

Theory of transformation for the diagonalization of quadratic Hamiltonians

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Abstract

A theory of transformation is presented for the diagonalization of a Hamiltonian that is quadratic in creation and annihilation operators or in coordinates and momenta. It is the systemization and theorization of Dirac and Bogoliubov-Valatin transformations, and thus provides us an operational procedure to answer, in a direct manner, the questions as to whether a quadratic Hamiltonian is diagonalizable, whether the diagonalization is unique, and how the transformation can be constructed if the diagonalization exists. The underlying idea is to consider the dynamic matrix. Each quadratic Hamiltonian has a dynamic matrix of its own. The eigenvalue problem of the dynamic matrix determines the diagonalizability of the quadratic Hamiltonian completely. In brief, the theory ascribes the diagonalization of a quadratic Hamiltonian to the eigenvalue problem of its dynamic matrix, which is familiar to all of us. That makes it much easy to use. Applications to various physical systems are discussed, with especial emphasis on the quantum fields, such as Klein-Gordon field, phonon field, etc..

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I. INTRODUCTION

In the preface to the first edition of “The Principles of Quantum Mechanics” [1], Dirac said: “The growth of the use of transformation theory, as applied first to relativity and later to the quantum theory, is the essence of the new method in theoretical physics.”

In this review, we shall present a theory of transformation, which can perform diagonalization to the Hamiltonian that is quadratic in creation and annihilation operators or in coordinates and momenta. Such transformations appear most frequently in classical and quantum mechanics, statistical mechanics, condensed-matter physics, nuclear physics, and quantum field theory.

For the sake of simplicity, let us begin with the so-called Bogoliubov-Valatin transformation.

A. Bogoliubov-Valatin transformation

In 1947, Bogoliubov [2] introduced a novel linear transformation to diagonalize the quantum quadratic Hamiltonian present in superfluidity. This method was later extended by Bogoliubov himself [3, 4, 5] and also by Valatin [6, 7] to the Fermi case in the theory of superconductivity. It has ever since got widely used in different fields [8, 9, 10], and known as Bogoliubov-Valatin (BV) transformation, including both the bosonic and fermionic versions.

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To show the underlying idea of the method due to Bogoliubov and Valatin, let us consider the quadratic Hamiltonian,

$$H = \sum_{i,j=1}^n (\alpha_{ij} c_i^\dagger c_j + \frac{1}{2} \gamma_{ij} c_i^\dagger c_j^\dagger + \frac{1}{2} \gamma_{ji}^* c_i c_j), \quad (1.1)$$

where $n \geq 1$ is a natural number, and c_i and c_i^\dagger are, respectively, the annihilation and creation operators for bosons or fermions. They satisfy the standard commutation or anticommutation relations,

$$[c_i, c_j^\dagger] = c_i c_j^\dagger \pm c_j^\dagger c_i = \delta_{ij}, \quad (1.2)$$

$$[c_i, c_j] = c_i c_j \pm c_j c_i = 0, \quad (1.3)$$

$$[c_i^\dagger, c_j^\dagger] = c_i^\dagger c_j^\dagger \pm c_j^\dagger c_i^\dagger = 0, \quad (1.4)$$

where δ_{ij} is the Kronecker delta function. The coefficients $\alpha_{ij} \in \mathbb{C}$ and $\gamma_{ij} \in \mathbb{C}$ have the following symmetries,

$$\alpha_{ij} = \alpha_{ji}^*, \quad \gamma_{ij} = \mp \gamma_{ji}, \quad (1.5)$$

where z^* denotes the complex conjugate of z . Throughout this review, the complex field \mathbb{C} will be used as the base field of the Hamiltonian H .

Using the form of matrix, Eq. (1.1) can be written as

$$(\star 1) \quad H = \frac{1}{2} \psi^\dagger M \psi \pm \frac{1}{2} \text{tr}(\alpha), \quad (1.6)$$

where $\text{tr}(A)$ denotes the trace of the matrix A . The ψ is a column vector and ψ^\dagger its Hermitian conjugate,

$$\psi = \begin{bmatrix} c \\ \tilde{c}^\dagger \end{bmatrix}, \quad \psi^\dagger = [c^\dagger, \tilde{c}], \quad (1.7)$$

where c and c^\dagger are the subvectors of size n ,

$$c = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}, \quad c^\dagger = [c_1^\dagger, c_2^\dagger, \dots, c_n^\dagger]. \quad (1.8)$$

Here \tilde{A} denotes the transpose of the matrix A . The coefficient matrix M has the form,

$$M = \begin{bmatrix} \alpha & \gamma \\ \gamma^\dagger & \mp \tilde{\alpha} \end{bmatrix}, \quad (1.9)$$

where α and γ are the submatrices with α_{ij} and γ_{ij} as their entries, respectively. Obviously, α can always be diag.

$$\alpha^\dagger = \alpha, \quad \tilde{\gamma} = \mp \gamma, \quad M^\dagger = M. \quad (1.10)$$

That is to say, α and M are both Hermitian matrices whereas γ is a symmetric or antisymmetric matrix, which is determined by whether the system is bosonic or

fermionic. Besides, the matrices α and γ will not vanish simultaneously; otherwise, the Hamiltonian H is zero trivially.

If we define a new product between the two operators c_i (or c_i^\dagger) and c_j (or c_j^\dagger) as

$$c_i \cdot c_j = [c_i, c_j], \quad (1.11)$$

then Eqs. (1.2)–(1.4) can be expressed compactly as

$$\psi \cdot \psi^\dagger = I_\pm, \quad (1.12)$$

where

$$I_\pm = \begin{bmatrix} I & 0 \\ 0 & \pm I \end{bmatrix}, \quad (1.13)$$

with I being the identity matrix of size n .

To diagonalize the Hamiltonian of Eq. (1.6), Bogoliubov and Valatin introduced a linear transformation,

$$c = Ad + B\tilde{d}^\dagger, \quad (1.14)$$

where A and B are two square matrices of size n , and d and \tilde{d}^\dagger are the vectors as follows,

$$d = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix}, \quad d^\dagger = [d_1^\dagger, d_2^\dagger, \dots, d_n^\dagger]. \quad (1.15)$$

Here d_i and \tilde{d}_j^\dagger are the new annihilation and creation operators respectively, they satisfy the standard commutation or anticommutation relations as in Eqs. (1.2)–(1.4), which means,

$$\varphi \cdot \varphi^\dagger = I_\pm, \quad (1.16)$$

where

$$\varphi = \begin{bmatrix} d \\ \tilde{d}^\dagger \end{bmatrix}, \quad \varphi^\dagger = [d^\dagger, \tilde{d}]. \quad (1.17)$$

From Eqs. (1.7), (1.17) and (1.14), it follows that

$$\psi = T\varphi, \quad (1.18)$$

where

$$T = \begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix}. \quad \begin{matrix} \curvearrowright \Leftrightarrow Z_x \top Z_x = \top \\ \text{[Lemma 10]} \end{matrix} \quad (1.19)$$

Here A^* denotes the complex conjugate of the matrix A . By the way, we note that such a form of T originates from the requirement that c and c^\dagger must be Hermitian conjugates of each other. For convenience, we shall call the operator vector such as ψ and φ the field operator.

Under the transformation of Eq. (1.18), the Hamiltonian of Eq. (1.6) becomes

$$H = \frac{1}{2} \varphi^\dagger T^\dagger M T \varphi \pm \frac{1}{2} \text{tr}(\alpha), \quad (1.20)$$

$$(*1) \quad \psi^\dagger = (c_1^\dagger \dots c_n^\dagger c_1 \dots c_n) \rightarrow 1 \times 2n$$

$$\psi = (c_1 \dots c_n c_1^\dagger \dots c_n^\dagger)^T \rightarrow 2n \times 1$$

$$\sum_{i,j} \alpha_{ij} c_i^\dagger c_j$$

$$\psi^\dagger \begin{pmatrix} \tilde{\alpha} & \tilde{0} \\ 0 & \pm \alpha^T \end{pmatrix} \begin{matrix} \{n \\ \{n \end{matrix} \psi$$

$$= \left(\sum_{i=1}^n c_i^\dagger \alpha_{i1}, \dots, \sum_{i=1}^n c_i^\dagger \alpha_{in}, \sum_{i=1}^n c_i \alpha_{s1}, \dots, \sum_{i=1}^n c_i \alpha_{ni} \right) \begin{pmatrix} c_1 \\ \vdots \\ c_n \\ c_1^\dagger \\ \vdots \\ c_n^\dagger \end{pmatrix}$$

$$= \sum_{i=1}^n \alpha_{i1} c_i^\dagger c_1 + \dots + \sum_{i=1}^n \alpha_{in} c_i^\dagger c_n +$$

$$\pm \sum_{i=1}^n \alpha_{s1} c_i c_1^\dagger \pm \dots \pm \sum_{i=1}^n \alpha_{ni} c_i c_n^\dagger = \leftarrow \text{comm. relations}$$

$$= \sum_{i=1}^n \alpha_{i1} c_i^\dagger c_1 + \dots + \sum_{i=1}^n \alpha_{in} c_i^\dagger c_n +$$

$$+ \sum_{i=1}^n \alpha_{s1} c_i c_1^\dagger + \dots + \sum_{i=1}^n \alpha_{ni} c_i c_n^\dagger \mp \alpha_{11} \mp \alpha_{22} \dots \mp \alpha_{nn}$$

$$= 2 \sum_{i,j} \alpha_{ij} c_i^\dagger c_j \mp \text{Tr}(\alpha)$$

$$\rightarrow \sum_{i,j} \alpha_{ij} c_i^\dagger c_j = \underbrace{\frac{1}{2} \psi^\dagger \begin{pmatrix} \alpha \\ \pm \alpha^T \end{pmatrix} \psi}_{\sum_{i,j} \alpha_{ij} c_i^\dagger c_j \mp \frac{1}{2} \text{Tr}(\alpha)} \pm \frac{1}{2} \text{Tr}(\alpha)$$

$$(*2) \quad \varphi \cdot \varphi^\dagger = I_\pm = \psi \cdot \psi^\dagger = T \varphi / \varphi T^\dagger \quad \mapsto \quad I_\pm = T I_\pm T^\dagger$$

where $T^\dagger MT$ is the new coefficient matrix. Meanwhile, Eq. (1.12) turns into

$$TI_\pm T^\dagger = I_\pm, \quad (\star_2) \quad (1.21)$$

where Eq. (1.16) has been used. Obviously, this is a condition for the transformation of Eq. (1.18).

For the Hamiltonian H to be diagonalized with respect to the new annihilation and creation operators, it is necessary that the new coefficient matrix $T^\dagger MT$ is diagonal, i.e.,

$$T^\dagger MT = \begin{bmatrix} \omega_1 & & 0 \\ & \omega_2 & \\ 0 & & \ddots \\ & & & \omega_{2n} \end{bmatrix}, \quad (1.22)$$

where ω_i for $i = 1, 2, \dots, 2n$ are the diagonal entries, they are real: $\omega_i \in \mathbb{R}$. Equation (1.22) means that all the off-diagonal entries of the matrix $T^\dagger MT$ must vanish identically. Under this condition, we have

$$H = \frac{1}{2} \sum_{i=1}^n (\omega_i \oplus \omega_{n+i}) d_i^\dagger d_i + \frac{1}{2} \sum_{i=1}^n \omega_{n+i} \pm \frac{1}{2} \text{tr}(\alpha). \quad (1.23)$$

comm.

This is the so-called diagonalized form for the Hamiltonian H .

To sum up, Eqs. (1.21) and (1.22) are the two conditions that must be fulfilled by the transformation matrix T . The former ensures the statistics of the system, i.e., the system will remain bosonic or fermionic after the transformation if it is bosonic or fermionic before the transformation, that is a physical requirement. The latter ensures the diagonalization of the Hamiltonian, it is just a mathematical requirement. According to Bogoliubov and Valatin, the transformation matrix T can be determined from Eqs. (1.21) and (1.22). After the determination of T , the diagonal entries ω_i for $i = 1, 2, \dots, 2n$ will be obtained, which accomplishes the diagonalization procedure. That is the main idea of the Bogoliubov-Valatin transformation.

As indicated by Eq. (1.10), the matrix M is Hermitian. So it can always be diagonalized by a unitary transformation. At first glance, it seems as if the Hamiltonian of Eq. (1.20) could be brought into diagonalization by the same unitary transformation. However, a close observation shows that such a unitary transformation can, in general, neither take the form of Eq. (1.19) nor meet the requirements of Eq. (1.21) although it always satisfies the condition of Eq. (1.22). Therefore, the unitary transformation for the diagonalization of the coefficient matrix M can not generally diagonalize the Hamiltonian of Eq. (1.20). That is because both the field ψ and the field φ are now the vectors of operators (quantum numbers) rather than the usual simple vectors of complex variables (classical numbers). For the latter, it is well known that a Hermitian quadratic form can always be diagonalized by the unitary transformation for the diagonalization of its coefficient matrix. In short, the BV

diagonalization for a quantum quadratic Hamiltonian is much more complicated than the unitary diagonalization for the usual Hermitian quadratic form of complex variables.

Finally, let us analyze the BV method in more detail. It can easily be seen from Eq. (1.19) that the transformation matrix T has $4n^2$ independent unknown entries. However, Eqs. (1.21) and (1.22) contain $4n^2$ and $4n^2 - 2n$ constraints on T , respectively. That is to say, the constraints are much more than the total number of the free unknown entries of T . Therefore, there are two possibilities: (1) Those constraints are consistent with the requirement of T , and thus T has solutions. (2) The constraints are inconsistent with the requirement of T , and T has no solution. Theoretically, it is very difficult to judge which case will happen because, as indicated by Eqs. (1.21) and (1.22), the constraints constitute $8n^2 - 2n$ coupled quadratic equations for $4n^2$ free unknowns. Furthermore, it will still be hard to solve for the multiple unknowns from the multiple equations of second degree even if there exist solutions for the matrix T . Mathematically, these difficulties arise from the well-known fact that there is no much knowledge about the multiple equations of second degree with multiple unknowns at present. In practice, one often has to rely on experience and tricks when he uses the BV method to resolve practical problems.

To overcome those difficulties, we intend to develop a new theory for BV transformation. We expect that this theory can not only judge straightforwardly whether a quantum quadratic Hamiltonian is BV diagonalizable but also yield the required transformation by a simple procedure if the Hamiltonian is BV diagonalizable. That is the main objective of this review.

B. Equation of motion

As shown in the preceding subsection, the diagonalization scheme adopted by Bogoliubov and Valatin is merely algebraic. That is to say, the scheme treats the diagonalization just as a pure algebraic problem, it does not consider the physics in diagonalization at all. We would like to complement it with physical contents so as to find the necessary and sufficient conditions for the diagonalization of a quantum quadratic Hamiltonian. Simply speaking, we shall take into account the equation of motion of the system, i.e., the Heisenberg equation.

To show the idea, let us consider the classical system of harmonic oscillators—the counterpart of the Bose system with a quadratic Hamiltonian [11],

$$\begin{aligned} H &= \frac{1}{2} \sum_{i,j=1}^n K_{ij} p_i p_j + \frac{1}{2} \sum_{i,j=1}^n V_{ij} q_i q_j \\ &= \frac{1}{2} \tilde{p} K p + \frac{1}{2} \tilde{q} V q, \end{aligned} \quad (1.24)$$

where q_i and p_i ($i = 1, 2, \dots, n$) are, respectively, the

generalized coordinates and momenta, with q and p being the corresponding column vectors,

$$q = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix}, \quad p = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{bmatrix}. \quad (1.25)$$

The K and V are the kinetic and potential matrices with K_{ij} and V_{ij} as their entries, respectively. They are both real and symmetric,

$$\tilde{K} = K > 0, \quad (1.26)$$

$$\tilde{V} = V \geq 0. \quad (1.27)$$

It is worthy to emphasize that K is a positive definite matrix, that is because the kinetic energy is always positive definite. In addition, the matrix V is only positive semidefinite, the bottom of potential being chosen as zero.

As well known, q_i and p_i ($i = 1, 2, \dots, n$) satisfy the following canonical relations,

$$\{q_i, q_j\} = 0, \quad (1.28)$$

$$\{p_i, p_j\} = 0, \quad (1.29)$$

$$\{q_i, p_j\} = \delta_{ij}, \quad (1.30)$$

or equivalently,

$$q \cdot \tilde{q} = 0, \quad (1.31)$$

$$p \cdot \tilde{p} = 0, \quad (1.32)$$

$$q \cdot \tilde{p} = I. \quad (1.33)$$

where $\{a, b\}$ denotes the Poisson bracket of a and b , and $a \cdot b = \{a, b\}$.

Of course, the Bogoliubov-Valatin scheme can be transplanted directly to diagonalize the classical quadratic Hamiltonian of Eq. (1.24) with respect to the new generalized coordinates and momenta. However, we would rather here turn to another way—the canonical equation of motion.

The canonical equation of motion can be deduced from the Hamiltonian of Eq. (1.24) and the Poisson brackets of Eqs. (1.28)–(1.30) as follows,

$$\frac{d}{dt}q = \{q, H\} = Kp, \quad (1.34)$$

$$\frac{d}{dt}p = \{p, H\} = -Vq. \quad (1.35)$$

where t denotes the time. As a result, we have

$$\frac{d^2}{dt^2}q = -KVq. \quad (1.36)$$

That is a homogeneous system of linear ordinary differential equations with constant coefficients.

From the theory of ordinary differential equations [12], we know that the solution of the homogeneous linear system above depends on the eigenvalue problem,

$$\omega^2 q = KVq. \quad (1.37)$$

This eigenvalue problem can be solved rigorously with the help of the Cholesky decomposition of K ,

$$K = Q\tilde{Q}, \quad (1.38)$$

where Q is an invertible matrix. The existence of such a decomposition stems mathematically from the positivity of K [13]. By introducing a temporal variable ξ ,

$$\xi = Q^{-1}q, \quad (1.39)$$

Eq. (1.37) can be transformed into

$$\omega^2 \xi = \Lambda \xi, \quad (1.40)$$

where

$$\Lambda = \tilde{Q}VQ = \tilde{\Lambda} \geq 0. \quad (1.41)$$

Just as V , the matrix Λ is still real, symmetric, and non-negative definite. So it can be orthogonally diagonalized,

$$\tilde{S}\Lambda S = \Gamma, \quad (1.42)$$

where

$$\tilde{S}S = S\tilde{S} = I, \quad (1.43)$$

$$\Gamma = \begin{bmatrix} \omega_1^2 & & 0 \\ & \omega_2^2 & \\ 0 & & \ddots \\ & & & \omega_n^2 \end{bmatrix}. \quad (1.44)$$

Here $\omega_i^2 \geq 0$ ($i = 1, 2, \dots, n$) are the eigenvalues of Λ , and S the orthogonal matrix with the eigenvectors of Λ as its column vectors.

From Eqs. (1.38), (1.41), (1.42), and (1.43), it follows that

$$T^{-1}KVT = \Gamma, \quad (1.45)$$

where

$$T = QS. \quad (1.46)$$

If we put

$$T = [v_1, v_2, \dots, v_n], \quad (1.47)$$

where v_i ($i = 1, 2, \dots, n$) denote the column vectors of T . Equation (1.45) shows that v_i are the eigenvectors of the matrix KV ,

$$\omega_i^2 v_i = KVv_i, \quad (1.48)$$

belonging to the eigenvalues ω_i^2 , respectively. In other words, they are the solutions of the eigenvalue problem of Eq. (1.37). Evidently, they are orthonormal and complete,

$$\tilde{T}GT = I, \quad (1.49)$$

$$T\tilde{T}G = I, \quad (1.50)$$

where $G = K^{-1}$. Namely, they constitute a n -dimensional Hilbert space with G as its metric tensor.

Just as usual, the general solution of Eq. (1.36) can be expanded in this Hilbert space as

$$q(t) = \sum_{i=1}^n \psi_i(t) v_i, \quad (1.51)$$

where $\psi_i(t)$ ($i = 1, 2, \dots, n$) are the expanding coefficients. But, not as usual, we do not care here how to determine those coefficients from the initial conditions. Instead, we would rather view this expansion as a linear transformation,

$$q(t) = T\psi(t), \quad (1.52)$$

where $\psi(t)$ is the column vector,

$$\psi(t) = \begin{bmatrix} \psi_1(t) \\ \psi_2(t) \\ \vdots \\ \psi_n(t) \end{bmatrix}. \quad (1.53)$$

As will be seen later, this view is crucial for the diagonalization of the Hamiltonian. Since T has full rank, the transformation is invertible. The inverse is

$$\psi(t) = T^{-1}q(t). \quad (1.54)$$

Physically, $\psi(t)$ represents the new generalized coordinates, and $q(t)$ the old ones.

The corresponding transformation for the generalized momenta can be deduced from Eq. (1.33). As is well known, a Poisson bracket is a bilinear function of its two arguments. This together with Eq. (1.33) indicates that there exists a duality relationship between $p(t)$ and $q(t)$ [14]. This duality implies that $p(t)$ will transform contravariantly with $q(t)$, i.e.,

$$\pi(t) = \tilde{T}p(t), \quad (1.55)$$

where $\pi(t)$ represents the new generalized momenta.

Under the transformation of Eqs. (1.54) and (1.55), the Hamiltonian of the system becomes as follows,

$$\begin{aligned} H &= \frac{1}{2}\tilde{\pi}\pi + \frac{1}{2}\tilde{\psi}\Gamma\psi \\ &= \frac{1}{2}\sum_{i=1}^n (\pi_i^2 + \omega_i^2 \psi_i^2), \end{aligned} \quad (1.56)$$

where

$$\psi \cdot \tilde{\psi} = 0, \quad (1.57)$$

$$\pi \cdot \tilde{\pi} = 0, \quad (1.58)$$

$$\psi \cdot \tilde{\pi} = I. \quad (1.59)$$

They are identical to the system of Eq. (1.24) and Eqs. (1.31)–(1.33), with the Hamiltonian being diagonalized with respect to the new generalized coordinates and momenta.

Proposition 1 *A classical quadratic Hamiltonian such as Eq. (1.24) can be diagonalized with respect to the generalized coordinates and momenta.*

This instance demonstrates clearly that the equation of motion is a very effective and powerful weapon for the diagonalization of a quadratic Hamiltonian, in comparison with the method of the preceding subsection. We see that the equation of motion can generate a linear transformation in a very natural way, which can then not only diagonalize the quadratic Hamiltonian but also ensure the invariance of Poisson brackets.

In the picture of diagonalization, the system is represented by the normal modes of motion. To diagonalize a quadratic Hamiltonian is therefore equivalent to seeking the normal modes of the system. Of course, the natural tool for seeking the normal modes is the equation of motion, from the point of view of physics. That is the physical interpretation for the diagonalization. All in all, the canonical equation of motion is a candidate way to the diagonalization of a classical quadratic Hamiltonian, in addition to the purely algebraic method due to Bogoliubov and Valatin.

Since Heisenberg equation is the quantum counterpart of the canonical equation of motion in the classical mechanics, it encourages us to try to employ Heisenberg equation to realize the diagonalization of the quantum quadratic Hamiltonian. That is the main idea of this review.

Complying with this idea, we shall first study the BV transformation and diagonalization of the Bose system, we find that a complete theory can be established using the Heisenberg equation (Sec. II). And then we study the BV transformation and diagonalization of the Fermi system (Sec. III), it is parallel to the Bose case. Their applications are discussed in the following two sections (Sec. IV and Sec. V). Afterwards, we would turn to studying the Dirac transformation and diagonalization, which concern coordinates and momenta. It is found that they are the generalizations of the BV transformation and diagonalization (Sec. VI). An advantage of the Dirac transformation and diagonalization is that they can be transplanted readily to the complex collective coordinates and momenta, and therefore have wide applications in field quantization (Sec. VII). Finally, we would like to clarify the mathematical essence of the transformation and diagonalization. We find that the equation of

(★₃) Alternative proof of Lemma 3 (Also showing lemma 4)

$$D = \begin{pmatrix} \alpha & \gamma \\ -\gamma^\dagger & -\tilde{\alpha} \end{pmatrix} \quad \begin{aligned} \alpha &= \alpha^\dagger \\ \gamma &= \tilde{\gamma} \end{aligned}$$

$$\Sigma_x = \begin{pmatrix} & \mathbb{1} \\ \mathbb{1} & \end{pmatrix}$$

$$\begin{aligned} \Sigma_x D \Sigma_x &= \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \alpha & \gamma \\ -\gamma^\dagger & -\tilde{\alpha} \end{pmatrix} \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} = \\ &= \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \gamma & \alpha \\ -\tilde{\alpha} & -\gamma^\dagger \end{pmatrix} = \begin{pmatrix} -\tilde{\alpha} & -\gamma^\dagger \\ \gamma & \alpha \end{pmatrix} \\ &= - \begin{pmatrix} \tilde{\alpha} & \gamma^\dagger \\ -\gamma & -\alpha \end{pmatrix} = - \begin{pmatrix} \alpha & \gamma \\ -\gamma^\dagger & -\tilde{\alpha} \end{pmatrix}^* = -D^* \end{aligned}$$

$$D\psi = \omega\psi$$

$$\Sigma_x D\psi = \omega \Sigma_x \psi$$

$$\Sigma_x D \Sigma_x \Sigma_x \psi = \omega \Sigma_x \psi \rightarrow -D^* (\Sigma_x \psi) = \omega (\Sigma_x \psi)$$

$$\rightarrow D (\Sigma_x \psi)^* = -\omega^* (\Sigma_x \psi)^*$$

$$\Rightarrow \text{If } \psi \mid D\psi = \omega \quad \text{then } \exists \psi' = (\Sigma_x \psi)^* \text{ s.t.}$$

$$D\psi' = -\omega^* \psi'$$

motion can be sublated. The transformation and diagonalization have nothing to do the equation of motion, but are the intrinsic and invariant property of a Hermitian quadratic form that is equipped with commutator or Poisson bracket (Sec. VIII).

Finally, it is worth noting that we shall confine our interest in this review only to the diagonalization of quadratic Hamiltonians. It will go out of our consideration as to whether and how a quadratic Hamiltonian can be derived and obtained for a real system.

II. DIAGONALIZATION THEORY OF BOSE SYSTEMS

In this section, we employ the Heisenberg equation of motion to study the quadratic Hamiltonian of bosons. It is found that a whole theory of diagonalization can be developed for the Bose system.

A. Dynamic matrix

The Heisenberg equation of motion can be derived from Eqs. (1.1)–(1.4),

$$i \frac{d}{dt} c = \alpha c + \gamma \tilde{c}^\dagger, \quad (2.1)$$

$$i \frac{d}{dt} \tilde{c}^\dagger = -\gamma^\dagger c - \tilde{\alpha} \tilde{c}^\dagger. \quad (2.2)$$

Here and hereafter, we shall apply the natural units of measurement, i.e., $\hbar = c = 1$, for convenience. The two equations above can be combined as

$$i \frac{d}{dt} \psi = D \psi, \quad (2.3)$$

where

$$D = \begin{bmatrix} \alpha & \gamma \\ -\gamma^\dagger & -\tilde{\alpha} \end{bmatrix}. \quad (2.4)$$

It should be pointed out that the matrix D is distinct from the matrix M of Eq. (1.9),

$$M = \begin{bmatrix} \alpha & \gamma \\ \gamma^\dagger & \tilde{\alpha} \end{bmatrix}, \quad (2.5)$$

except both $\alpha = 0$ and $\gamma = 0$, the trivial case that has been excluded, *ab initio*, in Sec. IA. As indicated by Eq. (1.6), the matrix M represents the constant coefficients of the Hamiltonian. In contrast, Eq. (2.3) demonstrates that the matrix D will control the dynamic behavior of the system.

Definition 2 We shall call the matrix present in the Hamiltonian, such as M , the coefficient matrix, and the matrix present in the Heisenberg equation, such as D , the dynamic matrix.

It is a characteristic feature of the Bose system that the dynamic matrix D is different from the coefficient matrix M .

On the other hand, it can be readily seen from Eqs. (2.4) and (2.5) that the dynamic matrix D and the coefficient matrix M have the relation,

$$D = I_- M. \quad (2.6)$$

This relation will play a fundamental role in the diagonalization of the Bose system. Besides, it is worth noting that D is generally not Hermitian whereas M is Hermitian forever.

Following Sec. IB, let us study the eigenvalue problem of Eq. (2.3),

$$\omega \psi = D \psi. \quad (2.7)$$

We expect that it would generate a linear transformation that could be used to diagonalize the quadratic Hamiltonian of bosons.

Now that $D \neq M$, there arises a question. As shown in Eqs. (1.20) and (1.22), the Hamiltonian requires a Hermitian congruence transformation to diagonalize the coefficient matrix M . However, the Heisenberg equation can, at most, generate a similarity transformation to diagonalize the dynamic matrix D , as can be seen from Eq. (2.7). Not only the matrices to be diagonalized but also the manners of diagonalization are different from each other. That is the key problem occurring in the Bose system.

To solve the problem, let us begin with a survey on the general properties of the dynamic matrix D .

Lemma 3 If ω is an eigenvalue of the dynamic matrix D , then $-\omega^*$ will also be an eigenvalue of D . (★₃)

Proof. The characteristic equation of Eq. (2.7) is

$$\det(\omega I_+ - D) = \begin{vmatrix} \omega I - \alpha & -\gamma \\ \gamma^\dagger & \omega I + \tilde{\alpha} \end{vmatrix} = 0. \quad (2.8)$$

First, let us perform some elementary row and column operations to the characteristic determinant,

$$\begin{aligned} \det(\omega I_+ - D) &= \begin{vmatrix} -I & 0 \\ 0 & -I \end{vmatrix} \begin{vmatrix} 0 & I \\ I & 0 \end{vmatrix} \\ &\times \begin{vmatrix} \omega I - \alpha & -\gamma \\ \gamma^\dagger & \omega I + \tilde{\alpha} \end{vmatrix} \begin{vmatrix} 0 & I \\ I & 0 \end{vmatrix} \\ &= \begin{vmatrix} -\omega I - \tilde{\alpha} & -\gamma^\dagger \\ \gamma & -\omega I + \alpha \end{vmatrix}. \end{aligned} \quad (2.9)$$

And then take complex conjugate,

$$\det(\omega I_+ - D)^* = \begin{vmatrix} -\omega^* I - \alpha & -\gamma \\ \gamma^\dagger & -\omega^* I + \tilde{\alpha} \end{vmatrix}, \quad (2.10)$$

where we have used the facts for the Bose system: $\alpha^\dagger = \alpha$ and $\tilde{\gamma} = \gamma$. Paying attention to

$$\det(\omega I_+ - D)^* = \det(\omega I_+ - D) = 0, \quad (2.11)$$

we have

$$\begin{vmatrix} -\omega^* I - \alpha & -\gamma \\ \gamma^\dagger & -\omega^* I + \tilde{\alpha} \end{vmatrix} = 0. \quad (2.12)$$

One reaches the lemma immediately by comparing this equation with Eq. (2.8). ■

This lemma shows that the eigenvalues of the dynamic matrix D will appear in pairs if they exist. When one of a pair is ω , the other is $-\omega^*$.

