Sparsity pattern of the self-energy for classical and quantum impurity problems

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Abstract

We prove that for various impurity models, in both classical and quantum settings, the self-energy matrix is a sparse matrix with a sparsity pattern determined by the impurity sites. In the quantum setting, such a sparsity pattern has been known since Feynman. Indeed, it underlies several numerical methods for solving impurity problems, as well as many approaches to more general quantum many-body problems, such as the dynamical mean field theory. The sparsity pattern is easily motivated by a formal perturbative expansion using Feynman diagrams. However, to the extent of our knowledge, a rigorous proof has not appeared in the literature. In the classical setting, analogous considerations lead to a perhaps less-known result, i.e., that the precision matrix of a Gibbs measure of a certain kind differs only by a sparse matrix from the precision matrix of a corresponding Gaussian measure. Our argument for this result mainly involves elementary algebraic manipulations and is in particular non-perturbative. Nonetheless, the proof can be robustly adapted to various settings of interest in physics, including quantum systems (both fermionic and bosonic) at zero and finite temperature, non-equilibrium systems, and superconducting systems.

1 Introduction

Consider the second-moment matrix \( G \in \mathbb{R}^{d \times d} \) of a Gibbs measure defined by a Hamiltonian \( H : \mathbb{R}^d \to \mathbb{R} \), i.e.,

\[
G = \frac{1}{Z} \int_{\mathbb{R}^d} xx^T e^{-H(x)} dx.
\]

Here the partition function

\[
Z = \int_{\mathbb{R}^d} e^{-H(x)} dx
\]

is the appropriate normalization factor.

We will write \( H \) in the form \( H = H_0 + U \), where \( H_0 = \frac{1}{2} x^T A x \) is a quadratic form. Assume that \( A \) and \( U \) are such that both \( Z \) and \( G \) are finite. Via the analogy with quantum many-body physics that will be discussed below, we refer to \( U \) as the interacting part of the Hamiltonian, or simply the interaction. Meanwhile \( H_0 \) represents the non-interacting part.

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If \( U \equiv 0 \) and \( A \) is a positive definite matrix, then immediately we have \( G = A^{-1} \). One seeks a generalization of this fact to the case in which \( U(x) \) depends only on a subset of the variables. We refer to this setting as the (classical) impurity model, by analogy to the quantum impurity model to be discussed below. Perhaps surprisingly, we have the following result:

**Theorem 1.1.** Let \( p \leq d \), and let \( A \in \mathbb{R}^{d \times d} \) be a symmetric matrix whose lower-right \((d-p) \times (d-p)\) block is positive definite. Let \( U : \mathbb{R}^d \to \mathbb{R} \) be a function that depends only on its first \( p \) arguments, i.e., \( U(x) = U_1(x_1, \ldots, x_p) \) for some \( U_1 : \mathbb{R}^p \to \mathbb{R} \), and assume that \( U_1 \) satisfies sufficient growth conditions such that the Gibbs measure with density proportional to \( e^{-\frac{1}{2}x^TAx-U(x)} \) has finite second-order moments. Then, with \( G \) defined as in (1.1),

\[
\Sigma := A - G^{-1} = \begin{pmatrix} \Sigma_p & 0 \\ 0 & 0 \end{pmatrix},
\]

where \( \Sigma_p \in \mathbb{R}^{p \times p} \) is a symmetric matrix.

In fact, Theorem 1.1 can be generalized by considering an arbitrary measure \( d\mu_1(x_1) \) of sufficient decay in the place of \( e^{-U_1(x_1)} \) \( d\mu_1 \), where we denote \( x_1 = (x_1, \ldots, x_p)^T \) and \( x_2 = (x_{p+1}, \ldots, x_d)^T \). In this setting the partition function is defined

\[
Z = \int_{\mathbb{R}^p} \int_{\mathbb{R}^{d-p}} e^{-\frac{1}{2}x^TAx} d\mu_1 d\mu_2(x_2),
\]

and the Green’s function is defined accordingly. The case

\[
\mu_1(x_1) = e^{-\sum_{i,j=1}^p J_{ij}x_i x_j} \sum_{\sigma \in \{-1,1\}^p} \delta(\cdot - \sigma)
\]

defines a notion of a classical impurity model for spin systems, in which a spin system is coupled to a Gaussian ‘bath.’ For such a spin impurity model, we can assume without loss of generality that the upper-left \( p \times p \) block of \( A \) is zero, and the ensemble is specified by the partition function

\[
Z = \sum_{\sigma \in \{-1,1\}^p} e^{-\frac{1}{2} \sum_{i,j=1}^p J_{ij} \sigma_i \sigma_j} \int_{\mathbb{R}^{d-p}} e^{-\frac{1}{2}y^TA_{22}y - y^TA_{21}\sigma} dy,
\]

where \( A_{21} \) and \( A_{22} \) denote the appropriate blocks of \( A \). We will stick to the original setting, in which the impurity is specified by a function \( U_1 \), to emphasize the analogy with the setting of the quantum many-body problem, but we comment that the proof of Theorem 1.1 is exactly the same in this broader context.

In statistics, \( G^{-1} \) is sometimes called the precision matrix. In our setting, if \( A \) is positive definite and \( U \equiv 0 \), then \( A \) is the precision matrix of the distribution in question. Hence Theorem 1.1 states that the difference of the precision matrices in the ‘interacting’ and ‘non-interacting’ settings, namely \( A - G^{-1} \), is a sparse matrix if the interaction \( U \) only depends on a subset of variables. The proof of the theorem is non-perturbative, and in fact \( A \) need not be positive definite (though, when \( U \) is independent of the last \( d-p \) variables, the lower-right \((d-p) \times (d-p)\) block of \( A \) must be positive definite to ensure that \( e^{-\frac{1}{2}x^TAx-U(x)} \) is normalizable). To the best of our knowledge, other than from the perspective of the Luttinger-Ward formalism to be discussed later [17, 10, 14, 15, 3], this basic linear-algebraic fact about Gibbs measures was not previously present in the literature.
As a matter of fact, we first observed a result of this type in a more complex setting, namely that of quantum impurity problems at zero temperature (as we shall discuss below, the analogous result is also true at finite temperature). Consider the Hamiltonian, denoted by $\hat{H}$, for a system of interacting fermions or bosons. Throughout we shall distinguish the cases of fermions and bosons via a parameter $\zeta$ given by $\zeta = -1$ in the case of fermions and $\zeta = +1$ in the case of bosons. In the second-quantized representation \[5\], $\hat{H}$ can be generally written as

$$\hat{H} = \hat{H}_0 + \hat{U},$$

where

$$\hat{H}_0 = \sum_{i,j=1}^{d} h_{ij} a_i^\dagger a_j$$

is viewed as the Hamiltonian for a system of non-interacting fermions or bosons. Here $a_i^\dagger, a_j$ are called the creation and annihilation operators, respectively, and $h \in \mathbb{C}^{d \times d}$ is a Hermitian matrix (in Appendix A we provide a brief introduction of the second-quantized representation).

Meanwhile, $\hat{U}$ is the interacting part of the Hamiltonian. Although $\hat{U}$ can be far more general, usually we have in mind the two-body interaction

$$\hat{U} = \sum_{i,j,k,l} (ij|U|kl) a_i^\dagger a_j^\dagger a_l a_k.$$

In this case, if there exists $p < d$ so that $(ij|U|kl) \neq 0$ only if $i, j, k, l \in \{1, \ldots, p\}$, then we call the Hamiltonian $\hat{H}$ an impurity Hamiltonian. More generally, we say that $\hat{H}$ is an impurity Hamiltonian if $\hat{U}$ can be written as a polynomial of the creation and annihilation operators $a_i^\dagger$ and $a_i$ for $i = 1, \ldots, p$ and is particle-number-conserving (see Appendix A for details). At a glance there is no connection between this impurity Hamiltonian and the type of Gibbs measure discussed earlier. Nonetheless, we claim that there is an analogy under which $h$ maps to $A$, the Green’s function of the quantum many-body problem maps to $G$, and the self-energy matrix associated with the Green’s function maps to $\Sigma$. Then the counterpart of Theorem 1.1 can be stated in words as: the self-energy matrix of a quantum impurity problem is a sparse matrix, with non-zero entries only on the block associated with the impurity sites.

The connection between the classical impurity model and the quantum impurity problem can be understood formally by writing quantum Green’s functions in terms of the coherent state path integral \[18\], which formally resembles a Gibbs measure. We remark that in the case of fermions, the resemblance should be noted with special caution because the coherent state path integral involves Grassmann integrals. In this sense, the setting of Theorem 1.1 can indeed be understood as the ‘classical impurity problem.’

Unlike the corresponding result for Gibbs measures, the quantum result has been well-known in the quantum physics literature since Feynman and Vernon in 1963 \[6\] at the latest, and it plays a central role in numerical algorithms for solving the quantum impurity problem, such as the quantum Monte Carlo (QMC) method \[8\]. The sparsity of the impurity self-energy matrix is also the starting point of various approximate methods—such as the dynamical mean field theory (DMFT) \[7, 11\] and its extensions \[22, 13\]—for solving general (i.e., non-impurity) quantum systems, especially those that are strongly correlated. Again somewhat surprisingly, this important statement is to the best of our knowledge a ‘folk theorem,’ in that we cannot find a rigorous proof of this result in the literature.

In this paper, we fill this gap by providing a rigorous proofs of the sparsity of the self-energy matrix of quantum impurity problems, in both the fermionic and bosonic cases at zero and finite temperature. We will also cover the non-equilibrium setting via the consideration of arbitrary
contour-ordered Green’s functions, as well as the anomalous setting, which is relevant to superconductivity. Excellent introductions to the non-equilibrium and anomalous formalisms can be found in [21] [2], respectively.

Our results in the non-equilibrium setting should be compared to those in a recent work [3], in which advanced/retarded non-equilibrium self-energies are rigorously constructed in the case of fermions. Though not noted explicitly in the work, the appropriate sparsity results for these quantities can be seen to follow from the construction itself. By contrast, our non-equilibrium sparsity result concerns the contour-ordered self-energy (for both fermions and bosons) and in particular recovers sparsity results for the advanced/retarded Green’s functions. Moreover, our result holds for arbitrary contour. However, we do not actually construct the contour-ordered self-energy, but rather phrase our sparsity result in terms of operators that we suggestively name ‘$G\Sigma$’ and ‘$\Sigma G$.’ In so doing we sidestep a considerable analytical challenge such as that encountered in [3]. Thus our result can be viewed as trying to parsimoniously illustrate the broadest possible formal picture of sparsity results for the self-energy, rather than focusing on the analytical question of the construction of the self-energy itself. Incidentally, in our view a rigorous construction of the contour-ordered self-energy (for arbitrary contour) seems to be an interesting and non-trivial matter.

We hope that this work will have pedagogical value, especially to the mathematical audience unfamiliar with the physics literature. Since it is difficult to find standard references in the mathematics literature that are appropriate to our setting, we have included appendices to put our results on firm footing. Via the appendices, we have also sought to make the work self-contained within reason, providing in particular some brief introduction to the theory of Green’s functions, both fermionic and bosonic, in the zero-temperature, finite-temperature, non-equilibrium, and anomalous settings. In all of these settings, the impurity model with $p = 0$ is precisely the non-interacting model, and our results on the sparsity pattern of the self-energy, applied in this special case, yield formulas for the non-interacting Green’s functions. In the non-equilibrium setting especially, such a formula seems to be non-trivial to establish by other means. Readers new to the subject may find this presentation of the non-interacting Green’s functions, as well as its embedding into a unified perspective, to be appealing in its own right.

Other formal perspectives:

We discuss several other ways of understanding the sparsity pattern of the self-energy for impurity problems. First, we remark by considering the coherent-state path integral representation [18] (in any of the quantum settings discussed in this paper), one can formally view the quantum many-body ensemble as a Gibbs measure. The proof of Theorem 1.1 can be mimicked in these settings at the formal level to derive the appropriate sparsity results, but we omit such formal manipulations here.

Secondly, the sparsity pattern can be most intuitively understood via the Feynman diagrammatic expansion, which provides another viewpoint on the formal unification of the classical and quantum settings. Indeed, due to the connection between the classical setting of Gibbs measures and the coherent state path integral, we limit our discussion the case of Gibbs models here for simplicity. We do not provide here a self-contained introduction to the diagrammatic expansion; instead we refer readers to [1] [18] [14] for a more detailed description. The reader will find that from the point of view of this paper, these objects can be thought of as more natural than the non-equilibrium self-energy itself, and indeed all of our sparsity results are proved by considering their analogs.
As before, define the partition function

\[ Z = \int_{\mathbb{R}^d} e^{-\frac{1}{2} x^T A x - \varepsilon U(x)} \, dx, \]  

where \( A \) is a positive definite matrix and where we have introduced the parameter \( \varepsilon > 0 \) as a prefactor for the interaction (referred to as the coupling constant). Then formally we may apply Taylor expansion for \( e^{-\varepsilon U(x)} \) to obtain a series expansion for \( Z \), as in

\[ Z = \int_{\mathbb{R}^d} \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} (-U(x))^n e^{-\frac{1}{2} x^T A x} \, dx \sim \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \int_{\mathbb{R}^d} (-U(x))^n e^{-\frac{1}{2} x^T A x} \, dx, \]  

where the ‘\( \sim \)’ is meant to indicate that the series is valid only in the asymptotic sense.

Assuming \( U(x) \) is a polynomial of \( x \), then each term on the right hand side of Eq. (1.5) requires the evaluation of a possibly large, but finite, number of moments of a Gaussian distribution. The expansion can be organized in terms of Feynman diagrams.

