

$$\begin{aligned} iG_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; t - t') = &- \lim_{\delta \to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \sum_n \\ &\times \left[e^{-i(E_n - E + \hbar\omega')(t - t')/\hbar} \frac{\langle \Psi_0 | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_0 \rangle}{\omega' + i\delta} \right. \end{aligned}$$

$$+e^{+i(E_n-E-\hbar\omega')(t-t')/\hbar}\frac{\langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle}{\omega'-i\delta}\Bigg]. \quad (161)$$

Moreover, we use the Fourier transform,

$$G_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)=\int_{-\infty}^{\infty}d\bar{t}\;G_{\alpha\beta}(\mathbf{r},\mathbf{r}';\bar{t})e^{+i\omega\bar{t}} \quad (162)$$

to yield

$$\begin{aligned}
iG_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) &= -\lim_{\delta\to0^+}\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega'\sum_n \\
&\times\Bigg[\int_{-\infty}^{\infty}d\bar{t}\;e^{-i(E_n-E+\hbar\omega'-\hbar\omega)\bar{t}/\hbar}\frac{\langle\Psi_0|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle}{\omega'+i\delta} \\
&+\int_{-\infty}^{\infty}d\bar{t}\;e^{+i(E_n-E-\hbar\omega'+\hbar\omega)\bar{t}/\hbar}\frac{\langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle}{\omega'-i\delta}\Bigg], \\
&= -\lim_{\delta\to0^+}\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega'\sum_n \\
&\times\Bigg[2\pi\delta((E_n-E+\hbar\omega'-\hbar\omega)/\hbar)\frac{\langle\Psi_0|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle}{\omega'+i\delta} \\
&+2\pi\delta((E_n-E-\hbar\omega'+\hbar\omega)/\hbar)\frac{\langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle}{\omega'-i\delta}\Bigg],
\end{aligned} \quad (163)$$

and evaluating the delta functions we arrive at the Lehmann representation of the single-particle Green's function:

$$G_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)=\lim_{\delta\to0^+}\sum_n\Bigg[\frac{\langle\Psi_0|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle}{\omega-(E_n-E)/\hbar+i\delta} +\frac{\langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle}{\omega+(E_n-E)/\hbar-i\delta}\Bigg]. \quad (164)$$

If $|\Psi_0\rangle$ is the ground state of an N fermion system, then the state $[\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle]$ must contain $N+1$ particles and the state $[\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle]$ must contain $N-1$ particles. Hence, by the orthogonality $\langle\Psi_n|$ must contain $N\pm1$ particles. This necessity to consider an assembly of particles is a new feature that is beyond the ordinary Schrödinger equation.

Lets examine the denominator in a bit more detail. In the first term, the intermediate state contains $N+1$ particles and we may rewrite the denominator as

$$\begin{aligned}
&\omega-[E_n(N+1)-E(N)]/\hbar = \\
&\quad\omega-[E_n(N+1)-E(N+1)]/\hbar-[E(N+1)-E(N)]/\hbar.
\end{aligned} \quad (165)$$

Now, it is clear that there are two distinct energetic contributions the energy difference $E_n(N+1)-E(N)$. The first, $[E(N+1)-E(N)]$ is the change in the ground-state energy of the system upon the addition of an extra particle. Since the volume

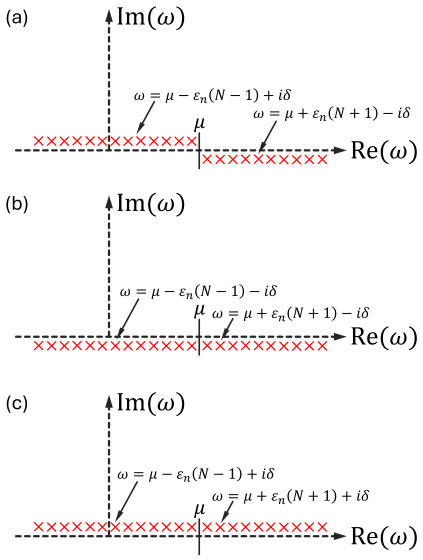

Figure 9
Pole structure of the (a) time-ordered, (b) retarded, and (c) advanced single-particle Green's Function.

of the system is kept constant this is just the chemical potential μ. Additionally, the quantity $[E_n(N+1) - E(N+1)] \equiv \varepsilon_n(N+1)$ is the *excitation energy* of the $N+1$ particle system. By definition $\varepsilon_n(N+1) \geq 0$.

Similarly for the second term, the intermediate state contains $N-1$ particles and we may rewrite the denominator as

$$\begin{aligned}\omega + [E_n(N-1) - E(N)]/\hbar &= \omega - [E(n) - E(N-1)]/\hbar + [E_n(N-1) - E(N-1)]/\hbar, \\ &= \omega - \mu/\hbar + \varepsilon_n(N-1)/\hbar \end{aligned} \tag{166}$$

Here, $[E(N) - E(N-1)]$ is chemical potential in the thermodynamic limit,[27,28] and $[E_n(N-1) - E(N-1)] \equiv \varepsilon_n(N-1)$ excitation energy of the $N-1$ particle system. The time ordered Green's function in the Lehmann representation may then be given by:

$$\begin{aligned} G_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{\delta \to 0^+} \sum_n \Bigg[&\frac{\langle \Psi_0 | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_0 \rangle}{\omega - \mu/\hbar - \varepsilon_n(N+1) + i\delta} \\ &+ \frac{\langle \Psi_0 | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_0 \rangle}{\omega - \mu/\hbar + \varepsilon_n(N-1)/\hbar - i\delta} \Bigg]. \end{aligned} \tag{168}$$

Since $G_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega)$ is the exact frequency dependent Green's function, it is interesting to consider the analytic properties of this function. The important observation is that $G_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega)$ *is a single-valued function of* ω *with simple poles at the exact excitation energies of the interacting system*. For frequencies below $\mu/\hbar$ the poles lie above the real line by $i\delta$, i.e., $\omega = \mu - \varepsilon_n(N-1) + i\delta$, with residue $\langle \Psi_0 | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_0 \rangle$, while for frequencies above $\mu/\hbar$ the poles lie below the real line by $i\delta$ with residue $\langle \Psi_0 | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_0 \rangle$, see Fig. 9(a).[29] For an interacting system the field operators connect the ground state with very many excited states of the systems containing $N+1$ particles.

It is clear that G is analytic in neither the upper ω-half plane nor the lower ω-half plane. As we have seen in the previous section, it is massively useful for contour integration to have functions that are analytic in either the upper or lower half ω-planes. Consequently, we therefore define the a new pair or functions the *retarded* and the *advanced* Green's functions.

$$iG^R_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = \langle \Psi_0 | \left\{ \hat{\psi}_{H\alpha}(\mathbf{r}t), \hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t') \right\} | \Psi_0 \rangle \, \theta(t - t') \tag{170}$$

$$iG^R_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = \langle \Psi_0 | \left\{ \hat{\psi}_{H\alpha}(\mathbf{r}t), \hat{\psi}^\dagger_{H\beta}(\mathbf{r}'t') \right\} | \Psi_0 \rangle \, \theta(t' - t) \tag{171}$$

where the curly braces denote the anti commutator and we have assumed $\langle \Psi_0 | \Psi_0 \rangle = 1$. Following the same steps as above we may obtain the Lehmann representation for the retarded and the advanced Green's functions:

$$\begin{aligned} G^{R,A}_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega) = \lim_{\delta \to 0^+} \sum_n \Bigg[&\frac{\langle \Psi_0 | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_0 \rangle}{\omega - \mu/\hbar - \varepsilon_n(N+1) \pm i\delta} \\ &+ \frac{\langle \Psi_0 | \, \hat{\psi}^\dagger_\beta(\mathbf{r}') \, | \Psi_n \rangle \, \langle \Psi_n | \, \hat{\psi}_\alpha(\mathbf{r}) \, | \Psi_0 \rangle}{\omega - \mu/\hbar + \varepsilon_n(N-1)/\hbar \pm i\delta} \Bigg]. \end{aligned} \tag{172}$$

[27] The chemical potential for the $N+1$ and N particle systems are not strictly the same. However, in the thermodynamic limit $(N \to \infty)$

$$\mu(N+1) = \mu(N) + O(N^{-1}). \tag{167}$$

Since we are mainly concerned with material systems that contain $\sim 10^{23}$ particles, $\mu(N+1) \approx \mu(N)$ is a reasonable approximation.