Physically, this property of the dynamic matrix D originates from the Hermitian symmetry of the Hamiltonian: $H^\dagger = H$. This symmetry implies that, if

$$c(t) = c_0 \exp(\mp i\omega t) \quad (2.13)$$

is a solution of Eq. (2.1), then

$$\tilde{c}^\dagger(t) = \tilde{c}_0^\dagger \exp(\pm i\omega^* t) \quad (2.14)$$

will be the solution of Eq. (2.2). That is to say, if

$$\psi(t) = \psi_0 \exp(-i\omega t) \quad (2.15)$$

is a solution of Eq. (2.3), the

$$\psi(t) = \psi_0 \exp(i\omega^* t) \quad (2.16)$$

must also be a solution of Eq. (2.3).

Lemma 4 *If $v(\omega)$ is an eigenvector belonging to the eigenvalue ω of the dynamic matrix D , then $v(-\omega^*)$ will be an eigenvector belonging to the eigenvalue $-\omega^*$. Here the vector $v(-\omega^*)$ is defined by*

$$v(-\omega^*) = \Sigma_x v^*(\omega) \quad (2.17)$$

with

$$\Sigma_x = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}. \quad (2.18)$$

Proof. Substituting $v(\omega)$ into Eq. (2.7), one has

$$(\omega I_+ - D)v(\omega) = 0. \quad (2.19)$$

It follows that

$$-\Sigma_x(\omega I_+ - D)\Sigma_x \Sigma_x v(\omega) = 0, \quad (2.20)$$

and that

$$[-\Sigma_x(\omega I_+ - D)\Sigma_x]^* [\Sigma_x v(\omega)]^* = 0. \quad (2.21)$$

From Eqs. (2.9) and (2.10), one can easily see that

$$[-\Sigma_x(\omega I_+ - D)\Sigma_x]^* = -\omega^* I_+ - D, \quad (2.22)$$

he thus gets

$$(-\omega^* I_+ - D)\Sigma_x v^*(\omega) = 0. \quad (2.23)$$

This means that $\Sigma_x v^*(\omega)$ is an eigenvector belonging to the eigenvalue $-\omega^*$. That is just Eq. (2.17). ■

This lemma shows that, for a given pair of eigenvalues $(\omega, -\omega^*)$, their eigenvectors can be formed into pairs according to Eq. (2.17).

In the classical case, the dynamic matrix D_{cl} of Eq. (1.36) is

$$D_{cl} = KV. \quad (2.24)$$

It indicates that D_{cl} is the production of a positive definite matrix K and a Hermitian matrix V . Although D_{cl} is not Hermitian in general, it is diagonalizable and all its eigenvalues are real. Mathematically, that is because the matrix K has Cholesky decomposition, as has been seen in Sec. IB. Now, as shown in Eq. (2.6), the dynamic matrix D for a Bose system is the production of an indefinite matrix I_- and a Hermitian matrix M . There exists no Cholesky decomposition for the matrix I_- , and there is no guarantee for D to be diagonalizable. Furthermore, the eigenvalues of D will, in general, be complex other than real even if D is diagonalizable. In a word, the present situation is much more involved than the classical case. To be clear, let us take a look at the simplest case, i.e., the Hamiltonian of Eq. (1.1) with $n = 1$.

Example 5

$$H = \alpha c^\dagger c + \frac{1}{2}\gamma c^\dagger c^\dagger + \frac{1}{2}\gamma^* cc. \quad (2.25)$$

Solution 6 Apparently, the dynamic matrix D is a 2×2 matrix,

$$D = \begin{bmatrix} \alpha & \gamma \\ -\gamma^* & -\alpha \end{bmatrix}. \quad (2.26)$$

The eigenvalue equation is

$$\begin{bmatrix} \alpha & \gamma \\ -\gamma^* & -\alpha \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \omega \begin{bmatrix} x \\ y \end{bmatrix}. \quad (2.27)$$

Obviously, the eigenvalues can be obtained from the characteristic equation,

$$\omega^2 - \alpha^2 + |\gamma|^2 = 0, \quad (2.28)$$

the results are

$$\omega = \begin{cases} \pm \sqrt{\alpha^2 - |\gamma|^2}, & |\alpha| > |\gamma| \\ 0, & |\alpha| = |\gamma| \\ \pm i \sqrt{|\gamma|^2 - \alpha^2}, & |\alpha| < |\gamma|. \end{cases} \quad (2.29)$$

Namely, there are two real eigenvalues when $|\alpha| > |\gamma|$, a zero eigenvalue when $|\alpha| = |\gamma|$, and two imaginary eigenvalues when $|\alpha| < |\gamma|$.

It is easy to show that, if $|\alpha| = |\gamma|$, there exists only one eigenvector,

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ \mp e^{-i\theta} \end{bmatrix}, \quad (2.30)$$

$$\Sigma_x \Sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{I} \quad (\text{obv from Pauli}) \quad \left(\begin{matrix} (!) \\ \rightarrow \varphi \text{ inherits inv. symm} \end{matrix} \right) \Sigma_x T^* \Sigma_x = T$$

where $\theta = \arg(\gamma)$ is the argument of γ , and the signs \mp correspond to $\alpha = \pm|\gamma|$, respectively. Therefore, the dynamic matrix D can not be diagonalized when $|\alpha| = |\gamma|$.

When $|\alpha| < |\gamma|$, the dynamic matrix D has two linearly independent eigenvectors. It is thus diagonalizable, but its eigenvalues are both imaginary.

When $|\alpha| > |\gamma|$, the dynamic matrix D has two linearly independent eigenvectors, it is also diagonalizable. In particular, its eigenvalues are both real.

In sum, the dynamic matrix of this Bose system has the same property as that of the classical system only when $|\alpha| > |\gamma|$: It is diagonalizable, and its eigenvalues are real.

This simple example exhibits clearly the complexity of Bose systems. To resolve this complexity, we shall study first the necessary and then the sufficient condition for the diagonalization of a quadratic Hamiltonian of bosons, which constitute the themes of the following two subsections, respectively.

B. Necessary condition for diagonalization

To be clear and definite in the following, we would first give three definitions here.

Definition 7 If an invertible matrix has the form as Eq. (1.19), we call it a **Bogoliubov-Valatin matrix**.

Definition 8 A linear transformation defined by Eq. (1.18) will be called a **Bogoliubov-Valatin transformation** if T is a BV matrix and ψ is a standard bosonic field, i.e., it satisfies Eq. (1.12).

Definition 9 The quadratic Hamiltonian defined in Eq. (1.1) is said to be **Bogoliubov-Valatinianly diagonalizable** if there is such a BV transformation that can fulfill both the conditions of Eqs. (1.21) and (1.22).

It should be pointed out that a BV transformation is not required to satisfy either the condition of Eq. (1.21) or the condition of Eq. (1.22), according to the definition 8

Lemma 10 The inverse of a BV matrix is also a BV matrix.

Proof. From Eq. (1.19), it is easy to show that a matrix T is a BV matrix if and only if

$$\Sigma_x T^* \Sigma_x = T. \quad (2.31)$$

Taking the inverses of the two sides, we obtain

$$\Sigma_x (T^{-1})^* \Sigma_x = T^{-1}. \quad (2.32)$$

This demonstrates that T^{-1} is also a BV matrix. ■

From Eq. (1.7), one can easily see that

$$\psi = (\widetilde{\Sigma_x \psi})^\dagger. \quad (2.33)$$



$$\underline{c} = (c_1, \dots, c_n), \quad c^\dagger = (c_1^\dagger, \dots, c_n^\dagger)^T \quad 8$$

$$\psi = (\underline{c}, \underline{\tilde{c}}^\dagger) \rightarrow \Sigma_x \psi = (\underline{\tilde{c}}^\dagger, \underline{c}) \rightarrow \widetilde{\Sigma_x \psi} = (\underline{c}^\dagger, \underline{\tilde{c}}) \rightarrow (\widetilde{\Sigma_x \psi})^\dagger = (\underline{c}, \underline{\tilde{c}}^\dagger) = \psi$$

This is a basic symmetry of the field operator, we shall call it the **involution symmetry**, for convenience. Mathematically, this symmetry roots from the fact that c_i and c_i^\dagger are not independent, but are the Hermitian conjugates of each other. Conversely, if a field has the involution symmetry as above, its component operators can not be independent, there must exist some relationship among them.

Now, consider the new field φ defined by the BV transformation of Eq. (1.18). It can be given by the inverse transformation,

$$\text{Mult. by } \Sigma_x \quad \varphi = T^{-1} \psi. \quad (2.34)$$

Obviously,

$$\Sigma_x \varphi = \Sigma_x T^{-1} \widetilde{\Sigma_x \psi} = \mathbb{I} \quad (2.35)$$

which results in \downarrow apply $(\widetilde{\cdot})^\dagger$ to both sides

$$(\widetilde{\Sigma_x \varphi})^\dagger = \underbrace{\Sigma_x (T^{-1})^*}_{= T^{-1}} \underbrace{\Sigma_x (\widetilde{\Sigma_x \psi})^\dagger}_{\psi} = \underbrace{\mathbb{I}}_{= T^{-1} \psi = \varphi} \quad (2.36)$$

This implies that

$$\varphi = (\widetilde{\Sigma_x \varphi})^\dagger. \quad (2.37)$$

where Eqs. (2.32)–(2.34) have been used. Therefore, the new field will have the same involution symmetry as the old one after a BV transformation.

Lemma 11 The involution symmetry of the field operator is conserved for the Bose system after a BV transformation. Namely, the involution symmetry is an invariant property of the BV transformation.

Suppose that φ is a new field, it thus has the involution symmetry. As mentioned above, its component operators will not be independent. In fact, it is easy to show that φ must have the same form as the old field ψ defined in Eq. (1.7). In other words, it can be represented as follows,

$$\varphi = \begin{bmatrix} d \\ \tilde{d}^\dagger \end{bmatrix}, \quad (2.38)$$

where

$$d = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix}, \quad d^\dagger = [d_1^\dagger, d_2^\dagger, \dots, d_n^\dagger]. \quad (2.39)$$

Here d_i and d_i^\dagger represent a new pair of operators, which are Hermitianly conjugate to each other. Their commutation rules can be derived from the inverse transformation,

$$\varphi \cdot \varphi^\dagger = T^{-1} \psi \cdot \psi^\dagger (T^{-1})^\dagger. \quad (2.40)$$

(*) H can be diagonalized by a BV transformation only if D is diagonalizable and if its eigenvalues are real | NECESSARY CONDITION

As stated in the definition 8 the old field ψ satisfies the standard commutation rule of Eq. (1.12). We therefore obtain

$$\varphi \cdot \varphi^\dagger = T^{-1} I_- (T^{-1})^\dagger. \quad (2.41)$$

The commutation rule for the new field φ is determined wholly by the BV matrix T , it may not be standard,

$$\varphi \cdot \varphi^\dagger \neq I_-. \quad (2.42)$$

It is standard if and only if T satisfies the condition of Eq. (1.21), which is equivalent to

$$T^{-1} I_- (T^{-1})^\dagger = I_-. \quad (2.43)$$

In a word, if a BV transformation satisfies the condition of Eq. (1.21), the new field is a standard bosonic field; if it further satisfies the condition of Eq. (1.22), the Hamiltonian of Eq. (1.1) gets BV diagonalized.

We shall leave it to the next subsection to discuss how to obtain a BV transformation and make it fulfill the two conditions of Eqs. (1.21) and (1.22). Here and now, we would, above all, show a basic property of the BV transformation, which will play the central role in the theory of diagonalization of quantum quadratic Hamiltonians.

Lemma 12 Under a BV transformation, the two dynamic matrices respectively for the old and new fields will be similar to each other.

Proof. Obviously, under a BV transformation as given in Eqs. (1.18) and (1.19), the equation of motion of the new field φ will still be linear in φ itself, i.e.,

$$i \frac{d}{dt} \varphi = [\varphi, H] = D_1 \varphi, \quad (2.44)$$

where D_1 is the dynamic matrix for the new field φ . Apparently, this equation has the same form as that for the old field ψ ,

$$i \frac{d}{dt} \psi = D \psi, \quad (2.45)$$

where D is the dynamic matrix for the old field ψ . On the other hand, it follows from Eq. (1.18) that

$$i \frac{d}{dt} \psi = T i \frac{d}{dt} \varphi. \quad (2.46)$$

With the above two equations of motion for ψ and φ , this equation can be expressed as

$$D \psi = T D_1 \varphi. \quad (2.47)$$

Substituting ψ further with Eq. (1.18), one has

$$(T^{-1} D T - D_1) \varphi = 0. \quad (2.48)$$

This equation is equivalent to

$$v_i \varphi = 0, \quad \forall i \in \{1, 2, \dots, 2n\}, \quad (2.49)$$

where v_i are the row vectors of the matrix $T^{-1} D T - D_1$. It implies that

$$v_i = 0, \quad \forall i \in \{1, 2, \dots, 2n\}. \quad (2.50)$$

That is

$$T^{-1} D T - D_1 = 0, \quad (2.51)$$

viz.,

$$D_1 = T^{-1} D T. \quad (2.52)$$

In other words, the dynamic matrix will vary in a similar manner under a BV transformation. ■

Proposition 13 If a quadratic Hamiltonian of bosons can be BV diagonalized, then its dynamic matrix is diagonalizable, and all the eigenvalues of the dynamic matrix will be real. (*)

Proof. Suppose that the diagonalized form of the Hamiltonian is

$$H = \sum_{i=1}^n \omega_i d_i^\dagger d_i + C, \quad (2.53)$$

where C is a real constant. Since H is Hermitian, all ω_i must be real, i.e., $\omega_i \in \mathbb{R}$. By definition, the new field φ satisfies the standard commutation rule,

$$\varphi \cdot \varphi^\dagger = I_-. \quad (2.54)$$

From the two equations above, the dynamic matrix D_1 for the new field φ can be found as

$$D_1 = \text{diag}(\omega_1, \omega_2, \dots, \omega_n, -\omega_1, -\omega_2, \dots, -\omega_n), \quad (2.55)$$

where $\text{diag}(a_1, a_2, \dots, a_m)$ denotes the diagonal matrix with a_1, a_2, \dots, a_m on the main diagonal. From this, one can reach the proposition by the lemma 12. (*)

Definition 14 A dynamic matrix is said to be physically diagonalizable if it is diagonalizable, and all its eigenvalues are real.

By this definition, the proposition can be restated as follows.

If a quadratic Hamiltonian of bosons can be BV diagonalized, its dynamic matrix is physically diagonalizable.

Corollary 15 The quadratic Hamiltonian of bosons defined in Eq. (1.1) can not be BV diagonalized if the coefficient submatrix α vanishes identically, i.e., $\alpha = 0$.

Proof. In this case, the dynamic matrix of Eq. (2.4) reduces to

$$D = \begin{bmatrix} 0 & \gamma \\ -\gamma^\dagger & 0 \end{bmatrix}. \quad (2.56)$$

Obviously, it is anti-Hermitian, and thus unitarily diagonalizable. Since $\gamma \neq 0$, the eigenvalues of D can not

(*) Spectrum is invariant under similarity transformations

all be zero, some of them must be purely imaginary. In other words, the dynamic matrix D is diagonalizable but not physically diagonalizable, which is inconsistent with the necessary condition for the BV diagonalization of a Hamiltonian. ■

This corollary shows that it is not all the quadratic Hamiltonians of bosons that can be BV diagonalized. What kind of Hamiltonians is BV diagonalizable? To answer it, one needs to study the sufficient condition for the BV diagonalization.

C. Sufficient condition for diagonalization

In the preceding subsection, we have already obtained the necessary condition for the BV diagonalization. Henceforth, we would presume that the necessary condition holds for the Bose system. Starting from this presumption, we shall search the sufficient condition for the BV diagonalization in this subsection.

By definition, the dynamic matrix D is of size $2n$. If D is physically diagonalizable, it has a complete set of totally $2n$ linearly independent eigenvectors. We have learned from the lemmas 3 and 4 that the eigenvalues and eigenvectors of D will appear in pairs. Let us continue this discussion about pairing.

Lemma 16 *If the dynamic matrix D is physically diagonalizable, then, for each pair of nonzero eigenvalues, i.e., $(\omega, -\omega)$ with $\omega \neq 0$, they have the same degeneracy. In other words, their eigenspaces have the same dimension.*

Proof. According to the lemma 4 if the eigenvalue ω has m eigenvectors,

$$v_l(\omega), \quad l = 1, 2, \dots, m, \quad (2.57)$$

the corresponding m vectors $v_l(-\omega)$,

$$v_l(-\omega) = \Sigma_x v_l^*(\omega), \quad l = 1, 2, \dots, m, \quad (2.58)$$

are the eigenvectors belonging to the eigenvalue $-\omega$. It can be readily confirmed that the vectors $v_l(-\omega)$ ($l = 1, 2, \dots, m$) are linearly independent if and only if the vectors $v_l(\omega)$ ($l = 1, 2, \dots, m$) are linearly independent.

In other words, if ω has m linearly independent eigenvectors, then $-\omega$ also has m linearly independent eigenvectors, and vice versa. That is to say, the eigenvalues ω and $-\omega$ have the same degeneracy, their eigenspaces have the same dimension. ■

The proof above shows that, if the basis vectors for the eigenspace of ω ($\omega \neq 0$) have been determined, the basis vectors for the eigenspace of $-\omega$ can be chosen as Eq. (2.58), and vice versa.

Lemma 17 *If the dynamic matrix D is physically diagonalizable and has zero eigenvalue, the eigenspace of zero eigenvalue is even dimensional. In particular, its basis vectors can be chosen and grouped as*

$$v_{m+l}(0) = \Sigma_x v_l^*(0), \quad l = 1, 2, \dots, m, \quad (2.59)$$

where $2m$ ($m \in \mathbb{N}$) is the dimension of the eigenspace of zero eigenvalue.

Proof. The first point is a direct result of the lemma 16

As to the second one, let us consider the eigenvalue equation,

$$Dv(0) = 0. \quad (2.60)$$

That is a homogeneous system of $2n$ linear equations, its solution set forms the eigenspace of zero eigenvalue.

Since the dimension of the eigenspace of zero eigenvalue is $2m$, we have $\text{rank}(D) = 2n - 2m$ where $\text{rank}(A)$ denotes the rank of the matrix A . It means that the vector $v(0)$ has $2m$ free unknown components. Therefore, we can choose the following $2m$ components of $v(0)$,

$$v^\alpha(0), \quad \alpha = 1, 2, \dots, m, n+1, n+2, \dots, n+m, \quad (2.61)$$

as the free unknowns. First, let the free unknowns be respectively as follows,

$$v_l^\alpha(0) = \delta_{\alpha l}, \quad (2.62)$$

where

$$l = 1, 2, \dots, m, \quad (2.63)$$

$$\alpha = 1, 2, \dots, m, n+1, n+2, \dots, n+m. \quad (2.64)$$

We obtain from Eq. (2.60) the first group of eigenvectors,

$$v_l(0), \quad l = 1, 2, \dots, m. \quad (2.65)$$

Clearly, they are linearly independent. Then, using the lemma 4 we have the other group of eigenvectors,

$$v_{m+l}(0) = \Sigma_x v_l^*(0), \quad l = 1, 2, \dots, m. \quad (2.66)$$

They are also linearly independent. The definitions for $v_{m+l}(0)$ show that

$$v_{m+l}^\alpha(0) = \delta_{\alpha, m+l}, \quad (2.67)$$

where

$$l = 1, 2, \dots, m, \quad (2.68)$$

$$\alpha = 1, 2, \dots, m, n+1, n+2, \dots, n+m. \quad (2.69)$$

Equations (2.62) and (2.67) imply that the two groups are also linearly independent. The combination of the two groups has $2m$ linearly independent eigenvectors, they form a basis for the eigenspace of zero eigenvalue. All in all, the basis vectors for the eigenspace of zero eigenvalue can be chosen and grouped as Eq. (2.59). ■

Following the two lemmas above, if the dynamic matrix D is physically diagonalizable, it is enough for us to find a half of the eigenvectors of D , the other half can be determined by Eqs. (2.58) and (2.59). In other words, the eigenvalues and eigenvectors of D can be formed into pairs according to Eqs. (2.58) and (2.59). Each pair has two linearly independent eigenvectors with opposite

eigenvalues. Such a pair will be called a **dynamic mode pair**. Consequently, **there are totally n dynamic mode pairs**. Henceforth, Eqs. (2.58) and (2.59) will be used as the conventions for the pairs of dynamic modes.

Suppose that the dynamic matrix D is physically diagonalizable. One can construct a linear transformation

as in Sec. IB

$$\psi = T\varphi, \quad (2.70)$$

where φ represents the new field operator, and **T is the matrix which consists of all the eigenvectors of D ,**

$$T = [v(\omega_1), v(\omega_2), \dots, v(\omega_n), v(-\omega_1), v(-\omega_2), \dots, v(-\omega_n)]. \quad (2.71)$$

Here each eigenvalue is counted up to its multiplicity, and the n dynamic mode pairs are separated and arranged sequentially into the left and right halves of the matrix T . Since the dynamic matrix D is supposed to be physically diagonalizable, the matrix T has full rank and is hence nonsingular and invertible. This analysis demonstrates that an invertible linear transformation can be derived from the equation of motion if the dynamic matrix of the system is physically diagonalizable.

Definition 18 *If the dynamic matrix D is physically diagonalizable, then a linear transformation can be defined by Eqs. (2.70) and (2.71). We shall call it the derivative transformation, and call the corresponding matrix T the derivative matrix.*

By use of both the conventions of Eqs. (2.58) and (2.59), we have

$$\Sigma_x T^* = [v(-\omega_1), v(-\omega_2), \dots, v(-\omega_n), v(\omega_1), v(\omega_2), \dots, v(\omega_n)]. \quad (2.72)$$

Paying attention to the fact that Σ_x is an elementary matrix, the right multiplication by it represents switching the left and right halves of the square matrix standing left to it. So we obtain

$$\text{T satisfies 2.58 and 2.59} \quad \mapsto \quad \Sigma_x T^* \Sigma_x = T. \quad (2.73)$$

That is an important property of the the derivative transformation, it implies that **the derivative matrix T has the same form as that of (1.19)**. According to the definitions 7 and 8 as well as the lemma 11, we obtain the lemma for the derivative transformation. *and (!)*

Lemma 19 *If the dynamic matrix D is physically diagonalizable, its derivative matrix is a BV matrix. The corresponding derivative transformation is a BV transformation, and thus it will conserve the involution symmetry of the field operator of the Bose system.*

As shown by the proof above, **it is the two conventions of Eqs. (2.58) and (2.59) that guarantee that the derivative transformation is a BV transformation**. Consequently, **one must comply with both of them when he constructs a BV transformation.**

Up to now, we have proved that a BV transformation can be generated by the Heisenberg equation of motion if the dynamic matrix of the system is physically diagonalizable.

Although the new field can inherit the involution symmetry through the derivative BV transformation, its commutation rule is not always standard. From now on, we shall turn to handling this problem. As already known, it is determined by Eq. (2.41). Usually, it does not matter what the magnitude of an eigenvector is. Above, when constructing the derivative BV transformation of Eqs. (2.70) and (2.71), we did not consider the magnitudes of the eigenvectors either. Nevertheless, Eq. (2.41) shows that the magnitudes of the eigenvectors can change the commutation rule of the new field heavily. Therefore, it is necessary for us to take into account the magnitudes of the eigenvectors if we want to make the new commutation rule standard. Mathematically, the magnitude of a vector concerns the metric on the linear space. Therefore, we introduce, first, a sesquilinear form [14, 15] for the Bose system.

Definition 20 *Using I_- , we define a sesquilinear form ϕ on the $2n$ -dimensional unitary space \mathbb{C}^{2n} as follows,*

$$\phi(|x\rangle, |y\rangle) = \langle x| I_- |y\rangle, \quad \forall |x\rangle, |y\rangle \in \mathbb{C}^{2n}, \quad (2.74)$$

where Dirac notations have been used for the vectors of \mathbb{C}^{2n} . The form ϕ will be directly referred to as the metric I_- , too.

The definition is proper because the matrix I_- is Hermitian with respect to the standard basis and standard

(*) So we know that if D is physically diag. \mapsto 2.58 and 2.59 are satisfied. But 2.83 shows that in general M will not be diagonalized by the arbitrary choice of eigenvectors of D but only by those orthonormal in the I_- metric.

\hookrightarrow Q. Are these compatible with 2.58 and 2.59?

inner product of the unitary space \mathbb{C}^{2n} . Besides, the metric vector space defined by the form ϕ is nondegenerate because the matrix I_- is nonsingular.

Although this form is indefinite, it is very useful for clarifying the properties of the eigenvectors of the dynamic matrix.

Lemma 21 *If the dynamic matrix D is physically diagonalizable, its eigenspaces will be orthogonal to each other with respect to the metric I_- .*

Proof. Since the dynamic matrix D is physically diagonalizable, the linear space \mathbb{C}^{2n} can be decomposed into the direct sum of the eigenspaces of D ,

$$\mathbb{C}^{2n} = E_1 \oplus E_2 \oplus \cdots \oplus E_m, \quad (2.75)$$

where E_k ($1 \leq k \leq m$ with $1 \leq m \leq 2n$) are the eigenspaces of D , which belong to the eigenvalues $\omega_k \in \mathbb{R}$ respectively,

$$D|k\mu\rangle = \omega_k |k\mu\rangle, \quad \forall |k\mu\rangle \in E_k. \quad (2.76)$$

Here a label μ is added to distinguish the vectors of the eigenspace E_k .

Using the relation of Eq. (2.6), the equation above can be reformulated as

$$M|k\mu\rangle = \omega_k I_- |k\mu\rangle. \quad (2.77)$$

As a result, we obtain

$$\langle l\nu|M|k\mu\rangle = \omega_k \langle l\nu|I_-|k\mu\rangle. \quad (2.78)$$

By complex conjugate, we have (M, I_- herm, $\omega_k \in \mathbb{R}$)

$$\langle k\mu|M|l\nu\rangle = \omega_k \langle k\mu|I_-|l\nu\rangle, \quad (2.79)$$

the eigenvalue ω_k being real. Again, from Eq. (2.78), we have

$$\langle k\mu|M|l\nu\rangle = \omega_l \langle k\mu|I_-|l\nu\rangle. \quad (2.80)$$

The combination of the two equations above leads to

$$\langle k\mu|I_-|l\nu\rangle = 0, \quad \text{if } \omega_k \neq \omega_l. \quad (2.81)$$

This equation demonstrates that the different eigenspaces of D are orthogonal to each other, i.e., $E_k \perp E_l$ ($k \neq l$), with respect to the metric I_- defined above. \blacksquare

The lemma shows that the whole space of \mathbb{C}^{2n} can be decomposed into an orthogonal direct sum of the eigenspaces of the dynamic matrix D if D is physically diagonalizable,

$$\mathbb{C}^{2n} = E_1 \oplus E_2 \oplus \cdots \oplus E_m. \quad (2.82)$$

Meanwhile, as indicated by Eqs. (2.78) and (2.81), the coefficient matrix M becomes block diagonal with respect to the eigenspaces of D ,

$$\langle l\nu|M|k\mu\rangle = \omega_k \langle l\nu|I_-|k\mu\rangle \delta_{kl}. \quad (2.83)$$

\hookrightarrow this is why M is block diagonal and not diagonal

(*)

Lemma 22 *If the dynamic matrix D is physically diagonalizable, then, for each eigenspace of D , there exists an orthonormal basis with respect to the metric I_- . That is,*

$$\langle k\mu|I_-|k\nu\rangle = \lambda_\mu \delta_{\mu\nu}, \quad |k\mu\rangle \in E_k, \quad |k\nu\rangle \in E_k, \quad (2.84)$$

where $1 \leq \mu, \nu \leq n_k$ with n_k being the dimension of the eigenspace E_k , and $\lambda_\mu = +1$ or -1 .

Proof. Taking notice of Eq. (2.82), the metric I_- must also be a nonsingular sesquilinear form on each eigenspace. Otherwise, it is singular on the whole space \mathbb{C}^{2n} , which leads to an evident contradiction. \blacksquare

Obviously, if

$$\mathcal{B}_k \triangleq \{|k\mu\rangle \in E_k | 1 \leq \mu \leq n_k\} \quad (2.85)$$

is an orthonormal basis for the eigenspace E_k , then the union of $\mathcal{B}_1, \mathcal{B}_2, \dots, \mathcal{B}_m$, i.e.,

$$\begin{aligned} \mathcal{B} &= \mathcal{B}_1 \cup \mathcal{B}_2 \cup \cdots \cup \mathcal{B}_m \\ &= \{|k\mu\rangle \in E_k | 1 \leq k \leq m, 1 \leq \mu \leq n_k\}, \end{aligned} \quad (2.86)$$

will form an orthonormal basis for \mathbb{C}^{2n} .

Now, for a nonzero eigenvalue ω ($\omega \neq 0$), we can choose an orthonormal basis for it,

$$v_l(\omega), \quad 1 \leq l \leq m, \quad (2.87)$$

where m is the dimension of the eigenspace of ω . Then, according to the lemma 16 and the convention of Eq. (2.58), we have a basis for the eigenspace of $-\omega$,

$$v_l(-\omega) = \Sigma_x v_l^*(\omega), \quad 1 \leq l \leq m. \quad (2.88)$$

It is also an orthonormal basis,

$$\begin{aligned} v_l^\dagger(-\omega)I_-v_k(-\omega) &= \left[v_l^\dagger(\omega)\Sigma_x I_- \Sigma_x v_k(\omega) \right]^* \\ &= -\lambda_l \delta_{lk}, \end{aligned} \quad (2.89)$$

where we have used the identity,

$$\Sigma_x I_- \Sigma_x = -I_-. \quad (2.90)$$

In sum, there are totally m dynamic mode pairs for the eigenenergy pair $(\omega, -\omega)$ where $\omega \neq 0$. Equation (2.89) shows that each mode pair has two linearly independent eigenvectors with opposite norms.