Feynman diagrammatic expansions can also be obtained for \( G \) and \( \Sigma \). In particular, the self-energy diagrams are truncated, one-particle irreducible Feynman diagrams [14]. To be concrete, one can keep in mind the quartic interaction

\[ U(x) = \frac{1}{8} \sum_{i,j=1}^{N} v_{ij} x_i^2 x_j^2, \]  

which mimics the two-body Coulomb interaction of quantum many-body physics. Here \( v \) is a symmetric positive definite matrix. In order to specify an impurity problem with fragment specified by indices \( 1, \ldots, p \) we take \( v_{ij} = 0 \) if \( i > p \) or \( j > p \). Then, it can readily be read from the diagrammatic expansion of \( \Sigma \) as in [14] that for each term in the expansion of \( \Sigma_{ij} \), the corresponding matrix element is nonzero only if \( 1 \leq i, j \leq p \). This observation suggests that the self-energy matrix \( \Sigma \), as the infinite sum of all of these terms, should follow the same sparsity pattern. We remark that the above diagrammatic argument can be applied to Gibbs models with rather general interaction form \( U(x) \), as well as in the quantum many-body setting, where the diagrammatic series can be derived directly in the second-quantized representation or via the coherent state path integral.

The major caveat to this argument is that the Feynman diagrammatic expansion often has zero radius of convergence and maintains validity only in the asymptotic sense. This is the case at least for the Gibbs models as well as bosonic systems. Hence the sparsity for each term of the expansion does not necessarily imply that the same is true of the self-energy itself when \( \varepsilon \) is positive. Even when the series does converge (such as for fermionic systems with finitely many states), the convergence radius may only be finite. Bootstrapping a positive radius of convergence via resummation or analytic continuation arguments [18] is one possible route to proving the sparsity result in such a setting, though the details seem to be cumbersome and the proof is not as simple or general as others considered above.

Finally, we discuss a route to the sparsity of the self-energy matrix via the so-called Luttinger-Ward formalism [17], which expresses the self-energy as a functional derivative

\[ \Sigma = \frac{\delta \Phi[G]}{\delta G}. \]  

Here \( \Phi[G] \) is a functional of the Green’s function, called the Luttinger-Ward functional. Recently, for the Gibbs model, we have proved [10, 15] that \( \Phi[G] \) is a well-defined for positive semidefinite
In particular, we have established a projection rule, which states that for the classical impurity problem when $U(x) = U_p(x_1, \ldots, x_p)$, we have

$$\Phi[G] = \Phi_p[G_p].$$

(1.8)

Here $G_p$ is the upper-left $p \times p$ block of $G$, and $\Phi_p$ is the Luttinger-Ward functional for the $p$-dimensional model. Combining Eq. (1.7) and (1.8), one immediately obtains the sparsity pattern for $\Sigma$.

However, establishing the existence of the Luttinger-Ward functional $\Phi[G]$ and its projection rule require a significant amount of work, and the rigorous proof is so far only applicable to the Gibbs model. In fact, the very existence of the Luttinger-Ward functional fermionic systems has been challenged over the past few years [12, 4, 9]. Although the Luttinger-Ward perspective offers additional insight, the direct proofs provided in this paper are at this point more generally applicable, and certainly much simpler.

Outline of the paper:

This paper is organized as follows. We use the classical impurity problem as a motivating example and prove Theorem 1.1 in section 2. Section 3 treats the quantum many-body case, including the settings of fermions and bosons in the equilibrium setting at zero and finite temperature, as well as the non-equilibrium setting specified by an arbitrary contour in the complex plane and the anomalous setting relevant to superconductivity.

Finally, in Appendix A we record self-contained background on second quantization. In Appendix B we discuss the zero-temperature ensemble for fermions and bosons and the construction of the frequency representation of Green's functions in this setting. In Appendix C we do the same for the finite-temperature ensemble. Some efforts must be made here to deal with analytical issues in the bosonic case, where the Fock space is infinite-dimensional, even for finitely many states. In Appendix D we discuss the technical conditions needed to define the appropriate objects in the bosonic non-equilibrium setting and provide some background on main non-equilibrium setting of interest, specified by the Kadanoff-Baym contour.

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2 The classical impurity problem (Proof of Theorem 1.1)

We now embark upon the proof of Theorem 1.1 stated above.

Recall the definitions:

$$Z = \int_{\mathbb{R}^d} e^{-\frac{1}{2} x^T Ax - U(x)} \, dx, \quad G = \frac{1}{Z} \int_{\mathbb{R}^d} x x^T e^{-\frac{1}{2} x^T Ax - U(x)} \, dx,$$
where the interaction $U$ only depends on the first $p \leq d$ variables. Let $q = d - p$. It is not hard to see that $G$ is positive definite, hence invertible.

We will indicate the blocks of $A$ via

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where the upper-left block is $p \times p$. For various integrals considered below to be convergent, we will require that $A_{22} > 0$. More generally, we adopt the notation that for any $d \times d$ matrix $M$, the notation $M_{21}$ indicates the lower-left block of $M$ (with respect to the above block structure), etc.

Then for the theorem, we want to show that the self-energy $\Sigma := A - G^{-1}$ satisfies $\Sigma_{12} = 0$, $\Sigma_{21} = 0$, and $\Sigma_{22} = 0$. In other words, we want to show that $(G^{-1})_{12} = A_{12}$, $(G^{-1})_{21} = A_{21}$, and $(G^{-1})_{22} = A_{22}$. Since $G$ and $A$ are symmetric, it suffices to show that $(G^{-1})_{12} = A_{12}$ and $(G^{-1})_{22} = A_{22}$, i.e., that

$$\begin{pmatrix} (G^{-1})_{12} \\ (G^{-1})_{22} \end{pmatrix} = \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix}.$$ Left-multiplying both sides by $G$ (invertible), we see that this is in turn equivalent to showing that $(GA)_{12} = 0_{p \times q}$ and $(GA)_{22} = I_q$.

In the following our notation will make use of the splitting

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

where $x \in \mathbb{R}^d$, $x_1 \in \mathbb{R}^p$, and $x_2 \in \mathbb{R}^q$. (For notational convenience, we do not use the notation $x_i$ as in the introduction. In this section, we will make no reference to the individual entries of $x$, so the notation is clear.) Then we can write $U(x) = U_1(x_1)$. Abusing notation slightly, we write $U_1 = U$.

Roughly speaking, the goal is to ‘integrate out’ the lower variables (i.e., the last $q$ variables). To this end, we expand $G$ as

$$G = \frac{1}{Z} \int_{\mathbb{R}^p} e^{-U(x_1)} \int_{\mathbb{R}^q} xx^T \exp \left[ -\frac{1}{2} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^T \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \right] \, dx_2 \, dx_1.$$

Observe that

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^T \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = (x_2 + A_{22}^{-1} A_{21} x_1)^T A_{22} \left( x_2 + A_{22}^{-1} A_{21} x_1 \right) + x_1^T (A_{11} - A_{12} A_{22}^{-1} A_{21}) x_1,$$

where $A_{22}^{-1}$ is understood always to indicate $(A_{22})^{-1}$ and where we have defined the Schur complement

$$A_{11}^S := A_{11} - A_{12} A_{22}^{-1} A_{21}.$$ Then it follows that

$$G = \frac{1}{Z} \int_{\mathbb{R}^p} e^{-\frac{1}{2} x_{1}^T A_{11}^{-1} x_1 - U(x_1)} \int_{\mathbb{R}^q} xx^T \exp \left[ -\frac{1}{2} \left( x_2 + A_{22}^{-1} A_{21} x_1 \right)^T A_{22} \left( x_2 + A_{22}^{-1} A_{21} x_1 \right) \right] \, dx_2 \, dx_1.$$
Recall that we want to show that \((GA)_{12} = 0\) and \((GA)_{22} = I_q\). Right-multiplying the integral in \((2.2)\) by \(A\), this motivates computing the upper-right and upper-left blocks of \(xx^T A\), as in
\[
(xx^T A)_{12} = x_1 \left( x_1^T \ x_2^T \right) \left( \begin{array}{c} A_{12} \\ A_{22} \end{array} \right), \quad (xx^T A)_{22} = x_2 \left( x_1^T \ x_2^T \right) \left( \begin{array}{c} A_{12} \\ A_{22} \end{array} \right).
\]
Now
\[
(x_1^T \ x_2^T) \left( \begin{array}{c} A_{12} \\ A_{22} \end{array} \right) = x_1 A_{12} + x_2 A_{22} = (x_1 A_{12} A_{22}^{-1} + x_2 A_{22}) y_2^T A_{22},
\]
where we have defined a new variable \(y_2 = x_2 + A_{22}^{-1} A_{21} x_1\), so
\[
(xx^T A)_{12} = x_1 y_2^T A_{22}, \quad (xx^T A)_{22} = x_2 y_2^T A_{22}.
\]
(2.3)
The remarkable thing is that \(x_2\) only appears in the exponent in the inner integrand of \((2.2)\) via the expression \(x_2 + A_{22}^{-1} A_{21} x_1 = y_2\). This motivates us to eliminate \(x_2\) from the second equation of \((2.3)\) to obtain
\[
(xx^T A)_{12} = x_1 y_2^T A_{22}, \quad (xx^T A)_{22} = y_2 y_2^T A_{22} - A_{22} A_{21} x_1 y_2^T A_{22}.
\]
(2.4)
Then consider the change of variables from \(x_1, x_2\) to \(x_1, y_2\), yielded by the linear transformation
\[
\left( \begin{array}{c} x_1 \\ y_2 \end{array} \right) = \left( \begin{array}{cc} I_p & 0 \\ A_{22}^{-1} A_{21} & I_q \end{array} \right) \left( \begin{array}{c} x_1 \\ x_2 \end{array} \right).
\]
Since the Jacobian determinant of this transformation is one, it follows from \((2.2)\) and \((2.4)\) that
\[
(GA)_{12} = \frac{1}{Z} \int_{\mathbb{R}^p} e^{-\frac{1}{2} x^T A_{11} x - U(x_1)} x_1 \left( \int_{\mathbb{R}^q} y_2^T e^{-\frac{1}{2} y_2^T A_{22} y_2} dy_2 \right) A_{22} dx_1.
\]
But evidently the inner integrand is zero, so \((GA)_{12} = 0\), as desired. It also follows from \((2.2)\) and \((2.4)\) that
\[
(GA)_{22} = \frac{1}{Z} \int_{\mathbb{R}^p} e^{-\frac{1}{2} x^T A_{11} x - U(x_1)} \left( \int_{\mathbb{R}^q} y_2^T e^{-\frac{1}{2} y_2^T A_{22} y_2} dy_2 \right) A_{22} dx_1
\]
\[
- \frac{1}{Z} \int_{\mathbb{R}^p} e^{-\frac{1}{2} x^T A_{11} x - U(x_1)} A_{22}^{-1} A_{21} x_1 \left( \int_{\mathbb{R}^q} y_2^T e^{-\frac{1}{2} y_2^T A_{22} y_2} dy_2 \right) A_{22} dx_1.
\]
The inner integrand in the second term of the last expression is once again zero. Meanwhile, the inner integrand of the first term yields \(Z_2 A_{22}^{-1}\), where
\[
Z_2 := \int_{\mathbb{R}^q} e^{-\frac{1}{2} y_2^T A_{22} y_2} dy_2.
\]
Then we have established
\[
(GA)_{22} = \frac{I_p}{Z} \int_{\mathbb{R}^p} \int_{\mathbb{R}^q} e^{-\frac{1}{2} x^T A_{11} x_1 - \frac{1}{2} y_2^T A_{22} y_2 - U(x_1)} dy_2 dx_1.
\]
Changing variables back to \(x_1, x_2\) and recalling from \((2.1)\) that \(x_1^T A_{11} x_1 + y_2^T A_{22} y_2 = x^T A x\), we see that
\[
(GA)_{22} = \frac{I_p}{Z} \int_{\mathbb{R}^d} e^{-\frac{1}{2} x^T A x - U(x)} dx = I_p,
\]
which completes the proof. \(\square\)
3 The quantum impurity problem

Our setting then is the Fock space $\mathcal{F}_{\zeta,d}$ of fermions ($\zeta = -1$) or bosons ($\zeta = +1$) with a finite number $d$ of states. The annihilation and creation operators are denoted $a_1, \ldots, a_d$ and $a_1^\dagger, \ldots, a_d^\dagger$, respectively. We refer the reader to Appendix A for further details of the construction of $\mathcal{F}_{\zeta,d}$ as well as other details of second quantization. For convenience we shall let $a = (a_1, \ldots, a_d)^T$ denote the vector of annihilation operators, and accordingly $a^\dagger = (a_1^\dagger, \ldots, a_d^\dagger)$.

For now we consider a particle-number-conserving self-adjoint Hamiltonian $\hat{H}$ on $\mathcal{F}_{\zeta,d}$, and we write $\hat{H}$ of the form $\hat{H} = \hat{H}_0 + \hat{U}$, where

$$\hat{H}_0 := a^\dagger h a = \sum_{i,j=1}^d h_{ij} a_i^\dagger a_j$$

is the single-particle (or non-interacting) part of the Hamiltonian, specified by a Hermitian $d \times d$ matrix $h$, and $\hat{U}$ is the interacting part, which is itself a self-adjoint operator on $\mathcal{F}_{\zeta,d}$ that conserves particle number.

In the case that $\hat{U}$ can be written as a polynomial of the $a_i^\dagger, a_i$ for $i = 1, \ldots, p$, we say that $\hat{H}$ is an impurity Hamiltonian, with a fragment specified by the indices $1, \ldots, p$. The rest of the indices correspond to the environment. In this case, since $\hat{U}$ conserves particle number, it follows that $\hat{U}$ commutes with $a_j$ and $a_j^\dagger$ for $j > p$.

Before proceeding, we state and prove a simple but useful lemma that will be used repeatedly throughout the following discussion.

**Lemma 3.1.** \([a^\dagger ha, a_j^\dagger] = \sum_{k=1}^d h_{kj} a_k^\dagger\) and \([a_j, a^\dagger hy] = \sum_{l=1}^d h_{jl} a_l].

