Time-dependent HFB in the quasiparticle representation

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Abstract

These notes present a derivation of the time-dependent Hartree-Fock-Bogoliubov (TDHFB) equation in the quasiparticle representation. That representation is also convenient for deriving some approximate treatments of TDHFB, namely adiabatic TDHFB, QRPA, and Nakatsukasa's method to solve the QRPA equations numerically.

I. NOTATION

The notation follows Ring and Schuck [1]. The Bogoliubov transformation between Fock-space operators $a^\dagger, a$ in the orbital space and quasiparticle operators $\beta^\dagger, \beta$ is given by

$$\begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{bmatrix} U & V^* \\ V & U^* \end{bmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \equiv \mathcal{W} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} . \tag{1}$$

Note that $\mathcal{W}$ is a unitary matrix. For an orbital space of dimension N, the U and V matrices have the same dimension and $\mathcal{W}$ has dimension $2N$. We will write $|uv\rangle$ for the quasiparticle vacuum wave function corresponding to the Bogoliubov transformation U, V.

The Hamiltonian[2] is of the form

$$\hat{H} = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{i>j,k>l} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + ... \tag{2}$$

In the quasiparticle representation, the Hamiltonian is expressed as a sum of terms, each containing a normally ordered product of $\beta^\dagger$ and β operators as

$$\hat{H} = H^{00} + (\sum_{i>j} H^{20}_{ij} \beta_i^\dagger \beta_j^\dagger + h.c.) + \sum_{ij} H^{11}_{ij} \beta_i^\dagger \beta_j + \sum_{ijkl} (H^{40}_{ijkl} \beta_i^\dagger \beta_j^\dagger \beta_k^\dagger \beta_l^\dagger + h.c.) + \tag{3}$$
$$+ \sum_{i>j,k>l} (H^{22}_{ijlk} \beta_i^\dagger \beta_j^\dagger \beta_l \beta_k + h.c.) + ...$$

The superscript shows the number of creation and annihilation operators associated with each term. The ellipses indicate higher order terms that are not needed in the derivations below. The formulas for the various terms in Eq. (3) are given in Ref. [1], Eq. (E.20-23). The specific matrix elements that will be needed are

$$\langle uv | \beta_j \beta_i \hat{H} | uv \rangle = H^{20}_{ij} \tag{4}$$

$$\langle uv | \beta_j \beta_i \hat{H} \beta_l^\dagger \beta_k^\dagger | uv \rangle = H^{22}_{ijkl} + \delta_{jl} H^{11}_{ik} + \delta_{ik} H^{11}_{jl} - \delta_{jk} H^{11}_{il} - \delta_{il} H^{11}_{jk} + \delta_{ik} \delta_{jl} H^{00} \tag{5}$$

$$\langle uv | \beta_l \beta_k \beta_j \beta_i \hat{H} | uv \rangle = \sum_P H^{40}_{ijkl}. \tag{6}$$

Here we have assumed $i > j$ and $k > l$ and the sum in the last equation is over permutations of $ijkl$. The compute code for evaluating H^{20} in terms of the U, V matrix in Eq. (4) is also at the heart of the gradient method for solving the static HFB equations[1, Sec. 7.3.3],[7].

II. DERIVATION OF THE TIME-DEPENDENT HFB APPROXIMATION

The time-dependent HFB equations are usually presented in the physical representation and that is indeed most convenient for computations. Pedagogically, the derivation in the quasiparticle representation is quite transparent and good starting point for various approximations. This method was used by Schütte in Ref. [3] as a basis for discussing the adiabaticity of nuclear collective dynamics.

and is also closely related to the gradient method for finding the HFB minima.