As pointed out after the lemma 19 the two conventions of Eqs. (2.58) and (2.59) must be obeyed in constructing a derivative BV transformation. The discussions above demonstrate that for a pair of nonzero eigenvalues, the orthonormalization is compatible with the convention of Eq. (2.58). If zero is an eigenvalue of the dynamic matrix, is the orthonormalization compatible with the convention of Eq. (2.59)? i.e., does there exist such a basis for the eigenspace of zero eigenvalue that is orthonormal and satisfies the convention of Eq. (2.59) simultaneously? The answer is yes.

so the question now is: Can I find an orthonormal basis for V_0 that still satisfies 2.59?

Lemma 23 *If the dynamic matrix D is physically diagonalizable and has zero eigenvalue, there exists such an orthonormal basis for the eigenspace of zero eigenvalue that meets the requirement of Eq. (2.59).*

Proof. According to the lemma 17 there always exists such a basis for the eigenspace V_0 of zero eigenvalue that satisfies the requirement of Eq. (2.59),

$$v_{m+k}(0) = \Sigma_x v_k^*(0), \quad k = 1, 2, \dots, m, \quad (2.91)$$

where $2m$ ($m \in \mathbb{N}$) is the dimension of V_0 , i.e., $\dim(V_0) = 2m$.

When $m = 1$,

$$v_1^\dagger(0)I_-v_1(0) \neq 0, \quad (2.92)$$

i.e., $v_1(0)$ can not be isotropic. Otherwise, one has

$$v_1^\dagger(0)I_-v_1(0) = 0, \quad v_2^\dagger(0)I_-v_2(0) = 0. \quad (2.93)$$

In addition,

$$\begin{aligned} v_1^\dagger(0)I_-v_2(0) &\stackrel{\text{Lemma 17}}{\downarrow} v_1^\dagger(0)I_- \Sigma_x v_1^*(0) \\ &= \tilde{v}_1^*(0)Jv_1^*(0) \\ &= 0, \end{aligned} \quad (2.94)$$

where J is the unit symplectic matrix,

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}. \quad (2.95)$$

That is to say, the two eigenvectors $v_1(0)$ and $v_2(0)$ are orthogonal to each other,

$$v_1^\dagger(0)I_-v_2(0) = 0, \quad v_2^\dagger(0)I_-v_1(0) = 0. \quad (2.96)$$

Equations (2.93) and (2.96) show that the matrix of the sesquilinear form I_- vanishes identically on V_0 . That is in contradiction with the fact that I_- is a nonsingular metric on V_0 . In a word, **the norm of $v_1(0)$ can not vanish.** So we can normalize it,

$$v_1^\dagger(0)I_-v_1(0) = 1 \text{ or } -1. \quad (2.97)$$

Accordingly,

$$v_2^\dagger(0)I_-v_2(0) = -1 \text{ or } 1. \quad (2.98)$$

Together with Eq. (2.96), one has

$$v_i^\dagger(0)I_-v_j(0) = -\lambda_i \delta_{ij}, \quad \lambda_i = \pm 1, \quad i, j = 1, 2. \quad (2.99)$$

This implies that the lemma holds when $m = 1$.

Suppose that the lemma holds when $m = l$ ($l \in \mathbb{N}$), we shall show that it also holds when $m = l + 1$.

If there exists at least one of the eigenvectors that is nonisotropic, assume without loss of generality that $v_1(0)$ is such a vector, i.e.,

$$v_1^\dagger(0)I_-v_1(0) \neq 0, \quad (2.100)$$

then we have

$$v_{l+2}^\dagger(0)I_-v_{l+2}(0) \neq 0, \quad (2.101)$$

namely, $v_{l+2}(0)$ is nonisotropic, too. That is because

$$v_{l+2}(0) = \Sigma_x v_1^*(0). \quad (2.102)$$

Consider the two-dimensional subspace W spanned by the linearly independent set $\{v_1(0), v_{l+2}(0)\}$, i.e.,

$$W = \text{span}(v_1(0), v_{l+2}(0)). \quad (2.103)$$

Analogous to the case of $m = 1$, we can obtain such an orthonormal basis for W ,

$$v_i^\dagger(0)I_-v_j(0) = -\lambda_i \delta_{ij}, \quad (2.104)$$

where $\lambda_i = \pm 1$, and $i, j = 1, l+2$. It satisfies the requirement of Eq. (2.59).

If all the eigenvectors are isotropic, there must exist at least two eigenvectors such that their inner product is nonvanishing. Otherwise, the form I_- will vanish identically on V_0 ,

$$v_i^\dagger(0)I_-v_j(0) = 0, \quad \forall i, j \in \{1, 2, \dots, 2l+2\}, \quad (2.105)$$

which is obviously impossible because the form I_- is nonsingular on V_0 . Without loss of generality, let us suppose that

$$v_1^\dagger(0)I_-v_2(0) \neq 0. \quad (2.106)$$

We can always adjust the phase of $v_1(0)$ or $v_2(0)$ so that $v_1^\dagger(0)I_-v_2(0)$ is purely imaginary,

$$v_1^\dagger(0)I_-v_2(0) \notin \mathbb{R}. \quad (2.107)$$

Now, set

$$w_1 = v_1(0) + iv_2(0), \quad (2.108)$$

$$w_2 = v_1(0) - iv_2(0), \quad (2.109)$$

and

$$w_{l+2} = \Sigma_x w_1^* = v_{l+2}(0) - iv_{l+3}(0), \quad (2.110)$$

$$w_{l+3} = \Sigma_x w_2^* = v_{l+2}(0) + iv_{l+3}(0). \quad (2.111)$$

From Eqs. (2.106) and (2.107), we obtain

$$\begin{aligned} w_1^\dagger I_- w_1 &= i [v_1^\dagger(0)I_-v_2(0) - v_2^\dagger(0)I_-v_1(0)] \\ &\neq 0. \end{aligned} \quad (2.112)$$

Obviously,

$$w_1(0), w_2(0), w_{l+2}(0), \text{ and } w_{l+3}(0) \in V_0. \quad (2.113)$$

Besides, they are linearly independent. For convenience, let us reset

$$v_1(0) = w_1, \quad v_2(0) = w_2, \quad (2.114)$$

$$v_{l+2}(0) = w_{l+2}, \quad v_{l+3}(0) = w_{l+3}, \quad (2.115)$$

and consider the new set,

$$\{v_1(0), v_2(0), \dots, v_{l+1}(0), v_{l+2}(0), v_{l+3}(0), \dots, v_{2l+2}(0)\}. \quad (2.116)$$

It is evident that this set forms a new basis for V_0 , and satisfies the requirement of Eq. (2.59). In particular, $v_1(0)$ is nonisotropic,

$$v_1^\dagger(0)I_-v_1(0) \neq 0. \quad (2.117)$$

Therefore, the new basis returns to the case discussed just above. All in all, we can always obtain a two-dimensional subspace W as given in Eqs. (2.102)–(2.104) whether the basis vectors of V_0 are isotropic or not.

Using the two basis vectors of W , we can put

$$\begin{aligned} \xi_i(0) &= v_{i+1}(0) - \frac{v_1^\dagger(0)I_-v_{i+1}(0)}{v_1^\dagger(0)I_-v_1(0)}v_1(0) \\ &\quad - \frac{v_{l+2}^\dagger(0)I_-v_{i+1}(0)}{v_{l+2}^\dagger(0)I_-v_{l+2}(0)}v_{l+2}(0), \end{aligned} \quad (2.118)$$

$$\begin{aligned} \xi_{l+i}(0) &= v_{l+i+2}(0) - \frac{v_1^\dagger(0)I_-v_{l+i+2}(0)}{v_1^\dagger(0)I_-v_1(0)}v_1(0) \\ &\quad - \frac{v_{l+2}^\dagger(0)I_-v_{l+i+2}(0)}{v_{l+2}^\dagger(0)I_-v_{l+2}(0)}v_{l+2}(0), \end{aligned} \quad (2.119)$$

where $i = 1, 2, \dots, l$. They are all orthogonal to $v_1(0)$ and $v_{l+2}(0)$,

$$v_i^\dagger(0)I_- \xi_j(0) = 0, \quad i = 1, l+2; \quad j = 1, 2, \dots, 2l. \quad (2.120)$$

Evidently, all those vectors $\xi_i(0)$ are still linearly independent and eigenvectors of zero eigenvalue, i.e.,

$$\xi_i(0) \in V_0, \quad i = 1, 2, \dots, 2l. \quad (2.121)$$

Now, consider the space W' ,

$$W' = \text{span}(\{\xi_i(0) \mid i = 1, 2, \dots, 2l\}). \quad (2.122)$$

It is a proper subspace of V_0 , $\dim(W') = 2l$. Obviously,

$$V_0 = W \oplus W'. \quad (2.123)$$

As shown above, $v_1(0)$ and $v_{l+2}(0)$ are both orthogonal to the set $\{\xi_i(0) \mid i = 1, 2, \dots, 2l\}$, therefore,

$$W' = W^\perp. \quad (2.124)$$

This implies that V_0 is the orthogonal direct sum of W and W' ,

$$V_0 = W \odot W'. \quad (2.125)$$

It is easy to show that

$$\left[v_1^\dagger(0)I_-v_{i+1}(0) \right]^* = -v_{l+2}^\dagger(0)I_-v_{l+i+2}(0), \quad (2.126)$$

$$\left[v_{l+2}^\dagger(0)I_-v_{i+1}(0) \right]^* = -v_1^\dagger(0)I_-v_{l+i+2}(0). \quad (2.127)$$

As a result, we obtain

$$\xi_{l+i}(0) = \Sigma_x \xi_i^*(0), \quad i = 1, 2, \dots, l. \quad (2.128)$$

This indicates that the basis for W' is exactly in accordance with the convention of Eq. (2.59). Since $\dim(W') = 2l$, by the induction hypothesis, the space W' has an orthonormal basis that satisfies the convention of Eq. (2.59). Suppose the basis is the set:

$$\{\zeta_1(0), \zeta_2(0), \dots, \zeta_{2l}(0)\}, \quad (2.129)$$

which satisfies

$$\zeta_{l+i}(0) = \Sigma_x \zeta_i^*(0), \quad (2.130)$$

where $i = 1, 2, \dots, l$, and

$$\zeta_i^\dagger(0)I_- \zeta_j(0) = -\lambda_i \delta_{ij}, \quad (2.131)$$

where $\lambda_i = \pm 1$ and $i, j = 1, 2, \dots, 2l$. It is evident that the set

$$\{v_1(0), v_{l+2}(0), \zeta_1(0), \zeta_2(0), \dots, \zeta_{2l}(0)\} \quad (2.132)$$

is a basis for V_0 . Upon ordering them as follows,

$$\eta_1(0) = v_1(0), \quad (2.133)$$

$$\eta_{l+2}(0) = v_{l+2}(0), \quad (2.134)$$

$$\eta_{i+1}(0) = \zeta_i(0), \quad i = 1, 2, \dots, l, \quad (2.135)$$

$$\eta_{l+i+2}(0) = \zeta_{l+i}(0), \quad i = 1, 2, \dots, l, \quad (2.136)$$

one has

$$\eta_{l+i}(0) = \Sigma_x \eta_i^*(0), \quad (2.137)$$

where $i = 1, 2, \dots, l+1$, and

$$\eta_i^\dagger(0)I_- \eta_j(0) = -\lambda_i \delta_{ij}, \quad (2.138)$$

where $\lambda_i = \pm 1$ and $i, j = 1, 2, \dots, 2(l+1)$. Here Eqs. (2.102), (2.104), (2.125), (2.130), and (2.131) have been used. The two equations above show that the new set

$$\{\eta_1(0), \eta_2(0), \dots, \eta_{2(l+1)}(0)\} \quad (2.139)$$

is an orthonormal basis for V_0 , and it satisfies the requirement of Eq. (2.59). In other words, the lemma holds for $m = l+1$.

Finally, by mathematical induction, the lemma is valid for any $m \in \mathbb{N}$. ■

In this proof, we present a modified version of the Gram-Schmidt orthogonalization process, which can maintain the satisfiability of the convention of Eq. (2.59). Put it another way, if one starts from a basis satisfying

Eq. (2.59), he can arrive finally at an orthonormal basis which will still satisfy Eq. (2.59) through this modified Gram-Schmidt orthogonalization process.

This lemma shows that there are totally m mode pairs for the zero eigenvalue $\omega = 0$, each mode pair has two linearly independent eigenvectors with opposite norms.

The total n dynamic mode pairs are thus selected, their eigenvectors form an orthonormal basis for the whole space of \mathbb{C}^{2n} ,

$$v^\dagger(\omega_i)I_-v(\omega_j) = \lambda_i\delta_{ij}, \quad (2.140)$$

where $\lambda_i = \pm 1$ and $1 \leq i, j \leq 2n$. Here each eigenvalue is counted up to its multiplicity. Each dynamic mode pair has two linearly independent eigenvectors with both opposite eigenenergies and opposite norms. Therefore, a half of the basis vectors have the norm 1, the other half have the norm -1 .

From Eq. (2.83) and the equation above, we obtain the following lemma.

Lemma 24 *With the orthonormal basis of \mathbb{C}^{2n} chosen as above, the coefficient matrix M is diagonalized,*

$$v^\dagger(\omega_i)Mv(\omega_j) = \lambda_i\omega_i\delta_{ij}, \quad 1 \leq i, j \leq 2n, \quad (2.141)$$

where $v^\dagger(\omega_i)$ is an eigenvector of the eigenvalue ω_i , with $\lambda_i = 1$ or -1 being the corresponding norm.

For each mode pair, its two eigenvectors have opposite norms, one is $+1$, the other is -1 . So we can stipulate an order for every mode pair: The first eigenvector has the norm of $+1$, and the second one has the norm of -1 . Under this stipulation, the derivative BV transformation of Eqs. (2.70) and (2.71) becomes

$$\psi = T_n\varphi, \quad (2.142)$$

$$T_n = [v(\omega_1), v(\omega_2), \dots, v(\omega_n), v(-\omega_1), v(-\omega_2), \dots, v(-\omega_n)], \quad (2.143)$$

where, for each mode pair of $(v(\omega_i), v(-\omega_i))$, the eigenvectors are ordered as follows,

$$v^\dagger(\omega_i)I_-v(\omega_i) = 1, \quad (2.144)$$

$$v^\dagger(-\omega_i)I_-v(-\omega_i) = -1. \quad (2.145)$$

That is to say, the left half of T_n is filled with the eigenvectors with the positive norms of $+1$; the right half of T_n is filled with the eigenvectors with the negative norms of -1 . For convenience, we shall call T_n the normal derivative BV matrix and Eq. (2.142) the normal derivative BV transformation. To sum up, a normal derivative BV transformation can always be generated by the Heisenberg equation of motion if the dynamic matrix of the system is physically diagonalizable.

According to the stipulation for the normal BV matrix T_n , one has

$$v^\dagger(\omega_i)I_-v(\omega_j) = \lambda_i\delta_{ij}, \quad 1 \leq i, j \leq 2n, \quad (2.146)$$

where

$$\lambda_i = \begin{cases} 1, & 1 \leq i \leq n \\ -1, & n+1 \leq i \leq 2n. \end{cases} \quad (2.147)$$

In terms of matrix, it can be expressed as

$$T_n^\dagger I_- T_n = I_-. \quad (2.148)$$

Thereby, we arrive at the following lemma.

Lemma 25 *If the dynamic matrix D is physically diagonalizable, the normal derivative BV matrix T_n satisfies the identity,*

$$T_n^\dagger I_- T_n = I_-. \quad (2.149)$$

In other words, T_n is a member of the group $U(n, n)$ [15]. The sesquilinear form I_- remains invariant under the transformation of T_n .

This lemma implies that the new field φ is a standard bosonic field, i.e.,

$$\varphi \cdot \varphi^\dagger = I_-. \quad (2.150)$$

Put it another way, the new component operators, d_i and d_i^\dagger ($i = 1, 2, \dots, n$) will satisfy the standard commutation rules for the annihilation and creation operators of bosons,

$$[d_i, d_j^\dagger] = \delta_{ij}, \quad [d_i, d_j] = 0, \quad [d_i^\dagger, d_j^\dagger] = 0. \quad (2.151)$$

Lemma 26 *If the dynamic matrix D is physically diagonalizable, the normal derivative BV matrix T_n will diagonalize the coefficient matrix M in the manner of Hermitian congruence. That is*

$$T_n^\dagger M T_n = \text{diag}(\omega_1, \dots, \omega_n, \omega_1, \dots, \omega_n). \quad (2.152)$$

Proof. It comes simply from the lemma 25 and Eq. (2.141). ■

This lemma shows that the dynamic matrix D and the coefficient matrix M can be diagonalized simultaneously if D is physically diagonalizable:

$$T_n^{-1} D T_n = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n), \quad (2.153)$$

$$T_n^\dagger M T_n = \text{diag}(\omega_1, \dots, \omega_n, \omega_1, \dots, \omega_n). \quad (2.154)$$

It is evident that the manners of diagonalization are different: The former is diagonalized by a similar transformation, and the latter by a Hermitian congruence transformation. In brief, the two different matrices have been

diagonalized by the two different manners of transformation simultaneously, that solves the key problem occurring in the Bose system.

With the two lemmas above, we obtain the sufficient condition for the diagonalization of the Bose system.

Proposition 27 *A quadratic Hamiltonian of bosons is BV diagonalizable if its dynamic matrix is physically diagonalizable.*

Proof. By replacing ψ with the φ of Eq. (2.142), Eq. (1.6) can be reformulated as

$$H = \frac{1}{2}\varphi^\dagger T_n^\dagger M T_n \varphi - \frac{1}{2}\text{tr}(\alpha). \quad (2.155)$$

Using the lemma 26 we have

$$H = \sum_{i=1}^n \omega_i d_i^\dagger d_i + \frac{1}{2} \sum_{i=1}^n \omega_i - \frac{1}{2}\text{tr}(\alpha), \quad (2.156)$$

where, as shown in Eq. (2.151), the d_i and d_i^\dagger ($i = 1, 2, \dots, n$) are the new annihilation and creation operators for the bosons. Equation (2.156) shows that a quadratic Hamiltonian of bosons can be BV diagonalized if its dynamic matrix is physically diagonalizable. ■

So far, we have found that the Heisenberg equation of motion is a natural generator of the normal BV transformation. This transformation can react on the Hamiltonian itself and brings it into a diagonalized form automatically. That is just what we expected.

Corollary 28 *The quadratic Hamiltonian of bosons of Eq. (1.1) is BV diagonalizable if the coefficient submatrix γ vanishes identically, i.e., $\gamma = 0$.*

Proof. When $\gamma = 0$, the dynamic matrix of Eq. (2.4) reduces to

$$D = \begin{bmatrix} \alpha & 0 \\ 0 & -\tilde{\alpha} \end{bmatrix}. \quad (2.157)$$

Since α is Hermitian, the $\tilde{\alpha}$ is Hermitian, $\tilde{\alpha}^\dagger = \tilde{\alpha}$, too. As a result, $D = D^\dagger$. It implies that D is unitarily diagonalizable and all its eigenvalues are real when $\gamma = 0$. Of course, the dynamic matrix D is BV diagonalizable if $\gamma = 0$, which proves the corollary. ■

On one hand, the corollary 28 shows that some quadratic Hamiltonians of bosons are BV diagonalizable. On the other hand, the corollary 15 indicates that there are also some quadratic Hamiltonians of bosons that can not be BV diagonalized. What is simultaneously the necessary and sufficient condition for the BV diagonalization? Evidently, the answer is just the combination of the two propositions 13 and 27

Theorem 29 *A quadratic Hamiltonian of bosons is BV diagonalizable if and only if its dynamic matrix is physically diagonalizable.*

This theorem is obviously consistent with our physical intuition: A system will behavior as a collective of quasi-particles if and only if there exists a complete set of linearly independent normal modes of motion in the system.

In particular, it converts the BV diagonalization into the eigenvalue problem of the dynamic matrix, whose theory is very clear and simple mathematically, and familiar to all of us. Therefore, this theorem makes it easy for us to find BV transformation and realize BV diagonalization.

Now, let us return to the example 5. If $|\alpha| < |\gamma|$, the dynamic matrix has two imaginary eigenvalues; the Hamiltonian is not BV diagonalizable. If $|\alpha| = |\gamma|$, the dynamic matrix is itself not diagonalizable; the Hamiltonian is not BV diagonalizable. If $|\alpha| > |\gamma|$, the dynamic matrix has two real eigenvalues, it is hence physically diagonalizable, therefore, the Hamiltonian is BV diagonalizable. To sum up, the Hamiltonian is BV diagonalizable only when $|\alpha| > |\gamma|$.

Further, let us find out the normal derivative BV transformation for the example 5 in the case of $|\alpha| > |\gamma|$.

Set

$$\omega = \sqrt{\alpha^2 - |\gamma|^2}. \quad (2.158)$$

The normalized eigenvector for ω can be obtained from Eq. (2.27),

$$v(\omega) = \begin{cases} \frac{1}{\sqrt{2\omega(\alpha-\omega)}} \begin{bmatrix} \gamma \\ \omega - \alpha \end{bmatrix}, & \alpha > 0 \\ \frac{1}{\sqrt{2\omega(\omega-\alpha)}} \begin{bmatrix} \gamma \\ \omega - \alpha \end{bmatrix}, & \alpha < 0, \end{cases} \quad (2.159)$$

with the norm being

$$v^*(\omega) I_- v(\omega) = \begin{cases} 1, & \alpha > 0 \\ -1, & \alpha < 0. \end{cases} \quad (2.160)$$

According to Eq. (2.143), the normal BV matrix is

$$T_n = \begin{cases} [v(\omega), v(-\omega)], & \alpha > 0 \\ [v(-\omega), v(\omega)], & \alpha < 0, \end{cases} \quad (2.161)$$

where the normalized eigenvector for $-\omega$ can be given according to the convention of Eq. (2.58). In detail, it reads,

$$T_n = \begin{cases} \frac{1}{\sqrt{2\omega(\alpha-\omega)}} \begin{bmatrix} \gamma & \omega - \alpha \\ \omega - \alpha & \gamma^* \end{bmatrix}, & \alpha > 0 \\ \frac{1}{\sqrt{2\omega(\omega-\alpha)}} \begin{bmatrix} \gamma & \omega - \alpha \\ \gamma^* & \omega - \alpha \end{bmatrix}, & \alpha < 0. \end{cases} \quad (2.162)$$

The following results can be readily verified,

$$T_n^\dagger I_- T_n = I_-, \quad (2.163)$$

$$T_n^{-1} D T_n = \begin{cases} \text{diag}(\omega, -\omega), & \alpha > 0 \\ \text{diag}(-\omega, \omega), & \alpha < 0, \end{cases} \quad (2.164)$$

$$T_n^\dagger M T_n = \begin{cases} \text{diag}(\omega, \omega), & \alpha > 0 \\ \text{diag}(-\omega, -\omega), & \alpha < 0, \end{cases} \quad (2.165)$$

$$H = \begin{cases} \omega d^\dagger d + \frac{1}{2}\omega - \frac{1}{2}\alpha, & \alpha > 0 \\ -\omega d^\dagger d - \frac{1}{2}\omega - \frac{1}{2}\alpha, & \alpha < 0, \end{cases} \quad (2.166)$$

where

$$[d, d^\dagger] = 1. \quad (2.167)$$

In this example, the eigenvalues are not degenerate. Let us look at a degenerate case.

Example 30

$$H = \alpha(c_1^\dagger c_1 + c_2^\dagger c_2) + \gamma c_1^\dagger c_2^\dagger + \gamma^* c_1 c_2. \quad (2.168)$$

Solution 31 The dynamic matrix D is a 4×4 matrix,

$$D = \begin{bmatrix} \alpha & 0 & 0 & \gamma \\ 0 & \alpha & \gamma & 0 \\ 0 & -\gamma^* & -\alpha & 0 \\ -\gamma^* & 0 & 0 & -\alpha \end{bmatrix}. \quad (2.169)$$

The characteristic equation is

$$(\omega^2 - \alpha^2 + |\gamma|^2)^2 = 0. \quad (2.170)$$

The solutions are

$$\omega = \begin{cases} \pm \sqrt{\alpha^2 - |\gamma|^2}, & |\alpha| > |\gamma| \\ 0, & |\alpha| = |\gamma| \\ \pm i \sqrt{|\gamma|^2 - \alpha^2}, & |\alpha| < |\gamma|. \end{cases} \quad (2.171)$$

If $|\alpha| < |\gamma|$, the dynamic matrix has imaginary eigenvalues. Of course, the Hamiltonian is not BV diagonalizable.

It can be readily verified that D has only two linearly independent eigenvectors if $|\alpha| = |\gamma|$,

$$v_1(0) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \mp e^{-i\theta} \end{bmatrix}, \quad v_2(0) = \begin{bmatrix} 0 \\ \mp e^{i\theta} \\ 1 \\ 0 \end{bmatrix}, \quad (2.172)$$

where $\theta = \arg(\gamma)$, and \mp correspond to $\alpha = \pm |\gamma|$ respectively. It means that D is itself not diagonalizable. Needless to say, the Hamiltonian is not BV diagonalizable when $|\alpha| = |\gamma|$.

If $|\alpha| > |\gamma|$, there are a pair of real eigenvalues, i.e., $(\omega, -\omega)$ where

$$\omega = \sqrt{\alpha^2 - |\gamma|^2}. \quad (2.173)$$

It is found that ω has two linearly independent eigenvectors, they can be chosen and orthonormalized as follows,

$$v_1(\omega) = \begin{cases} \begin{bmatrix} \frac{\gamma}{\sqrt{2\omega(\alpha-\omega)}} \\ 0 \\ 0 \\ \frac{\omega-\alpha}{\sqrt{2\omega(\alpha-\omega)}} \end{bmatrix}, & \alpha > 0 \\ \begin{bmatrix} \frac{\gamma}{\sqrt{2\omega(\omega-\alpha)}} \\ 0 \\ 0 \\ \frac{\omega-\alpha}{\sqrt{2\omega(\omega-\alpha)}} \end{bmatrix}, & \alpha < 0, \end{cases} \quad (2.174)$$

$$v_2(\omega) = \begin{cases} \begin{bmatrix} 0 \\ \frac{\omega+\alpha}{\sqrt{2\omega(\omega+\alpha)}} \\ -\gamma^* \\ \frac{\gamma}{\sqrt{2\omega(\omega+\alpha)}} \end{bmatrix}, & \alpha > 0 \\ \begin{bmatrix} 0 \\ \frac{\omega+\alpha}{\sqrt{-2\omega(\omega+\alpha)}} \\ \gamma^* \\ \frac{\gamma}{\sqrt{-2\omega(\omega+\alpha)}} \end{bmatrix}, & \alpha < 0, \end{cases} \quad (2.175)$$

their norms are

$$v_1^*(\omega) I_- v_1(\omega) = \begin{cases} 1, & \alpha > 0 \\ -1, & \alpha < 0, \end{cases} \quad (2.176)$$

$$v_2^*(\omega) I_- v_2(\omega) = \begin{cases} 1, & \alpha > 0 \\ -1, & \alpha < 0. \end{cases} \quad (2.177)$$

The orthonormal eigenvectors for $-\omega$, $v_1(-\omega)$ and $v_2(-\omega)$, can be obtained according to the convention of Eq. (2.58).

Evidently, each eigenvalue is two-fold degenerate. The four eigenvectors, $v_1(\omega)$, $v_2(\omega)$, $v_1(-\omega)$ and $v_2(-\omega)$, form an orthonormal basis for \mathbb{C}^4 , i.e.,

$$T_n^\dagger I_- T_n = I_-, \quad (2.178)$$

where T_n is the normal derivative BV matrix,

$$T_n = \begin{cases} [v_1(\omega), v_2(\omega), v_1(-\omega), v_2(-\omega)], & \alpha > 0 \\ [v_1(-\omega), v_2(-\omega), v_1(\omega), v_2(\omega)], & \alpha < 0. \end{cases} \quad (2.179)$$

Those facts demonstrate that the dynamic matrix D is physically diagonalizable if $|\alpha| > |\gamma|$.

To sum up, the Hamiltonian of Eq. (2.168) is BV diagonalizable only when $|\alpha| > |\gamma|$.

When $|\alpha| > |\gamma|$, the following results can be verified straightforwardly,

$$T_n^- D T_n = \begin{cases} \text{diag}(\omega, \omega, -\omega, -\omega), & \alpha > 0 \\ \text{diag}(-\omega, -\omega, \omega, \omega), & \alpha < 0, \end{cases}, \quad (2.180)$$

$$T_n^\dagger M T_n = \begin{cases} \text{diag}(\omega, \omega, \omega, \omega), & \alpha > 0 \\ \text{diag}(-\omega, -\omega, -\omega, -\omega), & \alpha < 0, \end{cases} \quad (2.181)$$

$$H = \begin{cases} \omega(d_1^\dagger d_1 + d_2^\dagger d_2) + \omega - \alpha, & \alpha > 0 \\ -\omega(d_1^\dagger d_1 + d_2^\dagger d_2) - \omega - \alpha, & \alpha < 0. \end{cases} \quad (2.182)$$

where

$$[d_i, d_j^\dagger] = \delta_{ij}, \quad [d_i, d_j] = 0, \quad [d_i^\dagger, d_j^\dagger] = 0. \quad (2.183)$$

The two examples above do not have zero eigenvalue. The following is an example with zero eigenvalue.

Example 32

$$H = c_1^\dagger c_1 + c_2^\dagger c_2 - c_1^\dagger c_2 - c_2^\dagger c_1. \quad (2.184)$$

Solution 33 The dynamic matrix D is

$$D = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}. \quad (2.185)$$

It has three eigenvalues,

$$\omega = 0, 2, -2. \quad (2.186)$$

For the pair of the nonzero eigenvalues, $(2, -2)$, they are nondegenerate,

$$v(2) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}, \quad v(-2) = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix}, \quad (2.187)$$

where the convention of Eq. (2.58) has been used. Their norms are

$$v^\dagger(2)I_-v(2) = 1, \quad v^\dagger(-2)I_-v(-2) = -1. \quad (2.188)$$

For the zero eigenvalue, it is two-fold degenerate, the orthonormal basis for this eigenspace can be chosen as follows,

$$v(0) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad v(-0) = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \quad (2.189)$$

where the convention of Eq. (2.59) has been used. Their norms are

$$v^\dagger(0)I_-v(0) = 1, \quad v^\dagger(-0)I_-v(-0) = -1. \quad (2.190)$$

Therefore, the dynamic matrix D has three real eigenvalues and four linearly independent eigenvectors, so it is physically diagonalizable. According to the theorem 29 the Hamiltonian of Eq. (2.184) is BV diagonalizable.

