The one dimensional semi-classical Bogoliubov-de Gennes Hamiltonian with PT symmetry: generalized Bohr-Sommerfeld quantization rules

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Abstract. We present a method for computing first order asymptotics of semiclassical spectra for 1-D Bogoliubov-de Gennes (BdG) Hamiltonian from Supraconductivity, which models the electron/hole scattering through two SNS junctions. This involves: 1) reducing the system to Weber equation near the branching point at the junctions; 2) constructing local sections of the fibre bundle of microlocal solutions; 3) normalizing these solutions for the “flux norm” associated to the microlocal Wronskians; 4) finding the relative monodromy matrices in the gauge group that leaves invariant the flux norm; 5) from this we deduce Bohr-Sommerfeld (BS) quantization rules that hold precisely when the fibre bundle of microlocal solutions (depending on the energy parameter $E$) has trivial holonomy. Such a semi-classical treatement reveals interesting continuous symetries related to monodromy. Details will appear elsewhere.

1. Bogoliubov-de Gennes Hamiltonian

BdG Hamiltonian describes the dynamics of a pair of quasi-particles electron/hole in the Theory of Supraconductivity [2]. We consider a narrow metallic 1-D wire (Normal Metal N) connected to Supraconducting bulks S through a SNS junction, and compute the excitation spectrum in the normal contact region as a function of gate voltage, when electronic levels transform into phase sensitive Andreev levels. The wire, or lead, is identified with a 1-D structure, the interval $x \in [-L,L]$ (case of a perfect junction) or $x \in [-L + \ell/2, L - \ell/2]$ (“dirty junction”), where $\ell \ll L$. The reference energy in the lead is Fermi level $E_F$. The pair electron/hole is acted upon by two kinds of potentials:

(1) the “order parameter” $\Delta(x)$ times a phase function $e^{i\phi(x)/2}$, which is the potential due to Cooper pairs in the superconducting bulk. This potential, subject to self-consistency relations, is priori unknown. Namely, inside S, $\Delta(x)e^{i\phi(x)/2}$ is a solution of Ginzburg-Landau (or Pitaevskiy) equations, and shows typically a vortex profile (in 2-D). In BdG Hamiltonian it is assumed, however, that $\Delta(x)e^{i\phi(x)/2}$ is an “effective” potential. Inside N, superconducting gap $\Delta(x) \equiv 0$: quasi-particles live in the “clean metal”. For $|x| \geq L + \ell$, $\Delta(x) = \Delta_0 > 0$.

We assume that the phase function $\phi(x)$ is constant near the junction, and gauge the interaction by $\phi_- = -\phi_+ = -\phi$ in the superconducting banks, so that $\phi(x) = \text{sgn}(x)\phi$. We
assume further that this equality holds everywhere: since $\Delta(x) = 0$ inside $N$, the discontinuity of $x \mapsto \phi(x)$ is irrelevant.

(2) a smooth chemical potential $\mu(x)$: typically $\mu(x)$ is flat in $N$ and drops smoothly to the band bottom in the superconducting banks $S$. In our model we assume again $\mu(x)$ to be constant in the superconducting bank, i.e. $\mu(x) = \mu_0$ when $|x| \geq L + \ell$. Andreev currents at energy $E$ occur only if $\mu(x) \geq E$ in $[-L, L]$.

The case of a perfect junction ($\Delta$ “hard-wall potential”) has been considered in [5], see also [4] for a SFS junction, and makes use scattering matrix techniques. In this work, justifying semi-classical techniques as in [8] (also in the multi-dimensional case) we rather consider an imperfect (or “dirty”) junction: $\Delta(x)e^{i\phi(x)/2}$ is a smooth function. In a neighborhood of $[-L, L]$, say $x \in [-L - \ell, L + \ell]$, the system is described at the classical level by BdG Hamiltonian

$$\mathcal{P}(x, \xi) = \begin{pmatrix} \xi^2 - \mu(x) & \Delta(x)e^{i\phi(x)/2} \\ \Delta(x)e^{-i\phi(x)/2} & -\xi^2 + \mu(x) \end{pmatrix}$$  \hspace{1cm} (1)$$

The energy surface: $\Sigma_E = \{ \det(\mathcal{P} - E) = -((\xi^2 - \mu(x))^2 - \Delta(x)^2 + E^2) = 0 \} = \Lambda_E^\pm \cup \Lambda_E^{E0}$ splits into 2 branches separated in momentum space, so consists of two microlocal wells. Interaction between these wells gives the imaginary parts of the resonances for the electron/hole scattering, and will be ignored in this paper. Because of smoothness of $x \mapsto \Delta(x)$, the reflections occur inside $[-L, L]$, we denote by $(\pm x_E, \xi_E) \in \Lambda_E^\pm$, the one-parameter family of “branching points” defined by $\Delta(\pm x_E) = E$ with $x_E$ near $x_0 \in [-L + \frac{\ell}{2}, L + \frac{\ell}{2}]$, $\Delta(x_0) > 0$. We do not consider the problem of “clustering” of eigenvalues as $E \to 0 = E_F$ (Fermi level). In the “hard wall potential” limit for $x$ near $x_0$, the potential $\Delta(x)$ can be safely approximated by a linear function such that $\Delta(x_0) = E_0$, and $\mu(x)$ by a constant $\mu$. So near $x_0$ we assume that

$$\phi(x) = \phi, \quad \mu(x) = \mu > E, \quad \Delta(x) = E + \alpha(x - x_E)$$

for large $\alpha > 0$. Condition $a_E = (x_E, \xi_E) \in \Sigma_E$ gives $\xi_E^2 = \mu > E, \Delta(x_E) = E$.