**Proof.** Simply compute

\[
(a^\dagger ha)^\dagger a_j^\dagger = \sum_{k,l=1}^d h_{kl} a_k^\dagger a_l^\dagger a_j^\dagger = \sum_{k,l=1}^d h_{kl} a_k^\dagger (\zeta a_j^\dagger a_l + \delta_{jl}) = \sum_{k,l=1}^d h_{kl} a_j^\dagger a_k^\dagger a_l + \sum_{k=1}^d h_{kj} a_k^\dagger = a_j^\dagger (a^\dagger ha) + \sum_{k=1}^d h_{kj} a_k^\dagger,
\]

which proves the first statement of the lemma. Similarly,

\[
(a^\dagger ha) a_j = \sum_{k,l=1}^d h_{kl} \zeta a_k^\dagger a_j a_l.
\]

---

2In sections 3.3 and 3.4 below, the notion of the Hamiltonian will be somewhat modified.

3See Appendix A for a details.
\[ \sum_{k,l=1}^{d} h_{kl} (a_j a_k^\dagger - \delta_{jk}) a_l \]
\[ = a_j (a^\dagger h a) - \sum_{l=1}^{d} h_{jl} a_l \]

which proves the lemma. \hfill \Box

### 3.1 Zero temperature

We consider the setting of zero temperature and fixed particle number \( N \). Let \( |\Psi_0^{(N)}\rangle \) denote a normalized \( N \)-particle ground state of \( \hat{H} \), and let the corresponding eigenvalue be \( E_0^{(N)} \). Then in this setting, the single-particle Green’s function can be understood as a rational function \( G : \mathbb{C} \rightarrow \mathbb{C}^{d \times d} \) defined by

\[ G^+(z) := \langle \Psi_0^{(N)} | a_i \frac{1}{z - (\hat{H} - E_0^{(N)})} a_j^\dagger | \Psi_0^{(N)} \rangle \]
\[ G^-(z) := -\zeta \langle \Psi_0^{(N)} | a_j \frac{1}{z + (\hat{H} - E_0^{(N)})} a_i | \Psi_0^{(N)} \rangle. \]

The self-energy is the rational function \( \Sigma : \mathbb{C} \rightarrow \mathbb{C}^{d \times d} \) defined by

\[ \Sigma(z) := z - h - G(z)^{-1}. \]

As we recover in Theorem 3.2, \( z - h \) is in fact the inverse of the non-interacting Green’s function, so this self-energy is defined analogously to the classical self-energy of Theorem 1.1. The reader should consult Appendix B for further details and justification of these definitions.

**Theorem 3.2.** Suppose that \( \hat{H} \) is an impurity Hamiltonian, with a fragment specified by the indices \( 1, \ldots, p \). Then the self-energy \( \Sigma : \mathbb{C} \rightarrow \mathbb{C}^{d \times d} \) is (up to the resolution of removable discontinuities) of the form

\[ \Sigma(z) = \begin{pmatrix} \Sigma_p(z) & 0 \\ 0 & 0 \end{pmatrix}. \]

**Remark 3.3.** Observe that if the fragment is of size zero, i.e., \( p = 0 \), then we are in the non-interacting setting, and Theorem 3.2 implies that \( \Sigma(z) \equiv 0 \), i.e., that \( G(z) = (z - h)^{-1} \). Thus we recover a clean proof of the formula for the non-interacting Green’s function. Usually this formula is proved by assuming, via a canonical transformation, that \( h \) is diagonal and then performing explicit computations \[5\].

**Proof.** We can write \( \hat{H} = \hat{H}_0 + \hat{U} \), where \( \hat{H}_0 = a^\dagger h a \) and \( \hat{U} \) commutes with \( a_j \) and \( a_j^\dagger \) for \( j > p \) is the interacting part, which is itself a self-adjoint operator on \( \mathcal{F}_{\xi,d} \) that conserves particle number.

It suffices to prove that the \( j \)-th column of \( G(z)\Sigma(z) \) is zero for \( j > p \) and that the \( i \)-th row of \( \Sigma(z)G(z) \) is zero for \( i > p \). We will only prove the first claim; the second follows by symmetric reasoning.

\[ ^4 \text{ Usually } G^\pm \text{ carry the extra information that their poles are viewed as being located infinitesimally below/above the real axis. The choices that yield the ‘time-ordered’ Green’s function are described in Appendix B.1. However, this extra information is irrelevant for the purpose of our results.} \]
Now $G(z)\Sigma(z) = zG(z) - G(z)h - I_d$, so we want to show that $zG_{ij}(z) = [G(z)h]_{ij} + \delta_{ij}$ for $j > p$.

Then we compute, using the fact that $(\hat{H} - E_0^{(N)})|\Psi_0^{(N)}\rangle = 0$,

\[
zG_{ij}^+(z) = \langle \Psi_0^{(N)}|a_ia_j \frac{1}{z - (\hat{H} - E_0^{(N)})}a_j^\dagger(z - (\hat{H} - E_0^{(N)}))|\Psi_0^{(N)}\rangle
\]
\[
= \langle \Psi_0^{(N)}|a_ia_j \frac{1}{z - (\hat{H} - E_0^{(N)})}(z - (\hat{H} - E_0^{(N)}))a_j^\dagger|\Psi_0^{(N)}\rangle
\]
\[
\quad + \langle \Psi_0^{(N)}|a_i \frac{1}{z - (\hat{H} - E_0^{(N)})}a_j^\dagger(z - (\hat{H} - E_0^{(N)}))|\Psi_0^{(N)}\rangle
\]
\[
= \langle \Psi_0^{(N)}|a_ia_j^\dagger|\Psi_0^{(N)}\rangle + \langle \Psi_0^{(N)}|a_i \frac{1}{z - (\hat{H} - E_0^{(N)})}a_j^\dagger(z - (\hat{H} - E_0^{(N)}))|\Psi_0^{(N)}\rangle.
\]

Now
\[
[a_i^\dagger, z - (\hat{H} - E_0^{(N)})] = [\hat{H}, a_i^\dagger] = [a_i^\dagger h, a_j^\dagger] + [\hat{U}, a_j^\dagger] = \sum_{k=1}^d h_{kj}a_k^\dagger,
\]
where we have used Lemma [3] as well as the fact that $j > p$ (so $[\hat{U}, a_j^\dagger] = 0$).

Then it follows that
\[
zG_{ij}^+(z) = \langle \Psi_0^{(N)}|a_ia_j^\dagger|\Psi_0^{(N)}\rangle + [G^+(z)h]_{ij}.
\]

Similarly, we compute
\[
zG_{ij}^-(z) = -\zeta\langle \Psi_0^{(N)}|(z + (\hat{H} - E_0^{(N)}))a_j^\dagger \frac{1}{z + (\hat{H} - E_0^{(N)})}a_i|\Psi_0^{(N)}\rangle
\]
\[
= -\zeta\langle \Psi_0^{(N)}|a_j^\dagger(z + (\hat{H} - E_0^{(N)})) \frac{1}{z + (\hat{H} - E_0^{(N)})}a_i|\Psi_0^{(N)}\rangle
\]
\[
\quad + (-\zeta)\langle \Psi_0^{(N)}|(z + (\hat{H} - E_0^{(N)}), a_j^\dagger) \frac{1}{z + (\hat{H} - E_0^{(N)})}a_i|\Psi_0^{(N)}\rangle
\]
\[
= -\zeta\langle \Psi_0^{(N)}|a_j^\dagger a_i|\Psi_0^{(N)}\rangle - \zeta\langle \Psi_0^{(N)}|a_j^\dagger(z + (\hat{H} - E_0^{(N)}), a_i^\dagger) \frac{1}{z + (\hat{H} - E_0^{(N)})}a_i|\Psi_0^{(N)}\rangle.
\]

Now
\[
[z + (\hat{H} - E_0^{(N)}), a_j^\dagger] = [\hat{H}, a_j^\dagger] = \sum_{k=1}^d h_{kj}a_k^\dagger.
\]

Then it follows that
\[
zG_{ij}^-(z) = -\zeta\langle \Psi_0^{(N)}|a_ia_j^\dagger|\Psi_0^{(N)}\rangle + [G^-(z)h]_{ij}.
\]

Therefore
\[
zG_{ij}(z) = [G(z)h]_{ij} + \langle \Psi_0^{(N)}|a_ia_j^\dagger - \zeta a_j^\dagger a_i|\Psi_0^{(N)}\rangle = [G(z)h]_{ij} + \delta_{ij},
\]
as was to be shown. \qed
3.2 Finite temperature

Now we consider the setting of finite inverse temperature $\beta \in (0, \infty)$ and chemical potential $\mu \in \text{int dom } Z$, where $Z(\mu) = \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}]$ (see Appendix C for further details). Note that int dom $Z$ is guaranteed to be non-empty under Assumption C.1.

We also let $|\Psi_m\rangle$ denote the normalized eigenstates of $\hat{H}$, where $m$ ranges from $0$ to $2^d - 1$ in the case of fermions and from $0$ to $\infty$ in the case of bosons. In this setting, the single-particle Green’s function can be understood as a rational function $G : \mathbb{C} \to \mathbb{C}^{d \times d}$ defined by

$$G_{ij}(z) = \sum_m e^{-\beta(E_m - \mu N_m)} \langle \Psi_m | a_i \frac{1}{z - (\hat{H} - E_m)} a_j^\dagger | \Psi_m \rangle$$

and these sums are absolutely convergent away from the poles. Here

$$Z = \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] = \sum_m e^{-\beta(E_m - \mu N_m)}.$$

Once again the self-energy is the rational function $\Sigma : \mathbb{C} \to \mathbb{C}^{d \times d}$ defined by

$$\Sigma(z) := z - h - G(z)^{-1}.$$

The reader should consult Appendix A for further details and justification of these definitions.

**Theorem 3.4.** Suppose that $\hat{H}$ is an impurity Hamiltonian, with a fragment specified by the indices $1, \ldots, p$. Then the self-energy $\Sigma : \mathbb{C} \to \mathbb{C}^{d \times d}$ is (up to the resolution of removable discontinuities) of the form

$$\Sigma(z) = \begin{pmatrix} \Sigma_p(z) & 0 \\ 0 & 0 \end{pmatrix}.$$

**Remark 3.5.** Once again (cf. Remark 3.3), we recover in the non-interacting setting the formula $G(z) = (z - h)^{-1}$.

**Remark 3.6.** There is a further object known as the Matsubara Green’s function [18], which in turn yields the Matsubara self-energy. Although it is not usually defined this way, the Matsubara Green’s function can be shown to be obtained from the finite-temperature Green’s function, as defined above, by restriction to points $i \omega_m + \mu$, where $\omega_m$ are the fermionic/bosonic Matsubara frequencies [18]. The Matsubara self-energy can be obtained from the finite-temperature self-energy defined above via similar restriction. Therefore Theorem 3.4 implies the same sparsity pattern for the Matsubara self-energy.

**Proof.** The proof is essentially the same as that of Theorem 3.2. Once again we want to show that the $j$-th column of $G(z)\Sigma(z)$ is zero for $j > p$ and that the $i$-th row of $\Sigma(z)G(z)$ is zero for $i > p$. We will only prove the first claim; the second follows by symmetric reasoning.

5The same comments as in section 3.1 apply here as well, though instead see Appendix C.1 for details relevant to this setting.
Define $G_m(z)$ by
\[ G_{m,ij}(z) := \langle \Psi_m | a_i z - (H - E_m) a_j | \Psi_m \rangle - \zeta \langle \Psi_m | a_j z + (H - E_m) a_i | \Psi_m \rangle. \]

Then by the same reasoning as in the proof of Theorem 3.2 (with the roles of $E_0^{(N)}$ and $|\Psi_0^{(N)}\rangle$ played by $E_m$ and $|\Psi_m\rangle$), we find that
\[ zG_{m,ij}(z) = [G_m(z)h]_{ij} + \delta_{ij}. \]

Now $G(z) = \frac{1}{Z} \sum_m e^{-\beta (E_m - \mu N_m)} G_{m,ij}(z)$, so the desired result follows.

### 3.3 Arbitrary contour

There is a more general perspective in which the time-ordering operation used in Appendices B and C to derive the Green’s functions considered above is generalized to an ordering operation on an arbitrary contour in the complex plane. This perspective adds significant value in the non-equilibrium setting, in which one considers a time-dependent Hamiltonian. For such time-dependent problems, passage to the frequency representation is not possible. Instead we consider kernels on the contour.

Let $\mathcal{C}$ denote a piecewise smooth contour in the complex plane (not necessarily closed). Technically one should think of $\mathcal{C}$ not as a subset of $\mathbb{C}$, but as a parametrized path, $\gamma : I \to \mathbb{C}$, where $I = (s_0, s_1)$ is some interval. Then for $s, s' \in I$ with $s < s'$, we define $\mathcal{C}(s, s')$ to be the ‘sub-contour’ defined by restriction of $\gamma$ to the interval $(s, s')$. If $s > s'$, we define $\mathcal{C}(s, s')$ to be the contour obtained from $\mathcal{C}(s', s)$ by reversing its orientation.

Additionally let $\hat{H}(z)$ denote an operator-valued function on a neighborhood of $\mathcal{C} = \gamma(I)$. Here $\hat{H}(z) = a^\dagger h(z) a + \hat{U}(z)$ is particle-number-conserving, and we say that $\hat{H}(z)$ is an impurity Hamiltonian with a fragment specified by indices $1, \ldots, p$ if, for every $z \in \mathcal{C}$, $\hat{U}(z)$ can be written as a polynomial of the $a_i^\dagger, a_i$ for $i = 1, \ldots, p$. As above, since $\hat{U}(z)$ must conserve particle number, it follows that $\hat{U}(z)$ commutes with $a_j$ and $a_j^\dagger$ for $j > p$. It is convenient to denote $z(s) := \gamma(s)$, and abusing notation slightly we will write $\hat{H}(s) := \hat{H}(z(s))$.