According to Eq. (2.143), the normal derivative BV matrix T_n has the form,

$$T_n = [v(2), v(0), v(-2), v(-0)]. \quad (2.191)$$

It is easy to show that

$$T_n^\dagger I_- T_n = I_-, \quad (2.192)$$

$$T_n^- D T_n = \text{diag}(2, 0, -2, -0), \quad (2.193)$$

$$T_n^\dagger M T_n = \text{diag}(2, 0, 2, 0), \quad (2.194)$$

$$H = 2d_1^\dagger d_1 + 0d_2^\dagger d_2, \quad (2.195)$$

where

$$[d_i, d_j^\dagger] = \delta_{ij}, \quad [d_i, d_j] = 0, \quad [d_i^\dagger, d_j^\dagger] = 0. \quad (2.196)$$

For this example, the eigenspace of the zero eigenvalue is two dimensional, it is the smallest and nondegenerate. Finally, we give an example whose eigenspace of the zero eigenvalue is more than two dimensional.

Example 34

$$H = 2c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3 + \sqrt{2}(c_1^\dagger c_2 + c_2^\dagger c_1) + \sqrt{2}(c_1^\dagger c_3 + c_3^\dagger c_1) + (c_2^\dagger c_3 + c_3^\dagger c_2). \quad (2.197)$$

Solution 35 The dynamic matrix D is

$$D = \begin{bmatrix} 2 & \sqrt{2} & \sqrt{2} & 0 & 0 & 0 \\ \sqrt{2} & 1 & 1 & 0 & 0 & 0 \\ \sqrt{2} & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & -\sqrt{2} & -\sqrt{2} \\ 0 & 0 & 0 & -\sqrt{2} & -1 & -1 \\ 0 & 0 & 0 & -\sqrt{2} & -1 & -1 \end{bmatrix}. \quad (2.198)$$

There are three eigenvalues,

$$\omega = 0, 4, -4. \quad (2.199)$$

For the pair of the nonzero eigenvalues, $(4, -4)$, they are nondegenerate,

$$v(4) = \begin{bmatrix} \frac{\sqrt{2}}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad v(-4) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{\sqrt{2}}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, \quad (2.200)$$

with the norms as follows

$$v^\dagger(4)I_-v(4) = 1, \quad v^\dagger(-4)I_-v(-4) = -1. \quad (2.201)$$

For the zero eigenvalue, it is four-fold degenerate, the orthonormal basis for the eigenspace can be chosen as follows,

$$v_1(0) = \begin{bmatrix} \sqrt{\frac{1}{3}} \\ -\sqrt{\frac{2}{3}} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad v_2(0) = \begin{bmatrix} \frac{1}{\sqrt{6}} \\ \frac{1}{2\sqrt{3}} \\ -\frac{\sqrt{3}}{2} \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad (2.202)$$

$$v_1(-0) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \sqrt{\frac{1}{3}} \\ -\sqrt{\frac{2}{3}} \\ 0 \end{bmatrix}, \quad v_2(-0) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{6}} \\ \frac{1}{2\sqrt{3}} \\ -\frac{\sqrt{3}}{2} \end{bmatrix}, \quad (2.203)$$

their norms are

$$v_1^\dagger(0)I_-v_1(0) = 1, \quad (2.204)$$

$$v_2^\dagger(0)I_-v_2(0) = 1, \quad (2.205)$$

$$v_1^\dagger(-0)I_-v_1(-0) = -1, \quad (2.206)$$

$$v_2^\dagger(-0)I_-v_2(-0) = -1. \quad (2.207)$$

In a word, the dynamic matrix D has three real eigenvalues and six linearly independent eigenvectors. The Hamiltonian is BV diagonalizable.

The normal derivative BV matrix T_n can be constructed according to Eq. (2.143),

$$T_n = [v(4), v_1(0), v_2(0), v(-4), v_1(-0), v_2(-0)]. \quad (2.208)$$

It can be verified straightforwardly that

$$T_n^\dagger I_- T_n = I_-, \quad (2.209)$$

$$T_n^- D T_n = \text{diag}(4, 0, 0, -4, -0, -0), \quad (2.210)$$

$$T_n^\dagger M T_n = \text{diag}(4, 0, 0, 4, 0, 0), \quad (2.211)$$

$$H = 4d_1^\dagger d_1 + 0d_2^\dagger d_2 + 0d_3^\dagger d_3, \quad (2.212)$$

where

$$[d_i, d_j^\dagger] = \delta_{ij}, \quad [d_i, d_j] = 0, \quad [d_i^\dagger, d_j^\dagger] = 0. \quad (2.213)$$

D. Uniqueness

The theorem 29 asserts that a quadratic Hamiltonian of bosons can be BV diagonalized if its dynamic matrix is physically diagonalizable. Apparently, there may exist many different BV transformations for a certain Hamiltonian that can all realize the diagonalization. This occurs especially when some eigenvalues of the dynamic matrix are degenerate because there are much orthonormal bases for the eigenspace of a degenerate eigenvalue, and accordingly there are much various choices for the column vectors of the normal derivative BV matrix. For instance, it is easy to show that, when $\alpha > 0$, the following two vectors,

$$v_1(\omega) = \begin{bmatrix} \frac{\gamma}{2\sqrt{2\omega(\alpha-\omega)}} \\ \frac{\omega+\alpha}{2\sqrt{2\omega(\omega+\alpha)}} \\ -\frac{\gamma^*}{2\sqrt{2\omega(\omega+\alpha)}} \\ \frac{\omega-\alpha}{2\sqrt{2\omega(\alpha-\omega)}} \\ \frac{\gamma}{2\sqrt{2\omega(\alpha-\omega)}} \\ \frac{\omega+\alpha}{2\sqrt{2\omega(\omega+\alpha)}} \\ -\frac{\gamma^*}{2\sqrt{2\omega(\omega+\alpha)}} \\ \frac{\omega-\alpha}{2\sqrt{2\omega(\alpha-\omega)}} \end{bmatrix}, \quad (2.214)$$

$$v_2(\omega) = \begin{bmatrix} \frac{\gamma}{2\sqrt{2\omega(\alpha-\omega)}} \\ \frac{\omega+\alpha}{2\sqrt{2\omega(\omega+\alpha)}} \\ -\frac{\gamma^*}{2\sqrt{2\omega(\omega+\alpha)}} \\ \frac{\omega-\alpha}{2\sqrt{2\omega(\alpha-\omega)}} \\ \frac{\gamma}{2\sqrt{2\omega(\alpha-\omega)}} \\ \frac{\omega+\alpha}{2\sqrt{2\omega(\omega+\alpha)}} \\ -\frac{\gamma^*}{2\sqrt{2\omega(\omega+\alpha)}} \\ \frac{\omega-\alpha}{2\sqrt{2\omega(\alpha-\omega)}} \end{bmatrix}, \quad (2.215)$$

also constitutes an orthonormal basis for the eigenspace of ω of the example 30. Substituting them into the BV matrix, one will find that this normal derivative BV matrix can diagonalize the Hamiltonian as the T_n given in Eq. (2.179). Even if all the eigenvalues are nondegenerate, the eigenvectors can choose their phases freely. In sum, the normal derivative BV transformation can never be unique.

That poses a natural question: Can different normal BV transformations give rise to different diagonalized forms for a certain quadratic Hamiltonian? Or, put it another way, is the diagonalized form of a quadratic Hamiltonian unique? The answer will be yes if one does not care the order of the quadratic terms present in a diagonal Hamiltonian.

Theorem 36 *If a quadratic Hamiltonian of bosons is BV diagonalizable, its diagonalized form will be unique up to a permutation of the quadratic terms.*

Proof. Suppose that there are two diagonalized forms for the Hamiltonian of Eq. (1.1). According to Eq. (2.156), they can be written as

$$H_1 = \sum_{i=1}^n \omega_i d_i^\dagger d_i + \frac{1}{2} \sum_{i=1}^n \omega_i - \frac{1}{2} \text{tr}(\alpha), \quad (2.216)$$

$$H_2 = \sum_{i=1}^n \omega'_i d_i^\dagger d_i + \frac{1}{2} \sum_{i=1}^n \omega'_i - \frac{1}{2} \text{tr}(\alpha). \quad (2.217)$$

We shall prove that the set $\{\omega_1, \omega_2, \dots, \omega_n\}$ is identical to the set $\{\omega'_1, \omega'_2, \dots, \omega'_n\}$. Here, if $\omega_i = \omega'_j$, they are both counted up to the same multiplicity.

According to the lemma 12 the dynamic matrices of H_1 and H_2 are both similar to that of the Hamiltonian H of Eq. (1.1),

$$T_{n1}^{-1} D T_{n1} = D_1, \quad (2.218)$$

$$T_{n2}^{-1} D T_{n2} = D_2, \quad (2.219)$$

where D_1 , D_2 , and D are, respectively, the dynamic matrices for H_1 , H_2 and H , and T_{n1} and T_{n2} are both the normal derivative BV matrices,

$$T_{n1}^\dagger I_- T_{n1} = I_-, \quad (2.220)$$

$$T_{n2}^\dagger I_- T_{n2} = I_-. \quad (2.221)$$

Thereby, D_1 and D_2 are similar to each other,

$$(T_{n1}^{-1} T_{n2})^{-1} D_1 (T_{n1}^{-1} T_{n2}) = D_2. \quad (2.222)$$

Observe

$$D_1 = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n), \quad (2.223)$$

$$D_2 = \text{diag}(\omega'_1, \dots, \omega'_n, -\omega'_1, \dots, -\omega'_n). \quad (2.224)$$

We have

$$\{\omega_1, \omega_2, \dots, \omega_n, -\omega_1, -\omega_2, \dots, -\omega_n\} = \{\omega'_1, \omega'_2, \dots, \omega'_n, -\omega'_1, -\omega'_2, \dots, -\omega'_n\}, \quad (2.225)$$

where each eigenenergy is counted up to its multiplicity. As a consequence,

$$\omega_1 \in \{\omega'_1, \omega'_2, \dots, \omega'_n\}, \quad (2.226)$$

or

$$\omega_1 \in \{-\omega'_1, -\omega'_2, \dots, -\omega'_n\}. \quad (2.227)$$

If

$$\omega_1 \in \{-\omega'_1, -\omega'_2, \dots, -\omega'_n\}, \quad (2.228)$$

let ω_1 be $-\omega'_1$, i.e., $\omega_1 = -\omega'_1$, without loss of generality. Thus, one obtains from Eq. (2.222)

$$v(\omega_1) = T_{n1}^{-1} T_{n2} v(-\omega'_1). \quad (2.229)$$

This gives rise to

$$v^\dagger(\omega_1) I_- v(\omega_1) = v^\dagger(-\omega'_1) I_- v(-\omega'_1), \quad (2.230)$$

where Eqs. (2.220) and (2.221) have been used. However,

$$v^\dagger(\omega_1) I_- v(\omega_1) = 1, \quad (2.231)$$

$$v^\dagger(-\omega'_1) I_- v(-\omega'_1) = -1. \quad (2.232)$$

Obviously, they contradict the equation (2.230). Therefore,

$$\omega_1 \notin \{-\omega'_1, -\omega'_2, \dots, -\omega'_n\}, \quad (2.233)$$

it must belong to the set $\{\omega'_1, \omega'_2, \dots, \omega'_n\}$, i.e.,

$$\omega_1 \in \{\omega'_1, \omega'_2, \dots, \omega'_n\}. \quad (2.234)$$

This implies that

$$\{\omega_1, \omega_2, \dots, \omega_n\} \subset \{\omega'_1, \omega'_2, \dots, \omega'_n\}. \quad (2.235)$$

For the same reason,

$$\{\omega'_1, \omega'_2, \dots, \omega'_n\} \subset \{\omega_1, \omega_2, \dots, \omega_n\}. \quad (2.236)$$

So

$$\{\omega_1, \omega_2, \dots, \omega_n\} = \{\omega'_1, \omega'_2, \dots, \omega'_n\}. \quad (2.237)$$

This means that H_1 and H_2 are identical up to a permutation of the members of the set $\{\omega_1, \omega_2, \dots, \omega_n\}$. In other words, the diagonalized form of a quadratic Hamiltonian is unique up to a permutation of the quadratic terms. ■

Up to now, the BV diagonalization is always meant to diagonalize a Hamiltonian with respect to the normal bosons, which fulfill the standard commutation rules.

Sometimes, e.g., in quantum electrodynamics, the so-called time-polarized bosons are needed, they satisfy the abnormal commutation relations,

$$[b_i, b_j^\dagger] = -\delta_{ij}, \quad [b_i, b_j] = 0, \quad [b_i^\dagger, b_j^\dagger] = 0. \quad (2.238)$$

If one exchanges the roles of b_i and b_i^\dagger , and interprets them respectively as a creator and annihilator, i.e.,

$$d_i = b_i^\dagger, \quad d_i^\dagger = b_i, \quad (2.239)$$

he has

$$[d_i, d_j^\dagger] = \delta_{ij}, \quad [d_i, d_j] = 0, \quad [d_i^\dagger, d_j^\dagger] = 0. \quad (2.240)$$

That is to say, the time-polarized bosons can always be transformed into the normal bosons, and vice versa. Hence, a Hamiltonian can also be diagonalized with respect to the time-polarized bosons. Accordingly, Eq. (2.156) will become

$$H = \sum_{i=1}^n -\omega_i (-b_i^\dagger b_i) - \frac{1}{2} \sum_{i=1}^n \omega_i - \frac{1}{2} \text{tr}(\alpha), \quad (2.241)$$

where $n_i = -b_i^\dagger b_i$ are the particle-number operators for the time-polarized bosons. Actually, a Hamiltonian can be diagonalized with respect to the normal bosons, or the time-polarized bosons, or the mixture of both the normal and time-polarized bosons as you wish, e.g.,

$$H = \sum_{i=1}^m \omega_i d_i^\dagger d_i + \sum_{i=m+1}^n \omega_i b_i^\dagger b_i + \frac{1}{2} \sum_{i=1}^m \omega_i - \frac{1}{2} \sum_{i=m+1}^n \omega_i - \frac{1}{2} \text{tr}(\alpha), \quad (2.242)$$

where $0 \leq m \leq n$. This fact will be used in Sec. VIII B. Anyway, the diagonalization is unique with respect to the normal bosons. The normal bosons will be used, by default, for the diagonalization of the Bose system unless otherwise specified.

By the way, we would like to note that the conclusions up to now are also valid for the Bose system whose Hamiltonian is represented quadratically with regard to the time-polarized bosons, or the mixture of both the normal and time-polarized bosons. That is because, as mentioned above, all the time-polarized bosons can be transformed into the normal bosons.

To conclude, a quadratic Hamiltonian of bosons has BV diagonalization if and only if its dynamic matrix is physically diagonalizable. If the diagonalization exists, its form is unique.

Thus far, a whole theory of diagonalization has been achieved for the Bose system.

III. DIAGONALIZATION THEORY OF FERMI SYSTEMS

In this section, we turn to the Fermi case. We shall study first the existence and then the uniqueness of the BV diagonalization for the Fermi system.

A. Existence

The Heisenberg equation for the fermionic field ψ can be derived from Eq. (1.1),

$$i \frac{d}{dt} \psi = D\psi, \quad (3.1)$$

where D is the dynamic matrix for the Fermi system,

$$D = \begin{bmatrix} \alpha & \gamma \\ \gamma^\dagger & -\tilde{\alpha} \end{bmatrix}. \quad (3.2)$$

In contrast to the Bose system where the dynamic matrix is distinct from the coefficient matrix, the dynamic matrix D is now identical to the coefficient matrix M ,

$$M = \begin{bmatrix} \alpha & \gamma \\ \gamma^\dagger & -\tilde{\alpha} \end{bmatrix}. \quad (3.3)$$

This demonstrates that the coefficient matrix M will control the dynamic behavior of the system, just as the dynamic matrix D . That is the radical difference between the Fermi and Bose systems. For the latter, as we know, the coefficient matrix does not control the dynamic behavior of the system. Now that $D = M$ and M is Hermitian, D is Hermitian, too. That is another feature of the Fermi system, which will bring us much convenience.

Similar to Eq. (2.6), the relation between D and M can be formally written as

$$D = I_+ M. \quad (3.4)$$

This relation is useful in the diagonalization of the Fermi system.

As before, let us consider the eigenvalue problem,

$$\omega \psi = D\psi. \quad (3.5)$$

Lemma 37 *For a quadratic Hamiltonian of fermions, its dynamic matrix is always BV diagonalizable.*

Proof. As mentioned above, the dynamic matrix for a Fermi system is Hermitian. It is well known that a Hermitian matrix is diagonalizable, and all its eigenvalues are real. Therefore, the dynamic matrix for a Fermi system is always BV diagonalizable. ■

This property is basically different from the Bose system. There, the dynamic matrix is not always diagonalizable. Needless to say, it is not always BV diagonalizable.

As $D = M$ and both are Hermitian, they can be diagonalized by an exactly identical unitary transformation. Mathematically, a unitary transformation is always

a similar transformation, the diagonalization manner of D is not inharmonious with that of M any longer. The problem present in the Bose system disappears spontaneously in the Fermi system.

Analogous to the Bose system, one can easily show that the lemmas 3, 4, 10, 11, and 12 are all valid for the Fermi system. Since the dynamic matrix is always BV diagonalizable now, the necessary condition for the BV diagonalization will hold automatically for a Fermi system. That guarantees further that the lemmas 16, 17 and 19 also hold for the Fermi system. All those eight lemmas stem from the Hermiticity of the Hamiltonian, and are irrespective of the statistics and metric of the system.

By introducing a sesquilinear form with I_+ and substituting I_- with I_+ , the lemmas 21 and 22 are both valid for the Fermi system, the only difference lies in that the norm with respect to I_+ is positive definite whereas the norm with respect to I_- is indefinite. The lemma 23 also holds for the Fermi case, but its proof needs quite a lot of modification, which we give below.

Proof. The eigenspace V_0 of zero eigenvalue is even dimensional, let the dimension be $2m$ ($m \in \mathbb{N}$). According to the lemma 17 there always exists a basis for V_0 that satisfies the requirement of Eq. (2.59), i.e.,

$$v_{m+l}(0) = \Sigma_x v_l^*(0), \quad l = 1, 2, \dots, m, \quad (3.6)$$

When $m = 1$, $\dim(V_0) = 2$, there are two basis vectors, i.e., $v_1(0)$ and $v_2(0)$, they are linearly independent.

First of all, we would make $v_1(0)$ normalized,

$$v_1^\dagger(0) I_+ v_1(0) = 1. \quad (3.7)$$

And then we consider $v_2(0)$. In fact, it is also normalized,

$$v_2^\dagger(0) I_+ v_2(0) = 1, \quad (3.8)$$

that is because

$$v_2(0) = \Sigma_x v_1^*(0). \quad (3.9)$$

There are two possible cases for $v_2(0)$: (1) It is orthogonal to $v_1(0)$. (2) It is not orthogonal to $v_1(0)$.

If $v_2(0) \perp v_1(0)$, i.e.,

$$v_1^\dagger(0) I_+ v_2(0) = 0, \quad (3.10)$$

we have

$$v_1^\dagger(0) I_+ v_1(0) = 1, \quad (3.11)$$

$$v_2^\dagger(0) I_+ v_2(0) = 1, \quad (3.12)$$

$$v_1^\dagger(0) I_+ v_2(0) = 0. \quad (3.13)$$

and

$$v_2(0) = \Sigma_x v_1^*(0), \quad (3.14)$$

So the basis $\{v_1(0), v_2(0)\}$ is itself orthonormal and satisfies the requirement of Eq. (2.59). In other words, the lemma holds if $v_2(0) \perp v_1(0)$.

If $v_2(0)$ is not orthogonal to $v_1(0)$, i.e.,

$$v_1^\dagger(0)I_+v_2(0) \neq 0, \quad (3.15)$$

we shall introduce two vectors $w_1(0)$ and $w_2(0)$ as follows,

$$w_1(0) = av_1(0) + bv_2(0), \quad (3.16)$$

$$w_2(0) = \Sigma_x w_1^*(0). \quad (3.17)$$

Here $a \in \mathbb{C}$ and $b \in \mathbb{C}$ are two coefficients, they will be determined by the orthonormal conditions,

$$w_1^\dagger(0)I_+w_1(0) = 1, \quad (3.18)$$

$$w_1^\dagger(0)I_+w_2(0) = 0. \quad (3.19)$$

Equations (3.16) and (3.17) show that both $w_1(0)$ and $w_2(0)$ are linear combinations of $v_1(0)$ and $v_2(0)$. Consequently, $w_1(0)$ and $w_2(0)$ are also the eigenvectors of zero eigenvalue, i.e., $w_1(0) \in V_0$ and $w_2(0) \in V_0$.

Observe

$$v_1^\dagger(0)I_+v_2(0) = [\tilde{v}_1(0)I_+\Sigma_x v_1(0)]^*. \quad (3.20)$$

We can adjust the phase of $v_1(0)$ anew so that

$$v_1^\dagger(0)I_+v_2(0) > 0. \quad (3.21)$$

By use of Cauchy inequality, we obtain

$$v_1^\dagger(0)I_+v_2(0) < \sqrt{v_1^\dagger(0)I_+v_1(0)}\sqrt{v_2^\dagger(0)I_+v_2(0)}, \quad (3.22)$$

where we have used the fact that $v_1(0)$ and $v_2(0)$ are linearly independent. Since

$$\sqrt{v_1^\dagger(0)I_+v_1(0)}\sqrt{v_2^\dagger(0)I_+v_2(0)} = 1, \quad (3.23)$$

we have

$$v_1^\dagger(0)I_+v_2(0) < 1. \quad (3.24)$$

In brief, we can always have

$$0 < v_1^\dagger(0)I_+v_2(0) < 1, \quad (3.25)$$

when $v_2(0)$ is not orthogonal to $v_1(0)$.

Under such choice, Eqs. (3.18) and (3.19) become

$$a^*a + b^*b + (a^*b + b^*a)v_1^\dagger(0)I_+v_2(0) = 1, \quad (3.26)$$

$$(a^*a^* + b^*b^*)v_1^\dagger(0)I_+v_2(0) + 2a^*b^* = 0. \quad (3.27)$$

It can be readily confirmed that there exists at least the following real solution for the coefficients a and b ,

$$a = \frac{1}{2\sqrt{1 + v_1^\dagger(0)I_+v_2(0)}} + \frac{1}{2\sqrt{1 - v_1^\dagger(0)I_+v_2(0)}}, \quad (3.28)$$

$$b = \frac{1}{2\sqrt{1 + v_1^\dagger(0)I_+v_2(0)}} - \frac{1}{2\sqrt{1 - v_1^\dagger(0)I_+v_2(0)}}. \quad (3.29)$$

With this solution, we have

$$w_1^\dagger(0)I_+w_1(0) = 1, \quad (3.30)$$

$$w_2^\dagger(0)I_+w_2(0) = 1, \quad (3.31)$$

$$w_1^\dagger(0)I_+w_2(0) = 0, \quad (3.32)$$

$$w_2(0) = \Sigma_x w_1^*(0). \quad (3.33)$$

That is to say, the set $\{w_1(0), w_2(0)\}$ will form an orthonormal basis for V_0 , and satisfy the requirement of Eq. (2.59). This implies that the lemma also holds if $v_2(0)$ is not orthogonal to $v_1(0)$.

To sum up, the lemma will always hold when $m = 1$.

Suppose that the lemma holds when $m = l$ ($l \in \mathbb{N}$). We consider then the case where $m = l + 1$. Obviously, it has a proper subspace W spanned by the linearly independent set $\{v_1(0), v_{l+2}(0)\}$, i.e.,

$$W = \text{span}(v_1(0), v_{l+2}(0)). \quad (3.34)$$

Taking notice of

$$v_{l+2}(0) = \Sigma_x v_1^*(0), \quad (3.35)$$

and following the same arguments as those for the case of $m = 1$, we can obtain an orthonormal basis for W ,

$$v_i^\dagger(0)I_-v_j(0) = -\lambda_i\delta_{ij}, \quad (3.36)$$

where $\lambda_i = \pm 1$ and $i, j = 1, l + 2$. It is evident that this basis satisfies the requirement of Eq. (2.59).

The rest steps of mathematical induction are simply similar to those for the Bose case. The convention of Eq. (2.59) can be kept by the modified Gram-Schmidt orthogonalization process. ■

The lemma 24 still holds for the Fermi system, with $\lambda_i \equiv 1$ for $i = 1, 2, \dots, 2n$.

Since all the eigenvectors are normalized to +1 now, one can not use the sign of the norm to stipulate an order within a mode pair. Here, we shall resort to the sign of the eigenvalue: The first eigenvalue in a pair is positive, and the second one negative; it is arbitrary if both the eigenvalues in a pair are equal to zero. Under such stipulation, the normal derivative BV transformation has the form,

$$\psi = T_n \varphi, \quad (3.37)$$

$$T_n = [v(\omega_1), v(\omega_2), \dots, v(\omega_n), v(-\omega_1), v(-\omega_2), \dots, v(-\omega_n)], \quad (3.38)$$

where

$$\omega_i \geq 0, \quad i = 1, 2, \dots, n. \quad (3.39)$$

That is to say, the left half of T_n is filled with the eigenvectors with nonnegative eigenvalues; the right half of T_n is filled with the eigenvectors with nonpositive eigenvalues.

With T_n ordered as above, the lemma 25 holds for the Fermi case,

$$T_n^\dagger I_+ T_n = I_+, \quad (3.40)$$

i.e., T_n is a member of the $U(2n)$ group 15. This lemma asserts that the new field is a standard fermionic field.

The lemma 26 must be modified as follows,

$$T_n^\dagger M T_n = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n). \quad (3.41)$$

That is because

$$\begin{aligned} T_n^\dagger M T_n &= T_n^\dagger I_+ D T_n \\ &= T_n^\dagger I_+ T_n T_n^{-1} D T_n \\ &= T_n^{-1} D T_n, \end{aligned} \quad (3.42)$$

where $T_n^\dagger I_+ T_n = I_+$ has been used.

At last, we arrive at the diagonalization theorem for the Fermi system.

Theorem 38 Any quadratic Hamiltonian of fermions is BV diagonalizable.

Apparently, the diagonalized form for the Hamiltonian is

$$H = \sum_{i=1}^n \omega_i d_i^\dagger d_i - \frac{1}{2} \sum_{i=1}^n \omega_i + \frac{1}{2} \text{tr}(\alpha), \quad (3.43)$$

where all the eigenenergies are nonnegative,

$$\omega_i \geq 0, \quad i = 1, 2, \dots, n. \quad (3.44)$$

Here, it is worth emphasizing that the BV diagonalization for a Fermi system is itself of unitary diagonalization, that is because T_n is, in fact, a unitary matrix, $T_n^\dagger T_n = I_+$.

All in all, the BV diagonalization for a quadratic Hamiltonian of fermions is much simpler than that for a quadratic Hamiltonian of bosons.

Example 39

$$H = \alpha(c_1^\dagger c_1 + c_2^\dagger c_2) + \gamma(c_1^\dagger c_2^\dagger - c_1 c_2). \quad (3.45)$$

Solution 40 The dynamic matrix D is

$$D = \begin{bmatrix} \alpha & 0 & 0 & \gamma \\ 0 & \alpha & -\gamma & 0 \\ 0 & -\gamma & -\alpha & 0 \\ \gamma & 0 & 0 & -\alpha \end{bmatrix}. \quad (3.46)$$

It has only a pair of eigenvalues, $(\omega, -\omega)$ where

$$\omega = \sqrt{\alpha^2 + \gamma^2}, \quad (3.47)$$

they are both two-fold degenerate. The normal BV matrix can be chosen as follows,

$$\begin{aligned} T_n &= [v_1(\omega), v_2(\omega), v_1(-\omega), v_2(-\omega)] \\ &= \frac{1}{\sqrt{(\omega - \alpha)^2 + \gamma^2}} \\ &\quad \times \begin{bmatrix} \gamma & 0 & 0 & \omega - \alpha \\ 0 & -\gamma & \omega - \alpha & 0 \\ 0 & \omega - \alpha & \gamma & 0 \\ \omega - \alpha & 0 & 0 & -\gamma \end{bmatrix}, \end{aligned} \quad (3.48)$$

where the convention of Eq. 2.58 has been used for $v_1(-\omega)$ and $v_2(-\omega)$. The diagonalized Hamiltonian has the form,

$$H = \omega(d_1^\dagger d_1 + d_2^\dagger d_2) - \omega + \alpha. \quad (3.49)$$

Example 41

$$H = \mu(c_1^\dagger c_2 + c_2^\dagger c_1) + \nu(c_1^\dagger c_2^\dagger - c_1 c_2), \quad (3.50)$$

where $\nu > 0$.

Solution 42 The dynamic matrix D is

$$D = \begin{bmatrix} 0 & \mu & 0 & \nu \\ \mu & 0 & -\nu & 0 \\ 0 & -\nu & 0 & -\mu \\ \nu & 0 & -\mu & 0 \end{bmatrix}. \quad (3.51)$$

There are two pairs of eigenvalues, $(\omega_1, -\omega_1)$ and $(\omega_2, -\omega_2)$ where

$$\omega_1 = \mu + \nu, \quad \omega_2 = \mu - \nu. \quad (3.52)$$

The eigenvectors $v(\omega_1)$ and $v(\omega_2)$ can be chosen as follows,

$$v(\omega_1) = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \\ -1 \\ 1 \end{bmatrix}, \quad v(\omega_2) = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}. \quad (3.53)$$

Correspondingly, $v(-\omega_1)$ and $v(-\omega_2)$ can be obtained from the convention of Eq. (2.58).

The normal BV matrix and the form of the diagonalized Hamiltonian are listed as follows.