The physical mechanism goes roughly as follows (see [5] for a detailed exposition): An electron $e^-$ moving in the metallic lead, say, to the right, with energy $0 < E \leq \Delta$ below the gap and kinetic energy $K_+(x) = \mu(x) + \sqrt{E^2 - \Delta(x)^2}$ is reflected back as a hole $e^+$ from the superconductor, injecting a Cooper pair into the superconducting contact. The hole has kinetic energy $K_-(x) = \mu(x) - \sqrt{E^2 - \Delta(x)^2}$, and a momentum of the same sign as this of the electron. When $\inf_{[-L,L]}K_-(x) > 0$ it bounces along the lead to the left and picks up a Cooper pair in the superconductor, transforming again to the original electron state, a process known as Andreev reflection. This works also the other way in $\Lambda_E^\pm$, since Hamiltonian system conserves both charge and energy. Actually, the hole can propagate throughout the lead only if $\inf_{[-L,L]}\mu(x) \geq E$. Otherwise, it is reflected from the potential $\mu(x)$ in the junction, and Andreev levels are quenched at higher energies, i.e. transform into localized electronic states.

For a rescaled “Planck constant” $h$ so that $h \ll \ell$, we consider Weyl $h$-quantization of BdG Hamiltonian $\mathcal{P}(x, hD_x)$ on $L^2(I) \otimes \mathbb{C}^2$, $I = [-L + \ell, L + \ell]$, which is self-adjoint when imposing Dirichlet boundary conditions at $\partial I$. Phase-sensitive Andreev states carry supercurrents that turn out to be proportional to the $\phi$-derivative of the eigen-energies of $\mathcal{P}(x, hD_x)$.

We have $\sigma^y \mathcal{P}(\phi)\sigma^y = -\mathcal{P}(-\phi)$, with $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, accounting for “negative energies”. We shall assume here $E > 0$. When potentials are even functions (typical for metals), $\mathcal{P}(x, hD_x)$ verifies PT symmetry $\mathcal{P}(x, hD_x) = \mathcal{P}(x, hD_x)\mathcal{I}^\prime$ which is essential for our approach to work.

At least formally, since BdG is only defined locally near $N$, removing boundary conditions leads to “resonances” (i.e. metastable states or quasi-particles with a finite life-time). Thus for simplicity we have assumed that [4,], together with its semi-classical quantization, describes the system not only in $I$, but on the whole real line, provided $h \ll \ell \ll L$. Thus $\mathcal{P}(x, hD_x)$ extends to $L^2(\mathbb{R}) \otimes \mathbb{C}^2$, I}
Our general goal is to give a precise mathematical meaning to these “resonances”. Here we content to compute their real parts through Bohr-Sommerfeld quantization rules.

2. Monodromy operator, scattering matrix: an outlook

a) Schrödinger operator: on the real line.

We first recall from [1] basic facts for a 1-D Schrödinger operator with a compactly supported potential $V$. The generalized wave-functions $u$ with energy $E = k^2 > 0$ satisfy

$$-\hbar^2 u''(x) + V(x)u(x) = Eu(x)$$

(2)

and outside supp $V$,

$$-\hbar^2 u''(x) = k^2 u(x)$$

(3)

defines the state space $\mathbb{Z} \cong \mathbb{C}^2$ of the “free particle”, spanned by $f_1(x) = e^{ikx/\hbar}$, $f_2(x) = e^{-ikx/\hbar}$.

The monodromy operator $M(k) : f_1 + Bf_2 \mapsto Af_1$ is such that

$$M(k) = \begin{pmatrix} 1/A & -B/A \\ -B/A & 1/A \end{pmatrix} \in \text{SU}(1,1)$$

In particular, $|A|^2 + |B|^2 = 1$. We call $|A|^2$ the transmission coefficient and $|B|^2$ the reflection coefficient. Along with the passage from the left to the right of the support of $V$, consider the passage from the right to the left. The corresponding solution $v$ of (2) is $e^{-ikx/\hbar} + B_2 e^{ikx/\hbar}$ to the right of supp $V$, and $A_2 e^{-ikx/\hbar}$ to the left. The scattering matrix is defined as

$$S(k) = \begin{pmatrix} A & B \\ -BA/A & B/A \end{pmatrix} \in \text{U}(2)$$

$S(k)$ remains unitary and symmetric for complex values of $k$. Resonances of (2) are then defined as $E = k^2 \in \mathbb{C}$, where $k$ is a pole of $S$, and physical resonances those with $\text{Im} k > 0$. Thus $E$ is a resonance iff the solution of (3) is purely outgoing as $x \to +\infty$ and $x \to -\infty$. The poles coincide with the poles of meromorphic extension of the resolvent $(P - k^2)^{-1}$ from the physical half-plane $\text{Im} E < 0$ to the second sheet $\text{Im} E > 0$.

b) Monodromy matrix for BdG equation: heuristics.