[28] Alexander L Fetter and John Dirk Walecka. *Quantum theory of many-particle systems*. Courier Corporation, 2012

[29] Note, the residue of a simple pole of order p at value c is given by:

$$\text{Res}(f, c) = \frac{1}{(p-1)!} \lim_{z \to c} \frac{d^{p-1}}{dz^{p-1}} \left((z-c)^p f(z) \right). \tag{169}$$

Again, G^R and G^A are meromorphic functions of ω. However, now all the poles in G^R lie in the lower ω-half plane so that G^R is analytic for $\mathrm{Im}\,\omega > 0$. In contrast all the poles of G^A lie in the upper ω-half plane so that G^A is analytic for $\mathrm{Im}\,\omega < 0$. See Fig. 9(b) and (c) for a plot of the corresponding pole structure of G^R and G^A, respectively. For real ω these two functions are related

$$\left[G^R_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)\right]^* = G^A_{\beta\alpha}(\mathbf{r}',\mathbf{r};\omega). \tag{173}$$

As we have seen above, the retarded Green's function is useful if we know the initial state of a system and want to know how it evolves forward in time. This is our link to experiment and most physical quantities of interest are given in terms of G^R. Simply put, it allows us to measure how the system evolves under external perturbation. Similarly, the advanced Green's function is useful if we know the end-point configuration and we want to figure out where it came from.

The only difference between G, G^R, and G^A are the convergence factors $\pm i\delta$ which are important near the singularities. This means we can link the retarded and advanced Green's function to G,

$$G^R_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = G_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) \quad \hbar\omega > \mu \tag{174}$$

$$G^A_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = G_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) \quad \hbar\omega < \mu. \tag{175}$$

This brings us to the special purpose of the time-ordered Green's function. In an interacting system we can expand G in the interaction potential and calculate G at each order. Then with this we can determine $G^{R,A}$ to relate to physical observables.

To make this connection more concrete, we can define the *spectral representation* of the single-particle Green's function as

$$G_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = \lim_{\delta\to 0^+}\int_0^\infty d\omega' \left[\frac{A^+(\mathbf{r},\mathbf{r}';\omega')}{\omega-\mu/\hbar-\omega'+i\delta} + \frac{A^-(\mathbf{r},\mathbf{r}';\omega)}{\omega-\mu/\hbar+\omega'-i\delta}\right], \tag{176}$$

where

$$A^+(\mathbf{r},\mathbf{r}';\omega) = \sum_n \langle\Psi_0|\,\hat\psi_\alpha(\mathbf{r})\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat\psi^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle\,\delta(\omega-\varepsilon_n(N+1)/\hbar), \tag{177}$$

$$A^-(\mathbf{r},\mathbf{r}';\omega) = \sum_n \langle\Psi_0|\,\hat\psi^\dagger_\beta(\mathbf{r}')\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat\psi_\alpha(\mathbf{r})\,|\Psi_0\rangle\,\delta(\omega-\varepsilon_n(N-1)/\hbar) \tag{178}$$

are the *probably distribution of energies* when a particle is added to the N particle ground state A^+ and when a particle is removed from the N particle ground state A^-. These are called *spectral functions*. What we have done? Well, now the Green's function has a *branch cut* along the whole of the real axis, thereby completely altering the analytic structure of the function. Physically, this means in the thermodynamic limit the density of levels ε_n have approached the point where the simple poles have merged to form a branch line, i.e., where the discrete index n labeling the various excited states has become a continuous variable.

Similarly the retarded and advanced Green's function can be written in the spectral representation with the *same* spectral functions,

$$G^{R,A}_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = \lim_{\delta\to 0^+}\int_0^\infty d\omega' \left[\frac{A^+(\mathbf{r},\mathbf{r}';\omega')}{\omega-\mu/\hbar-\omega'\pm i\delta} + \frac{A^-(\mathbf{r},\mathbf{r}';\omega)}{\omega-\mu/\hbar+\omega'\pm i\delta}\right]. \tag{179}$$

This shows that all Green's functions can be constructed if A^+ and A^- are known! The spectral functions are a density of excited states ε_n, positive-definite, and obey the sum rule:

$$\begin{aligned}
&\int_0^\infty d\omega\ A(\mathbf{r},\mathbf{r}';\omega) \\
&= \int_0^\infty d\omega\ A^+(\mathbf{r},\mathbf{r}';\omega) + A^-(\mathbf{r},\mathbf{r}';\omega) \\
&= \sum_n \left[\langle\Psi_0|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle + \langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_n\rangle\,\langle\Psi_n|\,\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle \right] \\
&= \langle\Psi_0|\,\hat{\psi}_\alpha(\mathbf{r})\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle + \langle\Psi_0|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\hat{\psi}_\alpha(\mathbf{r})\,|\Psi_0\rangle \\
&= \langle\Psi_0|\left\{\hat{\psi}_\alpha(\mathbf{r}),\hat{\psi}^\dagger_\beta(\mathbf{r}')\right\}|\Psi_0\rangle = \delta(\mathbf{r},\mathbf{r}'),
\end{aligned} \tag{180}$$

and

$$\int d\mathbf{r}\int_0^\infty d\omega\ A(\mathbf{r},\mathbf{r};\omega) = \int d\mathbf{r}\int_0^\infty d\omega\ A^+(\mathbf{r},\mathbf{r};\omega) + A^-(\mathbf{r},\mathbf{r};\omega) = 1. \tag{181}$$

Free Particle—- With these definitions, we take a moment to obtain the Green's functions for a Fermi gas. The ground state of a Fermi gas $|\Phi_0\rangle$, as we saw in the section on second quantization, is characterized by all the momentum states being filled up to some momentum p_F, the Fermi momentum. In second quantized notation we recall is given by,

$$|\Phi_0\rangle = \Pi_{|\mathbf{p}|\le p_F,\sigma}\ \hat{a}^\dagger_{\mathbf{p}\sigma}\,|0\rangle\,.$$

We evaluate Eq. 151 and 170 and find:

$$G_{\sigma\sigma'}(\mathbf{p},\omega) = \delta_{\sigma\sigma'}\frac{\theta(\mathbf{p}-p_F)}{\omega-\varepsilon_{\mathbf{p}}+i\delta} + \frac{\theta(p_F-\mathbf{p})}{\omega-\varepsilon_{\mathbf{p}}-i\delta}, \tag{182a}$$

$$G^R_{\sigma\sigma'}(\mathbf{p},\omega) = \frac{\delta_{\sigma\sigma'}}{\omega-\varepsilon_{\mathbf{p}}+i\delta}, \tag{182b}$$

$$G^A_{\sigma\sigma'}(\mathbf{p},\omega) = \frac{\delta_{\sigma\sigma'}}{\omega-\varepsilon_{\mathbf{p}}-i\delta}. \tag{182c}$$

We can also define a function that is analytic everywhere except on the real line,

$$g_{\sigma\sigma'}(\mathbf{p},z) = \frac{\delta_{\sigma\sigma'}}{z-\varepsilon_{\mathbf{p}}}, \tag{183}$$

to generate each Green's function:

$$G^R_{\sigma\sigma'}(\mathbf{p},\omega) = g_{\sigma\sigma'}(\mathbf{p},\omega+i\delta), \tag{184a}$$

$$G^A_{\sigma\sigma'}(\mathbf{p},\omega) = g_{\sigma\sigma'}(\mathbf{p},\omega-i\delta), \tag{184b}$$

$$G_{\sigma\sigma'}(\mathbf{p},\omega) = g_{\sigma\sigma'}(\mathbf{p},\omega+i\delta\bar{f}(\omega-\varepsilon_F)), \tag{184c}$$

$$\tag{184d}$$

where

$$\bar{f}(\omega-\varepsilon_F) = \begin{cases} 1 & \omega > \varepsilon_F \\ -1 & \omega < \varepsilon_F \end{cases}. \tag{185}$$

Exercise 11. Prove Eqs. 182.