1. If $\mu > \nu$,

$$T_n = [v(\omega_1), v(\omega_2), v(-\omega_1), v(-\omega_2)], \quad (3.54)$$

$$H = \omega_1 d_1^\dagger d_1 + \omega_2 d_2^\dagger d_2 - \frac{1}{2}(\omega_1 + \omega_2). \quad (3.55)$$

2. If $\mu < -\nu$,

$$T_n = [v(-\omega_1), v(-\omega_2), v(\omega_1), v(\omega_2)], \quad (3.56)$$

$$H = -\omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 + \frac{1}{2}(\omega_1 + \omega_2). \quad (3.57)$$

3. If $-\nu \leq \mu \leq \nu$,

$$T_n = [v(\omega_1), v(-\omega_2), v(-\omega_1), v(\omega_2)], \quad (3.58)$$

$$H = \omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 - \frac{1}{2}(\omega_1 - \omega_2). \quad (3.59)$$

B. Uniqueness

Following the same arguments as those for the Bose system, one can readily know that there exist much different BV transformations that can all realize BV diagonalization to the same Hamiltonian of fermions. Nevertheless, the diagonalized form will be unique up to a permutation of the quadratic terms.

Theorem 43 The diagonalized form for a quadratic Hamiltonian of fermions is unique up to a permutation of the quadratic terms.

Proof. Suppose that there are two diagonalized forms for the Hamiltonian of Eq. (1.1). According to Eq. (3.43), they can be written as

$$H_1 = \sum_{i=1}^n \omega_i d_i^\dagger d_i - \frac{1}{2} \sum_{i=1}^n \omega_i + \frac{1}{2} \text{tr}(\alpha), \quad (3.60)$$

$$H_2 = \sum_{i=1}^n \omega'_i d_i^\dagger d_i - \frac{1}{2} \sum_{i=1}^n \omega'_i + \frac{1}{2} \text{tr}(\alpha), \quad (3.61)$$

where

$$\omega_i \geq 0, \quad i = 1, 2, \dots, n, \quad (3.62)$$

$$\omega'_i \geq 0, \quad i = 1, 2, \dots, n. \quad (3.63)$$

Let D_1 and D_2 be the dynamic matrices for H_1 and H_2 , respectively. Obviously, they are both diagonal,

$$D_1 = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n), \quad (3.64)$$

$$D_2 = \text{diag}(\omega'_1, \dots, \omega'_n, -\omega'_1, \dots, -\omega'_n). \quad (3.65)$$

As D_1 and D_2 are similar to each other, one has

$$\{\omega_1, \omega_2, \dots, \omega_n, -\omega_1, -\omega_2, \dots, -\omega_n\} = \{\omega'_1, \omega'_2, \dots, \omega'_n, -\omega'_1, -\omega'_2, \dots, -\omega'_n\}. \quad (3.66)$$

Paying attention to Eqs. (3.62) and (3.63), he can further obtain

$$\{\omega_1, \omega_2, \dots, \omega_n\} = \{\omega'_1, \omega'_2, \dots, \omega'_n\}. \quad (3.67)$$

This demonstrates that the diagonalized form of a quadratic Hamiltonian is unique up to a permutation of the quadratic terms. ■

Since all the energies of quasiparticles are nonnegative in the Hamiltonian of Eq. (3.43), there will be no

quasiparticle in the ground state of the system, viz., the ground state is exactly the vacuum of quasiparticles. If one does not obey the stipulation given in Eqs. (3.37), (3.38), and (3.39), he can obtain other diagonalized forms for the Hamiltonian. Nevertheless, the ground states of the system will not be the vacuum of quasiparticles. For example, instead of Eqs. (3.37), (3.38), and (3.39), let us stipulate anew that

$$\psi = T_n \varphi, \quad (3.68)$$

$$T_n = [v(-\omega_1), v(-\omega_2), \dots, v(-\omega_n), v(\omega_1), v(\omega_2), \dots, v(\omega_n)], \quad (3.69)$$

where

$$\omega_i \geq 0, \quad i = 1, 2, \dots, n. \quad (3.70)$$

It is easy to show that the Hamiltonian has a new diagonalized form,

$$H = - \sum_{i=1}^n \omega_i d_i^\dagger d_i + \frac{1}{2} \sum_{i=1}^n \omega_i + \frac{1}{2} \text{tr}(\alpha). \quad (3.71)$$

Now, all the energies of quasiparticles are nonpositive, the ground state of the system will be the Fermi sea which is occupied fully by quasiparticles. Here, the elementary excitations of the system would be quasiholes rather than quasiparticles. Upon the particle-hole transformation,

$$f_i = d_i^\dagger, \quad f_i^\dagger = d_i, \quad i = 1, 2, \dots, n, \quad (3.72)$$

the new diagonalized form can be transformed into the old one,

$$H = \sum_{i=1}^n \omega_i f_i^\dagger f_i - \frac{1}{2} \sum_{i=1}^n \omega_i + \frac{1}{2} \text{tr}(\alpha). \quad (3.73)$$

and vice versa. Hence, both are essentially equivalent. Of course, you can also use the mixing picture if you like, e.g.,

$$H = \sum_{i=1}^m \omega_i f_i^\dagger f_i - \sum_{i=m+1}^n \omega_i d_i^\dagger d_i - \frac{1}{2} \sum_{i=1}^m \omega_i + \frac{1}{2} \sum_{i=m+1}^n \omega_i + \frac{1}{2} \text{tr}(\alpha), \quad (3.74)$$

where $0 < m < n$. The elementary excitations of the system include now both the quasiparticles and quasiholes. Usually, the hole and mixing pictures are less convenient than the particle picture. That is the reason why we stipulate the BV transformation as in Eqs. (3.37), (3.38), and (3.39). By default, the particle picture will be used for the diagonalization of the Fermi system unless otherwise specified. The diagonalization is unique in this picture.

To conclude, the BV diagonalization exists and is unique for every quadratic Hamiltonian of fermions.

IV. APPLICATION TO BOSE SYSTEMS

Now, we apply the diagonalization theory of bosons to real systems. We shall concentrate ourselves on the two typical Hamiltonians: the normal Hamiltonian and the pairing Hamiltonian. As a matter of fact, they are the prototypes of many practical models, and represent almost all the problems which we encounter frequently in practice.

A. The normal Hamiltonian

First, let us consider the normal Hamiltonian,

$$H = \sum_{i,j=1}^n \alpha_{ij} c_i^\dagger c_j. \quad (4.1)$$

In this Hamiltonian, there are only the normal terms such as $c_i^\dagger c_j$. The abnormal terms, such as $c_i^\dagger c_j^\dagger$ and $c_i c_j$, disappear completely. This kind of Hamiltonian has been discussed in the corollary 28 according to it, such a Hamiltonian is always BV diagonalizable. In fact, the result can be strengthened further as follows.

Proposition 44 *The normal Hamiltonian of Eq. (4.1) can be BV diagonalized by the unitary transformation generated by the coefficient matrix α .*

Proof. The eigenvalue equation is

$$Dv(\omega) = \omega v(\omega), \quad (4.2)$$

where D is the dynamic matrix,

$$D = \begin{bmatrix} \alpha & 0 \\ 0 & -\tilde{\alpha} \end{bmatrix}. \quad (4.3)$$

Let the eigenvector $v(\omega)$ be

$$v(\omega) = \begin{bmatrix} x(\omega) \\ y(\omega) \end{bmatrix}, \quad (4.4)$$

where $x(\omega)$ and $y(\omega)$ are the two subvectors of size n . The eigenvalue equation of D becomes

$$\begin{bmatrix} \alpha & 0 \\ 0 & -\tilde{\alpha} \end{bmatrix} \begin{bmatrix} x(\omega) \\ y(\omega) \end{bmatrix} = \omega \begin{bmatrix} x(\omega) \\ y(\omega) \end{bmatrix}. \quad (4.5)$$

It reduces to

$$\alpha x(\omega) = \omega x(\omega), \quad (4.6)$$

$$\tilde{\alpha} y(\omega) = -\omega y(\omega). \quad (4.7)$$

The first equation is exactly the eigenvalue equation of the coefficient matrix α . Since α is Hermitian, it can be unitarily diagonalized,

$$U^\dagger \alpha U = \text{diag}(\omega_1, \omega_2, \dots, \omega_n), \quad (4.8)$$

where $\omega_i \in \mathbb{R}$ ($i = 1, 2, \dots, n$) are the eigenvalues of α , and U the unitary matrix which consists of the eigenvectors of α ,

$$U^\dagger U = U U^\dagger = I, \quad (4.9)$$

$$U = [x(\omega_1), x(\omega_2), \dots, x(\omega_n)], \quad (4.10)$$

the $x(\omega_i)$ standing for the eigenvector of the eigenvalue ω_i , respectively. Obviously, Eqs. (4.6) and (4.7) have the solutions,

$$v(\omega_i) = \begin{bmatrix} x(\omega_i) \\ 0 \end{bmatrix}, \quad i = 1, 2, \dots, n, \quad (4.11)$$

they are all the eigenvectors of Eq. (4.5), and orthonormalized as follows,

$$v^\dagger(\omega_i) I_- v(\omega_j) = \delta_{ij}, \quad i, j = 1, 2, \dots, n, \quad (4.12)$$

which comes directly from Eq. (4.9). According to the convention for $v(-\omega_i)$, the rest half of the eigenvectors of Eq. (4.5) is

$$v(-\omega_i) = \begin{bmatrix} 0 \\ x^*(\omega_i) \end{bmatrix}, \quad i = 1, 2, \dots, n, \quad (4.13)$$

they are also orthonormalized,

$$v^\dagger(-\omega_i) I_- v(-\omega_j) = -\delta_{ij}, \quad i, j = 1, 2, \dots, n. \quad (4.14)$$

In fact, $x^*(\omega_i)$ is exactly the eigenvector of $\tilde{\alpha}$,

$$\tilde{\alpha} x^*(\omega_i) = -(-\omega_i) x^*(\omega_i), \quad (4.15)$$

with the eigenvalue being $-\omega_i$. Substituting them into Eq. (2.143), we obtain the normal BV matrix,

$$T_n = \begin{bmatrix} U & 0 \\ 0 & U^* \end{bmatrix}. \quad (4.16)$$

It can be readily confirmed that

$$T_n^\dagger I_- T_n = I_-, \quad (4.17)$$

$$T_n^- D T_n = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n), \quad (4.18)$$

$$T_n^\dagger M T_n = \text{diag}(\omega_1, \dots, \omega_n, \omega_1, \dots, \omega_n), \quad (4.19)$$

$$H = \sum_{i=1}^n \omega_i d_i^\dagger d_i, \quad (4.20)$$

where

$$[d_i, d_j^\dagger] = \delta_{ij}, \quad [d_i, d_j] = 0, \quad [d_i^\dagger, d_j^\dagger] = 0. \quad (4.21)$$

Equation (4.16) shows that the normal BV matrix T_n for the diagonalization of the Hamiltonian of (4.1) can be constructed using the unitary matrix U generated by the coefficient matrix α . Put it another way, the quadratic Hamiltonian of Eq. (4.1) can be BV diagonalized by the unitary transformation generated by the coefficient matrix α . ■

The proposition shows that, to diagonalize the Hamiltonian of Eq. (4.1), one should first find the unitary matrix U from the coefficient matrix α , and then construct the normal BV matrix T_n according to Eq. (4.16).

The above procedure is feasible but somewhat redundant, it can be further simplified. As a matter of fact, the BV transformation corresponding to T_n can be reduced to a simple unitary transformation,

$$c = U d, \quad c^\dagger = d^\dagger U^\dagger, \quad (4.22)$$

which can be verified readily from the substitution of T_n into Eq. (2.142). As a consequence, we obtain

$$d \cdot d^\dagger = I, \quad d \cdot d = 0, \quad d^\dagger \cdot d^\dagger = 0, \quad (4.23)$$

where the standard relations,

$$c \cdot c^\dagger = I, \quad c \cdot c = 0, \quad c^\dagger \cdot c^\dagger = 0, \quad (4.24)$$

have been used. Through the unitary transformation of Eq. (4.22), the Hamiltonian of Eq. (4.1) can be straightforwardly diagonalized as follows,

$$H = c^\dagger \alpha c = d^\dagger U^\dagger \alpha U d = \sum_{i=1}^n \omega_i d_i^\dagger d_i. \quad (4.25)$$

It is the same as Eq. (4.20).

Physically, this simple version arises directly from the fact that the Heisenberg equation of the field c ,

$$i \frac{d}{dt} c = \alpha c, \quad (4.26)$$

does not couple with its Hermitian field c^\dagger . If a unitary transformation U for the field c is generated by this equation of motion,

$$c = U d, \quad (4.27)$$

an adjoint transformation U^\dagger will be yielded meanwhile for the Hermitian field c^\dagger ,

$$c^\dagger = d^\dagger U^\dagger, \quad (4.28)$$

by the equation of motion,

$$-i \frac{d}{dt} c^\dagger = c^\dagger \alpha. \quad (4.29)$$

As shown by Eqs. (4.8), (4.23) and (4.25), they diagonalize the Hamiltonian exactly. The simple version makes it much easier to diagonalize the Hamiltonian of Eq. (4.1). It is unnecessary to solve the eigenvalue problem of the dynamic matrix D and construct the BV matrix T_n , but sufficient for us to find out the unitary matrix U from the Hermitian matrix α . In short, it reduces the eigenvalue problem of D , which is of size $2n$, to the eigenvalue problem of α , which is of size n .

Example 45

$$H = \varepsilon_1 c_1^\dagger c_1 + \varepsilon_2 c_2^\dagger c_2 + \mu(c_1^\dagger c_2 + c_2^\dagger c_1). \quad (4.30)$$

Solution 46 The coefficient matrix is

$$\alpha = \begin{bmatrix} \varepsilon_1 & \mu \\ \mu & \varepsilon_2 \end{bmatrix}. \quad (4.31)$$

It has two eigenvalues,

$$\omega_1 = \frac{1}{2} \left[\varepsilon_1 + \varepsilon_2 + \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\mu^2} \right], \quad (4.32)$$

$$\omega_2 = \frac{1}{2} \left[\varepsilon_1 + \varepsilon_2 - \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4\mu^2} \right]. \quad (4.33)$$

The unitary matrix can be found as follows,

$$U = \begin{bmatrix} v(\omega_1), & v(\omega_2) \end{bmatrix} \\ = \frac{1}{\sqrt{(\omega_1 - \varepsilon_1)^2 + \mu^2}} \\ \times \begin{bmatrix} \mu & \omega_2 - \varepsilon_2 \\ \omega_1 - \varepsilon_1 & \mu \end{bmatrix}, \quad (4.34)$$

The diagonalized Hamiltonian is

$$H = \omega_1 d_1^\dagger d_1 + \omega_2 d_2^\dagger d_2. \quad (4.35)$$

Example 47

$$H = \varepsilon(c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3) \\ + \mu(c_1^\dagger c_2 + c_2^\dagger c_1 + c_2^\dagger c_3 + c_3^\dagger c_2). \quad (4.36)$$

Solution 48 The coefficient matrix is

$$\alpha = \begin{bmatrix} \varepsilon & \mu & 0 \\ \mu & \varepsilon & \mu \\ 0 & \mu & \varepsilon \end{bmatrix}. \quad (4.37)$$

It has three eigenvalues,

$$\omega_1 = \varepsilon, \quad \omega_2 = \varepsilon + \sqrt{2}\mu, \quad \omega_3 = \varepsilon - \sqrt{2}\mu. \quad (4.38)$$

The corresponding unitary matrix is

$$U = \begin{bmatrix} v(\omega_1), & v(\omega_2), & v(\omega_3) \end{bmatrix} \\ = \frac{1}{2} \begin{bmatrix} \sqrt{2} & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ -\sqrt{2} & 1 & 1 \end{bmatrix}, \quad (4.39)$$

It is easy to show that

$$H = \omega_1 d_1^\dagger d_1 + \omega_2 d_2^\dagger d_2 + \omega_3 d_3^\dagger d_3. \quad (4.40)$$

By the way, we note that the examples [32](#) and [34](#) can also be diagonalized using the present method.

B. The pairing Hamiltonian

As shown above, the Heisenberg equation and dynamic matrix are reducible for a normal Hamiltonian. There is another reducible case, which we are going to handle below.

Consider the so-called pairing Hamiltonian,

$$H = \sum_{i,j=1}^n (\alpha_{ij} a_i^\dagger a_j + \varepsilon_{ij} b_i^\dagger b_j + \gamma_{ij} a_i^\dagger b_j^\dagger + \gamma_{ji}^* a_i b_j), \quad (4.41)$$

where a_i (a_i^\dagger) and b_i (b_i^\dagger) are both the annihilation (creation) operators of bosons, and

$$\alpha^\dagger = \alpha, \quad \varepsilon^\dagger = \varepsilon, \quad \tilde{\gamma} = \gamma. \quad (4.42)$$

In this Hamiltonian, the abnormal terms, such as $a_i b_j$ and $a_i^\dagger b_j^\dagger$, appear exactly in pairs, each pair has one a -boson and one b -boson, there are totally n pairs between a - and b -bosons. Simply speaking, the particles of the system are formed perfectly into boson pairs.

According to Eq. [\(2.3\)](#), the Heisenberg equation for the Hamiltonian above has the variables of a_i , a_i^\dagger , b_i , and b_i^\dagger where $i = 1, 2, \dots, n$, hence it has the multiplicity of $4n$. It is easy to show that the Heisenberg equation can be reduced to the equations of motion of the variables of a_i and b_i^\dagger ($i = 1, 2, \dots, n$),

$$i \frac{d}{dt} a_i = \alpha_{ij} a_j + \gamma_{ij} b_j^\dagger, \quad (4.43)$$

$$i \frac{d}{dt} b_i^\dagger = -\varepsilon_{ji} b_j - \gamma_{ij}^* a_j. \quad (4.44)$$

Clearly, that is just of multiplicity $2n$. We shall utilize those $2n$ multiple equations straightforwardly to study the diagonalization problem of the Hamiltonian of Eq. [\(4.41\)](#). It is equivalent to but will be simpler than from the primitive equation [\(2.3\)](#) and the theorem [29](#), as has already been seen from the discussions on the normal Hamiltonian. In particular, it will bring us a fairly simple algorithm for the diagonalization of the pairing Hamiltonian.

For the sake of convenience, we introduce the new operators c_i and c_i^\dagger as follows,

$$c_i = b_i^\dagger, \quad c_i^\dagger = b_i, \quad i = 1, 2, \dots, n. \quad (4.45)$$

Accordingly, the commutators will be

$$a \cdot a^\dagger = I, \quad a \cdot a = 0, \quad a^\dagger \cdot a^\dagger = 0, \quad (4.46)$$

$$c \cdot c^\dagger = -I, \quad c \cdot c = 0, \quad c^\dagger \cdot c^\dagger = 0, \quad (4.47)$$

$$a \cdot c = 0, \quad a \cdot c^\dagger = 0, \quad a^\dagger \cdot c = 0, \quad a^\dagger \cdot c^\dagger = 0. \quad (4.48)$$

In fact, the c -particles are just the so-called time-polarized bosons. Using those new operators, the Hamiltonian of Eq. [\(4.41\)](#) can be written as

$$H = \psi^\dagger M \psi - \text{tr}(\varepsilon), \quad (4.49)$$

where M is the coefficient matrix,

$$M = \begin{bmatrix} \alpha & \gamma \\ \gamma^\dagger & \varepsilon \end{bmatrix}, \quad (4.50)$$

and ψ the field operator,

$$\psi = \begin{bmatrix} a \\ c \end{bmatrix}, \quad \psi^\dagger = \begin{bmatrix} a^\dagger & c^\dagger \end{bmatrix}. \quad (4.51)$$

The commutator for ψ is

$$\psi \cdot \psi^\dagger = I_-. \quad (4.52)$$

Here, it is worth pointing out that there is no involution symmetry for the field ψ now, which is quite different

from that of Eq. (1.7). As can be seen latter, this property will make the diagonalization much easier: One need not ensure the involution symmetry for the new field any more.

The Heisenberg equation of motion for the field ψ can be derived from Eqs. (4.49) and (4.52),

$$i \frac{d}{dt} \psi = D\psi, \quad (4.53)$$

where D is the dynamic matrix,

$$D = \begin{bmatrix} \alpha & \gamma \\ -\gamma^\dagger & -\varepsilon \end{bmatrix}. \quad (4.54)$$

As regards M and D , one has

$$D = I_- M, \quad (4.55)$$

which is identical to Eq. (2.6). We note that the coefficient matrix M is Hermitian.

Different from the normal Hamiltonian, the pairing Hamiltonian is not always BV diagonalizable.

Proposition 49 *The boson pairing Hamiltonian of Eq. (4.41) is BV diagonalizable if and only if the dynamic matrix D is physically diagonalizable.*

Proof. The sufficiency can be proved as follows.

First, if the dynamic matrix D is BV diagonalizable, then its eigenspaces will be orthogonal to each other with respect to the metric I_- . The proof is the same as that for the lemma 21 which can be easily seen by comparing Eq. (4.55) with Eq. (2.6).

Second, for every eigenspace of the dynamic matrix D , there exists an orthonormal basis with respect to the metric I_- . The proof is completely the same as that for the lemma 22

Now, summing up all the orthonormal bases chosen as above, we obtain an orthonormal basis for the whole space \mathbb{C}^{2n} ,

$$v^\dagger(\omega_i) I_- v(\omega_j) = \lambda_i \delta_{ij}, \quad (4.56)$$

where $v(\omega_i)$ ($1 \leq i \leq 2n$) are the eigenvectors with $\lambda_i = \pm 1$ being the corresponding norms. It follows from Eq. (4.55) that

$$v^\dagger(\omega_i) M v(\omega_j) = \lambda_i \omega_i \delta_{ij}. \quad (4.57)$$

By introducing the matrix,

$$U = [v(\omega_1), v(\omega_2), \dots, v(\omega_{2n})], \quad (4.58)$$

the two equations above can be formulated as

$$U^\dagger I_- U = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_{2n}), \quad (4.59)$$

$$U^\dagger M U = \text{diag}(\lambda_1 \omega_1, \lambda_2 \omega_2, \dots, \lambda_{2n} \omega_{2n}). \quad (4.60)$$

Here, it is enough for us to take only into account of the orthonormalization of the eigenvectors because, as

pointed out above, the field ψ has no involution symmetry. One need not take care of both the orthonormalization and involution symmetry simultaneously as before, particularly as in the lemma 23. Obviously, that brings us much convenience.

Applying Sylvester's law of inertia [14] to the first equation above, we find that, of the total $2n$ norms (λ_i with $i = 1, 2, \dots, 2n$), there must be n positive norms and n negative norms. Upon rearranging the order of the eigenvectors, $v(\omega_i)$, $1 \leq i \leq 2n$, within the matrix U , the two equations above can be reformulated as

$$U^\dagger I_- U = I_-, \quad (4.61)$$

$$U^\dagger M U = \text{diag}(\omega_1, \dots, \omega_n, -\omega_{n+1}, \dots, -\omega_{2n}). \quad (4.62)$$

Now, defining a new field φ ,

$$\varphi = U^{-1} \psi, \quad (4.63)$$

we have from Eq. (4.52)

$$\varphi \cdot \varphi^\dagger = I_-. \quad (4.64)$$

Accordingly, the Hamiltonian of Eq. (4.49) can be written as

$$H = \varphi^\dagger U^\dagger M U \varphi - \text{tr}(\varepsilon). \quad (4.65)$$

If one expands φ as

$$\varphi = \begin{bmatrix} d \\ e \end{bmatrix}, \quad \varphi^\dagger = \begin{bmatrix} d^\dagger & e^\dagger \end{bmatrix}, \quad (4.66)$$

he obtains the commutation relations,

$$d \cdot d^\dagger = I, \quad d \cdot d = 0, \quad d^\dagger \cdot d^\dagger = 0, \quad (4.67)$$

$$e \cdot e^\dagger = -I, \quad e \cdot e = 0, \quad e^\dagger \cdot e^\dagger = 0, \quad (4.68)$$

$$d \cdot e = 0, \quad d \cdot e^\dagger = 0, \quad d^\dagger \cdot e = 0, \quad d^\dagger \cdot e^\dagger = 0, \quad (4.69)$$

and the corresponding Hamiltonian,

$$H = \sum_{i=1}^n (\omega_i d_i^\dagger d_i - \omega_{n+i} e_i^\dagger e_i) - \text{tr}(\varepsilon). \quad (4.70)$$

Heeding that the e -particles are the time-polarized bosons, we need perform the transformation,

$$f_i = e_i^\dagger, \quad f_i^\dagger = e_i, \quad i = 1, 2, \dots, n, \quad (4.71)$$

where the f -particles return to the normal bosons. At last, we obtain the diagonalized Hamiltonian,

$$H = \sum_{i=1}^n (\omega_i d_i^\dagger d_i - \omega_{n+i} f_i^\dagger f_i) - \sum_{i=1}^n \omega_{n+i} - \text{tr}(\varepsilon), \quad (4.72)$$

where the operators d_i (d_i^\dagger) and f_i (f_i^\dagger) ($i = 1, 2, \dots, n$) satisfy the standard commutation relations for bosons,

$$d \cdot d^\dagger = I, \quad d \cdot d = 0, \quad d^\dagger \cdot d^\dagger = 0, \quad (4.73)$$

$$f \cdot f^\dagger = I, \quad f \cdot f = 0, \quad f^\dagger \cdot f^\dagger = 0, \quad (4.74)$$

$$d \cdot f = 0, \quad d \cdot f^\dagger = 0, \quad d^\dagger \cdot f = 0, \quad d^\dagger \cdot f^\dagger = 0. \quad (4.75)$$

The proof for necessity is simply similar to that for the proposition 13. ■

Example 50

$$H = \varepsilon_1 c_1^\dagger c_1 + \varepsilon_2 c_2^\dagger c_2 + \gamma(c_1^\dagger c_2^\dagger + c_2 c_1), \quad (4.76)$$

where $\gamma > 0$.

Solution 51 The dynamic matrix is

$$D = \begin{bmatrix} \varepsilon_1 & \gamma \\ -\gamma & -\varepsilon_2 \end{bmatrix}. \quad (4.77)$$

Obviously, its characteristic equation is

$$\omega^2 + (\varepsilon_2 - \varepsilon_1)\omega + (\gamma^2 - \varepsilon_1\varepsilon_2) = 0. \quad (4.78)$$

1. If $|\varepsilon_1 + \varepsilon_2| < 2\gamma$, there are two imaginary eigenvalues,

$$\omega = \frac{1}{2} \left[\varepsilon_1 - \varepsilon_2 \pm i\sqrt{4\gamma^2 - (\varepsilon_1 + \varepsilon_2)^2} \right]. \quad (4.79)$$

The dynamic matrix D is not physically diagonalizable.

2. If $|\varepsilon_1 + \varepsilon_2| = 2\gamma$, there is only one real eigenvalue,

$$\omega = \frac{1}{2} (\varepsilon_1 - \varepsilon_2). \quad (4.80)$$

It is easy to show that ω has only one eigenvector. The dynamic matrix D is not physically diagonalizable.

3. If $|\varepsilon_1 + \varepsilon_2| > 2\gamma$, there are two real eigenvalues,

$$\omega_1 = \frac{1}{2} \left[\varepsilon_1 - \varepsilon_2 + \sqrt{(\varepsilon_1 + \varepsilon_2)^2 - 4\gamma^2} \right], \quad (4.81)$$

$$\omega_2 = \frac{1}{2} \left[\varepsilon_1 - \varepsilon_2 - \sqrt{(\varepsilon_1 + \varepsilon_2)^2 - 4\gamma^2} \right]. \quad (4.82)$$

The dynamic matrix D is thus physically diagonalizable. Meanwhile, the Hamiltonian H can be BV diagonalized, the corresponding transformation matrix is

$$U = \begin{cases} [v(\omega_1), v(\omega_2)], & \varepsilon_1 + \varepsilon_2 > 2\gamma \\ [v(\omega_2), v(\omega_1)], & \varepsilon_1 + \varepsilon_2 < -2\gamma, \end{cases} \quad (4.83)$$

where

$$v(\omega_1) = \frac{1}{\sqrt{\gamma^2 - (\omega_1 - \varepsilon_1)^2}} \begin{bmatrix} \gamma \\ \omega_1 - \varepsilon_1 \end{bmatrix}, \quad (4.84)$$

$$v(\omega_2) = \frac{1}{\sqrt{\gamma^2 - (\omega_1 - \varepsilon_1)^2}} \begin{bmatrix} \omega_2 + \varepsilon_2 \\ -\gamma \end{bmatrix}. \quad (4.85)$$

It is easy to show

$$U^\dagger I_- U = I_-, \quad (4.86)$$

$$U^\dagger M U = \begin{cases} \text{diag}(\omega_1, -\omega_2), & \varepsilon_1 + \varepsilon_2 > 2\gamma \\ \text{diag}(\omega_2, -\omega_1), & \varepsilon_1 + \varepsilon_2 < -2\gamma, \end{cases} \quad (4.87)$$

$$H = \begin{cases} \omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 - \omega_2 - \varepsilon_2, & \varepsilon_1 + \varepsilon_2 > 2\gamma \\ \omega_2 d_1^\dagger d_1 - \omega_1 d_2^\dagger d_2 - \omega_1 - \varepsilon_2, & \varepsilon_1 + \varepsilon_2 < -2\gamma. \end{cases} \quad (4.88)$$

Obviously, this example is an extension of the example 30. Besides, one can see that the present method is much more convenient than that adopted by the example 30.

Example 52

$$H = \sum_{i=1}^2 \varepsilon(a_i^\dagger a_i + b_i^\dagger b_i) + \sum_{i,j=1}^2 \gamma(a_i^\dagger b_j^\dagger + a_i b_j), \quad (4.89)$$

where $\varepsilon > 0$, and $\gamma > 0$.

Solution 53 The dynamic matrix is

$$D = \begin{bmatrix} \varepsilon & 0 & \gamma & \gamma \\ 0 & \varepsilon & \gamma & \gamma \\ -\gamma & -\gamma & -\varepsilon & 0 \\ -\gamma & -\gamma & 0 & -\varepsilon \end{bmatrix}. \quad (4.90)$$

There are four eigenvalues,

$$\omega_1 = \varepsilon, \quad \omega_2 = -\varepsilon, \quad \omega_3 = \omega_+, \quad \omega_4 = \omega_-, \quad (4.91)$$

where

$$\omega_{\pm} = \begin{cases} \pm i\sqrt{4\gamma^2 - \varepsilon^2}, & \varepsilon < 2\gamma \\ 0, & \varepsilon = 2\gamma \\ \pm\sqrt{\varepsilon^2 - 4\gamma^2}, & \varepsilon > 2\gamma. \end{cases} \quad (4.92)$$

If $\varepsilon < 2\gamma$, D has two imaginary eigenvalues, H is not BV diagonalizable.