Now we discuss BdG equation $(P(x, hD_x) - E)U = 0$ for large $|x|$, i.e. (within our approximation above) when $|x| \geq L + \ell$, so $\Delta(x) = \Delta_0$, $\mu(x) = \mu_0 > E$. Solutions are of the form

$$U(x; h) = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e^{ikx/\hbar} \\ e^{i\ell x/\hbar} \end{pmatrix}$$

$$\mu_0 + E \pm i\Delta_0 \in \{k^2, \ell^2\},$$

so eigenfrequencies are $(\pm k, \pm \ell)$, $k = \sqrt{\mu_0 + E + i\Delta_0}$, and the corresponding solutions as follows:

Let $\phi(x) = \text{sgn}(x)\phi$, $\mathcal{Z}$ be the 2-D complex line bundle spanned by $F^\pm_1(x) = \begin{pmatrix} e^{i\beta(x)/2} \\ -i \end{pmatrix} e^{\pm ikx/\hbar}$ (associated with the scattering process $e^+ \to e^-$), and $\overline{\mathcal{Z}}$ the 2-D complex line bundle spanned by $F^\pm_2(x) = \begin{pmatrix} e^{i\beta(x)/2} \\ i \end{pmatrix} e^{\pm ikx/\hbar}$ (associated with the scattering process $e^- \to e^+$).

The space of solutions of exponential type for BdG is $\mathcal{Z} \oplus \overline{\mathcal{Z}}$, and $\mathcal{Z}, \overline{\mathcal{Z}}$ are orthogonal for the usual pointwise Hermitian product in $\mathbb{C}^2$. Declare that $E \in \mathbb{C}$ is a $\mathcal{Z}$-resonance iff the $\mathcal{Z}$-component of the wave function solving BdG equation is outgoing and evanescent (“physical solution”) at infinity, i.e.

$$U(x, h) = A \begin{pmatrix} e^{i\beta/2} \\ -i \end{pmatrix} e^{ikx/\hbar}, x \to +\infty$$

$$U(x, h) = B \begin{pmatrix} e^{-i\beta/2} \\ -i \end{pmatrix} e^{-ikx/\hbar}, x \to -\infty$$
Similarly we say that $E$ is a $\mathbb{Z}$-resonance iff the $\mathbb{Z}$-component of the wave function is outgoing (and evanescent) at infinity, i.e.

$$U(x,h) = A\left(e^{i\phi/2}\right)e^{-iE/h}x \to +\infty$$

$$U(x,h) = B\left(e^{-i\phi/2}\right)e^{iE/h}x \to -\infty$$

So for both sets of resonances, the corresponding solution is simultaneously decaying, and outgoing at $\pm \infty$. These sets of resonances need not coincide (although they come up in pairs), but their real parts are given by Bohr-Sommerfeld quantization rules. Namely, define the monodromy operator $M^Z(k)$ acting on $Z$ according to the formula

$$\left(\begin{array}{c}
e^{-i\phi/2} \\
-i \end{array}\right)e^{ikx/h} + B\left(\begin{array}{c}
e^{-i\phi/2} \\
-i \end{array}\right)e^{-ikx/h} \to A\left(\begin{array}{c}
e^{i\phi/2} \\
-i \end{array}\right)e^{ikx/h}$$

and similarly for $M^\overline{Z}(k)$. It is plausible to expect that $M^Z(k), M^\overline{Z}(k) \in \mathbb{U}(1,1)$, and that the corresponding scattering matrices $S^Z(k), S^\overline{Z}(k)$ have a meromorphic extension to the complex plane, their poles defining the resonances $E^Z$ and $E^\overline{Z}$. Actually, we shall construct “relative monodromy operators” in the “classically allowed region”. In particular the relative monodromy operators are in $\mathbb{U}(1,1)$ for some specific Lorenzian form which is constructed below.

3. Bohr-Sommerfeld quantization rules

In this work, we content to determine the real parts of the resonances, extending to this setting the method of positive commutators elaborated in [12], [9] and [10]. Imaginary parts may be determined as in [11]. We obtain Bohr-Sommerfeld quantization rules for the quasi-particle, alternating even and odd quantum numbers associated with the electron and the hole. In the sequel we will sketch a proof of the following result:

**Theorem 1**: Let $\int_{y_0}^{y_0} \eta^\rho(y;h) dy$ be the semi-classical actions (see Proposition 8 below) $\rho = 1$ for the electron, $\rho = -1$ for the hole. Bohr-Sommerfeld quantization conditions near $E_0$ are given at first order by:

$$\oint_{\gamma_E} \eta^\rho(y;h) dy - h\phi + h\pi + O(h^2) = 2\pi nh; \quad n \in \mathbb{Z}$$

with even (resp. odd) quantum numbers $n$ for the electron (resp. the hole). Here $\oint_{\gamma_E}$ denotes integral over the loop $\gamma_E$ obtained by gluing together $\Lambda^\rho_E$ and $\Lambda^{\overline{\rho}}_E$, if we ignore tunneling in momentum space.

4. Microlocal solutions in Fourier representation near the branching points

a) Reduction of the system.

