Riccati equations and quasi-1D noninteracting problems

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We consider a general 1D matrix Schrödinger equation within a transfer matrix approach. For a quadratic kinetic term we discuss expressions for the local Green function in terms of solutions of equations of the Riccati type, and an associated formula for the operator determinant. For a linear kinetic term, the approach reduces to Eilenberger quasiclassical equations. In general, it derives from classical results in boundary value problems. We consider applications to illustrative problems, concentrating on superconductivity, and discuss a general gradient expansion for the free energy density.

I. INTRODUCTION

The Schrödinger equation and its Green functions remain a fundamental tool in many branches of physics. Many problems also involve a functional determinant of the associated linear operator. As such, considerable effort has been spent to find approaches for dealing with such calculations, and the problem is consequently overall well studied.

Here, I remark on a certain method that can be used to compute the local (or, “diagonal”) Green function \( g(x) = G(x,x) \) and a functional determinant of the linear operator, in quasi-1D settings often appearing especially in condensed-matter physics problems. The local Green function is the quantity needed for the local density of states and for mean-field type iterations in several models, e.g., in the auxiliary free-particle problem in Hartree or density functional theory or Bogoliubov equations. A perhaps surprising point is that for a common class of 1D Hamiltonians with a quadratic kinetic term, the operator determinant \( \det[\epsilon - \mathcal{H}] \) can be obtained from \( g(x) \).

Many aspects of the problem have been studied before. Several results can be conveniently obtained by considering the problem in a scattering theory perspective in terms of the transfer matrix. Results for the determinant can be obtained by standard methods for ordinary differential operators. I consider in particular a quadratic kinetic term, but extensions to other cases are possible, and in particular for linear spectrum quasiclassical equations well-known in superconducting transport are found. The Riccati equations obtained with a quadratic kinetic term can be understood as a matrix generalization of those discussed by Caroli et al.\(^{11-13}\) Several related methods for linear boundary value problems are also known, especially invariant imbedding methods and decoupling to Riccati systems bear similarity and have been discussed before.\(^{12-14}\) At least for the scalar case, similar trace formulas can be found in works on inverse scattering theory.\(^{20}\) and a related approach was used in Refs.\(^{21,22}\) to find gradient expansions for the superconducting free energy. A partially similar formula as here was recently discussed in Ref.\(^{23}\)

The final formulation for the quadratic kinetic term obtains a compact form, Eqs. (1)–(5). As such, and as the matrix formulation and its associated “trace formula” for the determinant in terms of \( g(x) \) appears to have received less attention, some further elaboration on the topic still seems of interest, from a physics application point of view. In this work, an elementary derivation of the results is outlined, and applications to simple physics problems are illustrated.

This manuscript is organized as follows. In Sec. II the expressions for \( g(x) \) and the determinant are derived. In Sec. III the results are applied to selected condensed-matter physics problems. Section IV concludes with discussion.

II. QUASI-1D LOCAL GREEN FUNCTIONS

The statement for the quadratic kinetic term obtains a compact form. Consider the “Hamiltonian”

\[
\mathcal{H} = \mathcal{T} + \mathcal{U}(x),
\]

\[
\mathcal{T} \equiv -\left[ \partial_x + i\mathcal{A}(x) \right] \frac{\hbar^2}{2M(x)} \partial_x + i\mathcal{A}(x),
\]

where \( M(x), \mathcal{A}(x) \) and \( \mathcal{U}(x) \) are \( n\times n \) complex matrices, not necessarily Hermitian, of which \( M(x) \) is invertible. Below, we set \( \hbar = 1 \). The local Green function and the \((\text{zeta-function regularized})\) determinant can then be expressed as

\[
g(x) = [a(x) + d(x)]^{-1}
\]

\[
\ln \det[\epsilon - \mathcal{H}] = -\int_{-\infty}^{\infty} dx \text{tr}[\mathcal{M}(x)g(x)^{-1}] + C,
\]

where \( C \) is a (possibly divergent) constant independent of \( \epsilon, \mathcal{U} \) and \( \mathcal{A} \), which is then canceled when considering ratios of determinants. The relation between the matrix inverse of the local Green function and the operator determinant is simple, and related trace formulas have been mentioned in works on inverse scattering theory at least for the scalar-valued problem. As seen below, this equation is valid also in finite-size systems.
when the wave function has zero boundary conditions. The matrix-valued “logarithmic derivatives” \( a(x), d(x) \) are determined as solutions to two decoupled matrix Riccati equations

\[
\begin{align*}
\partial_x d + ia[A, d] &= 2dM d - \mathcal{U} + \epsilon \\
\partial_x a + ia[A, a] &= \mathcal{U} - \epsilon - 2aMa,
\end{align*}
\]

with initial conditions provided by their bulk values at \( x \to \pm \infty \), which for \( A(\pm \infty) = 0 \) read \( d(-\infty) = -\frac{1}{2M(-\infty)} \sqrt{2M(-\infty)(\mathcal{U}(-\infty) - \epsilon)} \) and \( a(\infty) = -\frac{1}{2M(\infty)} \sqrt{2M(\infty)(\mathcal{U}(\infty) - \epsilon)} \), where \( \sqrt{\cdot} \) is the principal matrix square root. The equation for \( d \) can be integrated in the linearly stable direction from left to right and \( a \) from right to left, resembling the procedure for solving the quasiclassical Riccati transport equations in superconductors\textsuperscript{11}. The scalar case of the above Riccati equations was discussed in Ref. 11, although obtained with a different reasoning. Note also the resemblance to well-known Riccati transformations\textsuperscript{25,26} for the equation of the wave function.