As a technical point, we assume that $\hat{H}(s)$ is piecewise continuous. Since the Fock space is finite dimensional in the case of fermions, the meaning of this statement is unambiguous. In the case of bosons, note that since $\hat{H}(s)$ is particle-number-conserving, we can sensibly consider its restriction to each of the $N$-particle subspaces (see Appendix A), each of which is finite-dimensional. Then by the continuity of $\hat{H}(s)$ we mean the continuity of all of these restrictions individually.

Now define a (not necessarily unitary) evolution operator from contour time $s' \in I$ to $s \in I$ as the time-ordered exponential
\[ U(s, s') = \mathcal{T} \left\{ e^{-i \int_{s'}^{s} \hat{H}(z) dz} \right\}. \]

This simply means that $U(s, s')$ is taken as the solution of the differential equation
\[ \partial_s U(s, s') = -i \hat{z}(s) \hat{H}(s) U(s, s'), \quad U(s', s') = \text{Id}. \quad (3.1) \]

This initial-value problem indeed admits a unique solution in the bosonic case because the ODE can be viewed as describing the evolution of an operator on each of the (finite-dimensional) $N$-particle subspace separately.
From this definition it follows that
\[ U(s, s'')U(s'', s') = U(s, s') \]
for all \( s, s', s'' \in I \) and moreover that
\[ \partial_s U(s, s') = i \dot{z}(s)U(s, s')\hat{H}(s'). \]  
(3.2)
Abusing notation slightly by pretending that we can invert \( s = s(z) \), we can more cleanly write
\[ \partial_z U(z, z') = -i\hat{H}(z)U(z, z'), \quad \partial_{z'} U(z, z') = iU(z, z')\hat{H}(z'), \]
where \( \partial_z = (\dot{z}(s))^{-1} \partial_s \). We will sometimes adopt this notational convention, and the meaning should be clear from context.

The following assumption is adopted to ensure that the Green’s function can be defined in the bosonic case:

**Assumption 3.7.** We assume that for all \( s > s' \), \( U(s, s') \) is a bounded operator. Moreover, we assume that there exists \( s > s' \) such that the operator norm of the restriction of \( U(s, s') \) to the \( N \)-particle subspace decays exponentially in \( N \).

Define the partition function
\[ Z = \text{Tr}[U(s_1, s_0)]. \]
Note that Assumption 3.7 guarantees that \( U(s_1, s_0) \) is trace class, so \( Z \) is indeed well-defined. In order to define our ensemble, we must be able to divide by \( Z \). Hence we assume:

**Assumption 3.8.** \( Z \neq 0 \).

We show in Appendix D how Assumptions 3.7 and 3.8 are naturally satisfied in the major nonequilibrium setting of interest, which features the Kadano ff-Baym contour.

Then we define ‘pseudo-Heisenberg’ representations of the annihilation and creation operators via
\[ a_i(s) = U(s_0, s)a_i U(s, s_0), \quad a_i^\dagger(s) = U(s_0, s)a_i^\dagger U(s, s_0). \]
The contour-ordered, single-body Green’s function (which we call the Green’s function for short when the context is clear) is a function \( G : I \times I \to \mathbb{C}^{d \times d} \) defined by
\[ G_{ij}(s, s') = -\frac{i}{Z} \text{Tr}[\mathcal{T}\{a_i(s)a_j^\dagger(s')\}U(s_1, s_0)], \]
where \( \mathcal{T} \) is the contour-ordering operator, formally defined by
\[ \mathcal{T}\{a_i(s)a_j^\dagger(s')\} = \begin{cases} a_i(s)a_j^\dagger(s'), & s' < s \\ \zeta a_j^\dagger(s')a_i(s), & s' \geq s. \end{cases} \]
In other words we can write \( G = G^+ + G^- \), where
\[ iG_{ij}^+(s, s') = \frac{1}{Z} \text{Tr}[U(s_1, s)a_i U(s, s')a_j^\dagger U(s', s_0)]\theta(s - s') \]
and
\[ i G_{ij}^{-}(s, s') = \frac{\zeta}{Z} \text{Tr} [U(s_1, s') a_j U(s', s) a_i U(s, s_0)] (1 - \theta(s - s')). \]
Here
\[ \theta(s) := \begin{cases} 1, & s > 0 \\ 0, & s \leq 0. \end{cases} \]

In the bosonic case, Assumption 3.7 guarantees that the traces needed for this definition do indeed exist. For later reference, note that we can define a product of suitable functions \( A, B : I \times I \to \mathbb{C}^{d \times d} \) (with an appropriate notion of multiplicative inverse, at least formally) via
\[
(AB)(s, s') = \int_{s_0}^{s_1} A(s, s'') B(s'', s') \dot{z}(s'') \, ds'',
\]
chosen so that formally we have
\[
(AB)(z, z') = \int_{s_0}^{z_1} A(z, z'') B(z'', z') \, dz''.
\]
Notice that the appropriate identity \( \delta(z, z') \) is then given by \( \delta(z, z') = (\dot{z}(s))^{-1} \delta(s - s') \).

We remark that the zero-temperature and Matsubara Green’s functions discussed in sections 3.1 and 3.6, respectively, can be recovered as contour-ordered Green’s functions. By contrast, the real-time Green’s function at finite temperature considered in section 3.2 cannot be recovered directly as a contour-ordered Green’s function, though it can be obtained indirectly via analytic continuation of the Matsubara Green’s function. For this reason, diagrammatic expansion techniques at finite temperature are limited to the Matsubara Green’s function and must be carried over to the real-time Green’s function via analytic continuation. For further details, see [21].

One now wants to define the self-energy as
\[ \Sigma(z, z') = i \partial_z - h(z) \delta(z, z') - G^{-1}(z, z'). \]
However, this definition is not rigorous without further justification. Indeed, note that \( G \) can be viewed as an integral operator on \( L^2(I) \), and under reasonable assumptions \( G \) is Hilbert-Schmidt, hence in particular compact. Therefore its inverse is guaranteed to be an unbounded operator, if it can be constructed. Formally, one expects that the \( i(\dot{z}(s))^{-1} \partial_s \) in our definition of the self-energy will cancel an analogous term in the formal inverse \( G^{-1} \) and that the self-energy can be written as a sum of a static and dynamic part as
\[
\Sigma(s, s') = \Sigma_{\text{stat}}(s - s') + \Sigma_{\text{dyn}}(s, s'),
\]
where \( \Sigma_{\text{dyn}} \) is a properly defined integral operator.

In our view the mathematical construction of the self-energy seems to be a non-trivial matter, and we will sidestep it in this work. (By contrast, the construction in the equilibrium setting is more straightforward in the frequency domain; see Appendices B and C.)

How then to discuss the sparsity pattern of the self-energy? Observe that formally, we should have
\[
(\Sigma G)(z, z') = i \partial_z G(z, z') - h(z) G(z, z') - I_d \delta(z, z')
\]
\[
(G \Sigma)(z, z') = -i \partial_z G(z, z') - G(z, z') h(z') - I_d \delta(z, z'),
\]
or, more rigorously,

\[
(\Sigma G)(s, s') = i(\dot{z}(s))^{-1} \partial_s G(s, s') - h(s)G(s, s') - I_d(\dot{z}(s))^{-1} \delta(s - s')
\]

\[
(G \Sigma)(s, s') = -i(\dot{z}(s'))^{-1} \partial_{s'} G(s, s') - G(s, s')h(s') - I_d(\dot{z}(s))^{-1} \delta(s - s').
\]

(3.3)

Now instead of constructing the self-energy, we can define operators \(\Sigma G\) and \(G \Sigma\) via (3.3) (in the sense of distributions), with the ‘\(\Sigma\)’ appearing here merely as a notation. Now the desired sparsity pattern of \(\Sigma\) is formally equivalent to the statement that \([\Sigma G]_{ij} = 0\) (as a distribution on \(I\)) for \(i > p\) and \([G \Sigma]_{ij} = 0\) for \(j > p\).

**Theorem 3.9.** With notation and assumptions as in the preceding, if \(\hat{H}(z)\) is an impurity Hamiltonian with a fragment specified by the indices \(1, \ldots, p\), then \([\Sigma G]_{ij} = 0\) for \(i > p\) and \([G \Sigma]_{ij} = 0\) for \(j > p\).

**Remark 3.10.** In the non-interacting setting \(p = 0\), we recover the formulas

\[
i\partial_s G(z, z') - h(z) G(z, z') = I_d \delta(z, z'), \quad -i\partial_z G(z, z') - G(z, z') h(z') = I_d \delta(z, z'),
\]

where we have abused notation slightly in the manner described above. These formulas seem to be non-trivial to establish by any other means. By contrast with the equilibrium case, this formula cannot be established simply via a canonical transformation because it may not be possible to simultaneously diagonalize the \(h(z)\) for all \(z\). In fact, in [21], the non-interacting Green’s function is defined via the formula (subject to certain boundary conditions) and shown to give the appropriate perturbation theory within the Martin-Schwinger hierarchy.

**Proof.** We prove only the first statement, as the second follows from similar arguments. Recall

\[
iG_{ij}^+(s, s') = \frac{1}{Z} \text{Tr} \left[ U(s_1, s)a_i U(s, s') a_j^\dagger U(s', s_0) \right] \theta(s - s').
\]

Then compute, using Eqs. (3.1) and (3.2),

\[
i(\dot{z}(s))^{-1} \partial_s G_{ij}^+(s, s') = \frac{i}{Z} \text{Tr} \left[ U(s_1, s) \hat{H}(s)a_i U(s, s') a_j^\dagger U(s', s_0) \right] \theta(s - s')
\]

\[
- \frac{i}{Z} \text{Tr} \left[ U(s_1, s)a_i \hat{H}(s) U(s, s') a_j^\dagger U(s', s_0) \right] \theta(s - s')
\]

\[
+ (\dot{z}(s))^{-1} \frac{1}{Z} \text{Tr} \left[ U(s_1, s)a_i a_j^\dagger U(s, s_0) \right] \delta(s - s')
\]

\[
= \frac{i}{Z} \text{Tr} \left[ U(s_1, s)[a_i, \hat{H}(s)]U(s, s') a_j^\dagger U(s', s_0) \right] \theta(s - s')
\]

\[
+ (\dot{z}(s))^{-1} \frac{1}{Z} \text{Tr} \left[ U(s_1, s)a_i a_j^\dagger U(s, s_0) \right] \delta(s - s').
\]

Now for \(i > p\), \([a_i, \hat{H}(s)] = [a_i, a_j^\dagger h(s)a] = \sum_{l=1}^d h_{il}(s)a_i\), by Lemma 3.1 Therefore

\[
i(\dot{z}(s))^{-1} \partial_s G_{ij}^+(s, s') = -\frac{i}{Z} \sum_{l=1}^d h_{il}(s) \text{Tr} \left[ U(s_1, s)a_l U(s, s') a_j^\dagger U(s', s_0) \right] \theta(s - s')
\]

\[
+ (\dot{z}(s))^{-1} \frac{1}{Z} \text{Tr} \left[ U(s_1, s)a_i a_j^\dagger U(s, s_0) \right] \delta(s - s').
\]
\[
[i(\dot{z}(s))^{-1} \partial_s G_{ij}(s, s')] = \left[ h(s)G^+(s, s') \right]_{ij} + (\dot{z}(s))^{-1} \frac{1}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s) a_j a_i^\dagger U(s, s_0) \right] \delta(s - s').
\]

Similarly,
\[
\begin{align*}
\frac{i}{\mathcal{Z}} & \text{Tr} \left[ U(s_1, s') a_i^\dagger U(s', s) \hat{H}(s) a_i U(s, s_0) \right] (1 - \theta(s - s')) \\
& - \frac{i}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s') a_i^\dagger U(s', s) \hat{\Theta}(s) U(s, s_0) \right] (1 - \theta(s - s')) \\
& - (\dot{z}(s))^{-1} \frac{\zeta}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s) a_i^\dagger a_i U(s, s_0) \right] \delta(s - s') \\
& = - \frac{i}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s) a_i^\dagger a_i U(s, s_0) \right] \delta(s - s') \\
& = - \frac{i}{\mathcal{Z}} \sum_{l=1}^d h_{il}(s) \text{Tr} \left[ U(s_1, s) a_i U(s, s') a_j^\dagger a_i U(s', s_0) \right] \theta(s - s') \\
& - \frac{i}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s) a_i^\dagger a_i U(s, s_0) \right] \delta(s - s') \\
& = \left[ h(s)G^-(s, s') \right]_{ij} - (\dot{z}(s))^{-1} \frac{\zeta}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s) a_i^\dagger a_i U(s, s_0) \right] \delta(s - s').
\end{align*}
\]

Therefore, since \( G = G^+ + G^- \), we have
\[
\begin{align*}
\frac{i}{\mathcal{Z}} (\dot{z}(s))^{-1} \partial_s G_{ij}(s, s') &= \left[ h(s)G(s, s') \right]_{ij} \\
&+ \frac{1}{\mathcal{Z}} \text{Tr} \left[ U(s_1, s) (a_i a_j^\dagger - \zeta a_i^\dagger a_i) U(s, s_0) \right] (\dot{z}(s))^{-1} \delta(s - s') \\
&= \left[ h(s)G(s, s') \right]_{ij} + \delta_{ij} (\dot{z}(s))^{-1} \delta(s - s'),
\end{align*}
\]
which completes the proof. \( \square \)

3.4 Anomalous setting

Finally we will consider a sparsity result for the self-energy of anomalous impurity problems. These are impurity problems in which the Hamiltonian does not conserve particle number. Since the anomalous setting is of most interest for the study of superconductivity in fermions, we will restrict our attention to the fermionic setting. This allows us to avoid some further analytic difficulty since our rigorous definitions in the bosonic case (in which the Fock space is infinite-dimensional) relied on particle number conservation. It also eases the notational burden to keep track of \( \zeta \) to distinguish the bosonic and fermionic systems. In order to simply illustrate the points that are novel to this setting, we further restrict our attention to the zero-temperature equilibrium setting.