The full equation of motion, $i\partial/\partial t|\Psi\rangle = \hat{H}|\Psi\rangle$, cannot be solved exactly in the space of HFB wave functions. But within that space, we seek an approximation of the form

$$i\frac{\partial}{\partial t}|u_t v_t\rangle \approx \hat{H}|u_t v_t\rangle. \tag{7}$$

From now on we will label the HFB wave functions by the time variable, $|t\rangle = |u_t v_t\rangle$. By the generalized Thouless theorem, we can express the left-hand side as a 2-quasiparticle excitation of the instantaneous HFB wave function, i.e.

$$i\frac{\partial}{\partial t}|t\rangle = \sum_{i>j} Z_{ij}\beta_i^\dagger\beta_j^\dagger|t\rangle$$

for some matrix Z. To determine it, we take the overlap of Eq. (7) with a set of bra states and demand that the matrix elements are equal. This can be imposed for all bra states of the form of 2-quasiparticle excitations of the instantaneous vacuum, $\langle t|\beta_i\beta_j$. Thus

$$\langle t|\beta_i\beta_j i\frac{\partial}{\partial t}|t\rangle = Z_{ij} = \langle t|\beta_i\beta_j\hat{H}|t\rangle = H^{20}_{ij}. \tag{8}$$

The time-dependent wave function may be expanded for short times Δt as

$$|t+\Delta t\rangle = |t\rangle + i\Delta t\sum_{i>j} H^{20}_{ij}\beta_i^\dagger\beta_j^\dagger|0\rangle + ... \tag{9}$$

A formal expression for the integration to finite time is

$$|t\rangle = T\exp\left(i\int_0^t dt'\sum_{i>j} H^{20}_{ij}(t')\beta_i^\dagger(t')\beta_j^\dagger(t')\right)|0\rangle \tag{10}$$

where T is the time-ordering operator. Note that the quasiparticle operators depend on time since they are referenced to the instantaneous HFB state. If $|0\rangle$ is close to an HFB minimum, $H^{20} = Z$ will be parametrically small, and we can consider expanding the wave function in powers of Z. This leads to the QRPA, derived in the next section. Another approximation, the adiabatic TDHFB, may be derived by considering the evolution for small time intervals. This is treated in Section V below.

III. DERIVATION OF QRPA AS THE SMALL-AMPLITUDE LIMIT OF TDHFB

To derive the QRPA from the HFB equation of motion Eq. (8), we assume Z to be small and consider only terms in the wave function up to order Z. The resulting equations are linear and the solutions will be sinusoidal. Let us write the wave function associated with frequency ω as

$$|t\rangle \approx |0\rangle + \sum_{i>j} (Z^r_{ij}\cos\omega t + iZ^i_{ij}\sin\omega t)\beta^\dagger_i\beta^\dagger_j|0\rangle. \tag{11}$$

Here Z^r and Z^i are real matrices, and $|0\rangle$ is a static solution to the HFB equation[5]. The left-hand side of Eq. (8) takes the form

$$i\langle t|\tilde\beta_i\tilde\beta_j\frac{\partial}{\partial t}|t\rangle = \tag{12}$$

$$\omega\langle 0|\left(1+\sum_{k>l}(Z^r_{ij}\cos\omega t - iZ^i_{ij}\sin\omega t)\beta_l\beta^\dagger_k\right)\tilde\beta_i\tilde\beta_j\left(\sum_{k>l}(-Z^r_{kl}\sin\omega t + iZ^i_{kl}\cos\omega t)\beta^\dagger_i\beta^\dagger_j\right)|0\rangle.$$

Here a distinction was made between the quasiparticle operators associated with the instantaneous state $\tilde\beta$ and those associated with the static HFB state (without tildes). In fact they are the same to zeroth order in Z. We carry out the contractions on the right-hand side of Eq. (10) and find to linear order in Z

$$i\langle t|\tilde\beta_i\tilde\beta_j\frac{\partial}{\partial t}|t\rangle = -i\omega Z^r_{ij}\sin\omega t + \omega Z^i_{ij}\cos\omega t. \tag{13}$$