We can also interpret Eq. (3) as an expression for the free energy density of noninteracting fermions in 1D,

\[
f(x) = T \sum_{\omega_n} \text{tr} M(x) g(x, i\omega_n)^{-1}, \tag{6}
\]

where \( \omega_n = 2\pi T(n + \frac{1}{2}) \) are the Matsubara frequencies, and the sum over them is appropriately regularized to render it convergent. Solving the Riccati equations for \( \hbar \to 0 \) leads to a WKB-type gradient expansion for the free energy density, discussed in Sec. III C.

In numerical applications\textsuperscript{15,18,19} solutions to the Riccati equation system can be obtained directly by conventional ODE solvers, starting from the bulk values of \( d, a \) at the boundary of the inhomogeneous region, and directly yields \( g(x) \). The approach somewhat resembles the recursive Green function method\textsuperscript{25}

As evident in Eq. (2), the functions \( a, d \) have to diverge at points where \( g(x) \) is not invertible. This problem has been discussed in the literature on numerical boundary value problems\textsuperscript{18,19,28} and can in some cases be overcome. However, for Green functions of Hermitian Hamiltonians with \( \epsilon \) away from the real axis (as e.g. in imaginary time calculations), the issue appears to be less critical and the Riccati method can be useful as is. Based on Eq. (3), such divergences may also have physical meaning.

We now proceed to obtaining the above results. Questions about convergence and singularities are skipped in several steps.

### A. Continuum transfer matrix formulation

Let us first remind how to recast the Schrödinger equation \( \mathcal{H}\psi = \epsilon\psi \) as a first-order system\textsuperscript{25,26} and introduce notation used below. Considering Eq. (1), we first define the 2n size vector

\[
\mathbf{u}(x) = \left( \frac{1}{2M(x)} \partial_x + iA(x) \right) \psi(x). \tag{7}
\]

The Schrödinger equation can now be expressed as

\[
\partial_x \mathbf{u}(x) = \mathbf{W}(x) \mathbf{u}(x), \tag{8}
\]

\[
\mathbf{W}(x) = \left( \begin{array}{cc} -iA(x) & 2M(x) \\ \mathcal{U}(x) - \epsilon & -iA(x) \end{array} \right). \tag{9}
\]

The fundamental matrix \( \mathbf{Y}(x) \) of the problem, i.e. essentially the transfer matrix expressed in a specific basis, is now defined by

\[
\partial_x \mathbf{Y}(x, x') = \mathbf{W}(x) \mathbf{Y}(x, x') \quad \mathbf{Y}(x, x) = \mathbf{1}. \tag{10}
\]

It has the property \( \mathbf{u}(x) = \mathbf{Y}(x, x') \mathbf{u}(x') \). As well-known, \( \partial_x \det \mathbf{Y} = \text{tr} \mathbf{W} \det \mathbf{Y} \), so \( \mathbf{Y} \) is invertible, although usually numerically badly conditioned.

The Green function for the first-order problem (8) is defined by

\[
[\partial_x - \mathbf{W}(x)] \mathbf{G}(x, x') = \delta(x - x'). \tag{11}
\]

For the quadratic kinetic term\textsuperscript{11} we can relate this to the Green function \( \mathcal{G} = [\epsilon - \mathcal{H}]^{-1} \) by

\[
\mathbf{G}(x, x') = \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \mathcal{G}(x, x') \left( \begin{array}{c} 0 \\ 1 \end{array} \right). \tag{12}
\]

Indeed, direct calculation gives (omitting arguments for brevity)

\[
-T \mathcal{G} = [\partial_x + iA] \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \frac{1}{2M} (|\mathbf{W} + iA| \mathbf{G} + \delta) \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \tag{13}
\]

\[
= [\partial_x + iA] \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \mathbf{G} \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \tag{14}
\]

\[
= [\mathcal{U} - \epsilon] \mathbf{G} + \delta, \tag{15}
\]

so that \( [\epsilon - \mathcal{H}] \mathbf{G}(x, x') = \delta(x - x') \).

Due to reasons that become apparent below, it is useful to now define the first-order local Green function as a symmetrized sum

\[
g(x) = \mathbf{G}(x, x + 0^+) + \mathbf{G}(x + 0^+, x). \tag{16}
\]

The relation to the local Green function \( \mathcal{G} \) corresponding to \( \mathcal{H} \) obtains then an additional factor of 1/2:

\[
g(x) = \frac{1}{2} \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \mathcal{G}(x) \left( \begin{array}{c} 0 \\ 1 \end{array} \right). \tag{17}
\]

Note that \( \mathbf{G}(x, x') \) is continuous across \( x = x' \), even though other components of \( \mathbf{G}(x, x') \) are generally not.