Now consider a self-adjoint Hamiltonian \( \hat{H} \) on the fermionic Fock space \( \mathcal{F}_{-1, d} \), and we write \( \hat{H} \) of the form
\[
\hat{H} = \hat{H}_0 + \hat{U},
\]
where
\[
\hat{H}_0 := \hat{H}_{\text{NA}} + \hat{H}_A + \hat{H}_A^\dagger
\]
is the single-particle part of the Hamiltonian (no longer particle-number-conserving), specified by its non-anomalous and anomalous parts

\[ \hat{H}_{NA} := \sum_{i,j=1}^{d} h_{ij} a_i^\dagger a_j, \quad \hat{H}_{A} := \frac{1}{2} \sum_{i,j=1}^{d} \Delta_{ij} a_i^\dagger a_j. \]

Therefore, up to a scalar multiple of the identity operator, \( \hat{H}_0 \) is given by

\[
\left( \begin{array}{c} a \\ a^\dagger \end{array} \right)^\dagger \left( \begin{array}{cc} h & \Delta \\ -\Delta^\dagger & -h \end{array} \right) \left( \begin{array}{c} a \\ a^\dagger \end{array} \right),
\]

where we have abused notation slightly by using \( a \) to indicate both a row and a column vector of operators. Without loss of generality we assume that \( \Delta = (\Delta_{ij}) \) is a complex antisymmetric matrix. (Note that then \(-\Delta = \Delta^\dagger\), and since \( h \) is Hermitian, \(-h = -h^T\).) Meanwhile, the interacting part \( \hat{U} \) is itself a self-adjoint operator on \( \mathcal{F}_{-1,d} \), and we demand that it can be written as an even polynomial of the creation and annihilation operators, which includes the particle-number-conserving operators. In the case that \( \hat{U} \) can be written as a polynomial of the \( a_i^\dagger, a_i \) for \( i = 1, \ldots, p \), we say that \( \hat{H} \) is an anomalous impurity Hamiltonian, with a fragment specified by the indices \( 1, \ldots, p \). As in earlier settings, the rest of the indices correspond to the environment. Note that the evenness of the polynomial specifying \( \hat{U} \) guarantees that \( \hat{U} \) commutes with \( a_j \) and \( a_j^\dagger \) for \( j > p \).

To determine the expectations computed at the end of the last section, it suffices to determine the following Green’s functions, which are themselves desirable to know:

\[
G_{ij}^{hp}(z) := G_{ij}^{hp,+}(z) + G_{ij}^{hp,-}(z) := \langle \Phi_0|a_i | z - (\hat{H} - E_0) a_j^\dagger \Phi_0 \rangle + \langle \Phi_0|a_j^\dagger | z + (\hat{H} - E_0) a_i \Phi_0 \rangle
\]

\[
G_{ij}^{pp}(z) := G_{ij}^{pp,+}(z) + G_{ij}^{pp,-}(z) := \langle \Phi_0|a_i | z - (\hat{H} - E_0) a_j^\dagger \Phi_0 \rangle + \langle \Phi_0|a_j^\dagger | z + (\hat{H} - E_0) a_i \Phi_0 \rangle
\]

\[
G_{ij}^{hh}(z) := G_{ij}^{hh,+}(z) + G_{ij}^{hh,-}(z) := \langle \Phi_0|a_i | z - (\hat{H} - E_0) a_j^\dagger \Phi_0 \rangle + \langle \Phi_0|a_j^\dagger | z + (\hat{H} - E_0) a_i \Phi_0 \rangle
\]

\[
G_{ij}^{ph}(z) := G_{ij}^{ph,+}(z) + G_{ij}^{ph,-}(z) := \langle \Phi_0|a_i | z - (\hat{H} - E_0) a_j^\dagger \Phi_0 \rangle + \langle \Phi_0|a_j^\dagger | z + (\hat{H} - E_0) a_i \Phi_0 \rangle,
\]

where \( |\Phi_0\rangle \) is the ground state of \( \hat{H} \) and \( E_0 \) is the ground-state energy. The superscripts \( p \) and \( h \) stand for ‘particle’ and ‘hole’, respectively, so \( G^{hh} \) is called the hole-hole Green’s function, \( G^{ph} \) is the particle-hole Green’s function, etc.

Notice that the last two Green’s functions are actually redundant because \( G^{hp}(z) = -[G^{hp}(-z)]^T \) and \( G^{hh}(z) = [G^{pp}(z)]^\dagger \). We can further define the anomalous Green’s function by

\[
G(z) := \begin{pmatrix} G^{hp}(z) & G^{hh}(z) \\ G^{pp}(z) & G^{ph}(z) \end{pmatrix}
\]
and the anomalous self-energy by

\[ \Sigma(z) := z - \left( \begin{array}{cc} \frac{h}{\Delta} & \frac{\Delta}{-h} \\ -\frac{\Delta}{-h} & \frac{h}{\Delta} \end{array} \right) - G(z)^{-1}. \]

In fact we will show the following result:

**Theorem 3.11.** Suppose that \( \hat{H} \) is an anomalous impurity Hamiltonian, with a fragment specified by the indices 1, \ldots, \( p \). Then the anomalous self-energy \( \Sigma : \mathbb{C} \to \mathbb{C}^{d \times d} \) is (up to the resolution of removable discontinuities) of the form

\[ \Sigma(z) = \begin{pmatrix} \Sigma_p^{hp}(z) & 0 \\ 0 & 0 \\ \Sigma_p^{pp}(z) & 0 \\ 0 & 0 \end{pmatrix}. \]

**Remark 3.12.** Note that in the case \( p = 0 \) we recover the formula

\[ G(z) = \left[ z - \left( \begin{array}{cc} \frac{h}{\Delta} & \frac{\Delta}{-h} \\ -\frac{\Delta}{-h} & \frac{h}{\Delta} \end{array} \right) \right]^{-1} \]

for the non-interacting anomalous Green’s function.

Recall from Lemma 3.1 that

\[ [\hat{H}_{NA}, a^\dagger_j] = \sum_{\gamma} h_{kj} a^\dagger_k \]

and

\[ [\hat{H}_{NA}, a_j] = -\sum_{\gamma} h_{jk} a^\dagger_k. \]

Before proceeding with the proof of Theorem 3.11 we supplement this result with a further simple lemma:

**Lemma 3.13.** Let \( \hat{H}_A = \frac{1}{2} \sum_{i,j=1}^d \Delta_{ij} a^\dagger_i a^\dagger_j \) with \( \Delta = (\Delta_{ij}) \) being a complex antisymmetric matrix. Then

\[ [\hat{H}_A, a^\dagger_j] = 0, \quad [\hat{H}_A, a_j] = 0, \quad [\hat{H}_A, a^\dagger_j] = \sum_k \Sigma_{jk} a^\dagger_k, \quad [\hat{H}_A, a_j] = \sum_k \Sigma_{kj} a_k. \]

**Proof.** The first two identities are obvious, and the fourth follows from the third by taking Hermitian conjugates and using the antisymmetry of \( \Delta \). To see the claimed third identity, simply compute

\[ \hat{H}_A a_j = \frac{1}{2} \sum_{ik} \Delta_{ik} a^\dagger_i a^\dagger_k a_j = \frac{1}{2} \sum_{ik} \Delta_{ik} a^\dagger_i a^\dagger_k \delta_{jk} - \frac{1}{2} \sum_{ik} \Delta_{ik} a^\dagger_i a_j a^\dagger_k = \frac{1}{2} \sum_{ik} \Delta_{ij} a^\dagger_i a^\dagger_k - \frac{1}{2} \sum_{ik} \Delta_{ik} a^\dagger_i a^\dagger_j + \frac{1}{2} \sum_{ik} \Delta_{ik} a_j a^\dagger_k a^\dagger_i = \frac{1}{2} \sum_k \Sigma_{kj} a^\dagger_k + a_j \hat{H}_A. \]
\[ \sum_k \Delta_{kj} a_k^\dagger + a_j \hat{H}_\Lambda. \]

**Proof.** (Of Theorem 3.11) Throughout we will often use \( \langle \cdot \rangle \) to indicate the expectation \( \langle \Phi_0 | \cdot | \Phi_0 \rangle \).

Now it suffices to show the following sparsity pattern

\[
G(z) \Sigma(z) = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \Sigma(z)G(z) = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]

We will only prove the first of these claims; the other follows by similar reasoning. Note that this first claim is equivalent to the fact that each of the following equalities holds along the last \( d - p \) columns:

\[
G^{hp}[z - h] - G^{hh} \Delta^\dagger = I_d,
\]

\[-G^{hp} \Delta + G^{hh}[z + h^T] = 0,
\]

\[G^{pp}[z - h] - G^{ph} \Delta^\dagger = 0,
\]

\[-G^{pp} \Delta + G^{nh}[z + h^T] = I_d.
\]

Now we begin the computations. In the following we assume that \( j > p \). Since \( (\hat{H} - E_0) | \Phi_0 \rangle = 0 \), we have

\[
zG_{ij}^{hp, +}(z) = \langle \Phi_0| a_i \frac{1}{z - (\hat{H} - E_0)} a_j^\dagger (z - (\hat{H} - E_0)) | \Phi_0 \rangle
\]

\[
= \langle a_i a_j^\dagger \rangle + \langle a_i \frac{1}{z - (\hat{H} - E_0)} [\hat{H}, a_j^\dagger] \rangle
\]

\[
= \langle a_i a_j^\dagger \rangle + \langle a_i \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_{NA}, a_j^\dagger] \rangle + \langle a_i \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_\Lambda, a_j^\dagger] \rangle
\]

\[
= \langle a_i a_j^\dagger \rangle + \sum_k \langle a_i \frac{1}{z - (\hat{H} - E_0)} a_k^\dagger \rangle h_{kj} + \sum_k \langle a_i \frac{1}{z - (\hat{H} - E_0)} a_k \rangle \Delta_{jk}
\]

\[
= \langle a_i a_j^\dagger \rangle + [G^{hp, +}]_{ij} + [G^{hh, +}]_{ij}.
\]

Similarly,

\[
zG_{ij}^{hp, -}(z) = \langle \Phi_0| (z + (\hat{H} - E_0)) a_j^\dagger \frac{1}{z + (\hat{H} - E_0)} a_i | \Phi_0 \rangle
\]

\[
= \langle a_j^\dagger a_i \rangle + \langle [\hat{H}, a_j^\dagger] \frac{1}{z + (\hat{H} - E_0)} a_i \rangle
\]

\[
= \langle a_j^\dagger a_i \rangle + \langle [\hat{H}_{NA}, a_j^\dagger] \frac{1}{z + (\hat{H} - E_0)} a_i \rangle + \langle [\hat{H}_\Lambda, a_j^\dagger] \frac{1}{z + (\hat{H} - E_0)} a_i \rangle
\]

\[
= \langle a_j^\dagger a_i \rangle + \sum_k \langle a_j^\dagger \frac{1}{z + (\hat{H} - E_0)} a_i \rangle h_{kj} + \sum_k \langle a_k \frac{1}{z + (\hat{H} - E_0)} a_i \rangle \Delta_{jk}
\]

\[
= \langle a_j^\dagger a_i \rangle + \sum_k \langle a_k \frac{1}{z + (\hat{H} - E_0)} a_i \rangle \Delta_{jk}.
\]
\[\langle a_j^\dagger a_i \rangle + [G^{hp,-} h]_{ij} + [G^{hh,-} \Delta^1]_{ij}.\]

Therefore, adding our results and recognizing that \(\langle a_i a_j^\dagger \rangle + \langle a_j^\dagger a_i \rangle = \delta_{ij}\), we obtain

\[zG^{hp}_{ij} = \delta_{ij} + [G^{hp} h]_{ij} + [G^{hh} \Delta^1]_{ij}\]

for all \(j > p\), which implies our first desired result.

Next compute

\[zG^{hh,+}_{ij}(z) = \langle \Phi_0 | a_j \frac{1}{z - (\hat{H} - E_0)} - a_j (z - (\hat{H} - E_0)) | \Phi_0 \rangle\]

\[= \langle a_j a_i \rangle + \langle a_i \frac{1}{z - (\hat{H} - E_0)} [\hat{H}, a_j] \rangle\]

\[= \langle a_j a_i \rangle + \langle a_i \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_{NA}, a_j] \rangle + \langle a_i \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_A, a_j] \rangle\]

\[= \langle a_j a_i \rangle + \sum_k (a_i \frac{1}{z - (\hat{H} - E_0)} a_k H_{jk} + \sum_k (a_i \frac{1}{z - (\hat{H} - E_0)} a_k^\dagger \Delta_{kj})\]

\[= \langle a_j a_i \rangle - [G^{hh,+} h^T]_{ij} + [G^{hp,+} \Delta]_{ij},\]

and

\[zG^{hh,-}_{ij}(z) = \langle \Phi_0 | (z + (\hat{H} - E_0)) a_j \frac{1}{z + (\hat{H} - E_0)} a_i | \Phi_0 \rangle\]

\[= \langle a_j a_i \rangle + \langle [\hat{H}, a_j] \frac{1}{z + (\hat{H} - E_0)} a_i \rangle\]

\[= \langle a_j a_i \rangle + \langle [\hat{H}_{NA}, a_j] \frac{1}{z + (\hat{H} - E_0)} a_i \rangle + \langle [\hat{H}_A, a_j] \frac{1}{z + (\hat{H} - E_0)} a_i \rangle\]

\[= \langle a_j a_i \rangle - \sum_k (a_i \frac{1}{z + (\hat{H} - E_0)} h_{jk} + \sum_k (a_i \frac{1}{z + (\hat{H} - E_0)} a_k^\dagger \Delta_{kj})\]

\[= \langle a_j a_i \rangle - [G^{hh,-} h^T]_{ij} + [G^{hp,-} \Delta]_{ij}.\]

Adding our results and recognizing that \(\langle a_i a_j \rangle + \langle a_j a_i \rangle = 0\), we obtain our second desired result.