The right-hand side of Eq. (8) expands to

$$\langle t|\tilde\beta_i\tilde\beta_j\hat H|t\rangle = \tag{14}$$

$$\langle 0|\left(1+\sum_{k>l}(Z^r_{ij}\cos\omega t - iZ^i_{ij}\sin\omega t)\beta_l\beta^\dagger_k\right)\tilde\beta_i\tilde\beta_j\hat H\left(1+\sum_{k>l}(Z^r_{ij}\cos\omega t + iZ^i_{ij}\sin\omega t)\beta_l\beta^\dagger_k\right)|0\rangle$$

Here to keep all terms linear in Z we also have to expand $\tilde\beta\tilde\beta$,

$$\tilde\beta_i\tilde\beta_j = (\beta_i - \sum Z_{ik}\beta^\dagger_k)(\beta_j - \sum Z_{jl}\beta^\dagger_l) = \beta_i\beta_j - Z_{ij} + \text{higher order terms} \tag{15}$$

Carrying out the contractions gives

$$\langle t|\tilde\beta_i\tilde\beta_j\hat H|t\rangle = \cos\omega t\left(\sum_{k>l}(\bar H^{22}_{klij} + H^{40}_{klij})Z^r_{kl}\right) + i\sin\omega t\left(\sum_{k>l}(\bar H^{22}_{klij} - H^{40}_{klij})Z^i_{kl}\right) \tag{16}$$

where $\bar{H}^{22}_{ijkl}$ is a shorthand notation for $\langle 0|\beta_i\beta_j\hat{H}\beta^\dagger_k\beta^\dagger_l|0\rangle - H^{00}\delta_{ik}\delta_{kl}$. Equating the real and imaginary parts of L and R yields two matrix equations, one for the coefficient of $\cos\omega t$ and one for the coefficient of $\sin\omega t$. The equations are

$$\omega Z^i = \sum_{k>l}(\bar{H}^{22}_{klij} + H^{40}_{klij})Z^r_{kl} \quad \text{and} \tag{17}$$

$$\omega Z^r = \sum_{k>l}(\bar{H}^{22}_{klij} - H^{40}_{klij})Z^i_{kl} \tag{18}$$

To make the connection with the usual form of the RPA matrix equations, we change the notation to

$$X = Z^r + Z^i; \quad Y = Z^r - Z^i \tag{19}$$

$$A = \bar{H}^{22}; \quad B = H^{40}$$

X and Y are vectors indexed by the 2-quasiparticle label ij and A, B are matrices in that space. Note that the dimension of the space is $N(N-1)/2$ where N is the dimension of the orbital space.

The coupled equations Eq. (17,17) take the familiar form

$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}. \tag{20}$$

IV. SOLUTION OF QRPA BY THE FINITE AMPLITUDE METHOD

The straightforward implementation of the A, B matrix equations for QRPA requires very large computer resources due to the rank-4 tensor structure of the Hamiltonian operator together with the dense matrix character of A and B. In fact, the main interest is in the lowest few eigenstates and more efficient methods are possible. The method proposed by Avagadro and Nakatsukasa [4] is particularly promising. Like the method proposed for RPA in Ref. [6], it can directly use the computational modules that are used to solve the corresponding time-dependent equation. The connection is very simple in the quasiparticle basis. The basic idea is use numerical differentiation to compute the right-hand sides of Eq. (17). We may assume that the code carrying out the time-dependent evolution uses complex arithmetic. Then we need only H^{20} for the states $|re\rangle$ and $|im\rangle$ generated from $|0\rangle$ by the transformations Z^r and $+iZ^i$, respectively. The calculated H^{20} matrix elements are

$$\langle re|\beta_i\beta_j\hat{H}|re\rangle \approx \sum_{k>l}(\bar{H}^{22}_{klij} + H^{40}_{kl})Z^r_{kl} \tag{21}$$

$$\langle im|\beta_i\beta_j\hat{H}|im\rangle \approx \sum_{k>l}(\bar{H}^{22}_{klij} - H^{40}_{kl})Z^i_{kl}.$$

The left-hand sides are the vectors created by applying the QRPA A and B matrices to the vectors Z^r and Z^i as in Eq. (18). Then the eigenvectors and eigenenergy can be found by some iterative Krylov space method such as the Lanczos algorithm.