The spectral function is then given by

$$A_{\sigma\sigma'}(\mathbf{p},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G^R(\mathbf{p},\omega) = \delta_{\sigma\sigma'}\delta(\omega-\varepsilon_{\mathbf{p}}) \tag{186}$$

where the density of states is

$$A(\omega) = \sum_{\mathbf{p},\sigma} A_{\sigma\sigma}(\mathbf{p},\omega) = \sum_{\mathbf{p},\sigma}\delta(\omega-\varepsilon_{\mathbf{p}}) \tag{187}$$

and the total number of electrons in the system

$$N = \int_{-\infty}^{\infty} A(\omega). \tag{188}$$

What is a Quasi-particle?—- Many macroscopic systems, e.g., gases, liquids, and electrons in metals, behave as they are comprised of nearly independent particles.[30] How is this behavior manifest in the Green's function? Well in the absence of interactions G^R has a simple pole at $\omega = \varepsilon_{\mathbf{p}}$ and propagate undamped with a frequency of the free particle energy:

$$G^R(\mathbf{p},t-t') = -i(1-n_{\mathbf{p}})e^{-i\varepsilon_{\mathbf{p}}(t-t')}\theta(t-t'). \tag{189}$$

In the presence of interactions $A(\mathbf{p},\omega)$ will no longer be a simple delta function, but rather a broad distribution of energy and momenta determined by the magnitude of $\left|\langle\Psi_n|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle\right|^2$ and the energy spread of transitions $\langle\Psi_n|\,\hat{\psi}^\dagger_\beta(\mathbf{r}')\,|\Psi_0\rangle$. That is, since the system has many particles with excitation energy $\varepsilon_{\mathbf{p}}$ and momentum $\mathbf{p}$– think of the excitations about the Fermi surface–we expect these states to couple in the presence of interactions, yielding a spread of energies. As a result, the state must have a finite lifetime and its propagation in general must be damped.

So, under what circumstances is the notion of a quasi-particle viable? Well, we can say that if

$$G^R(\mathbf{p},t-t') = -iZ_{\mathbf{p}}e^{-i\tilde{\varepsilon}_{\mathbf{p}}(t-t')}e^{-\Gamma_{\mathbf{p}}(t-t')}\theta(t-t'). \tag{190}$$

for some positive length of time $(t-t')$ then the notion of a quasi-particle would appear justified since it describes the propagation of a state of energy $\tilde{\varepsilon}_{\mathbf{p}}$ and strength $Z_{\mathbf{p}}$ which persists for time $\tau \sim \Gamma_{\mathbf{p}}^{-1}$. Furthermore, to obtain Eq. 190 the spectral function must take the form,

$$A(\mathbf{p},\omega) = \frac{iZ_{\mathbf{p}}/2\pi}{\omega-\tilde{\varepsilon}_{\mathbf{p}}+i\Gamma_{\mathbf{p}}} + \text{incoherent background}, \tag{191}$$

a Lorentzian sitting on top of a incoherent background, similar to that in Fig. 10. If we now evaluate

$$G^R(\mathbf{p},t-t') = -i\int_0^\infty d\omega\; A(\mathbf{p},\omega)e^{-i(\omega+\mu)(t-t')}\theta(t-t'), \tag{192}$$

by closing the contour in the lower half ω-plane we obtain the contribution to $G(\mathbf{p},t-t')$ from the peak that is that given in Eq. 190 and an incoherent part from

[30] For a more detailed introduction, you are highly encouraged to read the short articles by J.R. Schrieffer[14] and David Pines[11].

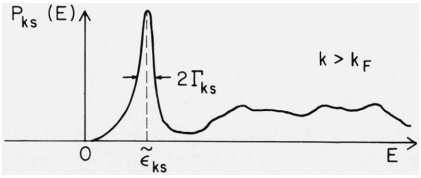

Figure 10
Probability distribution $A(\mathbf{p},\omega)$ for a quasi-particle corresponding to a bare Bloch state $\mathbf{p}$ for $\mathbf{p} > \mathbf{p}_F$. Adapted from [14].

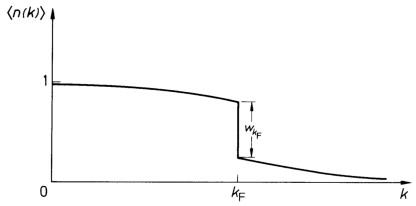

Figure 11
. The average particle number per unit volume in momentum space for a normal interacting Fermi system at $T = 0$ K. k_F is the Fermi momentum. Adapted from [3].

the background. This calculation is not trivial and is only sketched in many of the books listed at the beginning of these notes.

As a consequence, the discontinuity in the momentum distribution of particles [Fig. 11] is equal to $Z_{\mathbf{p}}$, implying that $0 \leq Z_{\mathbf{p}} \leq 1$, where $Z_{\mathbf{p}} = 1$ is the normal non-interacting system and as interactions are increased we find $Z_{\mathbf{p}} \to 0$ suggesting that the notion of a quasi-particle is lost. Additionally, this is also seen in

$$\int_{-\infty}^{\infty} A_{\text{Lorentzian}}(\mathbf{p}, \omega) = Z_{\mathbf{p}}, \tag{193}$$

suggesting that the peak, or quasi-particle, melts into the incoherent background as $Z_{\mathbf{p}} \to 0$.

Existence of the Self-Energy—- Let us examine the quasi-particle propagator (Eq. 190) in frequency space a bit further. can we connect the interacting Green's function to the free Green's function? Well we start with Eq. 190 in momentum space,

$$\begin{aligned} G^R(\mathbf{p}, \omega) &= \frac{Z_{\mathbf{p}}}{\omega - \tilde{\varepsilon}_{\mathbf{p}} + i\Gamma_{\mathbf{p}}} \\ &= \left[\frac{\omega}{Z_{\mathbf{p}}} - \frac{\tilde{\varepsilon}_{\mathbf{p}}}{Z_{\mathbf{p}}} + i\frac{\Gamma_{\mathbf{p}}}{Z_{\mathbf{p}}}\right]^{-1} \\ &= \left[\omega - \omega + \frac{\omega}{Z_{\mathbf{p}}} - \frac{\tilde{\varepsilon}_{\mathbf{p}}}{Z_{\mathbf{p}}} + i\frac{\Gamma_{\mathbf{p}}}{Z_{\mathbf{p}}}\right]^{-1} \\ &= \left[\omega - \left(1 - \frac{1}{Z_{\mathbf{p}}}\right)\omega - \frac{\tilde{\varepsilon}_{\mathbf{p}}}{Z_{\mathbf{p}}} + i\frac{\Gamma_{\mathbf{p}}}{Z_{\mathbf{p}}}\right]^{-1} \\ &= \left[\omega - \varepsilon_{\mathbf{p}} - \Sigma(\mathbf{p}, \omega)\right]^{-1} \\ &= \left[G_0(\mathbf{p}, \omega) - \Sigma(\mathbf{p}, \omega)\right]^{-1} \end{aligned} \tag{194}$$

where the last line connecting the interacting and free Green's function,

$$G_0^R(\mathbf{p}, \omega) = \frac{1}{\omega - \varepsilon_{\mathbf{p}} + i\delta}, \tag{195}$$

is the so-called Dyson's equation:

$$G^R(\mathbf{p}, \omega) = G_0^R(\mathbf{p}, \omega) + G_0^R(\mathbf{p}, \omega)\Sigma(\mathbf{p}, \omega)G^R(\mathbf{p}, \omega). \tag{196}$$

Importantly, the function connecting these two is the *self-energy*:

$$\Sigma(\mathbf{p}, \omega) = \left(1 - \frac{1}{Z_{\mathbf{p}}}\right)\omega + i\frac{\Gamma_{\mathbf{p}}}{Z_{\mathbf{p}}}. \tag{197}$$

The self energy connects the interacting and free Green's functions by describing the effect of the interacting many-particle environment on the single particle states. In particular, the real part of $\Sigma(\mathbf{p}, \omega)$ around $\omega = 0$ determines how the energy eigenvalues shift due to interactions, as compared to the non-interacting $\varepsilon_{\mathbf{p}}$, and the imaginary part determines the broadening of the spectral function, or how the excitation decays in time. The form found here may be obtained via perturbation theory, with the general self-energy being a complicated function.