In $\hbar$-Fourier representation, $\mathcal{F}_\hbar u(\xi) = (2\pi\hbar)^{-1/2}\int e^{-ix\xi/h}u(x) dx$ the local Hamiltonian near $a = a_E = (x_E,\xi_E)$, $\mathcal{P}^a$ takes the form:

$$\mathcal{P}^a(-\hbar D_\xi,\xi) = \left(\begin{array}{cc}
\xi^2 - \mu & e^{i\phi/2}(E - \alpha hD_\xi - \alpha x_E) \\
e^{-i\phi/2}(E - \alpha hD_\xi - \alpha x_E) & -\xi^2 + \mu
\end{array}\right)$$

(4)
By PT symmetry $P^a = T P^a T$ near $a = a^E_\xi = (-x_E, \xi_E)$. Solving the system $P^a(-hD_\xi, \xi)\hat{U} = 0, \hat{U} = (\hat{\xi}^1, \hat{\xi}^2)$ gives second order ODE for $u(\xi) = \exp[-i \int g(s)ds/h] \tilde{\varphi}_2(\xi)$,

$$P^a(-hD_\xi, \xi, h)u(\xi) = \frac{E^2}{\alpha^2}u(\xi) \tag{5}$$

$$P^a(-hD_\xi, \xi, h) = (hD_\xi)^2 + \alpha^{-2}(\xi^2 - \mu)^2 + h^2(\xi^2 - \mu - E)^2(2\xi^2 + \mu + E)$$

After $E$-dependent scalings $\beta = \sqrt{\alpha}(2\xi_E)^{-3/2} > 0$, $E_1 = (2\xi_E)^{-2}E_2 \xi = 2\xi_E\beta \omega \xi' + \xi_E, \omega = \pm 1$ ($\xi'$ is “local momentum”) we obtain $P^{a}(hD_\xi', \xi', h)u_\omega(\xi') = (\frac{E_1}{\beta})^2 u_\omega(\xi')$, where

$$P^{a}(hD_\xi', \xi', h) = (-hD_\xi')^2 + (\xi' + \beta \omega \xi'^2)^2 + h^2 \beta^2 f(\omega \beta \xi')$$

is an anharmonic Schrödinger operator. The lower order term $f(z) = (2z^2 + 2z + \frac{3}{4} + E_1)(z^2 + z - E_1)^{-2}$ has a pole on $\Lambda^E_2$ where the linear approximation of $\Delta(x)$ breaks down. The linear approximation only holds for small $\xi'$. Consider the map

$$\iota^a : \sum_{\omega = \pm 1} \text{Ker}_h(P^a_\omega - (\frac{E_1 \omega}{\beta})^2) \to \text{Ker}_h(P^a - E) \tag{6}$$

where $\text{Ker}_h$ denotes the microlocal kernel. The index $\omega$ is to be chosen carefully with the complex germ of solutions having the right decay beyond the branching points $\pm x_E$. We shall endow the RHS of (6) with a Lorentzian structure and “diagonalize” $\iota^a$ in some orthogonal subspaces.

b) The normal form of Helffer-Sjöstrand

When $E_1 < \frac{1}{4}$, we take $P^a_\omega$ microlocally to its normal form, namely:

**Proposition 2** [9]: There exists an analytic diffeomorphism $t \mapsto F_0(t)$ defined in a neighborhood of $0$, $F_0(0) = 0$, with inverse $G_0$, and a real analytic phase function $\phi_\beta(\xi', \theta)$, defined in a neighborhood of $(0,0)$, of the form $\phi_\beta(\xi', \theta) = \xi' \theta + g_\beta(\xi', \theta)$, $g_\beta(\xi', \theta) = O(|\xi'|^3)$, parametrizing the canonical transformation $\kappa_\beta : (\partial_{\phi_\beta(\xi', \theta)} \rightarrow (\xi', \partial_{\xi'} \phi_\beta)$, such that $F_0 \circ p_\beta \circ \kappa_\beta = p_0$. At the semi-classical level, there is a (formally) unitary FIO operator $A$ defined microlocally near $(0,0)$

$$A\nu(\xi', h) = (2\pi h)^{-1} \int e^{i\epsilon(\xi', \eta, \theta)/h} e^{ib(\xi', \eta, \theta, h)} v(\eta, h) d\eta d\theta$$

and a real valued analytic symbol

$$F(t, \beta, h) = F_0(t, \beta) + hF_1(t, \beta) + h^2F_2(t, \beta) + \cdots$$

with $F_1(t, \beta) = -\frac{1}{2}$ such that

$$A^* F(P_\omega, \beta, h)A = P_0(\eta, hD_\eta) = \frac{1}{2}((hD_\eta)^2 + \eta^2 - h), \quad A^* A \equiv \text{Id}$$

The function $F_0$, taking the period $T(E)$ of Hamilton vector flow for $P_\omega^a$ at energy $(E_1/\beta)^2$ to $2\pi$, involves an elliptic integral, which requires sometimes the use of formal calculus.

c) Weber equation and parabolic cylinder functions

Weber equation $P_0 v = -v'' + \frac{1}{4} \xi^2 v = (\nu + \frac{1}{2})\tilde{v}$ scales to

$$\tilde{v''} + \frac{1}{4} \xi^2 \tilde{v} = (\nu + \frac{1}{2})\tilde{v}$$
Fundamental solutions express as parabolic cylinder functions $D_\nu$, entire in $\mathbb{C}$. The systems 
$(D_\nu(\pm \xi), D_{-\nu-1}(\pm i\xi))$ are fundamental solutions for any choice of $\pm$. Integral representations

give asymptotic solutions of $(P_0 - \nu h)u(\eta) = 0$ by stationary phase for real $\nu$, $E_1^2 = 2\beta^2 F(\beta^2 E_1^2, \beta, h) = 2\beta^2 (\nu + 1) h$.

\[
D_\nu(\varepsilon(h/2)^{-1/2} \eta) = \frac{\Gamma(\nu + 1)}{2\pi i \sqrt{h}} h^{E_2/4h} f_0(i\nu) \exp[i \Phi^\nu(\eta)/h] \, ds
\]

\[
D_{-\nu-1}(i\varepsilon(h/2)^{-1/2} \eta) = \frac{\Gamma(-\nu)}{2\pi i \sqrt{h}} h^{-E_2/4h} f_\infty(i\nu) \exp[i \Phi^{-\nu}(\eta)/h] \, ds
\]

with $\varepsilon = \pm 1$, $E = \sqrt{2(\nu + 1)/h}$, see [13]. This normalization is called Whittaker normalization.