Next compute

\[zG^{pp,+}_{ij}(z) = \langle \Phi_0 | a_i^\dagger \frac{1}{z - (\hat{H} - E_0)} a_j^\dagger (z - (\hat{H} - E_0)) | \Phi_0 \rangle\]

\[= \langle a_i^\dagger a_j^\dagger \rangle + \langle a_i^\dagger \frac{1}{z - (\hat{H} - E_0)} [\hat{H}, a_j^\dagger] \rangle\]

\[= \langle a_i^\dagger a_j^\dagger \rangle + \langle a_i^\dagger \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_{NA}, a_j^\dagger] \rangle + \langle a_i^\dagger \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_A, a_j^\dagger] \rangle\]

\[= \langle a_i^\dagger a_j^\dagger \rangle + \sum_k (a_i^\dagger \frac{1}{z - (\hat{H} - E_0)} a_k^\dagger h_{kj} + \sum_k (a_i^\dagger \frac{1}{z - (\hat{H} - E_0)} a_k^\dagger \Delta_{jk})\]

\[= \langle a_i^\dagger a_j^\dagger \rangle + [G^{pp,+} h]_{ij} + [G^{hh,+} \Delta^1]_{ij},\]
and
\[
zG_{ij}^{pp-}(z) = \langle \Phi_0 | (z + (\hat{H} - E_0)) a_j \frac{1}{z + (\hat{H} - E_0)} a_i | \Phi_0 \rangle
\]
\[
= \langle a_j a_i \rangle + \langle [\hat{H} - E_0] a_j \rangle \frac{1}{z + (\hat{H} - E_0)} a_i
\]
\[
= \langle a_j a_i \rangle + \langle [\hat{H}_{NA} - E_0] a_j \rangle \frac{1}{z + (\hat{H} - E_0)} a_i + \langle [\hat{H}_A - E_0] a_j \rangle \frac{1}{z + (\hat{H} - E_0)} a_i
\]
\[
= \langle a_j a_i \rangle + \sum_k \langle a_j \frac{1}{z + (\hat{H} - E_0)} a_k \rangle h_{kj} + \sum_k \langle a_k \frac{1}{z + (\hat{H} - E_0)} a_j \rangle \Delta_{kj}
\]
\[
= \langle a_j a_i \rangle + [G_{ij}^{pp-} h^T]_{ij} + [G_{ij}^{pp-} \Delta]_{ij},
\]
yielding our third desired result.

Finally, compute
\[
zG_{ij}^{ph, \cdot +}(z) = \langle \Phi_0 | a_j \frac{1}{z - (\hat{H} - E_0)} a_j (z - (\hat{H} - E_0)) | \Phi_0 \rangle
\]
\[
= \langle a_j a_j \rangle + \langle a_j \frac{1}{z - (\hat{H} - E_0)} [\hat{H}, a_j] \rangle
\]
\[
= \langle a_j a_j \rangle + \langle a_j \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_{NA}, a_j] \rangle + \langle a_j \frac{1}{z - (\hat{H} - E_0)} [\hat{H}_A, a_j] \rangle
\]
\[
= \langle a_j a_j \rangle - \sum_k \langle a_j \frac{1}{z - (\hat{H} - E_0)} a_k \rangle h_{kj} + \sum_k \langle a_k \frac{1}{z - (\hat{H} - E_0)} a_j \rangle \Delta_{kj}
\]
\[
= \langle a_j a_j \rangle - [G_{ij}^{ph, \cdot +} h^T]_{ij} + [G_{ij}^{ph, \cdot +} \Delta]_{ij},
\]
and
\[
zG_{ij}^{ph, \cdot -}(z) = \langle \Phi_0 | (z + (\hat{H} - E_0)) a_j \frac{1}{z + (\hat{H} - E_0)} a_i | \Phi_0 \rangle
\]
\[
= \langle a_j a_j \rangle + \langle [\hat{H} - E_0] a_j \rangle \frac{1}{z + (\hat{H} - E_0)} a_i
\]
\[
= \langle a_j a_j \rangle + \langle [\hat{H}_{NA} - E_0] a_j \rangle \frac{1}{z + (\hat{H} - E_0)} a_i + \langle [\hat{H}_A - E_0] a_j \rangle \frac{1}{z + (\hat{H} - E_0)} a_i
\]
\[
= \langle a_j a_j \rangle - \sum_k \langle a_k \frac{1}{z + (\hat{H} - E_0)} a_j \rangle h_{kj} + \sum_k \langle a_k \frac{1}{z + (\hat{H} - E_0)} a_j \rangle \Delta_{kj}
\]
\[
= \langle a_j a_j \rangle - [G_{ij}^{ph, \cdot -} h^T]_{ij} + [G_{ij}^{ph, \cdot -} \Delta]_{ij},
\]
yielding the last desired result. \(\square\)

A Second quantization

Here we introduce the formalism of second quantization, with the aim of providing enough background and results to make the results of this paper rigorous. We limit our discussion to fermionic
and bosonic Fock spaces with finitely many states, i.e., finitely many creation and annihilation operators. This setting can directly describe lattice models such as the Hubbard model in addition to tight-binding approximations of continuum systems. In this sense we can view the set \(\{1, \ldots, d\}\) as indexing sites in a lattice model. More generally, one can reduce a continuum problem to this setting via the choice of a finite orbital basis \([18]\).

### A.1 The occupation number construction

Let \(N_{-1} = \{0, 1\}\) and \(N_{+1} = \{0, 1, 2, \ldots\}\). These are the sets of allowable occupation numbers of a state in the fermionic and bosonic cases, respectively. (Recall that the cases \(\zeta = -1\) and \(\zeta = +1\) indicate, respectively, the cases of fermions and bosons.)

Let \(d\) be a positive integer, the number of states, and consider the collection:

\[
B_{\zeta,d} = \{|n_1, n_2, \ldots, n_d\rangle : n_i \in N_{\zeta}\}.
\]

This set will be the occupation number basis for our Fock space \(F_{\zeta,d}\). For short, we may indicate the basis elements by \(|n\rangle\) for \(n \in N_{\zeta}^d\).

To define the Fock space, consider the set \(V_{\zeta,d}\) of finite formal linear combinations of elements of \(B_{\zeta,d}\). Then \(V_{\zeta,d}\) is a vector space, and it can be endowed with an inner product by stipulating that the elements of \(B_{\zeta,d}\) are orthonormal. (Hence \(B_{\zeta,d}\) is an orthonormal basis of \(V_{\zeta,d}\).) For fermions, \(V_{\zeta,d}\) is finite-dimensional and therefore a Hilbert space, but this is not the case for bosons. Therefore we define \(F_{\zeta,d}\) to be the completion of \(V_{\zeta,d}\) with respect to the metric induced by its inner product, so \(F_{\zeta,d}\) is a Hilbert space, and \(B_{\zeta,d}\) is a complete orthonormal set (in fact, a basis if \(\zeta = -1\)).

In accordance with Dirac’s bra-ket notation, we will denote elements of \(F_{\zeta,d}\) with the notation \(|\phi\rangle\) (where \(\phi\) can be thought of as a symbolic label), and we denote the adjoint of an element \(|\phi\rangle \in F_{\zeta,d}\) by \(\langle \phi|\). Inner products may then be denoted \(\langle \psi|\phi\rangle\), and we denote the induced norm on \(F_{\zeta,d}\) by \(\|\phi\| = \sqrt{\langle \phi|\phi\rangle}\).

The reader should be careful to distinguish between the vacuum state \(|0, \ldots, 0\rangle\), denoted \(|-\rangle\) for short, and the zero vector of \(F_{\zeta,d}\), denoted simply as \(0\), which is the linear combination of elements of \(B_{\zeta,d}\) in which all coefficients are zero. In particular the vacuum state has norm 1 and the zero vector has norm 0.

### A.2 Creation and annihilation operators

The annihilation operators \(a_i\) are linear operators \(V_{\zeta,d} \to V_{\zeta,d}\) defined by their action on the basis \(B_{\zeta,d}\):

\[
a_i|n\rangle = \begin{cases} 0, & n_i = 0 \\ \zeta \sum_{j<i} n_j \sqrt{n_i} |n_1, \ldots, n_{i-1}, n_i - 1, n_{i+1} \ldots n_d\rangle, & n_i \neq 0. \end{cases}
\]

Meanwhile the creation operators \(a_i^\dagger\) are linear operators \(V_{\zeta,d} \to V_{\zeta,d}\), defined by their action on the basis \(B_{\zeta,d}\):

\[
a_i^\dagger|n\rangle = \begin{cases} 0, & \zeta = -1, n_i = 1 \\ \zeta \sum_{j<i} n_j \sqrt{n_i + 1} |n_1, \ldots, n_{i-1}, n_i + 1, n_{i+1} \ldots n_d\rangle, & n_i \neq 0. \end{cases}
\]

\(^6\)For the zero vector we forgo the bra-ket notation here to avoid confusion.
In the case of fermions, $V_{\zeta,d} = F_{\zeta,d}$ is finite-dimensional, so the creation and annihilation operators are defined on $F_{\zeta,d}$, and they are in fact Hermitian adjoints of one another in the usual sense as the notation suggests. Moreover, $a_i$ and $a_i^\dagger$ have operator norm 1, which in particular remains bounded in the limit of infinitely many states. In fact, as this observation suggests, the appropriate creation and annihilation operators on fermionic Fock spaces generated by infinitely many states (which we do not define or consider these here) are bounded operators with operator norm 1.

By contrast, in the case of bosons, $a_i$ and $a_i^\dagger$ are unbounded operators, even for finite $d$. Thus $a_i$ and $a_i^\dagger$ are only densely defined (unbounded) operators on $F_{\zeta,d}$. In fact, adjoint operators can be defined even for operators that are only densely defined on a Hilbert space, and in this sense $a_i$ and $a_i^\dagger$ are Hermitian adjoints of one another. For the reader familiar only with adjoints of bounded operators, one can merely consider the '†' as a notation.

The most important feature of the creation and annihilation operators are the (anti)commutation relations. Denoting commutator of operators $A,B$ by $[A,B]_+ := AB - BA$ and the anticommutator by $[A,B]_- := AB + BA$, we have

$$[a_i, a_j]\zeta = [a_i^\dagger, a_j^\dagger]\zeta = 0, \quad [a_i, a_j^\dagger]\zeta = \delta_{ij} \text{Id},$$

A.1 on $V_{\zeta,d}$. These relations can be readily verified from the definitions of $a_i$ and $a_i^\dagger$.

We say that a composition of creation and annihilation operators such as $a_i^\dagger a_j$ is normally ordered if all of the creation operators appear to the left of all of the annihilation operators. Any composition of creation and annihilation operators can be converted to a linear combination of normally ordered operators via the (anti)commutation relations.

For a unitary transformation $T : \mathbb{R}^d \to \mathbb{R}^d$, one can define new operators $\tilde{a}_i^\dagger = \sum_{j=1}^d T_{ij} a_j^\dagger$ and $\tilde{a}_i = \sum_{j=1}^d T_{ij} a_j$. These can be viewed as creation and annihilation operators, respectively, in that they satisfy the same commutation relations as in A.1. One can in turn view these as generators for our Fock space inducing a different occupation number basis.

### A.3 Number operators and eigenspaces

For each state we define a number operator

$$\hat{n}_i := a_i^\dagger a_i,$$

which is a linear operator $V_{\zeta,d} \to V_{\zeta,d}$. In the case of bosons $\hat{n}_i$ can be viewed as an unbounded, self-adjoint, densely defined operator on $F_{\zeta,d}$. Note that the number operators all commute, i.e., $[n_i, n_j]_+ = 0$ for all $i,j$.

We also define the total number operator by

$$\hat{N} := \sum_{i=1}^d \hat{n}_i.$$

The set of eigenvectors of $\hat{n}$ (as a linear transformation $V_{\zeta,d} \to V_{\zeta,d}$) is precisely $B_{\zeta,d}$, and each eigenvector $|n\rangle$ has eigenvalue $\sum_{i=1}^d n_i$. Thus the set of eigenvalues is given by $\{0,1,\ldots,d\}$ in the case of fermions and $\{0,1,\ldots\}$ in the case of bosons.
Then we define the $N$-particle subspace to be the $N$-eigenspace of $\hat{N}$, which is finite-dimensional (even for bosons), and we denote it by $\mathcal{F}^{(N)}_{\zeta,d}$. Then we can write

$$\mathcal{V}_{\zeta,d} = \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)}_{\zeta,d}.$$ 

The $N$-eigenspace is understood to be $\{0\}$ for any integer $N \notin \{0, 1, \ldots, d\}$ in the case of fermions and for any $N \notin \{0, 1, \ldots\}$ in the case of bosons. Notice that $a_i$ maps $\mathcal{F}^{(N)}_{\zeta,d} \to \mathcal{F}^{(N-1)}_{\zeta,d}$ and $a_i^\dagger$ maps $\mathcal{F}^{(N)}_{\zeta,d} \to \mathcal{F}^{(N+1)}_{\zeta,d}$.

We say that an operator $A$ on $\mathcal{F}_{\zeta,d}$ conserves particle number if $A$ maps $\mathcal{F}^{(N)}_{\zeta,d} \to \mathcal{F}^{(N)}_{\zeta,d}$ for all integers $N$. Evidently any operator such as $a_i^\dagger a_j$ in which an equal number of creation and annihilation operators appear, as well as any sum of such operators, must conserve particle number.

### A.4 Hamiltonians

For convenience we shall let $a = (a_1, \ldots, a_d)$ denote the vector of annihilation operators, and accordingly $a^\dagger = (a_1^\dagger, \ldots, a_d^\dagger)^T$. Then consider a Hamiltonian $\hat{H} = H(a^\dagger, a)$ that is a normally ordered polynomial of creation and annihilation operators. As an operator on $\mathcal{V}_{\zeta,d}$, we stipulate that $\hat{H}$ commutes with the total number operator $\hat{N}$. Hence $\hat{H}$ conserves particle number and is an operator $\mathcal{F}^{(N)}_{\zeta,d} \to \mathcal{F}^{(N)}_{\zeta,d}$ for all $N$, and we demand that $\hat{H}$ is self-adjoint as such.