The above is essentially textbook scattering theory. For spatially uniform \( \mathcal{H} \), Eq. (11) is solved by \( \mathbf{Y}(x, x') = e^{(x-x')^T \mathbf{W}} \). Eigendecomposition \( \mathbf{W} \mathbf{u}_j = \lambda_j \mathbf{u}_j \) gives the modes propagating/decaying to the left (\( \text{Re} \lambda_j > 0 \) for
Im $\epsilon \neq 0$) and right ($\text{Re} \lambda_j < 0$). Considering transmission across an inhomogeneous region $[x_L, x_R]$ and expressing $Y(x_R, x_L)$ in terms of appropriately normalized eigenmodes of the leads $x < x_L, x > x_R$ gives the standard transfer matrix of the region.

For translationally uniform system, $i\partial_x \rightarrow k_x$, the bulk Green function is obtained as

$$G(k_x) = \frac{1}{i k_x - \mathbb{W}}, \quad (18)$$

$$g(x) = \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \sum_k e^{\pm ik_x 0^+} G(k_x) \quad (19)$$

$$= -P_+ + P_- = -\text{sgn} (\mathbb{W}), \quad (20)$$

where $\text{sgn}$ is the matrix sign function\textsuperscript{29} and $P_\pm$ projectors to eigenmodes with $\pm \text{Re} \lambda_j > 0$. For hermitian Hamiltonians and $\text{Im} \epsilon \neq 0$, generally $\text{Re} \lambda_j \neq 0$, so that $P_- \neq 0$. Here the Green function is obtained as

$$g(x) = Y(x) [2P - 1] Y(x)^{-1} \quad (27)$$

It then follows that $g(x)$ satisfies

$$\partial_x g(x) = [W(x), g(x)], \quad g(x)^2 = 1 \quad (28)$$

This has the same form as the Eilenberger quasiclassical transport equations\textsuperscript{22}. The similarity is not coincidental — it is related to general mathematical structure of linear boundary value problems\textsuperscript{31}.

It is important to note that Eq. (28), together with boundary conditions, forms a closed set of equations from which $g(x)$ can in principle be solved. Below, we follow a procedure similar to that often used with the quasiclassical equations, and use the nonlinear constraint $g^2 = 1$ to eliminate some of the variables\textsuperscript{10,24,31}. As opposed to Eilenberger equations, which involve a linearization of the spectrum, the results are exact for the quadratic Hamiltonian\textsuperscript{1}.

We look for solutions to Eq. (28) by introducing projection matrices similar to those used in Refs. 24 and 31

$$p_+ = \begin{pmatrix} 1 \\ a \\ a + d \end{pmatrix} \quad (29)$$

$$p_- = \begin{pmatrix} 1 \\ -a \\ -a - d \end{pmatrix} \quad (30)$$

so that $p_+ + p_- = 1$, $p_+ p_- = p_- p_+ = 0$. The solution Ansatz reads

$$g = p_+ - p_- \quad (31)$$

$$= \begin{pmatrix} -d^{-1}(a - d) & 2(a + d)^{-1} \\ 2a(a + d)^{-1} d & -(a + d)^{-1}(a - d)^{-1} \end{pmatrix} \quad (32)$$

It satisfies the condition $g^2 = 1$ automatically, and differential equations required for $d, a$ follow by substituting it in Eq. (28). For this, it is convenient to observe that

$$\pm \delta p_\pm = p_+ \begin{pmatrix} 0 & -d^{-1} (d a d^{-1}) \\ 0 & 0 \end{pmatrix} + p_- \begin{pmatrix} 0 & 0 \\ \delta a & 0 \end{pmatrix} p_+ \quad (33)$$

and use projector properties of $p_\pm$. Direct calculation then gives

$$\partial_x d(x) = - (d - 1) W(x) \begin{pmatrix} 1 \\ -d \end{pmatrix} \quad (34)$$

$$\partial_x a(x) = - (a - 1) W(x) \begin{pmatrix} 1 \\ a \end{pmatrix} \quad (35)$$

C. Eilenberger and Riccati equations

From Eq. (24), we see that the first-order local Green function\textsuperscript{16} can be expressed as

$$g(x) = Y(x) [2P - 1] Y(x)^{-1} \quad (27)$$

It then follows that $g(x)$ satisfies

$$\partial_x g(x) = [W(x), g(x)], \quad g(x)^2 = 1 \quad (28)$$

Below, we assume the problem is such that ($20$) applies.

B. Boundary conditions

We now consider an interval $[x_L, x_R]$, and recall standard results for such boundary value problems\textsuperscript{15-17}. Linear two-point boundary conditions can be generally expressed as

$$B_L u(x_L) + B_R u(x_R) = 0 \quad (22)$$

Equation (22) can also be written as

$$M(\epsilon) u(x_L) = 0, \quad M(\epsilon) = B_L + B_R Y(x_R), \quad (23)$$

where $Y(x) = Y(x, x_L)$. The eigenenergies $\epsilon_j$ are then determined by the condition $\det M(\epsilon) = 0$.