If $\varepsilon = 2\gamma$, the zero eigenvalue has only one eigenvector, H is not BV diagonalizable.

If $\varepsilon > 2\gamma$, D is physically diagonalizable, H can be BV diagonalized. The corresponding transformation matrix is

$$U = [v(\omega_1), v(\omega_3), v(\omega_2), v(\omega_4)], \quad (4.93)$$

where

$$v(\omega_1) = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{bmatrix}, \quad v(\omega_3) = \begin{bmatrix} \frac{2\gamma}{\sqrt{8\gamma^2 - 2(\omega_+ - \varepsilon)^2}} \\ \frac{2\gamma}{\sqrt{8\gamma^2 - 2(\omega_+ - \varepsilon)^2}} \\ \frac{\omega_+ - \varepsilon}{\sqrt{8\gamma^2 - 2(\omega_+ - \varepsilon)^2}} \\ \frac{\omega_+ - \varepsilon}{\sqrt{8\gamma^2 - 2(\omega_+ - \varepsilon)^2}} \end{bmatrix} \quad (4.94)$$

$$v(\omega_2) = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, \quad v(\omega_4) = \begin{bmatrix} \frac{\omega_- + \varepsilon}{\sqrt{8\gamma^2 - 2(\omega_- + \varepsilon)^2}} \\ \frac{\omega_- + \varepsilon}{\sqrt{8\gamma^2 - 2(\omega_- + \varepsilon)^2}} \\ -\frac{2\gamma}{\sqrt{8\gamma^2 - 2(\omega_- + \varepsilon)^2}} \\ -\frac{2\gamma}{\sqrt{8\gamma^2 - 2(\omega_- + \varepsilon)^2}} \end{bmatrix} \quad (4.95)$$

The diagonalized Hamiltonian is

$$H = \omega_1 d_1^\dagger d_1 + \omega_3 d_2^\dagger d_2 - \omega_2 d_3^\dagger d_3 - \omega_4 d_4^\dagger d_4 - \omega_2 - \omega_4 - 2\varepsilon. \quad (4.96)$$

The propositions and algorithms developed in this section can be applied to statistical as well as condensed-matter physics [2, 5, 8, 9, 16, 17, 18].

V. APPLICATION TO FERMI SYSTEMS

As in the preceding subsection, we shall also concentrate ourselves on the normal and pairing Hamiltonians. They represent the problems which we encounter most frequently in practice.

A. The normal Hamiltonian

The normal Hamiltonian reads

$$H = \sum_{i,j=1}^n \alpha_{ij} c_i^\dagger c_j. \quad (5.1)$$

The proposition 44 can be easily transplanted to the present case.

Proposition 54 *A normal Hamiltonian of fermions can be BV diagonalized by the unitary transformation generated by its coefficient matrix.*

That is also because the Heisenberg equation for the Hamiltonian of Eq. (5.1) is reducible. It can be reduced as

$$i \frac{d}{dt} c = \alpha c. \quad (5.2)$$

Since α is Hermitian, this equation of motion can generate a unitary transformation U for the field c ,

$$c = U d, \quad (5.3)$$

where

$$U^\dagger U = U U^\dagger = I, \quad (5.4)$$

$$U^\dagger \alpha U = \text{diag}(\omega_1, \omega_2, \dots, \omega_n). \quad (5.5)$$

The d represents the new field, it is easy to show that d is a standard fermionic field,

$$d \cdot d^\dagger = I, \quad d \cdot d = 0, \quad d^\dagger \cdot d^\dagger = 0. \quad (5.6)$$

Accordingly,

$$H = d^\dagger U^\dagger \alpha U d = \sum_{i=1}^n \omega_i d_i^\dagger d_i. \quad (5.7)$$

Besides, a particle-hole transformation will be needed if some eigenenergies are negative.

To sum up, a normal Hamiltonian can be BV diagonalized by the unitary transformation generated by its coefficient matrix no matter whether the system is bosonic or fermionic.

Example 55

$$H = \varepsilon(c_1^\dagger c_1 + c_2^\dagger c_2) + \mu(c_1^\dagger c_2 + c_2^\dagger c_1), \quad (5.8)$$

where $\mu > 0$.

Solution 56 *The coefficient matrix is*

$$\alpha = \begin{bmatrix} \varepsilon & \mu \\ \mu & \varepsilon \end{bmatrix}. \quad (5.9)$$

It has two eigenvalues,

$$\omega_1 = \varepsilon + \mu, \quad \omega_2 = \varepsilon - \mu. \quad (5.10)$$

The unitary matrix can be easily found,

$$U = [v(\omega_1), v(\omega_2)] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \quad (5.11)$$

1. *If $\varepsilon \geq \mu$, $\omega_1 > 0$ and $\omega_2 \geq 0$,*

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}, \quad (5.12)$$

$$H = \omega_1 d_1^\dagger d_1 + \omega_2 d_2^\dagger d_2. \quad (5.13)$$

2. *If $-\mu \leq \varepsilon < \mu$, $\omega_1 \geq 0$ and $\omega_2 < 0$,*

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2^\dagger \end{bmatrix}, \quad (5.14)$$

$$H = \omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 + \omega_2. \quad (5.15)$$

3. *If $\varepsilon < -\mu$, $\omega_1 < 0$ and $\omega_2 < 0$,*

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} d_1^\dagger \\ d_2^\dagger \end{bmatrix}, \quad (5.16)$$

$$H = -\omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 + \omega_1 + \omega_2. \quad (5.17)$$

Here, a particle-hole transformation is performed to the d_2 -particles if $-\mu \leq \varepsilon < \mu$, and to both the d_1 - and d_2 -particles if $\varepsilon < -\mu$.

B. The pairing Hamiltonian

The pairing Hamiltonian reads

$$H = \sum_{i,j=1}^n (\alpha_{ij} a_i^\dagger a_j + \varepsilon_{ij} b_i^\dagger b_j + \gamma_{ij} a_i b_j + \gamma_{ji}^* a_i^\dagger b_j^\dagger), \quad (5.18)$$

where

$$\alpha^\dagger = \alpha, \quad \varepsilon^\dagger = \varepsilon, \quad \tilde{\gamma} = -\gamma. \quad (5.19)$$

Following the Bose case, let us introduce the new operators c_i and c_i^\dagger as

$$c_i = b_i^\dagger, \quad c_i^\dagger = b_i, \quad i = 1, 2, \dots, n. \quad (5.20)$$

The new anticommutators will be

$$a \cdot a^\dagger = I, \quad a \cdot a = 0, \quad a^\dagger \cdot a^\dagger = 0, \quad (5.21)$$

$$c \cdot c^\dagger = I, \quad c \cdot c = 0, \quad c^\dagger \cdot c^\dagger = 0, \quad (5.22)$$

$$a \cdot c = 0, \quad a \cdot c^\dagger = 0, \quad a^\dagger \cdot c = 0, \quad a^\dagger \cdot c^\dagger = 0. \quad (5.23)$$

Obviously, they are still standard, which is rather different from the Bose case. In terms of these new operators, Eq. (5.18) can be expressed as

$$H = \psi^\dagger M \psi + \text{tr}(\varepsilon), \quad (5.24)$$

where M is the coefficient matrix,

$$M = \begin{bmatrix} \alpha & \gamma \\ \gamma^\dagger & -\varepsilon \end{bmatrix}, \quad (5.25)$$

and ψ the field operator,

$$\psi = \begin{bmatrix} a \\ c \end{bmatrix}, \quad \psi^\dagger = [a^\dagger, c^\dagger]. \quad (5.26)$$

It is evident that

$$M = M^\dagger, \quad (5.27)$$

$$\psi \cdot \psi^\dagger = I_+. \quad (5.28)$$

Namely, M is Hermitian, and ψ is a standard fermionic field. This means that Eq. (5.24) is, in fact, a normal Hamiltonian. Hence, we obtain the proposition.

Proposition 57 *A pairing Hamiltonian of fermions can be first transformed into a normal Hamiltonian, and then BV diagonalized by the unitary transformation generated by the corresponding coefficient matrix.*

As well known, Eq. (5.20) represents a particle-hole transformation in physics. So, the proposition says actually that a pairing Hamiltonian of fermions can be transformed into a normal Hamiltonian by a particle-hole transformation.

Example 58

$$H = \varepsilon_1 c_1^\dagger c_1 + \varepsilon_2 c_2^\dagger c_2 + \gamma(c_1^\dagger c_2^\dagger + c_2 c_1), \quad (5.29)$$

where $\gamma > 0$.

Solution 59 *The coefficient matrix is*

$$M = \begin{bmatrix} \varepsilon_1 & \gamma \\ \gamma & -\varepsilon_2 \end{bmatrix}. \quad (5.30)$$

It has two eigenvalues,

$$\omega_1 = \frac{1}{2} \left[\varepsilon_1 - \varepsilon_2 + \sqrt{(\varepsilon_1 + \varepsilon_2)^2 + 4\gamma^2} \right], \quad (5.31)$$

$$\omega_2 = \frac{1}{2} \left[\varepsilon_1 - \varepsilon_2 - \sqrt{(\varepsilon_1 + \varepsilon_2)^2 + 4\gamma^2} \right], \quad (5.32)$$

and generates a unitary transformation matrix,

$$\begin{aligned} U &= [v(\omega_1), v(\omega_2)] \\ &= \frac{1}{\sqrt{(\omega_1 - \varepsilon_1)^2 + \gamma^2}} \\ &\quad \times \begin{bmatrix} \gamma & \omega_2 + \varepsilon_2 \\ \omega_1 - \varepsilon_1 & \gamma \end{bmatrix}. \end{aligned} \quad (5.33)$$

1. If $\gamma^2 \leq -\varepsilon_1 \varepsilon_2$ and $\varepsilon_1 > 0$, the diagonalized Hamiltonian has the form,

$$H = \omega_1 d_1^\dagger d_1 + \omega_2 d_2^\dagger d_2 + \varepsilon_2, \quad (5.34)$$

where

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = U^{-1} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}. \quad (5.35)$$

2. If $\gamma^2 \leq -\varepsilon_1 \varepsilon_2$ and $\varepsilon_1 < 0$, the diagonalized Hamiltonian has the form,

$$H = -\omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 + \omega_1 + \omega_2 + \varepsilon_2, \quad (5.36)$$

where

$$\begin{bmatrix} d_1^\dagger \\ d_2^\dagger \end{bmatrix} = U^{-1} \begin{bmatrix} c_1^\dagger \\ c_2^\dagger \end{bmatrix}. \quad (5.37)$$

3. If $\gamma^2 > -\varepsilon_1 \varepsilon_2$, the diagonalized Hamiltonian has the form,

$$H = \omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 + \omega_2 + \varepsilon_2, \quad (5.38)$$

where

$$\begin{bmatrix} d_1 \\ d_2^\dagger \end{bmatrix} = U^{-1} \begin{bmatrix} c_1 \\ c_2^\dagger \end{bmatrix}. \quad (5.39)$$

Obviously, this example is an extension of the example 39. One can see that the present method is much simpler than that used by the example 39.

Example 60

$$H = \sum_{i=1}^2 \varepsilon(a_i^\dagger a_i + b_i^\dagger b_i) + \sum_{i,j=1}^2 \gamma(a_i^\dagger b_j^\dagger + a_i b_j), \quad (5.40)$$

where $\varepsilon > 0$, and $\gamma > 0$.

Solution 61 *The coefficient matrix is*

$$M = \begin{bmatrix} \varepsilon & 0 & \gamma & \gamma \\ 0 & \varepsilon & \gamma & \gamma \\ \gamma & \gamma & -\varepsilon & 0 \\ \gamma & \gamma & 0 & -\varepsilon \end{bmatrix}. \quad (5.41)$$

It has four eigenvalues,

$$\omega_1 = \varepsilon, \quad \omega_2 = -\varepsilon, \quad (5.42)$$

$$\omega_3 = \sqrt{\varepsilon^2 + 4\gamma^2}, \quad \omega_4 = -\sqrt{\varepsilon^2 + 4\gamma^2}. \quad (5.43)$$

The diagonalized Hamiltonian is

$$\begin{aligned} H &= \omega_1 d_1^\dagger d_1 - \omega_2 d_2^\dagger d_2 + \omega_3 d_3^\dagger d_3 - \omega_4 d_4^\dagger d_4 \\ &\quad + \omega_2 + \omega_4 + 2\varepsilon. \end{aligned} \quad (5.44)$$

The corresponding BV transformation has the form,

$$\begin{bmatrix} a_1 \\ a_2 \\ b_1^\dagger \\ b_2^\dagger \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{2\gamma}{\sqrt{8\gamma^2+2(\omega_3-\varepsilon)^2}} & \frac{\omega_4+\varepsilon}{\sqrt{8\gamma^2+2(\omega_4+\varepsilon)^2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{2\gamma}{\sqrt{8\gamma^2+2(\omega_3-\varepsilon)^2}} & \frac{\omega_4+\varepsilon}{\sqrt{8\gamma^2+2(\omega_4+\varepsilon)^2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{\omega_3-\varepsilon}{\sqrt{8\gamma^2+2(\omega_3-\varepsilon)^2}} & \frac{2\gamma}{\sqrt{8\gamma^2+2(\omega_4+\varepsilon)^2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{\omega_3-\varepsilon}{\sqrt{8\gamma^2+2(\omega_3-\varepsilon)^2}} & \frac{2\gamma}{\sqrt{8\gamma^2+2(\omega_4+\varepsilon)^2}} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2^\dagger \\ d_3 \\ d_4^\dagger \end{bmatrix}. \quad (5.45)$$

The propositions and algorithms developed in this section can be applied to statistical physics [3, 4, 5, 6, 7, 8], condensed-matter physics [9, 19, 20, 21], and nuclear physics [8, 22].

VI. GENERALIZED BOGOLIUBOV-VALATIN TRANSFORMATION

Historically, Dirac [1] and later Shrödinger [23, 24, 25, 26] found that a linear harmonic oscillator can be diagonalized with regard to the bosonic creation and annihilation operators,

$$\begin{aligned} H &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \\ &= \omega a^\dagger a + \frac{1}{2}\omega, \end{aligned} \quad (6.1)$$

where m and ω are the mass and (angular) frequency of the oscillator, respectively. The q and p are the coordinate and momentum operators. They are both Hermitian, and satisfy the canonical commutation rule,

$$[p, q] = -i. \quad (6.2)$$

The a and a^\dagger are the annihilation and creation operators. They are Hermitian conjugates of each other, and satisfy the bosonic commutation rule,

$$[a, a^\dagger] = 1. \quad (6.3)$$

Both a and a^\dagger are the linear functions of q and p ,

$$a = \sqrt{\frac{m\omega}{2}} \left(q + i \frac{p}{m\omega} \right), \quad (6.4)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2}} \left(q - i \frac{p}{m\omega} \right), \quad (6.5)$$

and vice versa. For convenience, we shall call such a transformation Dirac transformation, and call the corresponding diagonalization Dirac diagonalization.

In this section, we shall study the necessary and sufficient conditions for Dirac diagonalization. We find that Dirac diagonalization is actually a generalization of BV diagonalization.

A. Theory of Dirac diagonalization

Consider the Hamiltonian that is quadratic in coordinates and momenta,

$$\begin{aligned} H &= \sum_{i,j=1}^n \left(\frac{1}{2} \mu_{ij} p_i p_j + \frac{1}{2} \kappa_{ij} q_i q_j + \frac{1}{2} \gamma_{ij} p_i q_j + \frac{1}{2} \gamma_{ji} q_i p_j \right) \\ &= \frac{1}{2} p^\dagger \mu p + \frac{1}{2} q^\dagger \kappa q + \frac{1}{2} p^\dagger \gamma q + \frac{1}{2} q^\dagger \gamma^\dagger p, \end{aligned} \quad (6.6)$$

where the coefficients are all real, $\kappa_{il} \in \mathbb{R}$, $\mu_{ij} \in \mathbb{R}$, $\gamma_{ij} \in \mathbb{R}$, and

$$\mu = \mu^\dagger, \quad \kappa = \kappa^\dagger. \quad (6.7)$$

The coordinates and momenta satisfy the canonical commutation relations,

$$[p_i, q_j] = -i\delta_{ij}, \quad [p_i, p_j] = 0, \quad [q_i, q_j] = 0, \quad (6.8)$$

or equivalently,

$$p \cdot q^\dagger = -iI, \quad p \cdot p^\dagger = 0, \quad q \cdot q^\dagger = 0. \quad (6.9)$$

Let us put

$$\phi = \begin{bmatrix} p \\ q \end{bmatrix}, \quad \phi^\dagger = [p^\dagger, q^\dagger]. \quad (6.10)$$

The Hamiltonian can be written more compactly as

$$H = \frac{1}{2} \phi^\dagger M \phi, \quad (6.11)$$

where M is the coefficient matrix,

$$M = \begin{bmatrix} \mu & \gamma \\ \gamma^\dagger & \kappa \end{bmatrix}, \quad (6.12)$$

which is Hermitian. Equation (6.9) becomes

$$\phi \cdot \phi^\dagger = \Sigma_y, \quad (6.13)$$

where

$$\Sigma_y = \begin{bmatrix} 0 & -iI \\ iI & 0 \end{bmatrix}. \quad (6.14)$$

Obviously, Σ_y is a Hermitian matrix.

The Heisenberg equation of motion for the field ϕ can be derived from Eqs. (6.11) and (6.13),

$$i \frac{d}{dt} \phi = D\phi, \quad (6.15)$$

where D is the dynamic matrix,

$$D = \Sigma_y M. \quad (6.16)$$

Generally, D is not Hermitian. The above equation gives the relationship between the dynamic matrix D and the coefficient matrix M , it is the counterpart of Eq. (2.6).

The eigenvalue equation for Eq. (6.15) is,

$$\omega v(\omega) = Dv(\omega). \quad (6.17)$$

It can be rewritten as

$$i\omega v(\omega) = JMv(\omega), \quad (6.18)$$

where J is the unit symplectic matrix given in Eq. (2.95). Paying attention to the fact that JM is a real matrix, one realizes immediatly that the lemma 3 also holds now.

Lemma 62 *If ω is an eigenvalue of the dynamic matrix D , then $-\omega^*$ will also be an eigenvalue of D .*

Nevertheless, the lemma 4 should be modified as follows.

Lemma 63 *If $v(\omega)$ is an eigenvector belonging to the eigenvalue ω of the dynamic matrix D , then its complex conjugate $v^*(\omega)$ will be an eigenvector belonging to the eigenvalue $-\omega^*$.*

These two lemmas show that the dynamic mode pair appears now in the form of $\{\omega, v(\omega)\}$ and $\{-\omega^*, v^*(\omega)\}$ where the two eigenvectors are complex conjugates of each other.

Now, consider the Dirac transformation,

$$\phi = T\psi, \quad (6.19)$$

where ψ represents the bosonic field given in Eq. (1.7). Evidently, the Heisenberg equation of ψ is still linear and homogeneous,

$$i \frac{d}{dt} \psi = D_1 \psi, \quad (6.20)$$

where D_1 is the dynamic matrix for ψ . Following the proof for the lemma 12, we obtain the lemma below.

Lemma 64 *Under a Dirac transformation, the two dynamic matrices respectively for the old and new fields will be similar to each other.*

It is evident that D_1 is a real diagonal matrix if the Hamiltonian of Eq. (6.11) has been diagonalized Diracianly. As a result, the proposition 13 holds for Dirac diagonalization, too.

Proposition 65 *If a Hamiltonian quadratic in coordinates and momenta can be Diracianly diagonalized, its dynamic matrix is physically diagonalizable.*

Also, it can be readily confirmed that the lemma 16 holds for the present case.

Lemma 66 *If the dynamic matrix D is physically diagonalizable, then, for each pair of nonzero eigenvalues, i.e., $(\omega, -\omega)$ with $\omega \neq 0$, they have the same degeneracy. Namely, their eigenspace have the same dimension. Especially, their bases can be chosen as*

$$v_l(-\omega) = v_l^*(\omega), \quad l = 1, 2, \dots, m, \quad (6.21)$$

where m ($m \in \mathbb{N}$) is the dimension of the eigenspace of ω .

But the lemma 17 needs a few modifications.

Lemma 67 *If the dynamic matrix D is physically diagonalizable and has zero eigenvalue, the eigenspace of zero eigenvalue is even dimensional. In particular, its basis vectors can be chosen and grouped as*

$$v_{m+l}(0) = v_l^*(0), \quad l = 1, 2, \dots, m, \quad (6.22)$$

where $2m$ ($m \in \mathbb{N}$) is the dimension of the eigenspace of zero eigenvalue.

Proof. It just needs to prove the second point.

When $\omega = 0$, Eq. (6.18) becomes

$$JMv(0) = 0. \quad (6.23)$$

As pointed out above, JM is a real matrix, its eigenvectors can be chosen naturally as real vectors. In other words, there exists a real basis for the eigenspace of zero eigenvalue,

$$w_l(0) = w_l^*(0), \quad l = 1, 2, \dots, 2m. \quad (6.24)$$

Let us put

$$v_l(0) = w_l(0) + iw_{m+l}(0), \quad (6.25)$$

$$v_{m+l}(0) = w_l(0) - iw_{m+l}(0), \quad (6.26)$$

where $l = 1, 2, \dots, m$. They are obviously a basis that is in accordance with Eq. (6.22). ■

Instead of I_- , we can here introduce a sesquilinear form using Σ_y , it is also a nonsingular metric. Notice the similarity between Eqs. (6.16) and (2.6). We can transplant the lemmas 21 and 22 to the present case.

Lemma 68 *If the dynamic matrix D is physically diagonalizable, its eigenspaces will be orthogonal to each other with respect to the metric Σ_y .*

Lemma 69 *If the dynamic matrix D is physically diagonalizable, then, for each eigenspace of D , there exists an orthonormal basis with respect to the metric Σ_y .*

As to the lemma [23](#) it needs some modifications.

Lemma 70 *If the dynamic matrix D is physically diagonalizable and has zero eigenvalue, there exists such an orthonormal basis for the eigenspace of zero eigenvalue that*

$$v_{m+l}(0) = v_l^*(0), \quad l = 1, 2, \dots, m, \quad (6.27)$$

where $2m$ ($m \in \mathbb{N}$) is the dimension of the eigenspace of zero eigenvalue.

Proof. According to the lemma [67](#), the eigenspace V_0 of zero eigenvalue has a basis,

$$v_{m+l}(0) = v_l^*(0), \quad l = 1, 2, \dots, m, \quad (6.28)$$

where $\dim(V_0) = 2m$ ($m \in \mathbb{N}$).

When $m = 1$, $v_1(0)$ must be nonisotropic,

$$v_1^\dagger(0)\Sigma_y v_1(0) \neq 0. \quad (6.29)$$

Otherwise, one has

$$v_1^\dagger(0)\Sigma_y v_1(0) = 0, \quad v_2^\dagger(0)\Sigma_y v_2(0) = 0. \quad (6.30)$$

In addition,

$$\begin{aligned} v_1^\dagger(0)\Sigma_y v_2(0) &= v_1^\dagger(0)\Sigma_y v_1^*(0) \\ &= -i\widetilde{v}_1^*(0)Jv_1^*(0) \\ &= 0. \end{aligned} \quad (6.31)$$

That is to say,

$$v_1^\dagger(0)\Sigma_y v_2(0) = 0, \quad v_2^\dagger(0)\Sigma_y v_1(0) = 0. \quad (6.32)$$

Equations [\(6.30\)](#) and [\(6.32\)](#) contradict the fact that Σ_y is a nonsingular metric on V_0 . That is to say, $v_1(0)$ can not be isotropic. It can thus be normalized,

$$v_1^\dagger(0)\Sigma_y v_1(0) = 1 \text{ or } -1. \quad (6.33)$$

Correspondingly,

$$v_2^\dagger(0)\Sigma_y v_2(0) = -1 \text{ or } 1. \quad (6.34)$$

Those together with Eq. [\(6.32\)](#) show that

$$v_i^\dagger(0)\Sigma_y v_j(0) = -\lambda_i \delta_{ij}, \quad \lambda_i = \pm 1, \quad i, j = 1, 2. \quad (6.35)$$

Thereby, the lemma holds when $m = 1$.

The rest steps of mathematical induction are similar to the lemma [23](#) ■

The combination of the lemmas [\(66\)](#)–[\(70\)](#) shows that there are totally $2n$ dynamic mode pairs. Each mode pair takes the form of $\{\omega, v(\omega)\}$ and $\{-\omega, v^*(\omega)\}$, viz., it contains two opposite eigenenergies, and two complex conjugate eigenvectors. Most importantly, the two complex conjugate eigenvectors have opposite norms, one is $+1$, the other is -1 :

$$v^\dagger(-\omega_i)\Sigma_y v(-\omega_i) = -[v^\dagger(\omega_i)\Sigma_y v(\omega_i)]^* = \pm 1. \quad (6.36)$$

Thereby, we can stipulate an order for every mode pair as in Eqs. [\(2.142\)](#)–[\(2.145\)](#): The first eigenvector has the norm of $+1$, the second one has the norm of -1 . So, we obtain a derivative transformation T_d as follows,

$$\phi = T_d \psi, \quad (6.37)$$

$$T_d = [v(\omega_1), v(\omega_2), \dots, v(\omega_n), v(-\omega_1), v(-\omega_2), \dots, v(-\omega_n)], \quad (6.38)$$

where

$$v^\dagger(\omega_i)\Sigma_y v(\omega_i) = 1, \quad (6.39)$$

$$v^\dagger(-\omega_i)\Sigma_y v(-\omega_i) = -1. \quad (6.40)$$

Consequently, we obtain a new version of the lemma [25](#).

Lemma 71 *If the dynamic matrix D is physically diagonalizable, its derivative transformation T_d satisfies the identity,*

$$T_d^\dagger \Sigma_y T_d = I_-. \quad (6.41)$$

The lemma shows that

$$\psi \cdot \psi^\dagger = I_-. \quad (6.42)$$

The new field ψ has another important property.

Lemma 72 *The new field ψ defined in Eq. [\(6.37\)](#) has the involution symmetry,*

$$\psi = (\widetilde{\Sigma_x \psi})^\dagger. \quad (6.43)$$

Proof. As ϕ is a real field, one has

$$\phi = \widetilde{\phi}^\dagger. \quad (6.44)$$

From Eq. [\(6.37\)](#), it follows that

$$\widetilde{\phi}^\dagger = T_d^* \widetilde{\psi}^\dagger, \quad (6.45)$$

which means

$$T_d \psi = T_d^* \widetilde{\psi}^\dagger. \quad (6.46)$$

It is easy to show that

$$T_d^* = T_d \Sigma_x. \quad (6.47)$$

Substituting it into Eq. (6.46), one obtains

$$T_d \psi = T_d \Sigma_x \widetilde{\psi}^\dagger. \quad (6.48)$$

Since T_d is invertible, and $\Sigma_x^{-1} = \Sigma_x$, he arrives finally at

$$\Sigma_x \psi = \widetilde{\psi}^\dagger. \quad (6.49)$$

It is equivalent to Eq. (6.43). ■

This lemma shows that the new field ψ takes exactly the form of Eq. (1.7). Together with Eq. (6.42), it means that the new field ψ is a standard bosonic field.

Lemma 73 *If the dynamic matrix D is physically diagonalizable, its derivative transformation T_d will diagonalize the coefficient matrix M in the manner of Hermitian congruence,*

$$T_d^\dagger M T_d = \text{diag}(\omega_1, \dots, \omega_n, \omega_1, \dots, \omega_n). \quad (6.50)$$

Proof. From Eq. (6.16), it follows that

$$M = \Sigma_y D. \quad (6.51)$$

Therefore,

$$\begin{aligned} T_d^\dagger M T_d &= T_d^\dagger \Sigma_y D T_d \\ &= T_d^\dagger \Sigma_y T_d T_d^{-1} D T_d \\ &= I_- T_d^{-1} D T_d. \end{aligned} \quad (6.52)$$

As D is physically diagonalizable, we have

$$T_d^{-1} D T_d = \text{diag}(\omega_1, \dots, \omega_n, -\omega_1, \dots, -\omega_n). \quad (6.53)$$

The combination of the two equations above proves the lemma. ■

Theorem 74 *A Hamiltonian quadratic in coordinates and momenta is Diracianly diagonalizable if and only if its dynamic matrix is physically diagonalizable.*

Proof. The necessary condition has been proved by the proposition 65

The sufficient condition can be proved as follows.

Consider the quadratic Hamiltonian of Eq. (6.11). If its dynamic matrix is physically diagonalizable, it can generate a derivative transformation as given in Eq. (6.37). Under this transformation, Eq. (6.11) becomes

$$\begin{aligned} H &= \frac{1}{2} \psi^\dagger T_d^\dagger M T_d \psi \\ &= \sum_{i=1}^n \omega_i d_i^\dagger d_i + \frac{1}{2} \sum_{i=1}^n \omega_i, \end{aligned} \quad (6.54)$$

where Eqs. (1.7), (6.42), and (6.50) have been used. It is a Hamiltonian that is diagonal with respect to the bosonic operators d_i^\dagger and d_i ($i = 1, 2, \dots, n$). ■

This theorem shows that the derivative transformation defined in Eq. (6.37) is exactly a Dirac transformation, it brings a Hamiltonian quadratic in coordinates and momenta into the form diagonalized with respect to bosons. Just as BV transformation, Dirac transformation can be generated by the equation of motion of the system automatically.