In general we can write

$$\hat{H} = \hat{H}_0 + \hat{U},$$

where

$$\hat{H}_0 := a^\dagger h a = \sum_{i,j=1}^{d} h_{ij} a_i^\dagger a_j$$

is the single-particle (or non-interacting) part of the Hamiltonian, specified by a Hermitian $d \times d$ matrix $h$, and $\hat{U} = U(a^\dagger, a)$ is the interacting part. Here $\hat{U}$ is normally ordered and commutes with $\hat{N}$ (since $\hat{H}_0$ does), and moreover $\hat{U}$ is self-adjoint on $\mathcal{F}^{(N)}_{\zeta,d}$ for all $N$ (since $\hat{H}_0$ is).

Via a unitary transformation of the creation and annihilation operators, one can without loss of generality assume that $h$ is diagonal. However, the utility of this manipulation is limited outside of the non-interacting setting because such a transformation may complicate the representation of the interaction term $\hat{U}$.

Though we need not define $\hat{U}$ more explicitly for the purposes of this paper, for concreteness one might keep in mind the two-body interaction

$$\hat{U} = \frac{1}{2} \sum_{ijkl} (ij|kl)a_i^\dagger a_j^\dagger a_k a_l.$$  \hspace{1cm} (A.2)

We comment more concretely on how such a second-quantized two-body operator may arise from a two-body potential in real space. To construct a finite-state Fock space, one first replaces the single-particle Hilbert space $\mathcal{H} := L^1(\mathbb{R}^3, \pm \frac{1}{2}; \mathbb{C}) \subset L^2(\mathbb{R}^3, \pm \frac{1}{2}; \mathbb{C})$ with a finite-dimensional subspace $\mathcal{H}_D$ spanned by an orthonormal single-particle basis $\mathcal{D} := \{\varphi_1, \ldots, \varphi_d\}$. One then defines the $N$-particle space as $\mathcal{F}^{(N)}_{\zeta,D} := \Lambda^N(\mathcal{H}_D)$ if $\zeta = -1$ and as $\mathcal{F}^{(N)}_{\zeta,D} := S^N(\mathcal{H}_D)$ if $\zeta = +1$, where $\Lambda^N$ and $S^N$ denote
the $N$-th exterior and symmetric powers, respectively. Then $\mathcal{F}^{(N)}_{\xi,D}$ so constructed is isomorphic to $\mathcal{F}_{\xi,d}^{(N)}$ as above via, in the case $\zeta = -1$, the isomorphism $|n\rangle \mapsto \wedge_{i=1}^{d} \varphi_{i}^{\wedge n}$, where the wedge in the exponent indicates a wedge power. The analogous isomorphism holds in the case $\zeta = +1$, with wedges replaced by symmetric products. A change of the basis $\mathcal{D}$ to some $\tilde{\mathcal{D}} = \{ \tilde{\varphi}_{1}, \ldots, \tilde{\varphi}_{d} \}$ that is induced by a unitary transformation $T : \mathbb{R}^{d} \to \mathbb{R}^{d}$ corresponds to a transformation of the annihilation operators by $\tilde{a}_{i} = \sum_{j=1}^{d} T_{ij} a_{j}$.

Under this correspondence, a translation-invariant two-body potential $v(x - y)$ in real space yields the tensor elements $(ij|U|kl)$ can be computed via the following two-body integrals [18]:

$$\langle ij \rangle = \int_{\mathbb{R}^{3}} \int_{\mathbb{R}^{3}} v(x - y) \varphi_{i}^{\ast}(x) \varphi_{j}^{\ast}(y) \varphi_{k}(x) \varphi_{l}(y) \, dx \, dy. \quad (A.3)$$

The elements of $h$ are obtained by suitable one-body integrals; see, e.g., [18].

In the case that $\hat{U} = U(a^{\dagger}, a)$ depends only on $a_{i}^{\dagger}, a_{i}$ for $i = 1, \ldots, p$, we say that $\hat{U}$ is an impurity Hamiltonian, with a fragment specified by the indices $1, \ldots, p$. The rest of the indices correspond to the environment.

**B The zero-temperature ensemble**

At zero temperature, typically one first fixes a particle number $N$, and attention is restricted to the $N$-particle subspace. Let $|\Psi_{0}^{(N)}\rangle \in \mathcal{F}_{\xi,d}^{(N)}$ be the $N$-particle ground state of $\hat{H}$, i.e., the minimal normalized eigenvector of $\hat{H}$ considered as an operator on the $N$-particle subspace. The role of the density operator is assumed by the orthogonal projector $|\Psi_{0}^{(N)}\rangle \langle \Psi_{0}^{(N)}|$ onto the ground state $|\Psi_{0}^{(N)}\rangle$, i.e., the statistical average of a linear operator $\hat{A}$ (with respect to the $N$-particle canonical ensemble) is given by

$$\langle \hat{A} \rangle_{N} = \langle \Psi_{0}^{(N)} | \hat{A} | \Psi_{0}^{(N)} \rangle.$$  

**B.1 Green’s functions and the self-energy at zero temperature**

For $t \in \mathbb{R}$, we denote the annihilation and creation operators in the Heisenberg representation by

$$a_{i}(t) := e^{i\hat{H}t} a_{i} e^{-i\hat{H}t}, \quad a_{i}^{\dagger}(t) := e^{i\hat{H}t} a_{i}^{\dagger} e^{-i\hat{H}t}.$$  

Then for a zero-temperature ensemble with $N$ particles, the time-ordered, single-body, real-time Green’s function (which we call the Green’s function for short) is a function $G : \mathbb{R} \times \mathbb{R} \to \mathbb{C}^{d \times d}$ defined by

$$G_{ij}(t, t') = -i \langle \Psi_{0}^{(N)} | \mathcal{T} \{ a_{i}(t) a_{i}^{\dagger}(t') \} | \Psi_{0}^{(N)} \rangle,$$

where $\mathcal{T}$ is the time-ordering operator, formally defined by

$$\mathcal{T} \{ a_{i}(t) a_{i}^{\dagger}(t') \} = \begin{cases} a_{i}(t) a_{i}^{\dagger}(t'), & t' < t \\ a_{i}^{\dagger}(t') a_{i}(t), & t' \geq t. \end{cases}$$

Note that $\mathcal{T}$ is not really an operator and it is interpreted merely via the symbolic content of its argument.
We can write
\[ G(t, t') = G^+(t, t') + G^-(t, t'), \]
where
\[ iG^+(t, t') := \langle \Psi_0^{(N)} | a_i(t) a_j(t') \rangle | \Psi_0^{(N)} \rangle \theta(t - t'), \]
\[ iG^-(t, t') := \langle \Psi_0^{(N)} | a_j^\dagger(t') a_i(t) \rangle | \Psi_0^{(N)} \rangle (1 - \theta(t - t')), \]
with
\[ \theta(s) := \begin{cases} 1, & s > 0 \\ 0, & s \leq 0. \end{cases} \]

It is easy to show that \( G(t, t'), G^+(t, t'), \) and \( G^-(t, t') \) depend only on \( t - t' \), so we can define \( G(t) := G(t, 0), G^+(t) := G^+(t, 0), \) and \( G^-(t) := G^-(t, 0) \) and consider these objects without any loss of information. It is then equivalent to consider the Fourier transforms
\[ G(\omega) := \int_\mathbb{R} G(t) e^{i\omega t - \eta |t|} \, dt \]
and likewise \( G^+(\omega) \) and \( G^-(\omega) \) defined similarly, so
\[ G(\omega) = G^+(\omega) + G^-(\omega). \]

Here \( \eta \) is interpreted as a positive, infinitesimally small quantity needed to ensure the convergence of the relevant integrals, and \( G(\omega), G^+(\omega), \) and \( G^-(\omega) \) are not really functions, but rather distributions on \( \mathbb{R} \) defined via the limit \( \eta \to 0^+ \).

One can show that
\[ G^+_{ij}(\omega) = \langle \Psi_0^{(N)} | a_i \frac{1}{\omega - (\hat{H} - E_0^{(N)}) + i\eta} a_j^\dagger | \Psi_0^{(N)} \rangle \]
and
\[ G^-_{ij}(\omega) = -\zeta \langle \Psi_0^{(N)} | a_j^\dagger \frac{1}{\omega + (\hat{H} - E_0^{(N)}) - i\eta} a_i | \Psi_0^{(N)} \rangle, \]
where \( E_0^{(N)} \) is the energy of the N-particle ground state, i.e., \( \hat{H} | \Psi_0^{(N)} \rangle = E_0 | \Psi_0^{(N)} \rangle \).

Now we can think of \( G^\pm \) as the restriction to the real axis of the rational function \( G^\pm : \mathbb{C} \to \mathbb{C}^{d \times d} \) defined by
\[ G^+_{ij}(z) := \langle \Psi_0^{(N)} | a_i \frac{1}{z - (\hat{H} - E_0^{(N)})} a_j^\dagger | \Psi_0^{(N)} \rangle \]
\[ G^-_{ij}(z) := -\zeta \langle \Psi_0^{(N)} | a_j^\dagger \frac{1}{z + (\hat{H} - E_0^{(N)})} a_i | \Psi_0^{(N)} \rangle, \]
and we can define \( G(z) := G^+(z) + G^-(z) \) accordingly to be rational on \( \mathbb{C} \).

Note that here we have left out the \( \pm i\eta \) in the denominators, which specified whether poles should be viewed as being infinitesimally above or below the real axis. This erases the distinction between the time-ordered Green’s function and the advanced and retarded Green’s functions, which we do not define here, though see [18] for details. In fact the distinction does not matter for our sparsity results, which applies equally well in all of these cases.

The self-energy is the rational function \( \Sigma : \mathbb{C} \to \mathbb{C}^{d \times d} \) defined by
\[ \Sigma(z) := z - h - G(z)^{-1}. \]
The finite-temperature ensemble

At inverse temperature $\beta \in (0, \infty)$, the partition function is defined by

$$Z := \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}],$$

where ‘Tr’ indicates the Fock space trace. Here $\mu \in \mathbb{R}$ is the chemical potential, but before commenting on its role, some further elaboration on the trace is owed in the bosonic case, in which the Fock space is infinite-dimensional.

By assumption, $\hat{H}$ conserves particle number, i.e., it maps $\mathcal{F}_N^{(\zeta,d)}$ to itself for all $N$. Thus $e^{-\beta(\hat{H} - \mu \hat{N})}$ does as well and can be viewed as a positive-definite operator on each $\mathcal{F}_N^{(\zeta,d)}$. The trace can then be constructed as

$$\text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] = \sum_{N=0}^{\infty} \text{Tr}_N[e^{-\beta(\hat{H} - \mu \hat{N})}] = \sum_{N=0}^{\infty} e^{\beta \mu N} \text{Tr}_N[e^{-\beta \hat{H}}],$$

where ‘$\text{Tr}_N$’ indicates the trace on the $N$-particle subspace. Since each of the summands is positive, $\text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] \in (0, +\infty)$ is well-defined.

More generally, the trace is defined for all operators in the trace class of $\mathcal{F}_d^{(\zeta,d)}$, i.e., the set of bounded linear operators $\hat{O} : \mathcal{F}_d^{(\zeta,d)} \rightarrow \mathcal{F}_d^{(\zeta,d)}$ for which

$$\sum_{n \in N_d^{(\zeta)}} \langle n | (\hat{O}^\dagger \hat{O})^{1/2} | n \rangle < +\infty,$$

in which case

$$\text{Tr}[\hat{O}] = \sum_{n \in N_d^{(\zeta)}} \langle n | \hat{O} | n \rangle.$$

See, e.g., [19] for further details on trace class operators.

Now since the partition function can be viewed as a normalization factor, the scenario $Z = +\infty$ is to be avoided. It is now that we turn to the chemical potential. We can view $Z$ as defined above as a function of $\mu$. Evidently $\mu \mapsto Z(\mu)$ is non-decreasing.

First we want to rule out the case that $Z \equiv +\infty$. Unfortunately, this case cannot be ruled out without further assumptions! To see why, suppose that $d' = 1$ (so write $a = a_1$), and let $\hat{H} = -a^\dagger a - a^\dagger a a = -a^\dagger a a = -\hat{N}^2$. Then

$$\text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] = \sum_{N=0}^{\infty} e^{\beta(N^2 + \mu N)} \text{Tr}_N \left[ \text{Id}_{\mathcal{F}_N^{(\zeta,d)}} \right] = \sum_{N=0}^{\infty} e^{\beta(N^2 + \mu N)} \binom{N + d - 1}{d - 1} = +\infty,$$

for all $\mu \in \mathbb{R}$.

We conclude that such a choice of $\hat{H}$ is unphysical, and to rule out such pathologies, we adopt the following:

**Assumption C.1.** We assume, in the case of bosons, that there exist some positive integer $N_0$ and some $\mu \in \mathbb{R}$ such that $\hat{H} - \mu \hat{N} \geq 0$ as an operator on all $N$-particle subspaces for $N \geq N_0$. (It is equivalent to require that there exist $N_0, \mu$ such that $\hat{U} - \mu \hat{N} \geq 0$ on all $N$-particle subspaces for $N \geq N_0$.)
This condition is satisfied in particular if $\hat{U}$ is a two-body interaction as in (A.2) such that $U_{ij,kl} := (kj|U|il)$, interpreted as a $d^2 \times d^2$ matrix, is positive semidefinite. Indeed, in this case, $\hat{U}$ is equal to (up to a single-body term)

$$\frac{1}{2} \sum_{ijkl} U_{ik,jl} \left[ a_i^\dagger a_k \right] \left[ a_j^\dagger a_l \right] \geq 0.$$ 

If the $(ij|U|kl)$ are derived from a real-space two-body potential $v$ that is a positive semidefinite function (i.e., has nonnegative Fourier transform), then it follows from (A.3) that the matrix $(U_{ik,jl})$ is positive definite as desired. Note that it is possible for $v$ to be positive definite but take negative values at long ranges, i.e., $v$ can act attractively at long range.