Classically forbidden regions $|\eta| > E$ lie on Stokes lines, classically allowed region $|\eta| < E$ in between, and 3 Stokes lines stem from each “turning point” $\eta = \pm E$.

d) Microlocal solutions.

We apply asymptotic stationary phase to $AD_j$, $j \in \{\nu, -\nu - 1\}$. With $h' = \beta^2 h$ as a “rescaled” Planck constant, we get:

**Proposition 3:** In Fourier representation, the image $K^a_\hbar(E) = \text{Ker}_\hbar(\mathcal{P}_a(-hD_{\xi}, \xi) - E)$ of $\mathcal{P}_a$ is a 2-D vector space spanned by the spinors $\hat{U}_{\xi,\omega} = \left(\hat{\xi}_\omega, \hat{\xi}_\omega\right) \in \{\nu, -\nu - 1\} \times \{-1, 1\}^2$, of the form:

\[
\hat{U}_{\varepsilon,\omega} = C_{h'} \sum_{\theta_\omega = \pm \hat{\theta}_\omega(\xi)} \left(\frac{e^{i\theta_\omega(\xi)}}{(\xi^2 - h\omega^2)^{1/2}}\right) \left(\frac{e^{i\theta_\omega(\xi)}}{(\xi^2 - h\omega^2)^{1/2}}\right) \exp[i \left(\Phi^\nu_{\varepsilon,\omega} + h'R_{\varepsilon,\omega}/h'\right)] + \mathcal{O}(h')
\]

\[
\hat{U}_{\varepsilon,\omega}^{-\nu-1} = C_{h'}^{-\nu-1} \sum_{\theta_\omega = \pm \hat{\theta}_\omega(\xi)} \exp[\text{sgn}(\theta_\omega)\left(\frac{e^{i\theta_\omega(\xi)}}{(\xi^2 - h\omega^2)^{1/2}}\right) \left(\frac{e^{i\theta_\omega(\xi)}}{(\xi^2 - h\omega^2)^{1/2}}\right) \exp[i \left(\Phi^{-\nu}_{\varepsilon,\omega} + h'R_{\varepsilon,\omega}^{-\nu-1}/h'\right)] + \mathcal{O}(h')
\]

Here $\hat{\theta}_\omega(\xi)$ is a critical point (from stationary phase), $\Phi^\nu_{\varepsilon,\omega} + h'R_{\varepsilon,\omega}$ the $h'$-dependent phase functions, and $X_{\varepsilon,\omega}$, $\hat{a}_{\varepsilon,\omega}$ some positive amplitudes. Spinors $U_{\varepsilon,\omega}$ verify the symmetry $\hat{U}_{\varepsilon,-\omega} = \hat{U}_{\varepsilon,\omega}$ for the “local time” reversal operator $^t u(\xi) = u(-\xi)$, and the constants $C_{h'}$ (from Whittaker normalization of $D_\nu, D_{-\nu-1}$) are related by $C_{h'} C_{h'}^{-\nu-1} = (2\sqrt{R})^3 \pi^2 \sin \pi \nu^{-1}$.

5. Normalization

a) The microlocal Wronskian.

We extend to BdG Hamiltonian the classical “positive commutator method” using conservation of some quantity called a “quantum flux” ([12], [9], [11], [10]).

**Definition 4:** Let $\mathcal{P}$ be (formally) self-adjoint, and $U^a, V^a \in K_\hbar(E)$ be supported on $\Lambda E$. We call the sesquilinear form $W^a_\rho(U^a, V^a) = \frac{1}{2} [\mathcal{P}, \chi^a]_\rho U^a V^a = \frac{1}{2} [\mathcal{P}, \chi^a]_\rho \tilde{U}^a \tilde{V}^a$ the microlocal Wronskian of $(U^a, V^a)$ in $\omega_\rho^n$. Here $\frac{1}{2} [\mathcal{P}, \chi^a]_\rho$ denotes the part of the commutator supported microlocally on $\omega_\rho^n$ (a small neighborhood of $\text{supp} \, \mathcal{P}, \chi^a \cap \Lambda E$ near $\rho$).

A crucial property of the microlocal Wronskian is to be invariant by Fourier transformation: $W^a_\rho(U^a, V^a) = W^a_\rho(\tilde{U}^a, \tilde{V}^a)$. The relation $W^a_\rho(U^a, V^a) + W^a_\rho(\tilde{U}^a, \tilde{V}^a) = 0$ doesn’t readily follow as in the scalar case [10], the microlocal solutions being neither smooth in spatial of Fourier representation near the branching point, but from a careful inspection, involving also formal calculus. This is used essentially in Propositions 5 and 8 below. Choosing $\varepsilon, \omega$ such that $\varepsilon \omega = 1$
we define a Lorenzian metric $\mathcal{W}_\rho$ on the space of microlocal solutions near $a$. In the basis

\[
\hat{U}_{\xi,\omega}^j, j \in \{\nu, -\nu - 1\}\]

we have, up to a constant factor:

\[
\rho\mathcal{W}_\rho = \left(\frac{|C_{h'}^\nu|^2\mathcal{O}(h')}{C_{h'}^\nu C_{h'}^{-\nu-1}\exp[i\pi E_1^2/4h'](1 + \mathcal{O}(h')) } \right)^{1/2} \end{align*}