Assuming the boundary value problem is solvable, the first-order Green function can be expressed as\textsuperscript{16,17}

$$G(x, x') = Y(x)[P\theta(x - x') - (1 - P)\theta(x' - x)]Y(x')^{-1} \quad (24)$$

The matrix $P$ is defined by

$$P = M^{-1} B_L \quad (25)$$

Quite generally\textsuperscript{30} $P$ is a projection matrix,

$$P = P^2 \quad (26)$$

For example, assuming $n$ separated and non-degenerate boundary conditions at both ends, so that $\text{rank} B_L = \text{rank} B_R = n$, we can write singular value decompositions as $B_L = u_L s_L v_L^T$, $B_R Y(x_R) = u_R s_R v_R^T$, where $v_L/R$ are $2n \times n$ matrices. Then, $P = [v^T]^{-1} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} v^T$, $v = (v_L, v_R)$, so that $P^2 = P$, provided $v$ is not singular. Below, we assume the problem is such that ($20$) applies.
These are Eqs. (15). Note that with the chosen parametrization, the equations are decoupled. The structure of the problem is essentially the same as in invariant imbedding.15

Instead of finding the boundary conditions to these equations from suitable $B_{L/R}$, we can match the solutions to the bulk value of $g(x)$ in an infinite system, a generic situation often studied in condensed-matter scattering problems (the “bulk” can be also vacuum). We assume that $x_L \to -\infty$ and $x_R \to +\infty$. Moreover, the Hamiltonian $H(x)$ is assumed to be spatially constant (“bulk”) at $x < x_-$ and $x > x_+$ for some fixed $x_\pm$. For $x \to \pm \infty$, the local Green function $g(x)$ is assumed to approach its bulk value — in physical problems, this is true when all wave vectors in the spatially uniform bulk region have an imaginary component, which generally is the case for $\text{Im} \epsilon \neq 0$.

The convergence to a bulk value for $x \to \pm \infty$ is reflected in the fixed points of the Riccati equations. Comparing to Eq. (21), we find that for $A = 0$, the physical boundary conditions are given by

$$d(x_-) = -\frac{1}{2M(-\infty)} \sqrt{2M(-\infty)H(-\infty) - \epsilon}, \quad (36)$$

$$a(x_+) = -\frac{1}{2M(\infty)} \sqrt{2M(\infty)H(\infty) - \epsilon}. \quad (37)$$

Here, we also account for the fact that linear stability analysis shows that $d$ has a stable integration direction from left to right, and $a$ from right to left, for which perturbations from the above bulk solutions are decaying.

For $A \neq 0$, the bulk solutions are obtained by solving the algebraic Riccati equations (obtained by setting $\partial_d d = \partial_a a = 0$), which is a well-studied problem. It can be done with a Schur approach decomposing $W = UTU^*$ in the bulk region. The ordering of diagonal entries of $T$, which can be selected as appropriate in the decomposition, should be chosen such that $\text{Re} \text{diag}(T_{11}) < 0$ in the $n \times n$ upper left block $T_{11}$. Then $d(x_-) = U_{21}U_{11}^{-1}$. The bulk $a(x_+) = -U_{21}^{-1}U_{11}^{-1}$ is obtained by a decomposition choosing $\text{Re} \text{diag}(T_{11}) > 0$.

D. Trace formula

Known results for functional determinant indicate that with the assumptions here,

$$\ln \text{Det}[\epsilon - \mathcal{H}] = \ln \det M + \int_{x_L}^{x_R} dx \ i \ \text{tr} A, \quad (38)$$

up to a constant independent of $\epsilon$, $A$, $\mathcal{U}$. Consider now $W \rightarrow W_\lambda$, i.e., $\mathcal{U}_\lambda$ or $A_\lambda$ depend in some way on a scalar parameter $\lambda(x)$ in the interval $[x_L, x_R]$. Differentiation of Eq. (38) now gives the variational property

$$\frac{\delta}{\delta \lambda} \ln \det M_\lambda = \text{tr} M_\lambda^{-1}B_{L/R}Y_\lambda(x)\partial_\lambda W_\lambda(x)Y_\lambda(x), \quad (39)$$

$$= \text{tr} Y_\lambda(x)(1 - P)Y_\lambda(x)^{-1}\partial_\lambda W_\lambda(x)$$

$$= -\frac{1}{2} \text{tr} g_\lambda(x)\partial_\lambda W_\lambda(x) + \frac{1}{2} \text{tr} \partial_\lambda W_\lambda(x).$$

The second term exactly cancels the variation of the second term in Eq. (38).

We will now limit the discussion to the problem with zero boundary conditions (ZBC) for the wave functions. For the Green function, this implies $G(x_{L/R}, x') = 0$, so that $g(x) \rightarrow 0$ for $x \rightarrow x_{L/R}$.

