

Fredholm Determinant for a Bogoliubov Hamiltonian

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The Fredholm determinant associated with the Bogoliubov Hamiltonians H and H_0 (eigenvalues E_j and E_{j0}) is $D(\zeta) \equiv \prod_j (\zeta - E_j) / (\zeta - E_{j0})$, where ζ is a complex number. $D(\zeta)$ holds all possible information on the one-particle excitation spectra of the BCS superfluids described by H and H_0 . For three-dimensional systems with order parameters and potentials varying along the x axis, we show that $D(\zeta)$ may be calculated from a finite matrix that transports eigenfunctions along this axis. For piecewise-constant order parameters and potentials, $D(\zeta)$ can be found in closed form.

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Some important equilibrium quantities of superconductors and Fermi superfluids such as the heat capacity and free energy are, in the framework of BCS theory, determined from the spectrum of the first quantized Hamiltonian for the system, the Bogoliubov Hamiltonian [1]. In this work we provide a method of obtaining complete information on the spectrum of a Bogoliubov Hamiltonian for a class of interesting systems.

A possible way of finding the spectrum is to diagonalize a finite (and therefore truncated) matrix representation of H . This yields a finite subset of *approximate* eigenvalues of H which may then be used to approximate physical quantities. This procedure is useful if all important eigenvalues in the problem are calculable within the available computer time (particular problems may be posed by systems whose scattering states contribute significantly). A feature of the above approach is that, from the outset, the calculation lies in the realm of numerical evaluation with no analytical insight or approximations available.

Here we present an alternative, and in some cases analytic, route to the spectrum for a particular class of systems (arbitrarily taken to be three dimensional) in which the order parameter and potential depend only on a single coordinate. This is an effectively one-dimensional behavior and includes systems with layered structures as well as those with cylindrical or spherical symmetry. We find all the spectral information in a single attempt by determining the quantity $\prod_j ([\zeta - E_j] / [\zeta - E_{j0}]) \equiv \text{Det}([\zeta - H] / [\zeta - H_0])$, where E_j are the eigenvalues of H , E_{j0} are those of a suitable reference Hamiltonian H_0 , ζ is a complex number, and Det denotes a determinant taken over the Hilbert space of H and H_0 . The resulting determinant is known from its connection with integral equations as a Fredholm determinant and all possible information on the spectrum of H is contained within it. For example, the density of states may be extracted from it [2], but quite striking is the fact that the free energy of, e.g., an s -wave superconductor, relative to that of a system with Hamiltonian H_0 , is naturally expressed directly in terms of the Fredholm determinant itself [3]: $\sum_m \times \ln \text{Det}([i\omega_m - H] / [i\omega_m - H_0])$, where ω_m are the Mat-

subara frequencies.

For the purposes of presentation, we shall discuss only layered systems in which the order parameter and potential depend on the x coordinate. It turns out, perhaps remarkably, that for such systems in which the order parameter and potential are piecewise constant the Fredholm determinant can be found in closed form via a finite number of matrix multiplications. Thus full information on the spectrum of such a system is available.

The calculational procedure (see below) involves construction of a finite dimensional matrix $M(x)$ [$M_0(x)$] that transports eigenfunctions of H (H_0) from 0 to x . With L the length of the system, it turns out that knowledge of $M(L)$ and $M_0(L)$ is sufficient to completely determine the Fredholm determinant. Originally it was conjectured by the author and K. D. Ivanova-Moser that a relation between the Fredholm determinant and the matrix $M(L)$ applied to a variant of a Dirac Hamiltonian subject to periodic boundary conditions (the Dirac Hamiltonian resulted from the approximation of a Bogoliubov Hamiltonian by an operator linear in derivatives [2]). This was subsequently proved by the author [4] while Nakahara, using the theory of the Hill determinant, found a proof for the related problem of the Schrödinger equation subject to both periodic and hard wall (Dirichlet) boundary conditions [5].

Here we shall generalize the approach of [4] to Bogoliubov operators subject to Dirichlet boundary conditions. We stress that no approximation of the second derivative character of the Bogoliubov operator will be made so the results will be applicable to systems with rapid spatial variation, for example, short coherence-length superconductors.

For simplicity we assume that the system is described by a real s -wave order parameter that has no momentum dependence; generalizations to higher orbital pairings are possible.