V. ATDHFB

The adiabatic time-dependent HFB is a method to construct the inertial dynamics associated with a given path in the space of static HFB configurations. Usually the path is constructed by the generator coordinate method. One defines a collective variable by the expectation of some one-body operator. The configurations are generated by the constraining the HFB wave function appropriately.

We examine the short-time behavior of the wave function around a starting configuration located at some point along the collective coordinate. In the QRPA we assumed that the time dependence was sinusoidal, here we expand it in a power series in the time variable. The imaginary part of Z does not affect the density at $t = 0$ and so can be nonzero; we write $Z^i_{ij} = P_{ij} + \mathcal{O}(t^2)$. On the other hand, the real part of Z must be zero at $t + 0$ to preserve the starting density at $t = 0$; we write $Z^r_{ij} = tQ_{ij} + \mathcal{O}(t^3)$. Thus we take the wave function to be

$$|t\rangle = (1 + \sum_{i>j}(iP_{ij} + tQ_{ij})\beta^\dagger_i\beta^\dagger_j)|0\rangle \tag{22}$$

with P, Q real matrices. The wave function is inserted into the equation of motion and we follow the same steps as in the derivation of the QRPA equations. The result is very similar to Eq. (17),

$$(\bar{H}^{22} - H^{40})P^i = Q^r. \tag{23}$$

Since we were given the path, we can assume we know Q^r. Thus, we need to solve Eq. (23) for Z^i. This is equivalent to inverting the matrix $A - B$ from Eq. (20).

VI. CONSERVATION LAWS IN TDHFB

The quasiparticle representation is also convenient for deriving conservation laws that are satisfied in TDHFB or QRPA. The time derivative of the expectation value of an operator

$\hat{O}$ is given by

$$\frac{d}{dt}\langle t|\hat{O}\ |t\rangle = \langle t|\hat{O}\left(\frac{\partial}{\partial t}|t\rangle\right) + h.c. \tag{24}$$

For the HFB evolution, the expression in large parentheses is replaced by

$$\frac{1}{i}\sum_{ij} H^{20}_{ij}\beta^\dagger_i\beta^\dagger_j|t\rangle. \tag{25}$$

The operator $\hat{O}$ is now transformed to the quasiparticle representation and the Wick contractions are carried out. The result is

$$\frac{d}{dt}\langle t|\hat{O}\ |t\rangle = \frac{1}{i}(\mathrm{Tr}O^{02}H^{20} - \mathrm{Tr}H^{02}O^{20}) \tag{26}$$

The operator $\hat{O}$ is conserved if the right-hand side vanishes. This is the case if the operator commutes with the Hamiltonian and it is a one-body operator. For two-body and higher-order operators, the proof fails because the commutator with Hamiltonian involves the O^{40} tensor as well as the O^{20} matrix. The Hamiltonian itself is conserved because the right-side of Eq. 26 explicitly vanishes in that case.

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[2] The discussion also applies to energy density functionals, provided the functional depends only on the one-body density matrices ρ, κ and the densities matrices are the usual HFB functions of the U, V matrices.

[3] G. Schütte, Phys. Rep. **80** 113 (1981).

[4] P. Avogadro and T. Nakatsukasa, Phys. Rev. C **84** 014314 (2011).

[5] Recall that the stationary solutions of the HFB equation satisfy $H^{20} = 0$.

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[7] L.M. Robledo and G.F. Bertsch, Phys. Rev. C **84** 014312 (2011).