It is now convenient to obtain an expression for $\text{Det}[\epsilon - \mathcal{H}_\lambda]$ by integrating Eq. (39) via finding a functional that produces the same variations for any $\lambda$. To start, consider the expression

$$R[a, d, \lambda] = \frac{1}{2} \int_{x_L}^{x_R} dx \left( \text{tr}[(a + d)^{-1}\partial_x(a - d)] - \text{tr}[gW_\lambda]\right), \quad (40)$$

where the matrix $g = g[a, d]$ is now defined as in Eq. (32). Direct calculation, making use of Eq. (33), gives the variations

$$\frac{\delta R}{\delta a} = -\frac{1}{2} \text{tr}[g\partial_\lambda W_\lambda], \quad (41)$$

$$\frac{\delta R}{\delta d} = (a + d)^{-1}[-\partial_x a - (a - 1)W_\lambda \left(\frac{1}{a}\right)](a + d)^{-1}, \quad (42)$$

$$\frac{\delta R}{\delta \lambda} = (a + d)^{-1}[\partial_x d + (d - 1)W_\lambda \left(\frac{1}{d}\right)](a + d)^{-1}. \quad (43)$$

Observe that the variation of the derivative term in Eq. (40) also generates boundary terms $\propto |a(x) + d(x)|^{-1} = g(x), x \to x_{L/R}$, but they vanish under the zero boundary conditions.

A functional that has the same variation as Eq. (38) vs. $\lambda$ for any $\lambda(x)$ can then be written as:

$$\ln \text{Det}[\epsilon - \mathcal{H}_\lambda]_{ZBC} = R[a_\lambda, d_\lambda, \lambda] = -\int_{x_L}^{x_R} dx \text{tr}[Mg_\lambda^{-1}], \quad (44)$$

Here, $g_\lambda^{-1} = a_\lambda + d_\lambda$, and $a_\lambda$ and $d_\lambda$ are the solutions that satisfy the saddle-point equations $\frac{\delta}{\delta a(x)} R[a_\lambda, d_\lambda] = \frac{4}{\delta a(x)} R[a_\lambda, d_\lambda] = 0$, which are equivalent with the Riccati Eqs. (34, 35).

As the correspondence (44) to the determinant applies for any variations, the left and right-hand sides are equal up to a constant independent of $A$ and $\mathcal{U}$, provided no singularities are encountered on the integration path. The constant can be absorbed in the normalization of the functional determinant, which already contains other similar factors. Finally, taking $x_{L/R} \rightarrow \mp \infty$ we find Eq. (3).
III. APPLICATIONS

In this section, we obtain solutions to particular problems.

A. Finite potential well

To illustrate with an elementary example, we can consider a finite potential well, with $A = 0$ and potential $U(x) = 0$ for $|x| > L/2$ and $U(x) = -u_0$ for $|x| < L/2$. The solution to the Riccati equations matched to the bulk boundary conditions becomes

$$d(x) = \frac{1}{2m} \begin{cases} -\alpha \tanh[ik(x-z_0)] & \text{for } x < -L/2, \\ -ik \tanh[ik(x-z_1)] & \text{for } x > L/2, \\ -\alpha \tanh[ik(x-z_1)] & \text{for } x < L/2, \\ -ik \tanh[ik(x-z_0)] & \text{for } x > L/2, \end{cases}$$

(45)

where $\alpha = \sqrt{-2mu}$, $ik = \sqrt{-2m(\epsilon + u_0)}$, and $z_0, z_1$ are chosen so as to make the function continuous. By symmetry, $a(x) = d(-x)$. The trace formula now gives

$$\text{Det}[\epsilon - \mathcal{H}] = e^{-\int_{-\infty}^{\infty} dx [ma(x)+md(x)+\alpha]}$$

$$= e^{-\frac{L_0}{ak}[\alpha \sin \frac{kL}{2} + k \cos \frac{kL}{2}]\frac{\alpha \cos \frac{kL}{2} - k \sin \frac{kL}{2}}{2}},$$

where $\mathcal{H}$ is the Hamiltonian with $u_0 = 0$. The (analytical continuation of the) ratio of the determinants has zeros when either $\alpha = k \tan(kL/2)$ or $\alpha = -k \cot(kL/2)$, which are the well-known conditions for the bound-state energies of a finite well. Considering $u_0 \to \infty$, the Green function of an infinite potential well is $g(x) = -(\dot{\epsilon})^{-1/2}(\coth[\sqrt{-\dot{\epsilon}}(L/2-x)] + \coth[\sqrt{-\dot{\epsilon}}(L/2+x)])^{-1}$, where $\dot{\epsilon} = \epsilon - u_0$.