Working in dimensionless units [6], we write the Bogoliubov operators H and H_0 as

$$\begin{aligned} H &= [p_x^2 + \zeta_{\perp} + V(x)]\sigma^3 + \Delta(x)\sigma^1, \\ H_0 &= [p_x^2 + \zeta_{\perp} + V_0(x)]\sigma^3 + \Delta_0(x)\sigma^1, \end{aligned} \quad (1)$$

where p_x is the x component of the momentum operator; $\zeta_{\pm} \equiv k_y^2 + k_z^2 - 1$ with k_y, k_z eigenvalues of p_y, p_z ; $V(x)$ and $\Delta(x)$ are, respectively, the potential energy and order parameter; and $\sigma^i, i=0,1,2,3$ are the unit 2×2 matrix and the Pauli matrices which here span the particle hole space of an s -wave superconductor. Dirichlet boundary conditions are imposed on the eigenfunctions Ψ of H and H_0 at $x=0$ and $x=L$: $\Psi(0)=0, \Psi(L)=0$.

Using Dirac notation in which [7] $\text{Tr}_2[\dots] \equiv \text{tr}_2 \int_0^L dx \langle x | \dots | x \rangle$ with tr_d denoting the trace over $d \times d$ matrices, we employ the identity [8]

$$\begin{aligned} \text{Tr}_2 \left[\frac{1}{\zeta - H} - \frac{1}{\zeta - H_0} \right] &= \frac{d}{d\zeta} \text{Tr}_2 \ln \left[\frac{\zeta - H}{\zeta - H_0} \right] \\ &= \frac{d}{d\zeta} \ln \text{Det} \left[\frac{\zeta - H}{\zeta - H_0} \right]. \end{aligned} \quad (2)$$

Setting

$$G(x, x'; \zeta) = \langle x | (\zeta - H)^{-1} | x' \rangle \quad (\zeta \text{ complex}) \quad (3)$$

allows us to write (2) as

$$\int_0^L dx \text{tr}_2 [G(x, x; \zeta) - G_0(x, x; \zeta)] = \frac{d}{d\zeta} \ln \text{Det} \left[\frac{\zeta - H}{\zeta - H_0} \right], \quad (4)$$

and we shall proceed by finding $G(x, x'; \zeta)$ and then applying the above equation.

The equation obeyed by $G(x, x'; \zeta)$ is

$$\begin{aligned} (\zeta - \{[-\partial_x^2 + \xi_{\pm} + V(x)]\sigma^3 + \Delta(x)\sigma^1\})G(x, x'; \zeta) \\ = \delta(x - x')\sigma^0. \end{aligned}$$

On setting

$$Y(x, x'; \zeta) = \begin{bmatrix} G(x, x'; \zeta) \\ \partial_x G(x, x'; \zeta) \end{bmatrix} \quad (5)$$

the equation for $G(x, x'; \zeta)$ takes the form [9]

$$[\partial_x - N(x; \zeta)]Y(x, x'; \zeta) = \delta(x - x') \begin{bmatrix} 0 \\ \sigma^0 \end{bmatrix}, \quad (6)$$

$$N(x; \zeta) = \begin{bmatrix} 0 & \sigma^0 \\ \sigma^3 \{\Delta(x)\sigma^1 + [\xi_{\pm} + V(x)]\sigma^3 - \zeta\} & 0 \end{bmatrix}.$$

To solve for $Y(x, x'; \zeta)$ we introduce the 4×4 matrix $M(x; \zeta)$ with the properties [10]

$$[\partial_x - N(x; \zeta)]M(x; \zeta) = 0, \quad (7)$$

$$M(0; \zeta) = \begin{bmatrix} \sigma^0 & 0 \\ 0 & \sigma^0 \end{bmatrix}.$$

Then a form for $Y(x, x'; \zeta)$ that automatically incorporates the Dirichlet boundary conditions at $x=0$ and $x=L$, i.e., that forces $G(x, x'; \zeta)$ to vanish at these points, is

$$\begin{aligned} Y(x, x'; \zeta) = \Theta(x - x')M(x)M^{-1}(L) \begin{bmatrix} 0 \\ A \end{bmatrix} \\ + \Theta(x' - x)M(x) \begin{bmatrix} 0 \\ B \end{bmatrix}, \end{aligned} \quad (8)$$