The S Matrix

So far we have seen that observables may be written in terms of Green's functions and we have explored the resulting analytic properties. However, all of this has been pursued within the Heisenberg picture where $|\Psi_H\rangle$ state vectors are unknown because $\hat{H}$ is not solvable when interactions are present. In fact this is the very information we are trying to obtain from the Green's functions approach! To move forward, we recall that $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ is solvable. So we can use the interaction picture to recast the problem.

We know

$$|\Psi_H\rangle = |\Psi_S(0)\rangle = |\Psi_I(0)\rangle\,, \tag{198}$$

so we connect $|\Psi_H\rangle$ to that in the interaction picture at some time before to recover the ground state wave function. To accomplish this, we adiabatically switch the interactions on using

$$\hat{H} = \hat{H}_0 + e^{-|\varepsilon|t}V \tag{199}$$

so that

$$|\Psi_H\rangle = \hat{U}_I(0,-\infty)\,|\phi_0\rangle \tag{200}$$

where $|\phi_0\rangle$ is the ground state of $\hat{H}_0$. This means we can rewrite the Green's function as

$$\begin{aligned}
iG(\mathbf{r}t,\mathbf{r}'t') &= \frac{\langle\Psi_H|\,\mathcal{T}\left\{\hat{\psi}_H(\mathbf{r}t)\hat{\psi}_H^\dagger(\mathbf{r}'t')\right\}|\Psi_H\rangle}{\langle\Psi_H|\Psi_H\rangle} \\
&= \frac{\langle\phi_0|\,\hat{U}_I(\infty,0)\mathcal{T}\left\{\hat{\psi}_H(\mathbf{r}t)\hat{\psi}_H^\dagger(\mathbf{r}'t')\right\}\hat{U}_I(0,-\infty)\,|\phi_0\rangle}{\langle\phi_0|\hat{U}_I(\infty,-\infty)|\phi_0\rangle} \\
&= \frac{\langle\phi_0|\,\hat{U}_I(\infty,0)\mathcal{T}\left\{\hat{U}_I(0,t)\hat{\psi}_I(\mathbf{r}t)\hat{U}_I(t,0)\hat{U}_I(0,t')\hat{\psi}_I^\dagger(\mathbf{r}'t')\hat{U}_I(t',0)\right\}\hat{U}_I(0,-\infty)\,|\phi_0\rangle}{\langle\phi_0|\hat{U}_I(\infty,-\infty)|\phi_0\rangle} \\
&= \frac{\langle\phi_0|\,\mathcal{T}\left\{\hat{U}_I(\infty,t)\hat{\psi}_I(\mathbf{r}t)\hat{U}_I(t,t')\hat{\psi}_I^\dagger(\mathbf{r}'t')\hat{U}_I(t',-\infty)\right\}|\phi_0\rangle}{\langle\phi_0|\hat{U}_I(\infty,-\infty)|\phi_0\rangle} \\
&= \frac{\langle\phi_0|\,\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I(\mathbf{r}t)\hat{\psi}_I^\dagger(\mathbf{r}'t')\right\}|\phi_0\rangle}{\langle\phi_0|\hat{U}_I(\infty,-\infty)|\phi_0\rangle},
\end{aligned} \tag{201}$$

with

$$\hat{U}_I(\infty,-\infty) = \mathcal{T}\left\{e^{-i\int_{-\infty}^{\infty}d\bar{t}\;V_I(\bar{t})}\right\}. \tag{202}$$

Where we have used

$$\hat{O}_H(t) = \hat{U}_I(0,t)\hat{O}_I(t)\hat{U}_I(t,0) \tag{203}$$

and the definition of the time ordering operator to place all time evolution operators are the appropriate places.

Example 12. If $V = 0$, then $G \to G_0$,

$$\frac{\langle\phi_0|\,\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I(\mathbf{r}t)\hat{\psi}_H^\dagger(\mathbf{r}'t')\right\}|\phi_0\rangle}{\langle\phi_0|\hat{U}_I(\infty,-\infty)|\phi_0\rangle} \to \frac{\langle\phi_0|\,\mathcal{T}\left\{\hat{\psi}_I(\mathbf{r}t)\hat{\psi}_H^\dagger(\mathbf{r}'t')\right\}|\phi_0\rangle}{\langle\phi_0|\phi_0\rangle}. \tag{204}$$

So how do we calculate G? There are several methods including:

1. Perturbation Theory (Diagrammatics):

   Here, we expand $\hat{U}_I$ to various orders in $\hat{V}_I$,

$$\begin{aligned}\hat{U}_I(\infty,-\infty) &= \mathcal{T}\left\{e^{-i\int_{-\infty}^{\infty}d\bar{t}\;V_I(\bar{t})}\right\} \\ &= \sum_{n=0}^{\infty}(-i)^n\frac{1}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_n\;\mathcal{T}\left\{V_I(\bar{t}_1)\cdots V_I(\bar{t}_n)\right\}\end{aligned} \tag{205}$$

   yielding,

$$\begin{aligned}&iG(\mathbf{r}t,\mathbf{r}'t') = \\ &\sum_{n=0}^{\infty}(-i)^n\frac{1}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_n\;\frac{\langle\phi_0|\,\mathcal{T}\left\{V_I(\bar{t}_1)\cdots V_I(\bar{t}_n)\hat{\psi}_I(\mathbf{r}t)\hat{\psi}_H^\dagger(\mathbf{r}'t')\right\}|\phi_0\rangle}{\langle\phi_0|\hat{U}(\infty,-\infty)|\phi_0\rangle}.\end{aligned} \tag{206}$$

2. Equation of Motion
3. Functional Methods (in principle non-perturbative):
   (a) Coherent Path Integrals
   (b) Schwinger Derivative Technique

In the next section we will use the equation of motion of G in conjunction with Schwinger derivative technique to obtain a set of self-consistent equations for G.

Green's Function Equation of Motion & Hedin's Equations

As we have seen, the many-body Hamiltonian in second quantization takes the form:

$$H = \int d\mathbf{r}\;\hat{\psi}^\dagger(\mathbf{r})\left(\frac{-\hbar^2\nabla^2}{2m} + V_{ne}(\mathbf{r})\right)\hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}). \tag{207}$$

Where we have included the nuclear-electron potential V_{ne}. To find the equation of motion for G, we start by considering the Heisenberg equation of motion for the annihilation operator in the Heisenberg picture,

$$-i\frac{\partial\hat{\psi}_H(1)}{\partial t_1} = \left[\hat{H}_H(1),\hat{\psi}_H(1)\right] \tag{208}$$

where we have used the short hand $1 \equiv \mathbf{r}_1 t_1$. To evaluate this, we first inserting the definition of Heisenberg operators

$$\left[\hat{H}_H(1),\hat{\psi}_H(1)\right] = e^{i\hat{H}t_1}\left[\hat{H},\hat{\psi}(\mathbf{r}_1)\right]e^{-i\hat{H}t_1} \tag{209}$$

and then compute the commutator of $\hat{H}$ and $\hat{\psi}(\mathbf{r}_1)$ term by term:

$$\begin{aligned}
\left[\hat{H}_{\text{kinetic}}, \hat{\psi}(\mathbf{r}_1)\right] &= \int d\mathbf{r}\ \left[\hat{\psi}^\dagger(\mathbf{r})\hat{h}(\mathbf{r})\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}_1)\right] \\
&= \int d\mathbf{r}\ \left(\hat{\psi}^\dagger(\mathbf{r})\cancelto{0}{\left\{\hat{h}(\mathbf{r})\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}_1)\right\}} - \left\{\hat{\psi}^\dagger(\mathbf{r})\hat{h}(\mathbf{r}), \hat{\psi}(\mathbf{r}_1)\right\}\hat{\psi}(\mathbf{r})\right) \\
&= -\int d\mathbf{r}\ \delta(\mathbf{r}-\mathbf{r}_1)\hat{h}(\mathbf{r})\hat{\psi}(\mathbf{r}) \\
&= -\hat{h}(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_1) \qquad (210)
\end{aligned}$$