B. Piecewise constant potential scattering

Consider general spatially homogeneous $\mathcal{H}$ with $A = 0$. With Ansatz $d = \frac{1}{2m} \partial_x f$, a general solution to Eq. (4) can be found:

$$d(x) = -\frac{1}{2M} \sqrt{\frac{1 - R(x)}{1 + R(x)}},$$

$$R(x) = e^{-x\sqrt{w}} R_0 e^{-x\sqrt{w}}, \quad w = 2M(\epsilon - \epsilon),$$

(47)

(48)

where $R_0$ is a free parameter. Similar solution exists for $a(x)$, replacing $R(x) \to \tilde{R}(x) = e^{x\sqrt{w}} R_0 e^{x\sqrt{w}}$. Moreover,

$$\text{tr}[Md(x)] = -\frac{1}{2} \text{tr} \sqrt{w} - \frac{1}{2} \partial_x \text{tr} \ln[1 + R(x)],$$

$$\text{tr}[Ma(x)] = -\frac{1}{2} \text{tr} \sqrt{w} + \frac{1}{2} \partial_x \text{tr} \ln[1 + \tilde{R}(x)],$$

(49)

(50)

for the expressions appearing in Eq. (3). For a scattering problem with Hamiltonian constant except at $x = 0$, $R(0^-) = 0$ and $\tilde{R}(0^+) = 0$. As a consequence

$$-\int_{-x_c}^{x_c} dx \text{ tr}(a + d) \mathcal{M} = x_c \text{ tr} \left[ \sqrt{w(0^-)} + \sqrt{w(0^+)} \right],$$

$$+ \ln \frac{\det(1 + R(0^-)) \det(1 + \tilde{R}(0^+))}{\det(1 + R(x_c)) \det(1 + \tilde{R}(x_c))}. \quad (51)$$

The denominator in the second term $\to 1$ for $x_c \to \infty$.

The above enables finding closed-form expressions for $g(x)$ for piecewise constant scattering problems with $A = 0$,

$$U(x) = U_j, \quad x_j < x < x_{j+1},$$

(52)

for $j = 1, \ldots, N$ with $x_1 = -\infty$ and $x_{N+1} = \infty$. It is given by

$$g(x) = [a_j(x) + d_j(x)]^{-1}, \quad x_j < x < x_{j+1},$$

(53)

with $d_j(x) = -(2M_j)^{-1} \sqrt{w_0}, \quad a_N(x) = -(2M_N)^{-1} \sqrt{w_N}$, where $w_j = 2M_j(U_j - \epsilon)$. The other factors are defined recursively by

$$d_j(x) = \frac{1}{2M_j} \sqrt{\frac{1 - e^{(x-x_j)\sqrt{w}}} {1 + e^{(x-x_j)\sqrt{w}}} R_j e^{(x-x_j)\sqrt{w}}} R_j e^{(x-x_j)\sqrt{w}}$$

$$a_j(x) = \frac{1}{2M_j} \sqrt{\frac{1 - e^{(x-x_{j+1})\sqrt{w}} R_j e^{(x-x_{j+1})\sqrt{w}}} {1 + e^{(x-x_{j+1})\sqrt{w}} R_j e^{(x-x_{j+1})\sqrt{w}}}},$$

where

$$R_j = 1 + w_j^{-1/2} 2M_j d_{j-1}(x_j),$$

$$\tilde{R}_j = 1 + w_j^{-1/2} 2M_j a_{j+1}(x_{j+1}). \quad (56)$$

(57)

This enables straightforward semi-analytical (i.e. requiring matrix exponential and principal square root) computation of the LDOS $N(\epsilon, x) = -\frac{1}{\pi} \text{Im} \text{ tr} g(\epsilon + i0^+, x)$ for problems with quadratic dispersion in piecewise constant potential. Similar results of course can be found via other standard methods, e.g. concatenating transfer/scattering matrices. However, note that here all the matrix exponentials involve matrices with no eigenvalues on the right half-plane, and may avoid some of the numerical problems involved in a transfer matrix computation via Eq. (10).

1. Josephson junction

Consider now a Bogoliubov–de Gennes Hamiltonian for a Josephson junction with a $\delta$-function barrier

$$\mathcal{H} = [-\frac{1}{2m} \partial_x^2 - \mu] \tau_3 + \Delta(x) \tau_+ + \Delta(x)^* \tau_- + H \tau_3 \delta(x),$$

(58)
where \( \Delta(x) = |\Delta| e^{i \text{sgn}(x) \varphi/2} \) is the superconducting order parameter, and \( H \) the potential barrier height. Here, \( \tau_{1,2,3} \) are Pauli matrices in the Nambu space, and \( \tau_\pm = \frac{1}{2} \tau_1 \pm i \tau_3 \). We wish to find the supercurrent across the interface. This can be found via the expression connecting it to the free energy: \( I = -\frac{e}{h} \partial_\varphi F \). In particular,

\[
I = \frac{2e}{h} T \sum_{\omega_n} j(\omega_n), \quad j = -\partial_\varphi \ln \text{Det}[\omega_n - \mathcal{H}], \quad (59)
\]

where \( \omega_n = 2\pi T (n + \frac{1}{2}) \) are Matsubara frequencies and \( T \) is the temperature.