Now, let us return to the linear harmonic oscillator, the dynamic matrix is

$$D = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{m} & 0 \\ 0 & m\omega^2 \end{bmatrix}. \quad (6.55)$$

It has a pair of eigenenergies,

$$\varepsilon = \pm\omega. \quad (6.56)$$

If $\omega = 0$, there exists only one eigenvector,

$$v(0) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \quad (6.57)$$

It means that the Hamiltonian of a free particle,

$$H = \frac{p^2}{2m}, \quad (6.58)$$

is not Diracianly diagonalizable. If $\omega > 0$, D is physically diagonalizable, there are two linearly independent orthonormalized eigenvectors

$$v(\omega) = \frac{1}{\sqrt{2m\omega}} \begin{bmatrix} -im\omega \\ 1 \end{bmatrix}, \quad (6.59)$$

$$v(-\omega) = \frac{1}{\sqrt{2m\omega}} \begin{bmatrix} im\omega \\ 1 \end{bmatrix}, \quad (6.60)$$

where the convention of Eq. (6.21) has been used for $v(-\omega)$. They generate a Dirac transformation,

$$\begin{bmatrix} p \\ q \end{bmatrix} = \frac{1}{\sqrt{2m\omega}} \begin{bmatrix} -im\omega & im\omega \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a \\ a^\dagger \end{bmatrix}. \quad (6.61)$$

As a result, we have

$$p = -i\sqrt{\frac{m\omega}{2}}(a - a^\dagger), \quad (6.62)$$

$$q = \frac{1}{\sqrt{2m\omega}}(a + a^\dagger). \quad (6.63)$$

They are just the inverse of Eqs. (6.4) and (6.5). According to Eq. (6.54), the diagonalized Hamiltonian has the form,

$$H = \omega a^\dagger a + \frac{1}{2}\omega, \quad (6.64)$$

which is the same as Eq. (6.1).

Theorem 75 *If a Hamiltonian quadratic in coordinates and momenta is Diracianly diagonalizable, its diagonalized form will be unique up to a permutation of the quadratic terms.*

Proof. The proof is similar to that for the theorem [36](#)

Set

$$c_i = \frac{1}{\sqrt{2}}(q_i + ip_i), \quad (6.65)$$

$$c_i^\dagger = \frac{1}{\sqrt{2}}(q_i - ip_i), \quad (6.66)$$

where q_i and p_i ($i = 1, 2, \dots, n$) are the coordinates and momenta which satisfy the canonical commutation rules of Eq. [\(6.9\)](#). It is easy to show that c_i and c_i^\dagger are the annihilation and creation operators that satisfy the bosonic commutation rules of Eqs. [\(1.2\)](#)–[\(1.4\)](#). The inverse is also true. Upon such an invertible linear substitution, the two Hamiltonians of Eqs. [\(1.1\)](#) and [\(6.6\)](#) can be transformed into each other, up to a real constant. Thereby, the BV diagonalization of Eq. [\(1.1\)](#) is mathematically equivalent to the Dirac diagonalization of Eq. [\(6.6\)](#). However, Dirac diagonalization does not require, in physics, the initial field to be a standard bosonic field. Correspondingly, the transformation matrix does not need to ensure the invariance of the metric, and is no longer limited to be a member of the group $U(n, n)$, cf.,

$$T_n^\dagger I_- T_n = I_-, \quad (6.67)$$

$$T_d^\dagger \Sigma_y T_d = I_-. \quad (6.68)$$

In this sense, Dirac diagonalization is more general than BV diagonalization. In particular, it can be generalized easily to complex collective coordinates and momenta, so it is rather useful in the quantizations of Bose fields, which will be discussed in the next section.

Here and now, we would give an interesting example of Dirac diagonalization.

B. Landau quantization

Consider a charged particle moving in a uniform magnetic field. The Hamiltonian is

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2, \quad (6.69)$$

where q , m and \mathbf{p} denote the charge, mass and momentum of the particle, respectively. As to \mathbf{A} , it is the vector potential of the magnetic field, which can be expressed in the form [\[27\]](#),

$$\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}, \quad (6.70)$$

where \mathbf{B} represents the magnetic field, and \mathbf{r} the coordinates of the particle. Assume without loss of generality

that the magnetic field \mathbf{B} is set along the z -axis. Thus

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega_L^2(x^2 + y^2) + \omega_L(xp_y - yp_x) + \frac{1}{2m}p_z^2, \quad (6.71)$$

where $\omega_L = qB/2m$ is the Larmor frequency. Obviously, p_z commutes with H , it will be conserved. This means that p_z can be replaced by a constant, which brings a constant energy, $p_z^2/2m$, to the Hamiltonian. Since a constant energy is unimportant to a Hamiltonian, we shall concern ourselves with the simplified version,

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega_L^2(x^2 + y^2) + \omega_L(xp_y - yp_x). \quad (6.72)$$

As shown in the following, this Hamiltonian can be Diracianly diagonalized and yield the so-called Landau levels.

Solution 76 *The dynamic matrix is*

$$D = \Sigma_y M, \quad (6.73)$$

where M is the coefficient matrix,

$$M = \begin{bmatrix} \frac{1}{m} & 0 & 0 & -\omega_L \\ 0 & \frac{1}{m} & \omega_L & 0 \\ 0 & \omega_L & m\omega_L^2 & 0 \\ -\omega_L & 0 & 0 & m\omega_L^2 \end{bmatrix}. \quad (6.74)$$

The dynamic matrix D has three eigenvalues

$$\omega_1 = 2\omega_L, \quad \omega_2 = -2\omega_L, \quad \omega_3 = 0. \quad (6.75)$$

The first two constitute a dynamic mode, their eigenvectors are complex conjugate to each other,

$$v(2\omega) = \frac{1}{2\sqrt{m\omega_L}} \begin{bmatrix} -m\omega_L \\ -im\omega_L \\ -i \\ 1 \end{bmatrix}, \quad (6.76)$$

$$v(-2\omega) = \frac{1}{2\sqrt{m\omega_L}} \begin{bmatrix} -m\omega_L \\ im\omega_L \\ i \\ 1 \end{bmatrix}, \quad (6.77)$$

the corresponding norms are

$$v^\dagger(2\omega_L)\Sigma_y v(2\omega_L) = 1, \quad (6.78)$$

$$v^\dagger(-2\omega_L)\Sigma_y v(-2\omega_L) = -1. \quad (6.79)$$

The third is zero, it is two-fold degenerate, and has two linearly independent eigenvectors, e.g.,

$$v_1(0) = \begin{bmatrix} m\omega_L \\ 0 \\ 0 \\ 1 \end{bmatrix}, \quad v_2(0) = \begin{bmatrix} 0 \\ -m\omega_L \\ 1 \\ 0 \end{bmatrix}. \quad (6.80)$$

They can be linearly combined and orthonormalized into a dynamic mode,

$$v(+0) = \frac{1}{2\sqrt{m\omega_L}} \begin{bmatrix} m\omega_L \\ -im\omega_L \\ i \\ 1 \end{bmatrix}, \quad (6.81)$$

$$v(-0) = \frac{1}{2\sqrt{m\omega_L}} \begin{bmatrix} m\omega_L \\ im\omega_L \\ -i \\ 1 \end{bmatrix}, \quad (6.82)$$

with the norms being

$$v^\dagger(+0)\Sigma_y v(+0) = 1, \quad (6.83)$$

$$v^\dagger(-0)\Sigma_y v(-0) = -1. \quad (6.84)$$

The Dirac transformation is therefore obtained as follows,

$$\begin{bmatrix} p_x \\ p_y \\ x \\ y \end{bmatrix} = [v(2\omega_L), v(+0), v(-2\omega_L), v(-0)] \begin{bmatrix} a_1 \\ a_2 \\ a_1^\dagger \\ a_2^\dagger \end{bmatrix}. \quad (6.85)$$

Finally, the diagonalized Hamiltonian is

$$H = 2\omega_L a_1^\dagger a_1 + \omega_L. \quad (6.86)$$

This result is rigorous and exactly the same as that due to Landau [27], with $\omega_c = 2\omega_L$ being the cyclotron frequency.

C. Partial diagonalization

If $\gamma = 0$,

$$H = \frac{1}{2}p^\dagger \mu p + \frac{1}{2}q^\dagger \kappa q, \quad (6.87)$$

it reduces to the Hamiltonian of Eq. (1.24). As already known from Sec. IB the latter is identical to the Hamiltonian of Eq. (1.56). Thereby, we obtain the proposition.

Proposition 77 *The Hamiltonian of Eq. (6.87) is Diracianly diagonalizable when the matrices μ and κ are both positive definite. If μ is positive definite but κ is nonnegative definite, it is partially diagonalizable, i.e., except that the normal modes with zero frequencies are conserved quantities and hence not Diracianly diagonalizable, all the rest part can be Diracianly diagonalized.*

The Hamiltonian of such kind is quite important because it is frequently encountered in various physical problems, particularly, in small oscillations and field quantization. To handle it, one can first transform it into Eq. (1.56) and then perform a Dirac diagonalization

to the latter, the total Dirac transformation being the product of the two successive transformations. That will be easier than handling Eq. (6.87) directly.

In the end, it is worth noting that all the conclusions of this section are valid for the time-polarized commutation relations,

$$[p_i, q_j] = i\delta_{ij}, \quad [p_i, p_j] = 0, \quad [q_i, q_j] = 0, \quad (6.88)$$

which can be seen readily by exchanging the roles of the group of p_i ($\forall i \in S \subset \{1, 2, \dots, n\}$) and the group of q_i ($\forall i \in S \subset \{1, 2, \dots, n\}$). This kind of abnormal commutation relations occurs in the quantization of Maxwell field, and will be discussed in Sec. VIIB

VII. FIELD QUANTA

In this section, we intend to examine field quanta, including Klein-Gordon field, phonon field, and Dirac field. In references, such problems are less addressed by BV or Dirac transformation. We find that they are pretty good tools for those problems.

A. Klein-Gordon field

Let us begin with the neutral Klein-Gordon field $\phi(\mathbf{x})$ [28, 29, 30]. Its Hamiltonian reads as follows,

$$H = \int d\mathbf{x} \frac{1}{2} \left\{ \pi^2(\mathbf{x}) + [\nabla \phi(\mathbf{x})]^2 + m^2 \phi^2(\mathbf{x}) \right\}, \quad (7.1)$$

where $m > 0$ is the mass of the field. The $\pi(\mathbf{x})$ is the momentum density conjugate to the field $\phi(\mathbf{x})$, they satisfy the canonical commutation rules,

$$[\pi(\mathbf{x}), \phi(\mathbf{x}')] = -i\delta(\mathbf{x} - \mathbf{x}'), \quad (7.2)$$

$$[\pi(\mathbf{x}), \pi(\mathbf{x}')] = 0, \quad (7.3)$$

$$[\phi(\mathbf{x}), \phi(\mathbf{x}')] = 0, \quad (7.4)$$

where $\delta(\mathbf{x})$ denotes Dirac delta function.

As usual, we would expand $\phi(\mathbf{x})$ and $\pi(\mathbf{x})$ into plane waves,

$$\phi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \phi(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}}, \quad (7.5)$$

$$\pi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \pi(\mathbf{p}) e^{-i\mathbf{p} \cdot \mathbf{x}}, \quad (7.6)$$

where we used the duality between $\phi(\mathbf{x})$ and $\pi(\mathbf{x})$. Physically, the $\phi(\mathbf{p})$ and $\pi(\mathbf{p})$ represent the complex collective coordinates and momenta of the system, respectively. As $\phi(\mathbf{x})$ and $\pi(\mathbf{x})$ are both real-valued fields,

$$\phi^\dagger(\mathbf{p}) = \phi(-\mathbf{p}), \quad (7.7)$$

$$\pi^\dagger(\mathbf{p}) = \pi(-\mathbf{p}). \quad (7.8)$$

In terms of $\phi(\mathbf{p})$ and $\pi(\mathbf{p})$, the Hamiltonian and canonical commutation rules can be expressed as follows,

$$H = \int d\mathbf{p} \frac{1}{2} [\pi^\dagger(\mathbf{p})\pi(\mathbf{p}) + (m^2 + \mathbf{p}^2) \phi^\dagger(\mathbf{p})\phi(\mathbf{p})], \quad (7.9)$$

$$[\pi(\mathbf{p}), \phi(\mathbf{p}')] = -i\delta(\mathbf{p} - \mathbf{p}'), \quad (7.10)$$

$$[\pi(\mathbf{p}), \pi(\mathbf{p}')] = 0, \quad (7.11)$$

$$[\phi(\mathbf{p}), \phi(\mathbf{p}')] = 0. \quad (7.12)$$

First of all, let us take a look at the equations of motion for $\phi(\mathbf{p})$ and $\pi(\mathbf{p})$, which can be derived from Eq. (7.9) and Eqs. (7.10)–(7.12),

$$i \frac{d}{dt} \phi(\mathbf{p}) = i\pi^\dagger(\mathbf{p}), \quad (7.13)$$

$$i \frac{d}{dt} \pi^\dagger(\mathbf{p}) = -i(m^2 + \mathbf{p}^2) \phi(\mathbf{p}). \quad (7.14)$$

They can be combined as

$$i \frac{d}{dt} \varphi(\mathbf{p}) = D(\mathbf{p})\varphi(\mathbf{p}), \quad (7.15)$$

where $\varphi(\mathbf{p})$ is the field operator,

$$\varphi(\mathbf{p}) = \begin{bmatrix} \pi^\dagger(\mathbf{p}) \\ \phi(\mathbf{p}) \end{bmatrix}, \quad (7.16)$$

and $D(\mathbf{p})$ the the dynamic matrix,

$$D(\mathbf{p}) = \begin{bmatrix} 0 & -i(m^2 + \mathbf{p}^2) \\ i & 0 \end{bmatrix}. \quad (7.17)$$

Obviously, the commutation rule for $\varphi(\mathbf{p})$ is

$$\varphi(\mathbf{p}) \cdot \varphi^\dagger(\mathbf{p}') = \delta(\mathbf{p} - \mathbf{p}')\Sigma_y, \quad (7.18)$$

where Σ_y is defined in Eq. (6.14).

The form of Eq. (7.15) hints us that the Hamiltonian H should be formulated with the field $\varphi(\mathbf{p})$,

$$H = \int d\mathbf{p} \frac{1}{2} \varphi^\dagger(\mathbf{p})M(\mathbf{p})\varphi(\mathbf{p}), \quad (7.19)$$

where $M(\mathbf{p})$ is the coefficient matrix,

$$M(\mathbf{p}) = \begin{bmatrix} 1 & 0 \\ 0 & m^2 + \mathbf{p}^2 \end{bmatrix}. \quad (7.20)$$

It is evident that

$$\varphi(-\mathbf{p}) = \widetilde{[\varphi^\dagger(\mathbf{p})]}, \quad (7.21)$$

$$D(\mathbf{p}) = \Sigma_y M(\mathbf{p}). \quad (7.22)$$

With those relations on hand, the following conclusions become self-evident.

1. The Hamiltonian of Eq. (7.9) is Diracianly diagonalizable if and only if $D(\mathbf{p})$ is physically diagonalizable.

2. If $D(\mathbf{p})$ is physically diagonalizable, the dynamic mode pair takes the form of $(\omega, v(\omega))$ and $(\omega, v(-\omega))$ where $v(-\omega) = v^*(\omega)$.

3. If $D(\mathbf{p})$ is physically diagonalizable, there exists an orthonormal basis with respect to the metric Σ_y . It generates a Dirac transformation as follows,

$$\varphi(\mathbf{p}) = T_d \psi(\mathbf{p}), \quad (7.23)$$

$$T_d = [v(\omega), v(-\omega)], \quad (7.24)$$

where

$$v^\dagger(\omega)\Sigma_y v(\omega) = 1, \quad (7.25)$$

$$v^\dagger(-\omega)\Sigma_y v(-\omega) = -1. \quad (7.26)$$

This implies that

$$T_d^\dagger \Sigma_y T_d = I_-, \quad (7.27)$$

and that

$$\psi(\mathbf{p}) \cdot \psi^\dagger(\mathbf{p}') = \delta(\mathbf{p} - \mathbf{p}')I_-. \quad (7.28)$$

4. The new field $\psi(\mathbf{p})$ has the involution symmetry,

$$\psi(-\mathbf{p}) = \left(\widetilde{\Sigma_x \psi(\mathbf{p})} \right)^\dagger. \quad (7.29)$$

This together with Eq. (7.28) means that $\psi(\mathbf{p})$ is a standard bosonic field, and assumes the following form,

$$\psi(\mathbf{p}) = \begin{bmatrix} a(\mathbf{p}) \\ a^\dagger(-\mathbf{p}) \end{bmatrix}, \quad (7.30)$$

where

$$[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = \delta(\mathbf{p} - \mathbf{p}'), \quad (7.31)$$

$$[a(\mathbf{p}), a(\mathbf{p}')] = 0, \quad (7.32)$$

$$[a^\dagger(\mathbf{p}), a^\dagger(\mathbf{p}')] = 0. \quad (7.33)$$

Those discussions demonstrate that the theory of Dirac diagonalization is also suitable for the complex collective coordinates and momenta.

It is easy to show that $D(\mathbf{p})$ has a pair of real eigenvalues,

$$\omega = \pm \varepsilon(\mathbf{p}) = \pm \sqrt{m^2 + \mathbf{p}^2}. \quad (7.34)$$

Since $D(\mathbf{p})$ is a square matrix of size 2, this means that $D(\mathbf{p})$ is physically diagonalizable. According to the above statement 1, the neutral Klein-Gordon field is Diracianly diagonalizable.

According to the above statements 2 and 3, the corresponding orthonormal eigenvectors can be chosen as

$$v(\varepsilon(\mathbf{p})) = \frac{1}{\sqrt{2\varepsilon(\mathbf{p})}} \begin{bmatrix} -i\varepsilon(\mathbf{p}) \\ 1 \end{bmatrix}, \quad (7.35)$$

$$v(-\varepsilon(\mathbf{p})) = \frac{1}{\sqrt{2\varepsilon(\mathbf{p})}} \begin{bmatrix} i\varepsilon(\mathbf{p}) \\ 1 \end{bmatrix}, \quad (7.36)$$

with the norms being

$$v^\dagger(\varepsilon(\mathbf{p}))\Sigma_y v(\varepsilon(\mathbf{p})) = 1, \quad (7.37)$$

$$v^\dagger(-\varepsilon(\mathbf{p}))\Sigma_y v(-\varepsilon(\mathbf{p})) = -1. \quad (7.38)$$

Finally, according to the above statements 3 and 4, the Dirac transformation can be constructed as follows,

$$\begin{bmatrix} \pi^\dagger(\mathbf{p}) \\ \phi(\mathbf{p}) \end{bmatrix} = \begin{bmatrix} v_1(\varepsilon(\mathbf{p})), & v_2(-\varepsilon(\mathbf{p})) \end{bmatrix} \begin{bmatrix} a(\mathbf{p}) \\ a^\dagger(-\mathbf{p}) \end{bmatrix}. \quad (7.39)$$

As a result, we have

$$\phi(\mathbf{p}) = \sqrt{\frac{1}{2\varepsilon(\mathbf{p})}} [a(\mathbf{p}) + a^\dagger(-\mathbf{p})], \quad (7.40)$$

$$\pi(\mathbf{p}) = -i\sqrt{\frac{\varepsilon(\mathbf{p})}{2}} [a(-\mathbf{p}) - a^\dagger(\mathbf{p})], \quad (7.41)$$

and

$$H = \int d\mathbf{p} \left[\varepsilon(\mathbf{p}) a^\dagger(\mathbf{p}) a(\mathbf{p}) + \frac{1}{2} \varepsilon(\mathbf{p}) \right]. \quad (7.42)$$

Substituting Eqs. (7.40) and (7.41) into Eqs. (7.5) and (7.6), and complementing them with the variable of time, we have

$$\begin{aligned} \phi(\mathbf{x}, t) = & \int d\mathbf{p} \sqrt{\frac{1}{2(2\pi)^3 \varepsilon(\mathbf{p})}} \left\{ a(\mathbf{p}) e^{i[\mathbf{p} \cdot \mathbf{x} - \varepsilon(\mathbf{p})t]} \right. \\ & \left. + a^\dagger(\mathbf{p}) e^{-i[\mathbf{p} \cdot \mathbf{x} - \varepsilon(\mathbf{p})t]} \right\}, \end{aligned} \quad (7.43)$$

$$\begin{aligned} \pi(\mathbf{x}, t) = & -i \int d\mathbf{p} \sqrt{\frac{\varepsilon(\mathbf{p})}{2(2\pi)^3}} \left\{ a(\mathbf{p}) e^{i[\mathbf{p} \cdot \mathbf{x} - \varepsilon(\mathbf{p})t]} \right. \\ & \left. - a^\dagger(\mathbf{p}) e^{-i[\mathbf{p} \cdot \mathbf{x} - \varepsilon(\mathbf{p})t]} \right\}. \end{aligned} \quad (7.44)$$

They are explicitly Lorentz covariant.

Evidently, all those results are the same as Refs. [28, 29, 30]. The charged Klein-Gordon field can be handled similarly.

Besides, we note that other complete sets of orthonormal functions, e.g., spherical waves, can be used instead of the plane waves to expand the fields if necessary.

For the neutral Klein-Gordon field, one can deal with the real collective coordinates and momenta as in Sec. VI if he expands the fields $\phi(\mathbf{x})$ and $\pi(\mathbf{x})$ with the real plane waves, i.e., $\{\sin(\mathbf{p} \cdot \mathbf{x}), \cos(\mathbf{p} \cdot \mathbf{x})\}$. He can transform back to the complex representation at the end of the calculation. That is rather tedious. In quantum mechanics and quantum field theory, complex waves and fields are unavoidable. That is the reason why we generalize the diagonalization theory given in Sec. VI to the case of complex collective coordinates and momenta.

B. Phonon field

For the neutral Klein-Gordon field, Eq. (7.9) shows that it belongs to the case that the matrices μ and κ in Eq. (6.87) are both positive definite. Physically, that is because it is massive, i.e., $m > 0$. There are also fields that belong to the other case where μ is positive definite but κ is nonnegative definite. A familiar example is the phonon field.

For the sake of brevity, we shall consider a simple three-dimensional lattice. As usual, we take the harmonic approximation [31, 32, 33], under which the Hamiltonian of the system becomes

$$\begin{aligned} H = & \frac{1}{2m} \sum_{\mathbf{l}, \alpha} p^\alpha(\mathbf{l}) p^\alpha(\mathbf{l}) \\ & + \frac{1}{2} \sum_{\mathbf{l}, \alpha} \sum_{\mathbf{l}', \beta} \Phi_{\alpha\beta}(\mathbf{l} - \mathbf{l}') u^\alpha(\mathbf{l}) u^\beta(\mathbf{l}'), \end{aligned} \quad (7.45)$$

where m is the mass of the atoms or ions, α and β denotes the x -, or y -, or z -component, \mathbf{l} is shortened for the lattice vector. The $\mathbf{u}(\mathbf{l})$ represents the phonon field, and $\mathbf{p}(\mathbf{l})$ the conjugate momentum field. They satisfy the canonical commutation rules,

$$[p^\alpha(\mathbf{l}), u^\beta(\mathbf{l}')] = -i\delta_{\mathbf{l}\mathbf{l}'}\delta_{\alpha\beta}, \quad (7.46)$$

$$[p^\alpha(\mathbf{l}), p^\beta(\mathbf{l}')] = 0, \quad (7.47)$$

$$[u^\alpha(\mathbf{l}), u^\beta(\mathbf{l}')] = 0. \quad (7.48)$$

The matrix $\Phi_{\alpha\beta}(\mathbf{l} - \mathbf{l}')$ stands for the interaction between the atoms or ions,

$$\Phi_{\alpha\beta}(\mathbf{l} - \mathbf{l}') = \left(\frac{\partial^2 \Phi}{\partial u_\alpha(\mathbf{l}) \partial u_\beta(\mathbf{l}')} \right)_0 = \Phi_{\beta\alpha}(\mathbf{l}' - \mathbf{l}), \quad (7.49)$$

where Φ is the elastic potential of the lattice, and the suffix 0 denotes the equilibrium configuration of the atoms or ions. Since the equilibrium configuration corresponds to the minimum of the potential, the matrix $\Phi_{\alpha\beta}(\mathbf{l} - \mathbf{l}')$ is nonnegative definite. Moreover, it fulfils the condition,

$$\sum_{\mathbf{l}} \Phi_{\alpha\beta}(\mathbf{l} - \mathbf{l}') = 0, \quad (7.50)$$

due to the translational symmetry of the lattice.

Using the collective coordinates $u^\alpha(\mathbf{k})$ and momenta $p^\alpha(\mathbf{k})$,

$$u^\alpha(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} u^\alpha(\mathbf{l}) e^{-i\mathbf{k} \cdot \mathbf{l}}, \quad (7.51)$$

$$p^\alpha(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} p^\alpha(\mathbf{l}) e^{i\mathbf{k} \cdot \mathbf{l}}, \quad (7.52)$$

we obtain

$$\begin{aligned} H = & \frac{1}{2m} \sum_{\mathbf{k}, \alpha} [p^\alpha(\mathbf{k})]^\dagger p^\alpha(\mathbf{k}) \\ & + \frac{1}{2} \sum_{\mathbf{k}, \alpha, \beta} \Phi_{\alpha\beta}(\mathbf{k}) [u^\alpha(\mathbf{k})]^\dagger u^\beta(\mathbf{k}), \end{aligned} \quad (7.53)$$

where

$$[p^\alpha(\mathbf{k}), u^\beta(\mathbf{k}')] = -i\delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\beta}, \quad (7.54)$$

$$[p^\alpha(\mathbf{k}), p^\beta(\mathbf{k}')] = 0, \quad (7.55)$$

$$[u^\alpha(\mathbf{k}), u^\beta(\mathbf{k}')] = 0, \quad (7.56)$$

and

$$\Phi_{\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{l}} \Phi_{\alpha\beta}(\mathbf{l})e^{-i\mathbf{k}\cdot\mathbf{l}}. \quad (7.57)$$

Here and hereafter in this subsection, all the vectors \mathbf{k} belong to the first Brillouin zone.

Since a simple lattice always has inversion symmetry, $\Phi_{\alpha\beta}(\mathbf{k})$ gets the following properties,

$$\Phi_{\alpha\beta}(\mathbf{k}) = \Phi_{\alpha\beta}^*(\mathbf{k}), \quad (7.58)$$

$$\Phi_{\alpha\beta}(\mathbf{k}) = \Phi_{\beta\alpha}(\mathbf{k}), \quad (7.59)$$

$$\Phi_{\alpha\beta}(-\mathbf{k}) = \Phi_{\alpha\beta}(\mathbf{k}). \quad (7.60)$$

The first two properties indicate that $\Phi_{\alpha\beta}(\mathbf{k})$ is a real symmetric matrix. Besides, $\Phi_{\alpha\beta}(\mathbf{k})$ is also a nonnegative matrix, just as $\Phi_{\alpha\beta}(\mathbf{l})$.

The Hamiltonian of Eq. (7.53) can be handled using the field,

$$\varphi(\mathbf{k}) = \begin{bmatrix} p^1(\mathbf{k}) \\ p^2(\mathbf{k}) \\ p^3(\mathbf{k}) \\ [u^1(\mathbf{k})]^\dagger \\ [u^2(\mathbf{k})]^\dagger \\ [u^3(\mathbf{k})]^\dagger \end{bmatrix}, \quad (7.61)$$

as in the proceeding subsection. However, it will be more convenient to follow the propositions 1 and 77. We therefore perform, first, a linear transformation that will make H diagonalized with regard to the new collective coordinates and momenta. As in Sec. 1B this transformation can be produced by the equations of motion of the coordinates $u_\alpha(\mathbf{k})$, exactly speaking, the following eigenvalue equation,

$$\omega^2 u^\alpha(\mathbf{k}) = \frac{1}{m} \sum_{\beta} \Phi_{\alpha\beta}(\mathbf{k}) u^\beta(\mathbf{k}). \quad (7.62)$$

As $\Phi_{\alpha\beta}(\mathbf{k})/m$ is a real, symmetric, and nonnegative matrix, it has three eigenvalues,

$$\omega_\sigma^2(\mathbf{k}) \geq 0, \quad \sigma = 1, 2, 3, \quad (7.63)$$

and a complete set of three orthonormal eigenvectors,

$$\sum_{\alpha} e_\sigma^\alpha(\mathbf{k}) e_{\sigma'}^\alpha(\mathbf{k}) = \delta_{\sigma\sigma'}, \quad (7.64)$$

$$\sum_{\sigma} e_\sigma^\alpha(\mathbf{k}) e_\sigma^\beta(\mathbf{k}) = \delta_{\alpha\beta}. \quad (7.65)$$

They are the so-called polarization vectors. One can further adjust these eigenvectors such that

$$\mathbf{e}_\sigma(\mathbf{k}) = \mathbf{e}_\sigma(-\mathbf{k}), \quad (7.66)$$

that is because $\Phi_{\alpha\beta}(-\mathbf{k}) = \Phi_{\alpha\beta}(\mathbf{k})$. According to Eqs. (1.54) and (1.55), $u^\alpha(\mathbf{k})$ and $p^\alpha(\mathbf{k})$ should be expanded as

$$u^\alpha(\mathbf{k}) = \sum_{\sigma} \phi_\sigma(\mathbf{k}) \frac{1}{\sqrt{m}} e_\sigma^\alpha(\mathbf{k}), \quad (7.67)$$

$$p^\alpha(\mathbf{k}) = \sum_{\sigma} \pi_\sigma(\mathbf{k}) \sqrt{m} e_\sigma^\alpha(\mathbf{k}), \quad (7.68)$$

where $\phi_\sigma(\mathbf{k})$ and $\pi_\sigma(\mathbf{k})$ are the new collective coordinates and momenta of the system. In terms of these new collective coordinates and momenta, Eq. (7.53) can be expressed as

$$H = \sum_{\mathbf{k}, \sigma} \left[\frac{1}{2} \pi_\sigma^\dagger(\mathbf{k}) \pi_\sigma(\mathbf{k}) + \frac{1}{2} \omega_\sigma^2(\mathbf{k}) \phi_\sigma^\dagger(\mathbf{k}) \phi_\sigma(\mathbf{k}) \right], \quad (7.69)$$

where

$$[\pi_\sigma(\mathbf{k}), \phi_{\sigma'}(\mathbf{k}')] = -i\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}, \quad (7.70)$$

$$[\pi_\sigma(\mathbf{k}), \pi_{\sigma'}(\mathbf{k}')] = 0, \quad (7.71)$$

$$[\phi_\sigma(\mathbf{k}), \phi_{\sigma'}(\mathbf{k}')] = 0, \quad (7.72)$$

and

$$\phi_\sigma^\dagger(\mathbf{k}) = \phi_\sigma(-\mathbf{k}), \quad \pi_\sigma^\dagger(\mathbf{k}) = \pi_\sigma(-\mathbf{k}). \quad (7.73)$$

The Hamiltonian of Eq. (7.69) is the same in form as that of Eq. (7.9), it can thus be treated as the latter. However, the photon field is massless,

$$\omega_\sigma(\mathbf{k}) \rightarrow 0, \quad \mathbf{k} \rightarrow 0, \quad (7.74)$$

which can be readily seen from Eqs. (7.50) and (7.57). Therefore, the Hamiltonian H is only partially diagonalizable, the components of $\mathbf{k} = 0$ can not be diagonalized. For $\mathbf{k} \neq 0$, the Dirac transformation is the same as Eqs. (7.40) and (7.41),

$$\phi_\sigma(\mathbf{k}) = \sqrt{\frac{1}{2\omega_\sigma(\mathbf{k})}} [a_\sigma(\mathbf{k}) + a_\sigma^\dagger(-\mathbf{k})], \quad (7.75)$$

$$\pi_\sigma(\mathbf{k}) = -i\sqrt{\frac{\omega_\sigma(\mathbf{k})}{2}} [a_\sigma(-\mathbf{k}) - a_\sigma^\dagger(\mathbf{k})]. \quad (7.76)$$

Under this transformation, the Hamiltonian becomes

$$H = \frac{1}{2} \sum_{\sigma} \pi_\sigma^2(\mathbf{0}) + \sum_{\mathbf{k} \neq 0} \sum_{\sigma} \left[\omega_\sigma(\mathbf{k}) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{1}{2} \omega_\sigma(\mathbf{k}) \right]. \quad (7.77)$$

That is the partially diagonalized form for the Hamiltonian of the photon field.