Changing Whittaker normalization for the $D_\nu, D_{-\nu-1}$ functions, and the microlocal solutions by some constant phase factors, we can reduce to $\rho\mathcal{W}_\rho = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \mathcal{O}(h')$, and prove:

**Proposition 5:** Under PT symmetry above the microlocal Wronskians $\mathcal{W}_\rho^a$ endow $K_h^a(E)$ (mod $h'$) with a Lorenzian form $\mathcal{W}_\rho = \frac{1}{2}(\mathcal{W}_\rho^a - \mathcal{W}_\rho^a)$. The same holds at $a'$, and the corresponding structures on $K_h^a \times K_h^{a*}$ and $K_h^{a'} \times K_h^{a'*}$ are anti-isomorphic. The group of automorphisms preserving $\mathcal{W}_\rho$ and $\mathcal{W}_\rho^{a'}$ mod $\mathcal{O}(h')$ is therefore $U(1,1)$.

6. Spinors in the spatial representation

We compute $U_{\xi,\omega}^\nu$, $U_{\xi,\omega}^{\nu,j}$ in spatial representation, then extend along the branches $\rho = \pm 1$ of $\Lambda_E^>$ with WKB solutions.

**a) Spinors near the branching points.**

Near $a, a'$ we apply inverse $h$-Fourier transform and get:

**Proposition 6:** Up to a constant phase factor

\[
U_{\xi,\omega}^\nu(x, h) = 2\omega \beta_{\xi E}e^{i\pi \xi_\omega} \sum_{\rho = \pm \epsilon} \left( e^{i\phi/2} \left( \frac{1}{2} - \frac{1}{2} \right) X_{\xi,\omega}^\nu \right) a_{\xi,\omega}^\nu \theta_{\xi,\omega}^\nu \xi_\omega (x)
\times \left( \frac{\mathcal{L}_\rho^0(x)}{\rho} \right)^{-1/2} \exp \left[ i \left( \Psi_{\xi,\omega}^{\rho,p}(x) + h' R_{\xi,\omega}^{\rho,p}(x) \right) / h' \right] (1 + \mathcal{O}(h'))
\]

\[
U_{\xi,\omega}^{\nu-1}(x, h) = 2\omega \beta_{\xi E}e^{i\pi \xi_\omega} \sum_{\rho = \pm \epsilon} \left( e^{i\phi/2} \left( \frac{1}{2} - \frac{1}{2} \right) X_{\xi,\omega}^{\nu-1} \right) a_{\xi,\omega}^{\nu-1} \theta_{\xi,\omega}^{\nu-1} \xi_\omega (x)
\times \left( \frac{\mathcal{L}_\rho^0(x)}{\rho} \right)^{-1/2} \exp \left[ i \left( \Psi_{\xi,\omega}^{\rho,p}(x) + h' R_{\xi,\omega}^{\rho,p}(x) \right) / h' \right] (1 + \mathcal{O}(h'))
\]

Here $\left( \mathcal{L}_\rho^0(x) \right)^{-1/2}$ is a real density (singular at $x = x_E$), and $\rho$ labels the branch of the Lagrangian manifold. The phases $\Psi_{\xi,\omega}^{\rho,p}(x) + h' R_{\xi,\omega}^{\rho,p}(x)$, $j \in \{\nu, -\nu - 1\}$ differ only by a constant.

**b) WKB spinors away from the branching points.**

The Lagrangian manifold $\Lambda_E^>$ consists of 2 branches $\Lambda_E^{>,\rho}$ (or simply $\rho = \pm 1$ so that $\rho = +1$ belongs to the electronic state ($\xi_1 > 0$ in the local coordinates near $a$ above), resp. $\rho = -1$ to the hole state ($\xi_1 < 0$). These states mix up when $\Delta(x) \neq 0$, but we can sort them out semiclassically, outside $a, a'$. Call the vector space of $\mathcal{C}^2$ generated by $\begin{pmatrix} i \rho \\ 0 \end{pmatrix}$ the space of (pure) electronic states, or electronic spinors, and this by $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the space of (pure) hole states, or hole spinors.

The principal symbol $P(x, \xi)$ has eigenvalues $\lambda_\rho = \rho \lambda(x, \xi) = \rho \sqrt{\Delta(x)^2 + (\xi^2 - \mu(x))^2}$. By diagonalizing, we obtain a line bundle $\Lambda_E^\rho$ with fiber

\[
Y_\rho(x, \xi) = (\Delta^2 + (-\xi^2 + \mu + \rho \sqrt{\Delta^2 + (\xi^2 - \mu)^2})^{1/2} \left( -\xi^2 + \mu + \rho \sqrt{\Delta^2 + (\xi^2 - \mu)^2} \right)
\]
Looking at the electronic state, we choose $\rho = +1$ so that $\lambda_\rho(x, \xi_\rho) - E = 0$, while $\lambda_{-\rho}(x, \xi_\rho) - E$ is elliptic. and similarly when looking at the hole state.