where $\Theta(x)$ is the Heaviside step function, A and B are 2×2 matrices, and, for conciseness, the ζ dependence of M has been suppressed. A and B are found from the discontinuity in Y at $x=x'$ as follows from (6). After a little algebra we find that

$$A = ([M^{-1}(L)]_{12})^{-1}(\sigma^0, 0)M^{-1}(x') \begin{bmatrix} 0 \\ \sigma^3 \end{bmatrix}, \quad (9)$$

$$B = -([M(L)]_{12})^{-1}(\sigma^0, 0)M(L)M^{-1}(x') \begin{bmatrix} 0 \\ \sigma^3 \end{bmatrix},$$

where $[M^{-1}(L)]_{12}$ is the top right 2×2 block of $M(L)$, etc.

For our purposes it is sufficient to consider $Y(x, x'; \zeta)$ for $x < x'$. Using (8) and (9) it is possible to write

$$\begin{aligned} Y(x, x'; \zeta) &= -M(x) \begin{bmatrix} 0 \\ ([M(L)]_{12})^{-1}(\sigma^0, 0)M(L)M^{-1}(x') \begin{bmatrix} 0 \\ \sigma^3 \end{bmatrix} \end{bmatrix} \\ &\equiv -M(x) \begin{bmatrix} 0, & 0 \\ ([M(L)]_{12})^{-1}, & 0 \end{bmatrix} M(L)M^{-1}(x') \begin{bmatrix} 0 \\ \sigma^3 \end{bmatrix}. \end{aligned} \quad (10)$$

Equation (4) requires $\text{tr}_2[G(x, x; \zeta)]$ and from (5) we have $G(x, x'; \zeta) = (\sigma^0, 0)Y(x, x'; \zeta)$. Since G is continuous at $x=x'$ we can use (10) for $x < x'$ and obtain

$$\begin{aligned} \text{tr}_2[G(x, x; \zeta)] &= -\text{tr}_2 \left[(\sigma^0, 0)M(x) \begin{bmatrix} 0, & 0 \\ ([M(L)]_{12})^{-1}, & 0 \end{bmatrix} M(L)M^{-1}(x) \begin{bmatrix} 0 \\ \sigma^3 \end{bmatrix} \right] \\ &= -\text{tr}_4 \left[\begin{bmatrix} 0 & 0 \\ \sigma^3 & 0 \end{bmatrix} M(x) \begin{bmatrix} 0, & 0 \\ ([M(L)]_{12})^{-1}, & 0 \end{bmatrix} M(L)M^{-1}(x) \right]. \end{aligned} \quad (11)$$

We can write this last expression in a useful form by differentiating the equation of motion for $M(x)$, (7), with respect to ζ . It straightforwardly follows that

$$-M^{-1}(x) \begin{pmatrix} 0 & 0 \\ \sigma^3 & 0 \end{pmatrix} M(x) = \partial_x \left[M^{-1}(x) \frac{dM(x)}{d\zeta} \right]$$

and using this in (11) yields

$$\text{tr}_2[G(x,x;\zeta)] = \partial_x \text{tr}_4 \left[M^{-1}(x) \frac{dM(x)}{d\zeta} \begin{pmatrix} 0, & 0 \\ ([M(L)]_{12})^{-1}, & 0 \end{pmatrix} M(L) \right]. \quad (12)$$

This is a key result. We see that the quantity required in (4), $\int_0^L dx \text{tr}_2[G(x,x;\zeta)]$, depends only on the values of $M(x)$ at the boundaries, $x=0$ and $x=L$. Furthermore, since $M(0)$ is the 4×4 unit matrix, it follows that $dM(0)/d\zeta = 0$ [11]; thus $\int_0^L dx \text{tr}_2[G(x,x;\zeta)]$ depends only on $M(L)$. We can therefore write

$$\begin{aligned} \int_0^L dx \text{tr}_2[G(x,x;\zeta)] &= \text{tr}_4 \left[\frac{dM(L)}{d\zeta} \begin{pmatrix} 0, & 0 \\ ([M(L)]_{12})^{-1}, & 0 \end{pmatrix} \right] \\ &= \text{tr}_2 \left[\frac{d[M(L)]_{12}}{d\zeta} ([M(L)]_{12})^{-1} \right] \\ &= \frac{d}{d\zeta} \text{tr}_2 \{ \ln([M(L)]_{12}) \} = \frac{d}{d\zeta} \ln \det_2([M(L)]_{12}), \end{aligned} \quad (13)$$

where we have freely used $\text{tr} \ln = \ln \det$ and \det_2 denotes the determinant of a 2×2 matrix.