It is easy to show that $\pi_\sigma(\mathbf{0})$ ($\sigma = 1, 2, 3$) represent physically the momenta of the center of mass of the system. The partial diagonalization is thus not difficult to understand because the center of mass of the system behaviors as a free particle.

Remark 78 Usually, the components of $\mathbf{k} = 0$ are regarded to be diagonalizable as those of $\mathbf{k} \neq 0$. That is to say, the Dirac transformation,

$$\phi_\sigma(\mathbf{k}) = \sqrt{\frac{1}{2\omega_\sigma(\mathbf{k})}} [a_\sigma(\mathbf{k}) + a_\sigma^\dagger(-\mathbf{k})], \quad (7.78)$$

$$\pi_\sigma(\mathbf{k}) = -i\sqrt{\frac{\omega_\sigma(\mathbf{k})}{2}} [a_\sigma(-\mathbf{k}) - a_\sigma^\dagger(\mathbf{k})], \quad (7.79)$$

and the Hamiltonian

$$H = \sum_{\mathbf{k}, \sigma} \left[\omega_\sigma(\mathbf{k}) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{1}{2} \omega_\sigma(\mathbf{k}) \right]. \quad (7.80)$$

are taken to be appropriate for all \mathbf{k} [31, 32, 33]. Strictly speaking, that is not right, particularly in the discrete case (Notice that $\omega_\sigma(\mathbf{k})|_{\mathbf{k}=0} = 0$. The transformation becomes meaningless when $\mathbf{k} = 0$.) Nevertheless, it will cause no problem in the thermodynamic limit. That is because the state of $\mathbf{k} = 0$ has zero measure and contributes nothing to the integration over \mathbf{k} . You can change the values of an integrand on a null set at your will, that imposes no influence on the integration. Since one usually needs to take the thermodynamic limit finally in his calculation, it will be convenient to think that the total Hamiltonian is diagonalizable in this case. The same thing occurs in the photon field [28, 29, 30] and in the magnons of antiferromagnets [17, 18]. In the language of mathematics, those fields can be said to be diagonalizable almost everywhere.

All the discussions in this subsection are also valid for the diagonalization of the Maxwell field under Coulomb gauge. The diagonalization of the Maxwell field under Lorentz gauge will be discussed in Sec. VIII B.

C. Dirac field

Finally, let us consider the Dirac field [28, 29, 30]. It is a Fermi field, different from the two cases above. The Hamiltonian is

$$H = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) (-i\boldsymbol{\alpha} \cdot \nabla + \beta m) \psi(\mathbf{x}), \quad (7.81)$$

where m is the mass of the field, and

$$\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \quad (7.82)$$

with σ_i ($i = 1, 2, 3$) being Pauli's 2×2 matrices, and I the 2×2 unit matrix. The spinor fields, $\psi(\mathbf{x})$ and $\psi^\dagger(\mathbf{x})$, satisfy the anticommutation rules,

$$[\psi_\mu(\mathbf{x}), \psi_\nu^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}') \delta_{\mu\nu}, \quad (7.83)$$

$$[\psi_\mu(\mathbf{x}), \psi_\nu(\mathbf{x}')] = 0, \quad (7.84)$$

$$[\psi_\mu^\dagger(\mathbf{x}), \psi_\nu^\dagger(\mathbf{x}')] = 0. \quad (7.85)$$

As before, we can expand the fields $\psi(\mathbf{x})$ and $\psi^\dagger(\mathbf{x})$ with plane waves,

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \psi(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}}, \quad (7.86)$$

$$\psi^\dagger(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \psi^\dagger(\mathbf{p}) e^{-i\mathbf{p} \cdot \mathbf{x}}, \quad (7.87)$$

where

$$\psi(\mathbf{p}) = \begin{bmatrix} c_1(\mathbf{p}) \\ c_2(\mathbf{p}) \\ c_3(\mathbf{p}) \\ c_4(\mathbf{p}) \end{bmatrix}, \quad (7.88)$$

$$\psi^\dagger(\mathbf{p}) = [c_1^\dagger(\mathbf{p}), c_2^\dagger(\mathbf{p}), c_3^\dagger(\mathbf{p}), c_4^\dagger(\mathbf{p})]. \quad (7.89)$$

Substituting them into Eq. (7.81), we obtain

$$\begin{aligned} H &= \int d\mathbf{p} \psi^\dagger(\mathbf{p}) (\mathbf{p} \cdot \boldsymbol{\alpha} + m\beta) \psi(\mathbf{p}) \\ &= \int d\mathbf{p} \sum_{\mu, \nu} c_\mu^\dagger(\mathbf{p}) (\mathbf{p} \cdot \boldsymbol{\alpha} + m\beta)_{\mu\nu} c_\nu(\mathbf{p}), \end{aligned} \quad (7.90)$$

where

$$[c_\mu(\mathbf{p}), c_\nu^\dagger(\mathbf{p}')] = \delta(\mathbf{p} - \mathbf{p}') \delta_{\mu\nu}, \quad (7.91)$$

$$[c_\mu(\mathbf{p}), c_\nu(\mathbf{p}')] = 0, \quad (7.92)$$

$$[c_\mu^\dagger(\mathbf{p}), c_\nu^\dagger(\mathbf{p}')] = 0. \quad (7.93)$$

Since $\alpha_i^\dagger = \alpha_i$ and $\beta^\dagger = \beta$, H is a normal Hamiltonian that has been discussed in Sec. V A. According to the proposition 54, it can be diagonalized by the unitary transformation,

$$\psi(\mathbf{p}) = T_{\mathbf{p}} \varphi(\mathbf{p}), \quad (7.94)$$

where $T_{\mathbf{p}}$ is the unitary matrix,

$$T_{\mathbf{p}}^\dagger T_{\mathbf{p}} = T_{\mathbf{p}} T_{\mathbf{p}}^\dagger = I, \quad (7.95)$$

$$T_{\mathbf{p}}^\dagger (\mathbf{p} \cdot \boldsymbol{\alpha} + m\beta) T_{\mathbf{p}} = \text{diag}(\varepsilon(\mathbf{p}), \varepsilon(\mathbf{p}), -\varepsilon(\mathbf{p}), -\varepsilon(\mathbf{p})), \quad (7.96)$$

and $\varphi(\mathbf{p})$ the new field,

$$\varphi(\mathbf{p}) = \begin{bmatrix} d_1(\mathbf{p}) \\ d_2(\mathbf{p}) \\ d_3^\dagger(-\mathbf{p}) \\ d_4^\dagger(-\mathbf{p}) \end{bmatrix}, \quad (7.97)$$

Here, a particle-hole transformation has been performed for the negative energies.

After the transformation, H becomes

$$H = \int d\mathbf{p} \sum_{\mu=1}^4 \varepsilon(\mathbf{p}) d_\mu^\dagger(\mathbf{p}) d_\mu(\mathbf{p}), \quad (7.98)$$

where

$$[d_\mu(\mathbf{p}), d_\nu^\dagger(\mathbf{p}')] = \delta(\mathbf{p} - \mathbf{p}')\delta_{\mu\nu}, \quad (7.99)$$

$$[d_\mu(\mathbf{p}), d_\nu(\mathbf{p}')] = 0, \quad (7.100)$$

$$[d_\mu^\dagger(\mathbf{p}), d_\nu^\dagger(\mathbf{p}')] = 0. \quad (7.101)$$

As usual, the vacuum energy has been removed from the Hamiltonian [28, 29, 30].

In this section, the theory of transformation has been applied to examine totally three kinds of field quanta. As has been seen, it operates neatly and concisely.

VIII. MATHEMATICAL ESSENCE OF DIAGONALIZABILITY

Up to now, we regard BV or Dirac diagonalization as a physical consequence of the Heisenberg equation of motion. Diagonalization represents the normal modes of motion of a system. Such a view provides us a concrete picture and intuitive interpretation of diagonalization, and thus makes it easy to understand. However, there is yet another view, it is abstract but more fundamental. In this view, the diagonalization in itself is an intrinsic and invariant property of a Hermitian quadratic form that is equipped with commutator or Poisson bracket, neither Hamiltonian nor equation of motion will be needed any more.

A. Heisenberg operator

For simplicity, we shall take the Hamiltonian of Eq. (1.1) as an instance to explain this abstract view.

First, we regard Eq. (1.1) purely as a Hermitian form Q that is quadratic in creation and annihilation operators,

$$Q \triangleq \sum_{i,j=1}^n (\alpha_{ij} c_i^\dagger c_j + \frac{1}{2} \gamma_{ij} c_i^\dagger c_j^\dagger + \frac{1}{2} \gamma_{ji}^* c_i c_j). \quad (8.1)$$

And then we introduce a linear operator f to replace the Heisenberg equation of motion,

$$f(x) \triangleq i[Q, x], \quad (8.2)$$

where

$$x = \sum_{i=1}^n (z_i c_i + s_i c_i^\dagger), \quad z_i \in \mathbb{C}, \text{ and } s_i \in \mathbb{C}. \quad (8.3)$$

For convenience, we shall call f the Heisenberg operator. Obviously, we can define such a Heisenberg operator for each Hermitian quadratic form.

If one denotes the μ th component of the field ψ defined in Eq. (1.7) with ψ_μ , he obtains

$$if(\psi_\mu) = D_{\mu\nu} \psi_\nu, \quad (8.4)$$

where $D_{\mu\nu}$ are exactly the entries of the dynamic matrix D . In matrix notation, it can be written as

$$if(\psi) = D\psi, \quad (8.5)$$

which is the counterpart of Eq. (2.3).

By replacing H with Q and the Heisenberg equation with the Heisenberg operator f , one can readily show that all the lemmas, propositions, and theorems in Sec. II will still hold. Evidently, it is also true for the other cases, e.g., the Fermi system. Here and now, there is no Hamiltonian, no time, and no equation of motion. This demonstrates unambiguously that the BV or Dirac diagonalization is essentially the algebraic property of a quadratic Hermitian form. From this standpoint, any physical picture and interpretation are redundant and unnecessary, they have nothing to do with the self of the BV or Dirac diagonalization and can be completely removed away.

It follows immediately from this abstract view that all the conclusions of Sec. VI hold for classical systems, up to a real constant.

Such sublation enlarges the scope of the objects of diagonalization, it can be performed to all the Hermitian quadratic forms besides the physical Hamiltonians. To show this point of view more straightforwardly, let us look at the following example.

Example 79

$$J_z = xp_y - yp_x. \quad (8.6)$$

As well known, J_z is the orbital angular moment along the z -direction. It is quadratic in coordinates, i.e., x and y , and momenta, i.e., p_x and p_y . Since J_z is not a Hamiltonian, the Heisenberg equation of motion becomes meaningless. Nevertheless, it can be Diracianly diagonalized.

Solution 80 The dynamic matrix is

$$D = \Sigma_y M, \quad (8.7)$$

where M is the coefficient matrix,

$$M = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}. \quad (8.8)$$

There exists a pair of eigenvalues for D ,

$$\omega = \pm 1. \quad (8.9)$$

It is easy to show that each eigenvalue has two linearly independent eigenvectors, for example,

$$v_1(1) = \begin{bmatrix} 1 \\ i \\ 0 \\ 0 \end{bmatrix}, \quad v_2(1) = \begin{bmatrix} 0 \\ 0 \\ 1 \\ i \end{bmatrix}. \quad (8.10)$$

They can be linearly combined and orthonormalized as follows,

$$v_1(1) = \frac{1}{2} \begin{bmatrix} 1 \\ i \\ i \\ -1 \end{bmatrix}, \quad v_2(1) = \frac{1}{2} \begin{bmatrix} 1 \\ i \\ -i \\ 1 \end{bmatrix}, \quad (8.11)$$

with the norms being

$$v_1^\dagger(1)\Sigma_y v_1(1) = 1, \quad v_2^\dagger(1)\Sigma_y v_2(1) = -1. \quad (8.12)$$

Correspondingly, the Dirac transformation will be

$$\begin{bmatrix} p_x \\ p_y \\ x \\ y \end{bmatrix} = [v_1(1), v_2(-1), v_1(-1), v_2(1)] \begin{bmatrix} a_1 \\ a_2 \\ a_1^\dagger \\ a_2^\dagger \end{bmatrix}, \quad (8.13)$$

where

$$v_1(-1) = v_1^*(1), \quad v_2(-1) = v_2^*(1). \quad (8.14)$$

Finally, the diagonalized form of J_z is

$$J_z = a_1^\dagger a_1 - a_2^\dagger a_2. \quad (8.15)$$

This result is quite similar to the coupled boson representation for angular momentum due to Schwinger [34, 35]. It is rigorous, concise, and agrees exactly with the familiar result about the orbital angular momentum, i.e., the eigenvalues of J_z consists of all the integers.

There is another interesting example.

Example 81

$$H = -\frac{p^2}{2m} - \frac{1}{2}m\omega^2 q^2, \quad (8.16)$$

where $m > 0$ and $\omega > 0$.

Formally, it looks like a “negative harmonic oscillator”. Of course, it can not represent a real physical system. Thereby we treat it just as a Hermitian quadratic form. It is ready to conjecture that this quadratic form would be diagonalized, by the same Dirac transformation as for the normal harmonic oscillator.

Solution 82 The dynamic matrix is

$$D = \Sigma_y M, \quad (8.17)$$

where M is the coefficient matrix,

$$M = \begin{bmatrix} -\frac{1}{m} & 0 \\ 0 & -m\omega^2 \end{bmatrix}. \quad (8.18)$$

The dynamic matrix D has a pair of eigenvalues,

$$\varepsilon = \pm\omega. \quad (8.19)$$

and two orthonormal eigenvectors,

$$v(\omega) = \frac{1}{\sqrt{2m\omega}} \begin{bmatrix} im\omega \\ 1 \end{bmatrix}, \quad (8.20)$$

$$v(-\omega) = \frac{1}{\sqrt{2m\omega}} \begin{bmatrix} -im\omega \\ 1 \end{bmatrix}, \quad (8.21)$$

$$v^\dagger(\omega)\Sigma_y v(\omega) = -1, \quad (8.22)$$

$$v^\dagger(-\omega)\Sigma_y v(-\omega) = 1. \quad (8.23)$$

They generate a Dirac transformation,

$$p = -i\sqrt{\frac{m\omega}{2}}(a - a^\dagger), \quad (8.24)$$

$$q = \frac{1}{\sqrt{2m\omega}}(a + a^\dagger). \quad (8.25)$$

They are the same as Eqs. (6.62) and (6.63). The diagonalized form is

$$H = -\omega a^\dagger a - \frac{1}{2}\omega. \quad (8.26)$$

Those results confirm our conjecture completely.

This example reminds us that the two propositions [1] and [77] also hold for the case where μ is negative definite and κ is nonpositive definite, no matter whether the commutation rules are standard, or time-polarized, or mixing. This fact will be useful in the following subsection.

B. Time-polarized photons

In this subsection, we shall concern ourselves with the diagonalization of the Maxwell field under Lorentz gauge.

As well known, the Maxwell field contains two spurious degrees of freedom in Lorentz gauge, viz., the longitudinal and time-polarized components. Because these degrees of freedom are not of physical quantity, the Hamiltonian is merely a Hermitian quadratic form. The abstract view of diagonalization finds its way and role here.

In Lorentz gauge, the Hamiltonian of Maxwell field has the form [28, 29, 30],

$$H = -\frac{1}{2} \int d\mathbf{x} [\pi^\mu(\mathbf{x})\pi_\mu(\mathbf{x}) + \nabla A^\mu(\mathbf{x}) \cdot \nabla A_\mu(\mathbf{x})], \quad (8.27)$$

where $A^\mu(\mathbf{x})$ ($\mu = 0, 1, 2, 3$) are the vector potentials, and $\pi^\mu(\mathbf{x})$ the corresponding canonical conjugate fields. They satisfy the following commutation rules,

$$[A^\mu(\mathbf{x}), \pi^\nu(\mathbf{x}')] = ig^{\mu\nu}\delta(\mathbf{x} - \mathbf{x}'), \quad (8.28)$$

$$[A^\mu(\mathbf{x}), A^\nu(\mathbf{x}')] = 0, \quad (8.29)$$

$$[\pi^\mu(\mathbf{x}), \pi^\nu(\mathbf{x}')] = 0, \quad (8.30)$$

where $g^{\mu\nu}$ is the metric tensor,

$$g^{\mu\nu} = \begin{bmatrix} 1 & & 0 \\ & -1 & \\ 0 & & -1 & \\ & & & -1 \end{bmatrix}. \quad (8.31)$$

Equations (8.28)–(8.30) indicate that the Hamiltonian H belongs to the mixing case where there are both the standard and time-polarized commutation relations simultaneously. Physically, that roots from the requirement of Lorentz covariance.

Expanding these fields with plane waves,

$$A^\mu(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} A^\mu(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}}, \quad (8.32)$$

$$\pi^\mu(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \pi^\mu(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}}, \quad (8.33)$$

we obtain

$$H = -\frac{1}{2} \int d\mathbf{x} \left\{ [\pi^\mu(\mathbf{p})]^\dagger \pi_\mu(\mathbf{p}) + \mathbf{p}^2 [A^\mu(\mathbf{p})]^\dagger A_\mu(\mathbf{p}) \right\}, \quad (8.34)$$

where

$$[A^\mu(\mathbf{p}), \pi^\nu(\mathbf{p}')] = ig^{\mu\nu} \delta(\mathbf{p} - \mathbf{p}'), \quad (8.35)$$

$$[A^\mu(\mathbf{p}), A^\nu(\mathbf{p}')] = 0, \quad (8.36)$$

$$[\pi^\mu(\mathbf{p}), \pi^\nu(\mathbf{p}')] = 0, \quad (8.37)$$

and

$$[A^\mu(\mathbf{p})]^\dagger = A^\mu(-\mathbf{p}), \quad (8.38)$$

$$[\pi^\mu(\mathbf{p})]^\dagger = \pi^\mu(-\mathbf{p}). \quad (8.39)$$

Just like the phonon field, the polarization vectors can be obtained from the eigenvalue equation for the fields $A^\mu(\mathbf{p})$,

$$\omega^2 \phi(\mathbf{p}) = D(\mathbf{p}) \phi(\mathbf{p}), \quad (8.40)$$

where

$$\phi(\mathbf{p}) = \begin{bmatrix} A^0(\mathbf{p}) \\ A^1(\mathbf{p}) \\ A^2(\mathbf{p}) \\ A^3(\mathbf{p}) \end{bmatrix}, \quad (8.41)$$

and

$$D(\mathbf{p}) = \begin{bmatrix} \mathbf{p}^2 & & 0 \\ & \mathbf{p}^2 & \\ 0 & & \mathbf{p}^2 & \\ & & & \mathbf{p}^2 \end{bmatrix}. \quad (8.42)$$

Paying attention to the fact that $D(\mathbf{p}) = \mathbf{p}^2 I$, the orthonormal basis for the polarization vectors can be chosen, except $\mathbf{p} = 0$, as follows,

$$\epsilon(\mathbf{p}, 0) = (1, 0, 0, 0), \quad (8.43)$$

$$\epsilon(\mathbf{p}, i) = (0, \mathbf{e}_i(\mathbf{p})), \quad (8.44)$$

where

$$\mathbf{e}(\mathbf{p}, 3) = \frac{\mathbf{p}}{|\mathbf{p}|}, \quad (8.45)$$

$$\mathbf{e}_i(\mathbf{p}) \cdot \mathbf{e}_j(\mathbf{p}) = \delta_{ij}, \quad i = 1, 2, 3. \quad (8.46)$$

That is to say, $\epsilon(\mathbf{p}, 0)$ is the time-like polarization vector, $\epsilon(\mathbf{p}, i)$ ($i = 1, 2$) the space-like transverse polarization vectors, and $\epsilon(\mathbf{p}, 3)$ the space-like longitudinal polarization vector. Obviously,

$$\epsilon^\mu(\mathbf{p}, \lambda) \epsilon_\mu(\mathbf{p}, \lambda') = g_{\lambda\lambda'}, \quad (8.47)$$

i.e., the polarization vectors form a four-dimensional orthonormal system. Using this new basis, the Hamiltonian can be expressed as

$$H = \frac{1}{2} \int d\mathbf{p} \left\{ \sum_{\lambda=1}^3 \left([\pi_\lambda(\mathbf{p})]^\dagger \pi_\lambda(\mathbf{p}) + \mathbf{p}^2 [A_\lambda(\mathbf{p})]^\dagger A_\lambda(\mathbf{p}) \right) - \left([\pi_0(\mathbf{p})]^\dagger \pi_0(\mathbf{p}) + \mathbf{p}^2 [A_0(\mathbf{p})]^\dagger A_0(\mathbf{p}) \right) \right\}, \quad (8.48)$$

where

$$[A_\lambda(\mathbf{p}), \pi_{\lambda'}(\mathbf{p}')] = ig_{\lambda\lambda'} \delta(\mathbf{p} - \mathbf{p}'), \quad (8.49)$$

$$[A_\lambda(\mathbf{p}), A_{\lambda'}(\mathbf{p}')] = 0, \quad (8.50)$$

$$[\pi_\lambda(\mathbf{p}), \pi_{\lambda'}(\mathbf{p}')] = 0, \quad (8.51)$$

and

$$[A_\lambda(\mathbf{p})]^\dagger = A_\lambda(-\mathbf{p}), \quad (8.52)$$

$$[\pi_\lambda(\mathbf{p})]^\dagger = \pi_\lambda(-\mathbf{p}). \quad (8.53)$$

It is worth noting that the time-like components, $A_0(\mathbf{p})$ and $\pi_0(\mathbf{p})$, constitute a “negative harmonic oscillator”.

According to Sec. VII A, H can be diagonalized by the following Dirac transformation,

$$A_\lambda(\mathbf{p}) = \sqrt{\frac{1}{2\varepsilon(\mathbf{p})}} \left[a_\lambda(\mathbf{p}) + a_\lambda^\dagger(-\mathbf{p}) \right], \quad (8.54)$$

$$\pi_\lambda(\mathbf{p}) = i\sqrt{\frac{\varepsilon(\mathbf{p})}{2}} \left[a_\lambda(-\mathbf{p}) - a_\lambda^\dagger(\mathbf{p}) \right], \quad (8.55)$$

where

$$\varepsilon(\mathbf{p}) = |\mathbf{p}|, \quad (8.56)$$

and

$$[a_\lambda(\mathbf{p}), a_{\lambda'}^\dagger(\mathbf{p}')] = -g_{\lambda\lambda'} \delta(\mathbf{p} - \mathbf{p}'), \quad (8.57)$$

$$[a_\lambda(\mathbf{p}), a_{\lambda'}(\mathbf{p}')] = 0, \quad (8.58)$$

$$[a_\lambda^\dagger(\mathbf{p}), a_{\lambda'}^\dagger(\mathbf{p}')] = 0. \quad (8.59)$$

Here, as usual, the commutation rules for the transverse and longitudinal polarizations ($\lambda = 1, 2, 3$) are chosen as normal or standard; those for the time-like polarizations ($\lambda = 0$) are chosen as abnormal or time-polarized. The

abnormal bosons here are usually called scalar or time-polarized photons. That is also the reason why we call the particles satisfying Eq. (2.238) the time-polarized bosons. The diagonalized form of the Hamiltonian is

$$H = \int d\mathbf{p} \varepsilon(\mathbf{p}) \left[\sum_{\lambda=1}^3 a_{\lambda}^{\dagger}(\mathbf{p}) a_{\lambda}(\mathbf{p}) - a_0^{\dagger}(\mathbf{p}) a_0(\mathbf{p}) \right], \quad (8.60)$$

where the vacuum energy has been removed from the Hamiltonian. This equation holds in the sense that the Hamiltonian is Diracian diagonalizable almost everywhere in momentum space (except $\mathbf{p} = 0$).

Finally, the quantized fields can be written as

$$A^{\mu}(x) = \int d\mathbf{p} \sqrt{\frac{1}{2(2\pi)^3 \varepsilon(\mathbf{p})}} \sum_{\lambda=0}^3 \epsilon^{\mu}(\mathbf{p}, \lambda) \times \left[a_{\lambda}(\mathbf{p}) e^{ip \cdot x} + a_{\lambda}^{\dagger}(\mathbf{p}) e^{-ip \cdot x} \right], \quad (8.61)$$

$$\pi^{\mu}(x) = i \int d\mathbf{p} \sqrt{\frac{\varepsilon(\mathbf{p})}{2(2\pi)^3}} \sum_{\lambda=0}^3 \epsilon^{\mu}(\mathbf{p}, \lambda) \times \left[a_{\lambda}(\mathbf{p}) e^{ip \cdot x} - a_{\lambda}^{\dagger}(\mathbf{p}) e^{-ip \cdot x} \right]. \quad (8.62)$$

It can be readily seen that all those results are the same as Refs. [28, 29, 30].

The diagonalization of the Maxwell field under Lorentz gauge is rather complicated. First, it contains unphysical degrees of freedom. Second, it needs mixing commutation relations, both for initial and final fields. And third, it is not diagonalizable everywhere but almost everywhere. One sees that those problems can be resolved naturally by the diagonalization theory developed in this review.

IX. CONCLUSIONS

In this review, a theory of transformation is set up for the diagonalization of the Hermitian quadratic form that

is equipped with commutator or Poisson bracket.

The theory is dynamic matrix oriented.

The dynamic matrix can be derived from the Hermitian quadratic form through the Heisenberg operator. Each Hermitian quadratic form has a dynamic matrix of its own.

The Bogoliubov-Valatinian or Diracian diagonalizability of a Hermitian quadratic form is equivalent to the physical diagonalizability of its dynamic matrix. That is to say, the diagonalization of a Hermitian quadratic form is essentially an eigenvalue problem of its dynamic matrix.

The dynamic matrix is always physically diagonalizable for a fermionic form. It may or may not be physically diagonalizable for a bosonic form. Accordingly, the diagonalization exists and is unique for a fermionic form, forever. It exists and is unique for a bosonic form only if the dynamic matrix is physically diagonalizable.

The dynamic matrix is the generator of the Bogoliubov-Valatin or Dirac transformation. The transformation required for diagonalization can be constructed immediately from the complete set of the orthonormal eigenvectors of the dynamic matrix, according to a standard algebraic procedure.

In a word, the eigenvalue problem of the dynamic matrix determines the diagonalizability of a Hermitian quadratic form, definitely and completely.

Finally, it is worth emphasizing that the quadratic Hamiltonian is just regarded as a Hermitian quadratic form in this review, i.e., only its mathematical properties are considered here. The physical instability as well as phase transitions of a system has not been concerned at all. That in itself is another intriguing problem, please refer to Ref. [36].

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I want a basis $\{\eta_0, \dots, \eta_{2m-1}\}$ of V_0 st

- orthonormal $\phi(\eta_i, \eta_j) = \lambda_i \delta_{ij}$ with $\lambda_i = \pm 1$

- $\eta_i = \sum_{\substack{x \\ x \in \{0, \dots, m-1\}}} \eta_{i+m}$ $i = 0, \dots, m-1$

— 0 —

$\mu=1$

$$V_0 = \langle v_0, v_1 \rangle$$

$$J = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\text{Lemma 17} \rightarrow v_1 = \sum_x v_0^*$$

$$\begin{aligned} \phi(v_0, v_1) &= v_0^+ \mathbb{I} \sum_x v_0^* = \widetilde{v_0}^* (\mathbb{I} \sum_x) v_0^* = \\ &= \widetilde{v_0}^* \begin{bmatrix} v_{0,2/2}^* \\ -v_{0,1/2}^* \end{bmatrix} = v_{0,1/2}^* v_{0,2/2}^* - v_{0,2/2}^* v_{0,1/2}^* = 0 \end{aligned}$$

$$\uparrow v_0^* = \begin{bmatrix} v_{0,1/2}^* \\ v_{0,2/2}^* \end{bmatrix}$$

$$\mapsto \phi(v_0, v_0) \neq 0 \rightarrow \phi(v_i, v_i) \neq 0 \quad (\text{otherwise } \mathbb{I} \text{ null on } V_0)$$

\rightarrow As soon as normalize all props are sat.

$\mu=2$

- Assume $\exists v_0 \mid \|v_0\| \neq 0 \rightarrow$ can construct $\eta_2 = \sum_x v_0^*$

Now want to build η_1 and $\eta_3 \mid \begin{cases} \text{orthogonal to } v_{0,2} \text{ and } e_0 \\ \eta_3 = \sum_x \eta_1^* \end{cases}$

$$\eta_1 \equiv v_1 - \frac{\phi(v_1, v_0)}{\phi(v_0, v_0)} v_0$$

$$\begin{aligned} \hookrightarrow \phi(\eta_2, \eta_1) &= \eta_2^+ \mathbb{I} \eta_1 = \widetilde{\eta_2}^* \mathbb{I} \eta_1 = (\sum_x v_0) \mathbb{I} \eta_1 = \\ &= \widetilde{v_0} \sum_x \mathbb{I} \eta_1 = -\widetilde{v_0} \mathbb{I} \sum_x \eta_1 = \\ &= -\widetilde{v_0} J v_1 + \frac{\phi(v_1, v_0)}{\phi(v_0, v_0)} \widetilde{v_0} J v_0 = -\widetilde{v_0} J v_1 \end{aligned}$$