and

$$\begin{aligned}
&\left[\hat{H}_{\text{int}}, \hat{\psi}(\mathbf{r}_1)\right] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\left[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}_1)\right] \\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\left(\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\cancelto{0}{\left[\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}_1)\right]} + \left[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}'), \hat{\psi}(\mathbf{r}_1)\right]\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\right) \\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\left(\hat{\psi}^\dagger(\mathbf{r})\left\{\hat{\psi}^\dagger(\mathbf{r}'), \hat{\psi}(\mathbf{r}_1)\right\} - \left\{\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}(\mathbf{r}_1)\right\}\hat{\psi}^\dagger(\mathbf{r}')\right)\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) \\
&= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\ \left(V(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\delta(\mathbf{r}'-\mathbf{r}_1) - V(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_1)\right) \\
&= \frac{1}{2}\int d\mathbf{r}\ V(\mathbf{r},\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}_1)\hat{\psi}(\mathbf{r}) - \frac{1}{2}d\mathbf{r}'\ V(\mathbf{r}_1,\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}_1) \\
&= \int d\mathbf{r}\ V(\mathbf{r},\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}_1)\hat{\psi}(\mathbf{r}) \qquad (211)
\end{aligned}$$

where moving to the last line we changed dummy variables $\mathbf{r}' \to \mathbf{r}$, used particle indistinguishability and hermiticity of $V(\mathbf{r},\mathbf{r}') = V(\mathbf{r}',\mathbf{r})$, and swapped the annihilation operators in the second term to combine integrands.

The equation of motion for $\hat{\psi}(1)$ then becomes

$$\begin{aligned}
&-i\frac{\partial\hat{\psi}_H(1)}{\partial t_1} = e^{i\hat{H}t_1}\left(-\hat{h}(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_1) + \int d\mathbf{r}\ V(\mathbf{r},\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}_1)\hat{\psi}(\mathbf{r})\right)e^{-i\hat{H}t_1} \\
&= -e^{i\hat{H}t_1}\hat{h}(\mathbf{r}_1)e^{-i\hat{H}t_1}e^{i\hat{H}t_1}\hat{\psi}(\mathbf{r}_1)e^{-i\hat{H}t_1} \\
&+ \int d\mathbf{r}\ V(\mathbf{r},\mathbf{r}_1)e^{i\hat{H}t_1}\hat{\psi}^\dagger(\mathbf{r})e^{-i\hat{H}t_1}e^{i\hat{H}t_1}\hat{\psi}(\mathbf{r}_1)e^{-i\hat{H}t_1}e^{i\hat{H}t_1}\hat{\psi}(\mathbf{r})e^{-i\hat{H}t_1} \\
&= -\hat{h}_H(1)\hat{\psi}_H(1) + \int d\mathbf{r}\ V(\mathbf{r},\mathbf{r}_1)\hat{\psi}_H^\dagger(\mathbf{r}t_1)\hat{\psi}_H(1)\hat{\psi}_H(\mathbf{r}t_1) \\
&= -\hat{h}_H(1)\hat{\psi}_H(1) + \int d\mathbf{r}\int dt_3\ V(\mathbf{r},\mathbf{r}_1)\delta(t_1-t_3)\hat{\psi}_H^\dagger(\mathbf{r}t_3)\hat{\psi}_H(1)\hat{\psi}_H(\mathbf{r}t_3) \\
&= -\hat{h}_H(1)\hat{\psi}_H(1) + \int d3\ V(3,1)\hat{\psi}_H^\dagger(3)\hat{\psi}_H(1)\hat{\psi}_H(3) \qquad (212)
\end{aligned}$$

where we introduced the shorthands $V(3,1) \equiv V(\mathbf{r},\mathbf{r}_1)\delta(t_1-t_3)$ and $\int d\mathbf{r}\int dt_3 \equiv \int d3$. Now, we multiply from the right hand side by $\hat{\psi}_H^\dagger(2)$ and take the time ordered expectation value of this expression to yield:

$$-i\left\langle\Psi_H\right|\mathcal{T}\left\{\frac{\partial\hat{\psi}_H(1)}{\partial t_1}\hat{\psi}_H^\dagger(2)\right\}\left|\Psi_H\right\rangle = -\hat{h}_H(1)\left\langle\Psi_H\right|\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}\left|\Psi_H\right\rangle$$

$$+\int d3\; V(3,1)\,\langle\Psi_H|\,\mathcal{T}\left\{\hat{\psi}_H^\dagger(3)\hat{\psi}_H(1)\hat{\psi}_H(3)\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle\,. \tag{213}$$

Here, we recognize the single-particle Green's function

$$iG(1,2) = \langle\Psi_H|\,\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle \tag{214}$$

and define the 2-particle Green's function

$$i^2G^{(2)}(1,3,3^+,2) = \langle\Psi_H|\,\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H(3)\hat{\psi}_H^\dagger(3^+)\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle \tag{215}$$

where $3^+ = t_3 + 0^+$ to ensure we recover the correct ordering $\hat{\psi}_H^\dagger(3)\hat{\psi}_H(3)$ under the time ordering operator. To obtain G on the left-hand side of Eq. 213 we examine the action of the time derivative on the single particle Green's function. That is,

$$\begin{aligned}
i\frac{\partial}{\partial t_1}G(1,2) &= \frac{\partial}{\partial t_1}\left(\langle\Psi_H|\,\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\,|\Psi_H\rangle\,\theta(1,2) - \langle\Psi_H|\,\hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\,|\Psi_H\rangle\,\theta(2,1)\right)\\
&= \langle\Psi_H|\,\frac{\partial}{\partial t_1}\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\,|\Psi_H\rangle\,\theta(1,2) + \langle\Psi_H|\,\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\,|\Psi_H\rangle\,\frac{\partial}{\partial t_1}\theta(1,2)\\
&- \langle\Psi_H|\,\hat{\psi}_H^\dagger(2)\frac{\partial}{\partial t_1}\hat{\psi}_H(1)\,|\Psi_H\rangle\,\theta(2,1) - \langle\Psi_H|\,\hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\,|\Psi_H\rangle\,\frac{\partial}{\partial t_1}\theta(2,1)\\
&= \delta(t-t')\,\langle\Psi_H|\left(\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) + \hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\right)|\Psi_H\rangle\\
&+ \langle\Psi_H|\,\frac{\partial}{\partial t_1}\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\,|\Psi_H\rangle\,\theta(1,2) - \langle\Psi_H|\,\hat{\psi}_H^\dagger(2)\frac{\partial}{\partial t_1}\hat{\psi}_H(1)\,|\Psi_H\rangle\,\theta(2,1)\\
&= \delta(t_1-t_2)\,\langle\Psi_H|\left\{\hat{\psi}_H(1),\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle + \langle\Psi_H|\,\mathcal{T}\left\{\frac{\partial}{\partial t_1}\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle\\
&= \delta(t_1-t_2)\delta(\mathbf{r}_1-\mathbf{r}_2) + \langle\Psi_H|\,\mathcal{T}\left\{\frac{\partial}{\partial t_1}\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle
\end{aligned} \tag{216}$$

where we used $\frac{\partial\theta(1,2)}{\partial t_1} = -\frac{\partial\theta(2,1)}{\partial t_1} = \delta(t_1-t_2)$ and the canonical quantization of the creation and annihilation operators. Inserting this into Eq. 213,

$$\begin{aligned}
-i\left(i\frac{\partial}{\partial t_1}G(1,2) - \delta(1,2)\right) &= -\hat{h}_H(1)iG(1,2) + \int d3\; V(3,1)(i)^2G(1,3,3^+,2)\\
i\left(\frac{\partial}{\partial t_1}G(1,2) + i\hat{h}_H(1)G(1,2) &= -i\delta(1,2) + \int d3\; V(3,1)(i)^2G(1,3,3^+,2)\right)\\
\left(i\frac{\partial}{\partial t_1} - \hat{h}_H(1)\right)G(1,2) &= \delta(1,2) - i\int d3\; V(3,1)G(1,3,3^+,2).
\end{aligned} \tag{217}$$

Here G is defined in terms of $G^{(2)}$ and if we derived the equation of motion for $G^{(2)}$ it will depend on $G^{(3)}$, and so on. This is the so-called Martin-Schwinger hierarchy. To move forward, we could truncate this hierarchy, but this is not a controlled approximation. Alternatively, we could expand each $G^{(n)}$ into its non-interacting parts and do diagrammatic perturbation theory. Here, we will take an alterative path originally used by Julian Schwinger in QED and adapted by Lars Hedin in condensed matter.