Now that we have argued that Assumption C.1 is natural, let us see how it guarantees that $\hat{Z}$ is equal to (up to a single-body term) $U$.

We will always assume in the finite-temperature setting that $\mu \in \mathrm{int} \, \mathrm{dom} \, Z$. It can be shown that if $\hat{U} = 0$, then $\mathrm{dom} \, Z = \{ \mu : \mu > \mu I_d \}$. Moreover, if there exist $N_0, \delta > 0$ such that $\hat{U} \geq \delta N^2$ on all $N$-particle subspaces for $N \geq N_0$ (which holds in particular if $\hat{U}$ is a two-body interaction as in (A.2) where the $d^2 \times d^2$ matrix $U_{ij,kl} := (ij|U|kl)$ is positive definite), then $\mathrm{dom} \, Z = \mathbb{R}$.

Notice that if $\mathrm{dom} \, Z$ is open, then since $Z$ is increasing we can write $\mathrm{dom} \, Z = (-\infty, \mu_c)$ for some $\mu_c$ possibly infinite. If $\mu_c < +\infty$, then by Fatou’s lemma we have that $\liminf_{\mu \to \mu_c^+} Z(\mu) \geq Z(\mu_c) = +\infty$, so $Z(\mu) \to +\infty$ as $\mu \to \mu_c^+$. (And in any case it follows from the definition of $Z$ that $Z(\mu) \to +\infty$ as $\mu \to +\infty$, so we can write more compactly that $Z(\mu) \to +\infty$ as $\mu \to \mu_c$, no matter whether $\mu_c$ is finite or infinite.)

The grand canonical ensemble is defined by the density operator

$$\rho := Z^{-1} e^{-\beta (H - \mu N)},$$

and the statistical average of an operator $\hat{A}$ with respect to the grand canonical ensemble is denoted

$$\langle \hat{A} \rangle_{\beta,\mu} = \mathrm{Tr}[\hat{A} \rho]$$

whenever $\hat{A} \rho$ is in the trace class. Note that if $\hat{A}$ conserves particle number then

$$\mathrm{Tr}[\hat{A} \rho] = \sum_{N=0}^{\infty} \mathrm{Tr}_N[\hat{A} \rho] = Z^{-1} \sum_{N=0}^{\infty} e^{\beta \mu N} \mathrm{Tr}_N[\hat{A} e^{-\beta H}]$$

is defined under the condition that the sum is absolutely convergent, which holds in particular if the norm of $\hat{A}$ as an operator on the $N$-particle subspace grows only polynomially with $N$, via the assumption that $\mu \in \mathrm{int} \, \mathrm{dom} \, Z$. When the context is clear we simply write $\langle \cdot \rangle$.

Of particular interest is the expected particle number

$$\langle \hat{N} \rangle = \frac{\sum_{N=0}^{\infty} N e^{\beta \mu N} \mathrm{Tr}_N[ e^{-\beta H}] }{ \sum_{N=0}^{\infty} e^{\beta \mu N} \mathrm{Tr}_N[ e^{-\beta H}] }.$$
Observe that $\langle \hat{N} \rangle_{\beta,\mu} \to 0$ as $\mu \to -\infty$. Also note that if $\text{dom } Z = \mathbb{R}$, then $\langle \hat{N} \rangle_{\beta,\mu} \to +\infty$. Defining the free energy $\Omega(\mu) := \beta^{-1} \log Z(\mu)$, we see that $\langle \hat{N} \rangle_{\beta,\mu} = \Omega'(\mu)$.

It is not hard to check that $\Omega$ is (strictly) convex, i.e., $\langle \hat{N} \rangle_{\beta,\mu}$ is increasing in $\mu$ for $\mu \in \text{int dom } Z$. Recall that if $\text{dom } Z = (0, \mu_c)$, then $Z(\mu) \to +\infty$ as $\mu \to \mu_c$, hence $\Omega(\mu) \to +\infty$ as $\mu \to \mu_c$. If $\mu_c < +\infty$, it follows that $\Omega'(\mu) \to +\infty$ as $\mu \to \mu_c$. (Otherwise, since $\Omega'$ is increasing, it approaches a finite limit $\mu \to \mu_c$. But in this case it would follow from the fundamental theorem of calculus that $\Omega$ approaches a finite limit as well: contradiction.) In summary we have established that if $\text{dom } Z$ is open, then $Z(\mu) \to +\infty$ as $\mu \to \mu_c$, no matter whether $\mu_c$ is finite or infinite. It follows that in this case $\mu \mapsto \langle \hat{N}_{\beta,\mu} \rangle$ is a bijection from $\text{dom } Z = (-\infty, \mu_c)$ to $(0, +\infty)$. Thus one can select the chemical potential $\mu$ to yield a predetermined expected particle number.

### C.1 Green’s functions and the self-energy at finite temperature

As above, for $t \in \mathbb{R}$, we denote the annihilation and creation operators in the Heisenberg representation by

$$a_i(t) := e^{iHt}a_ie^{-iHt}, \quad a_i^\dagger(t) := e^{iHt}a_i^\dagger e^{-iHt}.$$  

Then at finite inverse temperature $\beta \in (0, \infty)$ and chemical potential $\mu \in \text{int dom } Z$, the time-ordered, single-body, real-time Green’s function (which we call the Green’s function for short when the context is clear) is a function $G : \mathbb{R} \times \mathbb{R} \to \mathbb{C}^{d \times d}$ defined by

$$G_{ij}(t,t') = -i \langle \mathcal{T}\{a_i(t) a_j^\dagger(t')\} \rangle_{\beta,\mu}.$$  

We can write

$$G(t,t') = G^+(t,t') + G^-(t,t'),$$  

where

$$iG^+(t,t') = \frac{1}{Z} \text{Tr} \left[ a_i(t) a_i^\dagger(t') e^{-\beta(H - \mu N)} \right] \theta(t - t'),$$  

$$iG^-(t,t') = -\frac{\zeta}{Z} \text{Tr} \left[ a_i^\dagger(t') a_i(t) e^{-\beta(H - \mu N)} \right] (1 - \theta(t - t')),$$

with

$$\theta(s) := \begin{cases} 1, & s > 0 \\ 0, & s \leq 0. \end{cases}$$

as above.

Once again it is easy to show that $G(t,t')$, $G^+(t,t')$, and $G^-(t,t')$ depend only on $t - t'$, so we can define $G(t) := G(t,0)$, $G^+(t) := G^+(t,0)$, and $G^-(t) := G^-(t,0)$ and consider these objects without any loss of information. It is then equivalent to consider the Fourier transforms

$$G(\omega) := \int_\mathbb{R} G(t)e^{i\omega t} dt$$

and likewise $G^+(\omega)$ and $G^-(\omega)$ defined similarly, so

$$G(z) = G^+(\omega) + G^-(\omega).$$

Now since $\hat{H}$ preserves particle number, we can safely diagonalize $\hat{H}$ as an operator on each of the $N$-particle subspaces separately. Then the spectrum of $\hat{H}$ consists of the union of its spectra.
on the $N$-particle subspaces. It follows from Assumption C.4 that $\hat{H} - \mu \hat{N}$ has a ground state, i.e., that its spectrum is bounded from below, for $\mu \in \text{int dom } Z$. Let $m = 0, 1, \ldots$ (terminating at $m = 2^d$ in the case of fermions) index the spectrum of $\hat{H}$, and let $|\Psi_m\rangle$ denote the $m$-th eigenstate. Let $N_m$ be the particle number of $|\Psi_m\rangle$ (which is an eigenstate of $\hat{N}$), and let $E_m$ be defined by $\hat{H}|\Psi_m\rangle = E_m|\Psi_m\rangle$.

One can show that

$$G^+_{ij}(\omega) = \frac{1}{Z} \sum_m e^{-\beta(E_m - \mu N_m)} \langle \Psi_m | a_i | \frac{1}{\omega - (H - E_m) + i\eta} a_j^\dagger | \Psi_m \rangle$$

and

$$G^-_{ij}(\omega) = -\zeta \frac{1}{Z} \sum_m e^{-\beta(E_m - \mu N_m)} \langle \Psi_m | a_i | \frac{1}{\omega + (H - E_m) - i\eta} a_j^\dagger | \Psi_m \rangle.$$

Recall that

$$Z = \sum_m e^{-\beta(E_m - \mu N_m)}.$$

Now we can think of $G^{\pm}$ as the restriction to the real axis of the rational function $G^{\pm} : \mathbb{C} \to \mathbb{C}^{d \times d}$ defined by

$$G^+_{ij}(z) := \frac{1}{Z} \sum_m e^{-\beta(E_m - \mu N_m)} \langle \Psi_m | a_i | \frac{1}{z - (H - E_m)} a_j^\dagger | \Psi_m \rangle$$

and

$$G^-_{ij}(z) := -\zeta \frac{1}{Z} \sum_m e^{-\beta(E_m - \mu N_m)} \langle \Psi_m | a_i | \frac{1}{z + (H - E_m)} a_j^\dagger | \Psi_m \rangle,$$

and we can define $G(z) := G^+(z) + G^-(z)$ accordingly to be rational on $\mathbb{C}$. Once again we have ignored the infinitesimal $\eta$ in this definition; the same comments made in Appendix B apply here.

The self-energy is the rational function $\Sigma : \mathbb{C} \to \mathbb{C}^{d \times d}$ defined by

$$\Sigma(z) := z - h - G(z)^{-1}.$$

## D Non-equilibrium setting and the Kadanoff-Baym contour

Here we briefly discuss one main non-equilibrium setting of interest, called the Kadanoff-Baym formalism. One considers an initial time $t_0$ and a final time $t_1$, with $t_1 > t_0$, and for $t \in [t_0, t_1]$, $\hat{H}(t)$ denotes the Hamiltonian at time $t$. This Hamiltonian determines the evolution, starting at time $t_0$, of a prepared grand canonical ensemble defined by a density operator $\rho$, i.e., a positive semi-definite operator on the Fock space of unit trace. Assuming, for simplicity, strict positive definiteness, we can write

$$\rho = \frac{1}{\text{Tr}[e^{-\beta \hat{H}}]} e^{-\beta \hat{H}}$$

for some Hamiltonian $\overline{H}$ and inverse temperature $\beta$. Of course, this form leaves freedom in choosing $\beta$, but it is good to think of $\beta$ as a free parameter. Often $\overline{H}$ may be thought of as $\hat{H}(t_0) - \mu \hat{N}$, but this need not be the case. To ensure that Assumption B.4 holds, it will suffice to assume that $\text{Tr}[e^{-\beta \overline{H} + \varepsilon \hat{N}}] < +\infty$ for some $\varepsilon > 0$ sufficiently small. This condition is analogous to the condition $\mu \in \text{int dom } Z$ discussed in Appendix C for the equilibrium finite-temperature ensemble. Assuming
the condition, let \( \hat{O}_N \) denote the restriction of \( e^{-\beta \overline{H}} \) to the \( N \)-particle subspace. Then it follows that \( \text{Tr}[\hat{O}_N] \) decays exponentially in \( N \), hence \( \|\hat{O}_N\|_2 \) does as well.

Here the contour is the Kadanoff-Baym contour \( C^{KB} \), specified by the path \( \gamma^{KB} \), which can be written as a concatenation

\[
\gamma^{KB} = \gamma^- + \gamma^+ + \gamma^M.
\]

Here \( \gamma^- : (0, t_1 - t_0) \to \mathbb{C} \) is defined by \( s \mapsto s + t_0 \), \( \gamma^+ : (0, t_1 - t_0) \to \mathbb{C} \) is defined by \( s \mapsto t_1 - s \), and \( \gamma^M : (0, \beta) \to \mathbb{C} \) is defined by \( s \mapsto t_0 - is \). Accordingly we define sub-contours, \( C_\pm \) and \( C_{KB} \). The concatenation \( \gamma^{KB} \) is viewed as a function \( (s_0, s_1) \to \mathbb{C} \), where \( s_0 = 0 \) and \( s_1 = 2(t_1 - t_0) + \beta \).

We have already defined the contour Hamiltonian \( \hat{H}(z) \) for \( z \in C_+ \). To complete the specification of our ensemble we stipulate that \( \hat{H}(z) = \overline{H} \) for \( z \in C_M \). For contour times \( s, s' < t_1 - t_0 \), the contour-ordered Green’s function \( G(s, s') \) recovers the appropriate notion of the real-time-ordered Green’s function; similarly, appropriate notions of advanced and retarded Green’s functions can be recovered from the contour-ordered Green’s function. However, only the contour-ordered Green’s function admits a favorable perturbation theory, and this remarkable fact is one motivation for considering it. See [21] for further details. In this work we additionally see that the contour-ordered setting is also the natural setting in which to recover a sparsity result for the self-energy of impurity problems in the non-equilibrium setting.

Now one can readily check that the partition function is given by \( Z = \text{Tr}[e^{-\beta \overline{H}}] > 0 \) (so Assumption 3.8 is satisfied). Now we verify Assumption 3.7. For \( s' \leq s \leq s_1 - \beta \), note that \( U(s, s') \) is unitary, hence bounded. Moreover, for \( s_1 - \beta \leq s' \leq s \), we have \( U(s, s') = e^{-(s-s')\overline{H}} \), which is trace class (by our assumption), hence bounded. It follows that for any \( s_0 \leq s' \leq s \leq s_1 \), the operator \( U(s, s') \) is bounded. In fact, \( U(s_1, s_1 - \beta) = e^{-\beta \overline{H}} \), and as mentioned above, the operator norm of this operator restricted to the \( N \)-particle subspace decays exponentially in \( N \). Thus Assumption 3.7 is satisfied.

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