As \( \mathcal{H} \) is piecewise constant, the analytical solutions have the form of Eq. (17), with \( R(0^-) = R(0^+) = 0 \). The unknown \( R(0^+) = R_+ \), \( R(0^-) = R_- \) are determined by the matching conditions obtained by integrating the Riccati equations across the \( \delta \)-barrier at the interface:

\[
d(0^+) - d(0^-) = -\tau_3 H, \quad a(0^+) - a(0^-) = +\tau_3 H. \quad (60)
\]

They give \( R_\pm \) as:

\[
R_\pm = [\sqrt{w_+} + \sqrt{w_-} + 2mH]^{-1} [\sqrt{w_+} - \sqrt{w_-} - 2mH],
\]

where \( w_\pm = w(x \gtrless 0) \). These quantities are similar to the reflection matrix of the interface in scattering theory. The local Green function (2) now reads:

\[
g(x) = [1 + e^{-|x|\sqrt{w_0}} R_0 e^{-|x|\sqrt{w_0}} - \frac{m}{\sqrt{w_0}} \tau_3],
\]

where \( \alpha = \text{sgn}(x) = \pm \). The LDOS is \( N(\epsilon, x) = -\frac{1}{\pi} \text{Im \, tr} \, g(x; \epsilon + i0+) \).

The summand in Eq. (59) can be found from Eq. (51):

\[
j = -\partial_\varphi \ln \text{det}[(1 + R_+)(1 - R_-)].
\]

Factoring out remaining parts independent of \( \varphi \) using

\[
w_\pm = e^{\pm i \varphi \tau_3/4} w \pm e^{i \varphi \tau_3/4},
\]

we get

\[
j = \partial_\varphi \ln \text{det} \left( 2mH + \sqrt{w} + e^{i \varphi \tau_3/2} \sqrt{w} e^{i \varphi \tau_3/2} \right). \quad (65)
\]

The matrix square root is:

\[
\sqrt{w} = \frac{\kappa_+ + \kappa_-}{2} + \frac{\kappa_+ - \kappa_-}{2} \left( \frac{\omega}{\sqrt{\omega^2 + \Delta^2}} \right) \left( -i \Delta \begin{array}{c} \omega \\ -i \Delta \end{array} \right),
\]

where \( \kappa_\pm = \sqrt{-2m\mu \pm 2mi \sqrt{\omega^2 + \Delta^2}} \). Evaluating the determinant gives the result

\[
j = \partial_\varphi \ln \left[ \omega^2 + (1 - \tau(\omega) \sin^2 \frac{\varphi}{2}) \Delta^2 \right],\quad \tau(\omega) \equiv \frac{1}{1 + Z(\omega)^2}, \quad Z(\omega) \equiv -i \frac{2mH + \kappa_+ + \kappa_-}{\kappa_+ - \kappa_-}. \quad (66)
\]

We can consider the limit \( \mu \to \infty \):

\[
\kappa_\pm \simeq \mp i \sqrt{2m|\mu|} \equiv \mp i k_F, \quad Z \simeq \frac{H}{k_F} \equiv \frac{H}{\hbar v_F}. \quad (69)
\]

Here, \( Z \) is the dimensionless barrier strength and \( \tau \) is the normal-state transmission coefficient of the interface. Neglecting the \( \omega_n \) dispersion of \( \tau(\omega) \), the Matsubara sum can be evaluated in closed form,

\[
I(\varphi) = \frac{2e}{h} T \sum_{\omega_n} j(\omega_n) = -\frac{2e}{h} \varepsilon(\varphi) \tanh \left( \frac{\varepsilon(\varphi)}{2T} \right). \quad (70)
\]

where \( \varepsilon(\varphi) = \Delta \sqrt{1 - \tau \sin^2 \frac{\varphi}{2}} \). This \( \mu \to \infty \) result is well-known for the single-channel supercurrent.

### 2. Magnetic impurity in a superconductor

A magnetic impurity in a quasi-1D superconductor can be described with the Hamiltonian in Eq. (68), replacing \( H \tau_3 \to J \tau_3 \). For simplicity we also now set \( \varphi = 0 \). From Eqs. (63, 64), the Green function has poles when \( \text{det}(\sqrt{w + mM \tau_3} \tau_3) |_{\omega = m} = 0 \). Taking the limit \( \mu \to \infty \) and using Eqs. (64, 65), this bound state condition gives \( \epsilon = \pm \Delta(1 - \gamma^2)/(1 + \gamma^2) \), \( \gamma = mJ / k_F = \pi N_0 J \), where \( N_0 = m/(\pi k_B) \) is the 1D density of states at the Fermi level. These are the Yu–Shiba–Rusinov \( A \) states.

### C. WKB expansion for free energy density

We can now pursue a WKB-type expansion for the noninteracting fermion free energy density in \( \hbar \to 0 \), taking \( A = 0 \) for simplicity, and expanding \( d = \sum_{k=0}^{\infty} \hbar^k d_k \) and similarly for \( a \).