Namely, we convert $iG(1,2) = \langle\Psi_H|\,\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}|\Psi_H\rangle$ to the interaction picture, but we do not partition the Hamiltonian into non-interacting and interacting,

instead we insert a perturbing field:

$$\hat{H} \to \hat{\tilde{H}} = \hat{H} + \hat{\pi} \tag{218}$$

where $\hat{H}$ is the full interacting Hamiltonian and $\hat{\pi}$ is the perturbing field. $\hat{\pi}$ is arbitrary and will be set to zero at the end of the analysis so that $\hat{U}_I(\infty, -\infty) \to 1$, $\hat{\psi}_I \to \hat{\psi}_H$, and $|\Psi_I\rangle \to |\Psi_H\rangle$. So,

$$iG(1,2) = \frac{\langle \Psi_I | \mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I(1)\hat{\psi}_I^\dagger(2)\right\}|\Psi_I\rangle}{\langle \Psi_I|\hat{U}(\infty,-\infty)|\Psi_I\rangle} \tag{219}$$

with

$$\hat{U}_I(\infty,-\infty) = \mathcal{T}\left\{e^{-i/\hbar\int_{-\infty}^{\infty} d4\ \hat{\psi}_I^\dagger(4)\pi(4)\hat{\psi}_I(4)}\right\}. \tag{220}$$

We will now take the functional derivative of G with respect to π. To do this we just need $\frac{\delta \hat{U}_I}{\delta\pi}$ since the operators do not depend on π. So we have,

$$\begin{aligned}
\frac{\delta \hat{U}_I(\infty,-\infty)}{\delta\pi(3)} &= \frac{\delta}{\delta\pi(3)}\mathcal{T}\left\{e^{-i/\hbar\int_{-\infty}^{\infty} d4\ \hat{\psi}_I^\dagger(4)\pi(4)\hat{\psi}_I(4)}\right\} \\
&= \mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\,(-i/\hbar)\int_{-\infty}^{\infty} d4\ \hat{\psi}_I^\dagger(4)\frac{\delta\pi(4)}{\delta\pi(3)}\hat{\psi}_I(4)\right\} \\
&= (-i/\hbar)\,\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I^\dagger(3)\hat{\psi}_I(3)\right\}
\end{aligned} \tag{221}$$

and

$$\begin{aligned}
i\frac{\delta G(1,2)}{\delta\pi(3)} &= \frac{\delta}{\delta\pi(3)}\left(\frac{\langle\Psi_I|\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I(1)\hat{\psi}_I^\dagger(2)\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle}\right) \\
&= \frac{\langle\Psi_I|\mathcal{T}\left\{\frac{\delta\hat{U}_I(\infty,-\infty)}{\delta\pi(3)}\hat{\psi}_I(1)\hat{\psi}_I^\dagger(2)\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle} \\
&- \frac{\langle\Psi_I|\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I(1)\hat{\psi}_I^\dagger(2)\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle}\frac{\langle\Psi_I|\mathcal{T}\left\{\frac{\delta\hat{U}_I(\infty,-\infty)}{\delta\pi(3)}\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle} \\
&= -i\frac{\langle\Psi_I|\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I^\dagger(3)\hat{\psi}_I(3)\hat{\psi}_I(1)\hat{\psi}_I^\dagger(2)\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle} \\
&- (-i)\frac{\langle\Psi_I|\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I(1)\hat{\psi}_I^\dagger(2)\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle}\frac{\langle\Psi_I|\mathcal{T}\left\{\hat{U}_I(\infty,-\infty)\hat{\psi}_I^\dagger(3)\hat{\psi}_I(3)\right\}|\Psi_I\rangle}{\langle\Psi_I|\hat{U}_I(\infty,-\infty)|\Psi_I\rangle} \\
&= -i(-1)i^2G^{(2)}(1,3,3^+,2) - (-i)iG(1,2)(-1)iG(3,3^+) \\
&= -iG^{(2)}(1,3,3^+,2) + iG(1,2)G(3,3^+)
\end{aligned} \tag{222}$$

We have re-written the 2-particle Green's function in terms of the single-particle Green's function and its derivative! This means the equation of motion is:

$$\left(i\frac{\partial}{\partial t_1} - \hat{h}_H(1) - \pi(1)\right)G(1,2) = \delta(1,2) - i\int d3\ V(3,1)\left(G(1,2)G(3,3^+) - \frac{\delta G(1,2)}{\delta\pi(3)}\right)$$

$$= \delta(1,2) - i\int d3\; V(3,1)G(1,2)G(3,3^+) + i\int d3\; V(3,1)\frac{\delta G(1,2)}{\delta\pi(3)} \tag{223}$$

To massage this further, we use two facts, (i) since $G(1,4)G^{-1}(4,2) = \delta(1,2)$ we can rewrite the functional derivative in terms of G^{-1},

$$\begin{aligned}\frac{\delta\left(G(1,4)G^{-1}(4,2)\right)}{\delta\pi(3)} &= 0 \\ \implies \frac{\delta G(1,2)}{\delta\pi(3)} &= -G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)}G(5,2),\end{aligned} \tag{224}$$

and (ii) we recognize $iG(3,3^+) = -\rho(3)$ as the particle density, with

$$\int d3\; \rho(3)V(3,1) = V_H(1) \tag{225}$$

being the Hartree Potential. Thus the equation of motion can be written as:

$$\begin{aligned}&\left(i\frac{\partial}{\partial t_1} - \hat{h}_H(1) - \pi(1)\right)G(1,2) = \delta(1,2) \\ &+ \left(V_H(1)\delta(1,5) - i\int d3\; V(3,1)G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)}\right)G(5,2).\end{aligned} \tag{226}$$

Comparing Eq. 226 to Eq. 196 we find the free Green's function to be

$$G_0^{-1}(1,2) = \left(i\frac{\partial}{\partial t_1} - \hat{h}_H(1) - \pi(1)\right)\delta(1,2) \tag{227}$$

with the exact self-energy given by

$$\bar{\Sigma}(1,4) = \; V_H(1)\delta(1,5) - i\int d3\; V(3,1)G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)} \tag{228}$$

where $\bar{\Sigma}(1,4)$ is composed of a Hartree self-energy $\Sigma_H(1,4)$ and a self-energy arising from exchange-correlation effects $\Sigma_{xc}(1,4)$. Therefore, Dyson's equation is

$$\begin{aligned}&G_0^{-1}(1,3)G(3,2) = \delta(1,2) + \bar{\Sigma}(1,5)G(5,2), \\ &G(3,2) = G_0(1,2) + G_0(1,4)\bar{\Sigma}(4,5)G(5,2).\end{aligned} \tag{229}$$

Typically, the Hartree contribution is included with the free Green's function

$$G_H^{-1}(1,2) = \left(i\frac{\partial}{\partial t_1} - \hat{h}_H(1) - \pi(1) - V_H(1)\right)\delta(1,2) \tag{230}$$

the with the self-energy defined in this case as

$$\Sigma(1,4) = -i\int d3\; V(3,1)G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)}. \tag{231}$$

Furthermore, we can set up an iterative solution for Σ by,

$$\Sigma(1,4) = -i\int d3\; V(3,1)G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)}$$

$$
\begin{aligned}
&= -i \int d3\; V(3,1) G(1,4) \frac{\delta \left(G_0^{-1}(4,5) - \Sigma(4,5) \right)}{\delta \pi(3)} \\
&= -i \int d3\; V(3,1) G(1,4) \left(\frac{\delta G_0^{-1}(4,5)}{\delta \pi(3)} - \frac{\delta \Sigma(4,5)}{\delta \pi(3)} \right) \\
&= -i \int d3\; V(3,1) G(1,4) \left(-\frac{\delta V_H(4)}{\delta \pi(3)} \delta(4,5) - \delta(4,3)\delta(4,5) - \frac{\delta \Sigma(4,5)}{\delta \pi(3)} \right) \\
&= +iV(5,1)G(1,5) + i \int d3\; V(3,1) G(1,5) \frac{\delta V_H(5)}{\delta \pi(3)} + i \int d3\; V(3,1) G(1,4) \frac{\delta \Sigma(4,5)}{\delta \pi(3)}.
\end{aligned} \tag{232}
$$

This is an iterative equation for the self-energy which provides a procedure for making an expansion of the self-energy in powers of the Coulomb interaction.