Equation (13) can now be used directly in (4), leading to the conclusion that $\ln \text{Det}[(\zeta - H)/(\zeta - H_0)]$ and $\ln \det_2([M(L)]_{12}/[M_0(L)]_{12})$ differ at most by an additive constant whose value may be pinned down by investigating the large $|\zeta|$ behavior of these quantities. This is a high energy limit where the first Born approximation is applicable. Both quantities are, for large $|\zeta|$, given in leading order by $(1/\sqrt{-\zeta} + 1/\sqrt{\zeta}) \int_0^L dx [V(x) - V_0(x)]$ indicating that the constant is unity; thus [12]

$$\text{Det} \begin{pmatrix} \zeta - H \\ \zeta - H_0 \end{pmatrix} = \det_2 \begin{pmatrix} [M(L)]_{12} \\ [M_0(L)]_{12} \end{pmatrix}. \quad (14)$$

We thus have proved that for Bogoliubov operators subject to Dirichlet boundary conditions [13] and describing structures with variation along a single direction, the Fredholm determinant may be found from the 4×4 matrix $M(L)$. This indicates that the Fredholm determinant may be found from computations on determinants of finite matrices, rather than attempting approximations on the determinant of infinite matrices (i.e., operators).

In the particular case of potentials and order parameters that are piecewise constant in nature (or *approximated* as so), it is evident from (7) that the matrix $M(x)$ is a product of the matrices associated with the separate strata of the system. Thus for a finite number of strata the Fredholm determinant may be found in closed form [14].

The calculations that have been presented hold for a system of finite length L , along the x direction. It follows that finite size effects are contained within the results. We note further that the thermodynamic limit $L \rightarrow \infty$ is achievable by using a generalization of the projection techniques used in [4].

The motivation for this work arose from considerations of the free energy and density of states of Fermi

superfluids and superconductors and elsewhere we intend to apply the results presented here.

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- [1] P. G. de Gennes, *Superconductivity of Metal and Alloys* (Benjamin, New York, 1966).
- [2] D. Waxman and K. D. Ivanova-Moser, *Ann. Phys.* (N.Y.) **226**, 271 (1993).
- [3] The free energy F (or strictly, grand potential) of an s -wave superconductor follows from the expression

$$\begin{aligned} \exp(-\beta F) &= \sum_{\{n_j\}} \exp \left[-\beta \sum_j n_j E_j \right] \\ &\quad \times \exp \left[-\beta \int d^3r |\Delta(\mathbf{r})|^2/g \right], \end{aligned}$$

where E_j are eigenvalues of the Bogoliubov Hamiltonian H , $\Delta(\mathbf{r})$ is the order parameter (with electron-phonon coupling g), the occupation numbers n_j take the values 0 and 1, and β^{-1} is the temperature. Summing over all allowed n_j and taking into account that the spectrum is symmetric (E_j is always accompanied by $-E_j$ if $\Delta \neq 0$) quickly leads to

$$F = -\frac{1}{\beta} \sum_j \ln[2 \cosh(\beta E_j/2)] + \int d^3r |\Delta(\mathbf{r})|^2/g.$$

Then

$$\begin{aligned} &\sum_j \ln[2 \cosh(\beta E_j/2)] \\ &= \text{Tr} \ln[2 \cosh(\beta H/2)] \\ &= \frac{1}{2} \text{Tr} \ln[(i\omega_m - H)(-i\omega_m - H)/\omega_m^2] \\ &= \frac{1}{2} \sum_m \ln \text{Det}[(i\omega_m - H)(-i\omega_m - H)/\omega_m^2], \end{aligned}$$

where $\omega_m = (2m+1)\pi/\beta$, $m = \dots -1, 0, 1, \dots$. Thus the difference in free energies of two systems with Hamiltonians H and H_0 is

$$F - F_0 = -\frac{1}{\beta} \sum_m \ln \text{Det}[(i\omega_m - H)/(i\omega_m - H_0)] + \int d^3r [|\Delta(\mathbf{r})|^2 - |\Delta_0(\mathbf{r})|^2]/g.$$