**Proposition 7** The microlocal kernel $\text{Ker}_h(\mathcal{P} - E)$ on $\Lambda_{E}^{>\rho}$ is one-dimensional space spanned by

$$W^\rho(x, h) = e^{iS_{\rho}(x, h)/h}(w^\rho_0(x, h)Y_\rho(x, \partial_x S_\rho) + \mathcal{O}(h)) = e^{iS_{\rho}(x, h)/h}\tilde{W}^\rho(x, h)$$

where $w^\rho_0(x)|dx|^{1/2}$ is a smooth half-density. By the uniqueness property of WKB solutions along simple bicharacteristics, the $h$ (or $h'$)-dependent phase function $S_\rho(x, h)$ should coincide, up to a constant (in a punctured neighborhood of $a$) with either one of $\Psi^{\rho}_j(x) + h'R^{\rho}_j(x)$ above, $j \in \{\nu, -\nu - 1\}$, and similarly for the half-densities.

### 7. Relative monodromy matrices

Now we look for connexion formulas. For each $\varepsilon, \omega, \rho = \pm 1, j \in \{\nu, -\nu - 1\}$, the normalized microlocal solutions $U^a, j, \rho_{\varepsilon, \omega}$ are related to the extension $U^-_{-\varepsilon, -\omega, \text{ext}}$ of the normalized microlocal solutions $U^a, k, \rho_{\varepsilon, \omega}$ along the bicharacteristics by a monodromy matrix

$$\mathcal{M}^{a, \alpha', \rho} = \left( \begin{array}{cc} d_{11}^\rho & d_{12}^\rho \\ d_{21}^\rho & d_{22}^\rho \end{array} \right) \in U(1, 1)$$

(defined at least mod $\mathcal{O}(h')$) which we call a relative monodromy matrix. Since there is a pair of particles, the symmetry between the $\mathcal{M}^{a, \alpha', \rho}$ and $\mathcal{M}^{a, \alpha, \rho}$ is order 4; $\mathcal{M}^{a, \alpha, \rho} \in U(1, 1)$ is obtained by extending from the left to the right, and applying symmetry

$$\rho \mathcal{M}^{a, \alpha, \rho} = \mathcal{I}(\mathcal{M}^{a, \alpha', \rho})^{-1} \mathcal{I} =, \rho = \pm 1$$

where $\mathcal{I}$ denotes complex conjugation. We compute the coefficients $d_{ij} = d_{ij}^\rho$. Considering behavior of $U^a, j, \rho_{\varepsilon, \omega}$ in the classically forbidden region (according to scattering process $e^+ \rightarrow e^-$ or $e^- \rightarrow e^+$) we obtain

$$\mathcal{M}^{a, \alpha', \rho} = \left( \begin{array}{cc} 0 & d_{12}^\rho \\ d_{21}^\rho & 0 \end{array} \right), \quad \overline{d_{12}^\rho} d_{21}^\rho = 1$$

Note that if we do not look too closely at the relevant complex branches, as is the case when computing BS, it makes no difference to choose instead $\mathcal{M}^{a, \alpha', \rho} = \left( \begin{array}{cc} d_{11}^\rho & 0 \\ 0 & d_{22}^\rho \end{array} \right)$, with $d_{11}^\rho d_{22}^\rho = 1$.

As in [12], [9], [11], [10], the argument consists now in extending microlocal solutions obtained above from $a$ to $a'$, and computing the resulting semi-classical action. So take first $U_1^a = U^\nu_{\varepsilon, \omega}$ near $a$, extend it along to $a'$ along the bicharacteristics $\rho = \pm 1$ by WKB. Evaluating on $\rho$ near $a'$ we find $U_1^{a', \rho} = U^\nu_{\varepsilon, \omega, \text{ext}} = d_{21}^\rho U^\nu_{\varepsilon, \omega, \varepsilon, \omega}$. Similarly, take $U_2$ starting at $a'$ and with $-\nu - 1$ instead of $\nu$, we get $U_2^{a', \rho} = U^{-\nu-1}_{-\varepsilon, -\omega, \varepsilon, \omega} = e_{12}^\rho U^\nu_{\varepsilon, \omega, \varepsilon, \omega}$, where $e_{12}^\rho = \rho(d_{21}^\rho)^{-1}$ is the matrix element of $\mathcal{M}^{a, \alpha, \rho}$ given in (7). We compute $d_{21}^\rho$ in two different ways and compare the result.

(1) Using time-reversal and PT symmetries in the microlocal Wronskians, we get

$$\left( \frac{i}{h} [\mathcal{P}, \chi^\alpha]_\rho U_1^\nu_{\varepsilon, \omega} \right) d_{21}^\rho = \left( \frac{i}{h} [\mathcal{P}, \chi^\alpha]_\rho U^\nu_{\varepsilon, \omega} \right) d_{21}^\rho = d_{21}^\rho W^\nu_{\rho} U^\nu_{\varepsilon, \omega, \varepsilon, \omega} = d_{21}^\rho W^\nu_{\rho} U^\nu_{\varepsilon, \omega, \varepsilon, \omega} = -d_{21}^\rho W^\nu_{\rho} U^\nu_{\varepsilon, -\omega, \varepsilon, \omega} = -d_{21}^\rho W^\nu_{\rho} U^\nu_{\varepsilon, -\omega, \varepsilon, \omega} = -d_{21}^\rho$$

(2) Using the extensions described in Proposition 7. Near $a'$ we have $U^\rho_{1,\text{ext}} = e^{i\phi/2}W^\rho(x,h) = d^{21}\chi_{\xi,-\nu}^{-1,a',\rho}$ (by solving transport equation along $\rho$ the amplitude picks up the phase factor $e^{i\phi/2}$, so we need to compute $(\frac{i}{\hbar}[\mathcal{P}^{\alpha'},\chi^{\alpha'}],_\rho W^\rho(x,h))U_{\xi,-\nu}^\rho$. The amplitude $W^\rho(x,h)$ is actually defined up to a real, constant factor $\tilde{C}^\rho$.