Example 13. Find Σ to second order in V?

First, we need to determine $\frac{\delta V_H}{\delta \pi}$,

$$
\begin{aligned}
\frac{\delta V_H(5)}{\delta \pi(3)} &= \int d9\; \frac{\delta \rho(9)}{\delta \pi(3)} V(9,5) = -i \int d9\; \frac{\delta G(9,9^+)}{\delta \pi(3)} V(9,5) \\
&= +i \int d9\; G(9,10) \frac{\delta G^{-1}(10,11)}{\delta \pi(3)} G(11,9^+) V(9,5)
\end{aligned} \tag{233}
$$

to first order in V, $\frac{\delta G^{-1}(10,11)}{\delta \pi(3)} \approx -\delta(10,3)\delta(10,11)$, meaning

$$
\frac{\delta V_H(5)}{\delta \pi(3)} \approx -i \int d9\; G(9,3) G(3,9^+) V(9,5). \tag{234}
$$

Then $\frac{\delta \Sigma(4,5)}{\delta \pi(3)}$ to first order in V is

$$
\begin{aligned}
\frac{\delta \Sigma(4,5)}{\delta \pi(3)} &= +iV(5,4) \frac{\delta G(4,5)}{\delta \pi(3)} \\
&= -iV(5,4) G(4,13) \frac{\delta G^{-1}(13,14)}{\delta \pi(3)} G(14,5) \\
&\approx +iV(5,4) G(4,3) G(3,5).
\end{aligned} \tag{235}
$$

Therefore, Σ to second order in V is given by:

$$
\begin{aligned}
\Sigma^{(2)}(1,4) \approx &+ iV(5,1)G(1,5) \\
&+ i \int d3\; V(3,1) G(1,5) \left(-i \int d9\; G(9,3) G(3,9^+) V(9,5) \right) \\
&+ i \int d3\; V(3,1) G(1,4) \left(+iV(5,4) G(4,3) G(3,5) \right), \\
= &+ iV(5,1)G(1,5) \\
&- \int d3 \int d9\; iV(3,1) G(1,5) G(9,3) G(3,9^+) iV(9,5) \\
&+ \int d3\; iV(3,1) G(1,4) iV(5,4) G(4,3) G(3,5).
\end{aligned} \tag{236}
$$

A diagrammatic representation of $\Sigma(1,4)$ is given in Fig. 12.

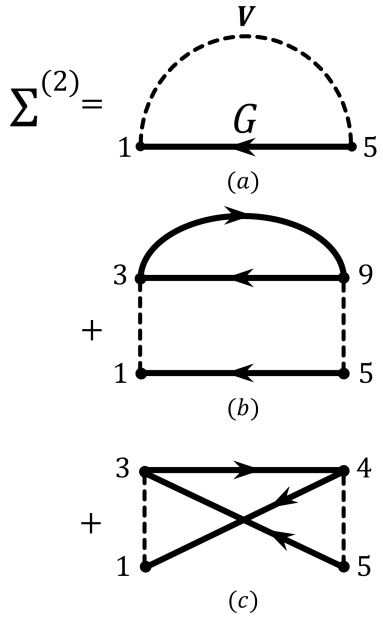

Figure 12
Diagrammatic representation of the various contributions to the second order in V self-energy: (a) first-order exchange, (b) 2-rung ladder, and (c) second-order exchange.

The Schwinger derivative technique has several advantages over the conventional diagrammatic technique. The iterative equation for the self-energy is *exact* and it allows us to generate all the terms of in the perturbation expansion without the need to enumerate the topologically distinct and connected diagrams, and employ Wick's Theorem. Moreover, the ground state in the definition of the green's function in the interacting picture is the exact interacting ground state. There is no assumption of adiabatic switching of the Coulomb interaction from $t = \pm\infty$ to $t = 0$ needed to make a one-to-one connection between the non-interacting and the interacting ground state. The probing field in the functional derivative technique can be large and rapidly varying in time. Its role is to perturb the system to elicit a response, not to connect non-interacting and interacting ground states. Thus, the Schwinger derivative technique provides a simple and elegant way of deriving the Self-energy.

The self-energy in Eq. 232 is given in terms of the bare Coulomb interaction V. This requires a large number of terms which converge very slowly in solids, thereby leading to nonphysical results. The reason is that screening effects in solids are of great importance. It was proposed by Lars Hedin to expand the self-energy in powers of the *screened* interaction W rather than the bare Coulomb interaction. The resulting set of equations provide a powerful basis for the examination of the electronic structure of quantum matter from first principles.

The key is to take the derivative with respect to the total potential $\Phi = \pi + V_H$ rather than π alone. This means,

$$\begin{aligned}\Sigma(1,4) &= -i\int d3\; V(3,1)G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)},\\ &= -i\int d3\; V(3,1)G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\Phi(6)}\frac{\delta\Phi(6)}{\delta\pi(3)}\end{aligned} \tag{237}$$

where the ratio of the total field to the applied field $\frac{\delta\Phi(6)}{\delta\pi(3)}$ is the longitudinal dielectric function $\varepsilon^{-1}(6,3)$. Furthermore, we can define the screened interaction as

$$W(6,1) = \frac{\delta\Phi(6)}{\delta\pi(3)}V(3,1) = \varepsilon^{-1}(6,3)V(3,1), \tag{238}$$

and if we use the chain rule, we can obtain an iterative equation for W as,

$$\begin{aligned}W(6,1) &= \left(\frac{\delta\pi(6)}{\delta\pi(3)} + \frac{\delta V_H(6)}{\delta\pi(3)}\right)V(3,1),\\ &= \left(\delta(6,3) + \frac{\delta\rho(4)}{\delta\pi(3)}V(4,6)\right)V(3,1),\\ &= \left(\delta(6,3) + V(6,4)\frac{\delta\rho(4)}{\delta\Phi(7)}\frac{\delta\Phi(7)}{\delta\pi(3)}\right)V(3,1),\\ &= V(6,1) + V(6,4)P(4,7)W(7,1).\end{aligned} \tag{239}$$

In the process of obtaining W, we defined the polarizability

$$P(4,7) = \frac{\delta\rho(4)}{\delta\Phi(7)} = -i\frac{\delta G(4,4^+)}{\delta\Phi(7)}$$

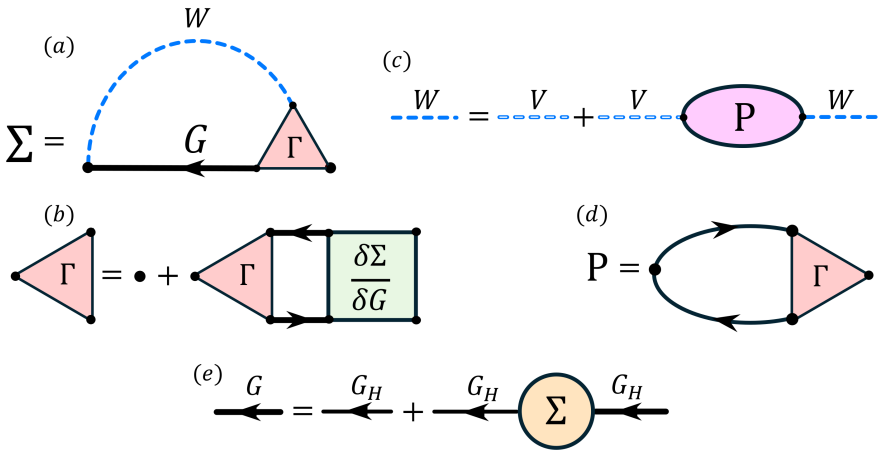

Figure 13: Diagrammatic representation of Hedin's five equations: (a) self-energy, (b) vertex function, (c) screen interaction, (d) polarizability, and (e) Dyson's equation.