- [4] D. Waxman, "The Fredholm Determinant for a Dirac Operator," *Ann. Phys. (N.Y.)* (to be published).
- [5] M. Nakahara, Physics Department, Kinki University, Higashi-Osaka 577, Japan, report (unpublished).
- [6] We work in dimensionless units where momenta are measured in units of the Fermi momentum k_F , distances in units of k_F^{-1} , and energy in units of $k_F^2/2m$.
- [7] In what follows we shall use Tr and Det to refer to a restricted trace and determinant where the good quantum numbers k_y and k_z are held fixed. Thus, for example, a complete trace over all degrees of freedom requires the restricted trace, Tr, as defined above to be supplemented by an integration over k_y and k_z .
- [8] B. Sakita, *Quantum Theory of Many-Variable Systems and Fields* (World Scientific, Singapore, 1985).
- [9] A related transformation of the Bogoliubov equation to a system of ordinary differential equations underlies the work of N. Schopohl and D. Waxman, *J. Phys. Condensed Matter* **4**, L639 (1992).
- [10] If we denote eigenfunctions of the Bogoliubov operator by $\Psi(x)$ [with the property $H\Psi(x) = \zeta\Psi(x)$] then $M(x)$ may be defined as the matrix that transports the "eigenfunctions"

$$\begin{pmatrix} \Psi(x) \\ \partial_x \Psi(x) \end{pmatrix}$$

from 0 to x :

$$\begin{pmatrix} \Psi(x) \\ \partial_x \Psi(x) \end{pmatrix} = M(x) \begin{pmatrix} \Psi(0) \\ \partial_x \Psi(0) \end{pmatrix}.$$

- [11] Strictly speaking, the lower limit of the integral delivers not $dM(0)/d\zeta$ but rather $\lim_{x \rightarrow 0^+} dM(x)/d\zeta$. For $x \approx 0$,

however, $M(x) \approx M(0) + \int \delta dx' N(x'; \zeta)$ and the assignment $dM(0)/d\zeta = 0$ yields the same result as the limit.

- [12] Equation (14) may be viewed as a generalization of a result for Schrödinger operators (subject to Dirichlet boundary conditions) as stated by S. Coleman in *The Uses of Instantons*, Proceedings of the International School of Subnuclear Physics, Ettore Majorana, edited by A. Zichichi (Plenum, New York, 1977). Coleman's result for the Fredholm determinant of a Schrödinger operator can be written in the form $[M(L)]_{12}/[M_0(L)]_{12}$ where here $M(x)$ is a 2×2 matrix that transports solutions of the Schrödinger equation from 0 to x (cf. Ref. [10]). See Ref. [5] for more details on Schrödinger operators.
- [13] By a straightforward application of the method presented here, Fredholm determinants with eigenfunctions subject to Neumann or periodic boundary conditions may be also expressed in terms of $M(L)$ and $M_0(L)$. We find that for Neumann boundary conditions ($\partial_x \Psi = 0$ at $x=0$ and L): $\text{Det}[(\zeta - H)/(\zeta - H_0)] = \det_2\{[M(L)]_{21}/[M_0(L)]_{21}\}$. For periodic boundary conditions ($\Psi(L) = u\Psi(0)$; $u = \exp[i\lambda\sigma^3 + i\mu\sigma^0]$, λ, μ real): $\text{Det}[(\zeta - H)/(\zeta - H_0)] = \det_4\{[U - M(L)]/[U - M_0(L)]\}$, where

$$U = \begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix}.$$

- [14] There is a simple result that is useful in this context. From (6), the factor in the matrix $M(x)$ associated with a stratus of width a is

$$\exp \begin{pmatrix} 0 & \sigma^0 \\ a & b \end{pmatrix},$$

where b is a 2×2 matrix. Then in 2×2 block form

$$\exp \begin{pmatrix} 0 & \sigma^0 \\ a & b \end{pmatrix} = \begin{pmatrix} \cosh(a\sqrt{b}), & \frac{\sinh(a\sqrt{b})}{\sqrt{b}} \\ \sqrt{b} \sinh(a\sqrt{b}), & \cosh(a\sqrt{b}) \end{pmatrix}$$

indicating that the matrix multiplications required are really only those of 2×2 matrices.