Proposition 8: Let $	ilde{\Psi}_{\xi,-\nu}^{\alpha',\rho}(x) = x\xi E + \frac{(2\xi E)^3}{\alpha}\Psi_{\xi,-\nu}^{\alpha',\rho}(x)$. We have

$$\left(\frac{i}{\hbar}[\mathcal{P}^{\alpha'},\chi^{\alpha'}],_\rho W^\rho(x,h)\right) = 2\tilde{C}^\rho e^{i\pi/4} \int \exp[i(\tilde{S}_\rho(x,h)/\hbar)] \beta(x,h)(\chi_{\xi,-\nu}^{\alpha'})(x) \, dx$$

where the amplitude $\beta(x,h)$, real mod $O(h)$, is computed from the WKB solutions in Proposition 7, and

$$\tilde{S}_\rho(x,h) = S_\rho(x,h) - \left(x\xi E + \tilde{\Psi}_{\xi,-\nu}^{\alpha',\rho}(x) - hR_{-\omega}(\theta_{-\omega}(\xi_{-\omega}(-x)))\right) = \frac{(2\xi E)^3}{\alpha}\Psi_{\xi,-\nu}^{\alpha',\rho}(x_0) - \int_{x_0}^{x_0} \eta^\rho(y;h) \, dy + hR_{-\omega}(\theta_{-\omega}(0))$$

Moreover, $\beta(x,h)$ is also independent of $x$, so that, comparing the former expression (1) and (8) for a suitable choice of $\tilde{C}^\rho$, we get

$$d^{21}_\rho = -e^{i\tau^\rho(h)/h} \int (\chi_{\xi,-\nu}^{\alpha'})(x) \, dx = e^{i\tau^\rho(h)/h}$$

Here $\tau^\rho(h) = h \frac{\phi}{2} + h \frac{\tau}{2} - \int_{x_0}^{x_0} \eta^\rho(y;h) \, dy + \text{Const.},$ where Const. is evaluated at the boundaries $x = \pm x_E$, and depends only on $E_1'$. It will eventually disappear from the final formula, by adding to BS the contribution of the lower branch $\Lambda_{E}^{-\rho}$. Note that $\int_{x_0}^{x_0} \eta^\rho(y;h) \, dy, \eta^\rho(y;h)$ being the derivative of the $h'$-depending phase function, is the semi-classical action.

8. Bohr-Sommerfeld quantization rules

We set $F_{\xi,-\nu}^{\alpha',\rho} = \frac{i}{\hbar}[\mathcal{P}^{\alpha'},\chi^{\alpha'}],_\rho U_{\xi,-\nu}^{\alpha',\rho}$, and similarly with $a'$. The set $\{G_{\xi,-\nu}^{\alpha',\beta} = F_{\xi,-\nu}^{\alpha',\beta} - F_{\xi,-\nu}^{\alpha',\beta} : j \in \{\nu - \nu - 1\}, b \in \{a, a'\}\}$ (or their h-Fourier transform) can be interpreted as a basis of the microlocal co-kernel of $\mathcal{P}$ near $a, a'$. Following [10], we introduce Gram matrix $G^\rho$ of vectors $\hat{U}_{1,\alpha'}$ and $\hat{U}_{2,\alpha'}$ in this basis, namely $G = \left(\begin{array}{cc} \hat{U}_1\hat{G}_{\xi,-\nu}^{\alpha',\alpha'} & \hat{U}_2\hat{G}_{\xi,-\nu}^{\alpha',\alpha'} \\ \hat{U}_1\hat{G}_{\xi,-\nu}^{\alpha',\alpha'} & \hat{U}_2\hat{G}_{\xi,-\nu}^{\alpha',\alpha'} \end{array}\right)$. Using symmetries we get

$$G = G^\rho = 2\left(\begin{array}{cc} 1 & e^{i\theta}\rho(d^{21}_\rho) \\ -d^{21}_\rho & -1 \end{array}\right)$$

The condition $\det(G^\rho) = 0$ means that $U_1$ is colinear to $U_2$, i.e. there is a global section of $\text{Ker}_{h}(\mathcal{P} - E)$. Recall $e^{i\theta}_\rho = \rho(d^{21}_\rho)^{-1};$ for $\rho = +1$ (electronic state) we get $\text{Im}d^{21}_\rho = 0$, that is $\sin\left(\frac{\tau^\rho(h)}{\hbar}\right) = 0$. We eventually obtain BS by “surgery”: namely (ignoring tunneling) we cut and paste the half-bicharacteristic $\Lambda_{\frac{\xi}{2}}^{-\nu}$ in the upper-half plane $\xi > 0$ with its symmetric part $\Lambda_{\frac{-\xi}{2}}^{\nu}$ in $\xi < 0$ and add together the contributions. By symmetry, the constant term Const. in $\tau^\rho(h)$ drops out, while the other terms $h \frac{\phi}{2} + h \frac{\tau}{2} - \int_{x_0}^{x_0} \eta^\rho(y;h) \, dy$ add up, which yields BS for the electronic state. We argue similarly for the hole state. This eventually gives Theorem 1.

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