$$= +iG(4,8)\frac{\delta G^{-1}(8,9)}{\delta\Phi(7)}G(9,4^+)$$
$$= -iG(4,8)\Gamma(8,9;7)G(9,4^+) \tag{240}$$

and the vertex function $\frac{\delta G^{-1}}{\delta\Phi}$ in Σ and P can be written as:

$$\begin{aligned}
\Gamma(4,5;6) &= -\frac{\delta G^{-1}(4,5)}{\delta\Phi(6)} = -\left(\frac{\delta G_H^{-1}(4,5)}{\delta\Phi(6)} - \frac{\delta\Sigma(4,5)}{\delta\Phi(6)}\right) \\
&= -\left(\frac{\delta G_H^{-1}(4,5)}{\delta\Phi(6)} - \frac{\delta\Sigma(4,5)}{\delta\Phi(6)}\right) \\
&= \delta(4,6)\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta\Phi(6)} \\
&= \delta(4,6)\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}\frac{\delta G(7,8)}{\delta\Phi(6)} \\
&= \delta(4,6)\delta(4,5) - \frac{\delta\Sigma(4,5)}{\delta G(7,8)}G(7,9)\frac{\delta G^{-1}(9,10)}{\delta\Phi(6)}G(10,8) \\
&= \delta(4,6)\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}G(7,9)G(10,8)\Gamma(9,10,6).
\end{aligned} \tag{241}$$

So all together, we have a set of 5 self consistent equations, the so-called Hedin's equations:

$$\Sigma(1,5) = -iW(6,1)G(1,4)\Gamma(4,5;6), \tag{242}$$
$$\Gamma(4,5;6) = \delta(4,6)\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}G(7,9)G(10,8)\Gamma(9,10,6), \tag{243}$$
$$W(6,1) = V(6,1) + V(6,4)P(4,7)W(7,1), \tag{244}$$
$$P(4,7) = -iG(4,8)\Gamma(8,9;7)G(9,4^+), \tag{245}$$
$$G(1,2) = G_H(1,2) + G_H(1,3)\Sigma(3,4)G(4,2). \tag{246}$$

Figure 13 gives a diagrammatic representation of Hdin's equations and Fig. 14 illustrates how the various equations are coupled.

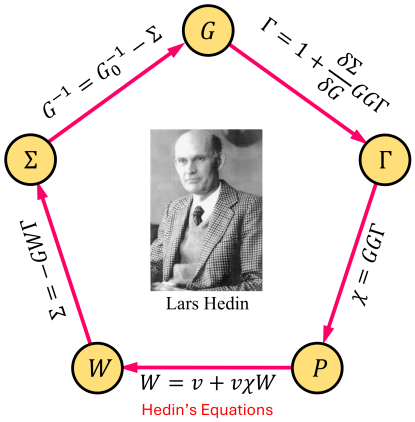

Figure 14
The five coupled integro-differential equations that compose Hedin's equations.

There are several approximations employed in the literature, including:

1. Assume $\Gamma = \delta$:
   (a) $scGW$
   (b) G_0W_0
   (c) $qpGW4$
2. Assume a diagrammatic form for Γ:
   (a) $GW\Gamma_1$
   (b) $GW\Gamma_{GW}$
   (c) GT
   (d) GWT
3. Assume $\Gamma = \delta$ and $W = V$:
   (a) Hartree-Fock
4. Assume $\Sigma = \Sigma_{loc}$:
   (a) Dynamical Mean-field Theory
5. Assume $\Gamma = \Gamma_{loc}$:
   (a) DΓA

We have achieved a major reduction of the equations needed to determine G: from an infinite set in the Martin-Schwinger hierocracy to the five Hedin's equations.

Example 14. Determine the GW correction to the vertex Γ and the next iteration of Σ beyond the GW approximation.

In the GW approximation, we have $\Sigma(1,5) - i = G(1,5)W(5,1)$, since $\Gamma = \delta(4,6)\delta(4,5)$. To get the next iteration of Γ we need $\frac{\delta\Sigma}{\delta G}$,

$$\begin{aligned}\frac{\delta\Sigma(4,5)}{\delta G(7,8)} &= -i\left(\frac{\delta W(5,4)}{\delta G(7,8)}G(4,5) + W(5,4)\frac{\delta G(4,5)}{\delta G(7,8)}\right)\\ &= -i\left(\frac{\delta W(5,4)}{\delta G(7,8)}G(4,5) + W(5,4)\delta(4,7)\delta(5,8)\right)\end{aligned} \tag{247}$$

where

$$\begin{aligned}\frac{\delta W(5,4)}{\delta G(7,8)} &= V(5,6)\frac{\delta P(6,9)}{\delta G(7,8)}W(9,4) + V(5,6)P(6,9)\frac{\delta W(9,4)}{\delta G(7,8)}\\ \frac{\delta W(5,4)}{\delta G(7,8)} - V(5,6)P(6,9)\frac{\delta W(9,4)}{\delta G(7,8)} &= V(5,6)\frac{\delta P(6,9)}{\delta G(7,8)}W(9,4)\\ \left(\delta(5,9) - V(5,6)P(6,9)\right)\frac{\delta W(9,4)}{\delta G(7,8)} &= V(5,6)\frac{\delta P(6,9)}{\delta G(7,8)}W(9,4)\\ \frac{\delta W(9,4)}{\delta G(7,8)} &= \varepsilon^{-1}(9,5)V(5,6)\frac{\delta P(6,9)}{\delta G(7,8)}W(9,4)\end{aligned}$$

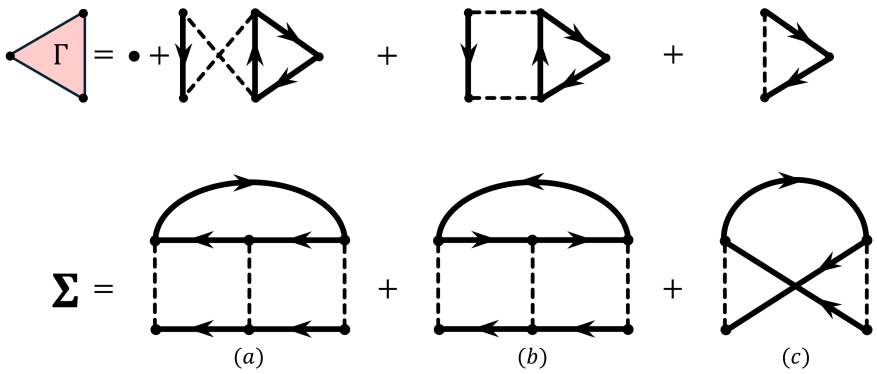

Figure 15: Diagrammatic representation of the GW correction to Γ and the corresponding beyond GW self-energy corrections: (a) three-rung particle-paricle ladder, (b) three-rung particle-hole ladder, (c) second-order exchange.

$$\frac{\delta W(9,4)}{\delta G(7,8)} = W(9,6)\frac{\delta P(6,9)}{\delta G(7,8)}W(9,4) \tag{248}$$

and

$$\begin{aligned}\frac{\delta P(6,9)}{\delta G(7,8)} &= -i\frac{\delta}{\delta G(7,8)}\left(G(6,10)G(10,6^+)\right)\\ &= -i\left(\delta(7,6)\delta(8,10)G(10,6^+) + G(6,10)\delta(10,7)\delta(6^+,8)\right).\end{aligned} \tag{249}$$

giving,

$$\frac{\delta W(5,4)}{\delta G(7,8)} = -iW(5,7)G(8,7)W(8,4) - iW(5,8)G(8,7)W(7,4) \tag{250}$$

Finally,

$$\begin{aligned}\frac{\delta \Sigma(4,5)}{\delta G(7,8)} &= -iW(5,7)G(8,7)(-i)W(8,4)\\ &\quad + (-i)W(5,8)G(8,7)(-i)W(7,4)\\ &\quad + (-i)W(5,4)\delta(4,7)\delta 5,8\end{aligned} \tag{251}$$

$$\Gamma(4,5;6) = \delta(4,6)\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}G(7,8)G(6,8) \tag{252}$$

$$\Sigma(1,5) = -iW(6,1)G(1,4)\Gamma(4,5;6). \tag{253}$$

Figure 15 Gives the diagrammatic representation of the GW correction to Γ and the corresponding beyond GW self-energy corrections.

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