Substituting the perturbation expansion into the Riccati equations gives

\[
d_0 = 0, \quad d_1 = -\frac{1}{2M} \sqrt{2M(U(x) - i\epsilon_n)} \quad (71),
\]

\[
d_{k+1} M d_1 + d_1 M d_{k+1} = \frac{1}{2} \partial_x d_k - \sum_{l=2}^{k} d_l M d_{k+2-l}, \quad (72)
\]

and similarly for \( a_k \) with replacement \( \partial_x \to -\partial_x \). Hence, \( a_k = (-1)^{k+1} d_k \). The Sylvester equation (72) for \( d_{k+1} \) has a unique solution when \( i\epsilon_n \) is not equal to an eigenvalue of \( U(x) \), i.e., it is always solvable for Hermitian Hamiltonians. Hence, \( d_k \) can be all solved recursively. Generally, \( d_k \propto \partial_x^{k-1} \). Substituting the result to the trace formula produces a gradient expansion for the free energy density

\[
f(x) = \sum_{k=0}^{\infty} \hbar^{2k-1} k_B T \sum_{n} \left[ \text{tr} M d_{2k+1} + \text{const} \right] \quad (73),
\]

\[
f_0(U(x)) + \sum_{k=1}^{\infty} \hbar^{2k-1} k_B T \sum_{n} \left[ \text{tr} M d_{2k+1} \right], \quad (74)
\]
with $\epsilon_n = 2\pi k_B T (n + \frac{1}{2})$. Here,
\[
f_0(U_0) = -\frac{k_B T}{h} \sum_n \text{tr} \sqrt{2M(U_0 - i\epsilon_n)}
\] (75)
is the free energy density of a uniform Fermi system with constant matrix-valued potential. For scalar $M = m > 0$ the result becomes
\[
f_0(U_0) = -k_B T \int_{-\infty}^{\infty} \frac{dp}{2\pi \hbar} \ln \det[1 + e^{-\frac{a^2}{m}+U_0}/(k_B T)],
\] (76)
as usual for noninteracting fermions.

Assuming constant $M$, the lowest-order correction can be solved. Writing $z_n = M d_n^\dagger$,
\[
\text{tr} 2z_3 = \frac{1}{16} \text{tr} [\partial_x((\partial_x z_1)z_{1}^{-1})z_{1}^{-1} + \partial_x(z_1^{-2}\partial_x z_1)].
\] (77)
This can be obtained e.g. solving Eq. (72) formally via $z_{k+1} = \sum_{n=0}^{k} (-\lambda)^n z_1^n [\partial_x z_k - \sum_{l=2}^{k} z_{l}z_{k+2-l}]z_1^{n-1}$ with suitable analytic continuation in $\lambda \to 1$.

When $M = m > 0$ is a constant and $U(x)$ is scalar-valued, the Sylvester equation does not pose a problem, and $d_k$ can be solved in a straightforward manner, generally producing terms $\propto (\partial_x^2 U) d_1^\alpha$ in the expression for $f$. Noting Eq. (75), the Matsubara sum of each term can be expressed in terms of an $U$-derivative of $f_0(U)$. This results to the gradient expansion
\[
f(x) = f_0 - \frac{1}{4}U_2 f_2 - \frac{5}{24}U_3 f_3 + \frac{1}{48}U_4 f_4 + \frac{7}{120}U_5 f_5 + \frac{19}{480}U_6 f_6 + \ldots,
\] (78)
or, by going to higher order and integrating by parts and discarding total $x$-derivative (i.e. boundary) terms, which do not contribute to the total free energy if $\partial_x U \to 0$ for $x \to \pm\infty$,
\[
f(x) = f_0 + \frac{U_2^2 f_3}{24} + \frac{U_2^2 f_4}{480} + \frac{U_3^2 f_5}{3456} + \frac{U_3^2 f_6}{13440} - \frac{U_2 f_6}{12096} - \frac{U_2^2 f_7}{11520} + \frac{U_4^2 f_5}{414720} + \ldots,
\] (79)
where $U_n = m^{-n/2}\partial_x^n U(x)$ and $f_n = \partial^{n} f_0(U)|_{U=U(x)}$.

For $T \to 0$, $f_0(U_0) = -\theta(-U_0)(-2mU_0)^{3/2}/(3\pi m)$.

For $T \to 0$, the above results can be compared to the somewhat different approach to the scalar problem in Ref. [40] $F = \text{Tr}[\theta(-\mathcal{H})]$, in which the step function $\theta$ is expressed as a contour integral and the trace written in terms of $G(x, x)$. Looking at the specific results, Eq. (76) for $T \to 0$ indeed coincides with the result in Ref. [40] up to a total $x$-derivative.

IV. SUMMARY AND CONCLUSIONS

The 1D local matrix Green function $G(x, x)$ satisfies a certain differential equation, which can be decoupled to two matrix Riccati equations. The functional determinant $\text{Det} G^{-1}$ can be obtained from $G(x, x)$ and the mass matrix $\mathcal{M}(x)$ in the quadratic kinetic term, up to an overall constant prefactor. The mathematical structure is essentially a reflection of the standard scattering theory in 1D. The results here are obtained by making use of several known facts about boundary value problems, and functional determinants, and applying methods that have proved useful when dealing with the quasi-classical transport equations in superconductivity. Analytical calculations are tractable for dealing with simple problems, and a general gradient expansion for the free energy of noninteracting fermions can be obtained in this way. The results apply for a fairly generic class of Hamiltonians, and similar results probably can be obtained also for different forms of the kinetic term.
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