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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 supraconducting 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 $\phi(x) = \operatorname{sgn}(x)\phi$. 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 $|x| \ge L + \ell$. Andreev currents at energy E occur only if $\mu(x) \ge E$ in [-L, L].

The case of a perfect junction (Δ "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 semiclassical 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

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

The energy surface: $\Sigma_E = \{\det(\mathcal{P} - E) = -(\xi^2 - \mu(x))^2 - \Delta(x)^2 + E^2 = 0\} = \Lambda_E^{\leq} \cup \Lambda_E^{\geq} \text{ splits}$ 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 $(\pm x_E, \xi_E) \in \Lambda_E^{\geq}$, 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 μ . 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 supraconductor, 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 supraconductor, transforming again to the original electron state, a process known as Andreev reflection. This works also the other way in $\Lambda_E^<$, 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 ∂I . Phase-sensitive Andreev states carry supercurrents that turn out to be proportional to the ϕ -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 ${}^{\vee}\mathcal{IP}(x, hD_x) = \mathcal{P}(x, hD_x)\mathcal{I}^{\vee}$ 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 (1), 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 $L^2(\mathbf{R}) \otimes \mathbf{C}^2$, 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

$$-h^{2}u''(x) + V(x)u(x) = Eu(x)$$
(2)

and outside supp V,

$$-h^2 u''(x) = k^2 u(x)$$
(3)

defines the state space $\mathcal{Z} \approx \mathbb{C}^2$ of the "free particle", spanned by $f_1(x) = e^{ikx/h}$, $f_2(x) = e^{-ikx/h}$. The monodromy operator $M(k) : f_1 + Bf_2 \mapsto Af_1$ is such that

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

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 $e^{-ikx/h} + B_2e^{ikx/h}$ to the right of suppV, and $A_2e^{-ikx/h}$ to the left. The scattering matrix is defined as

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

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 Imk > 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 ImE < 0 to the second sheet ImE > 0.

b) Monodromy matrix for BdG equation: heuristics.

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

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

 $\mu_0 + E \pm i\Delta_0 \in \{k^2, \ell^2\}$, so eigenfrequencies are $(\pm k, \pm \overline{k})$, $k = \sqrt{\mu_0 + E + i\Delta_0}$, and the corresponding solutions as follows:

Let $\phi(x) = \operatorname{sgn}(x)\phi$, \mathcal{Z} be the 2-D complex line bundle spanned by $F_1^{\pm}(x) = \binom{e^{i\phi(x)/2}}{-i}e^{\pm ikx/h}$ (associated with the scattering process $e^+ \to e^-$), and $\overline{\mathcal{Z}}$ the 2-D complex line bundle spanned by $F_2^{\pm}(x) = \binom{e^{i\phi(x)/2}}{i}e^{\pm i\overline{kx}/h}$ (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.

$$U(x,h) = A\binom{e^{i\phi/2}}{-i}e^{ikx/h}, x \to +\infty$$
$$U(x,h) = B\binom{e^{-i\phi/2}}{-i}e^{-ikx/h}, x \to -\infty$$

Similarly we say that E is a \overline{Z} -resonance iff the \overline{Z} -component of the wave function is outgoing (and evanescent) at infinity, i.e.

$$U(x,h) = A\binom{e^{i\phi/2}}{i}e^{-i\overline{k}x/h}, x \to +\infty$$
$$U(x,h) = B\binom{e^{-i\phi/2}}{i}e^{i\overline{k}x/h}, x \to -\infty$$

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 $M^{\mathbb{Z}}(k)$ acting on \mathbb{Z} according to the formula

$$\binom{e^{-i\phi/2}}{-i}e^{ikx/h} + B\binom{e^{-i\phi/2}}{-i}e^{-ikx/h} \mapsto A\binom{e^{i\phi/2}}{-i}e^{ikx/h}$$

and similarly for $M^{\overline{Z}}(k)$. It is plausible to expect that $M^{\mathbb{Z}}(k), M^{\overline{Z}}(k) \in U(1,1)$, and that the corresponding scattering matrices $S^{\mathbb{Z}}(k), S^{\overline{Z}}(k)$ have a meromorphic extension to the complex plane, their poles defining the resonances $E^{\mathbb{Z}}$ and $E^{\overline{Z}}$. Actually, we shall construct "relative monodromy operators" in the "classically allowed region". In particular the relative monodromy operators are in 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 $\int_{-x_0}^{x_0} \eta^{\rho}(y;h) dy$ 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:

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

Here \oint_{γ_E} denotes integral over the loop γ_E obtained by gluing together $\Lambda_E^>$ and $\Lambda_E^<$, if we ignore tunneling in momentum space.

4. Microlocal solutions in Fourier representation near the branching points

a) Reduction of the system.

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

$$\mathcal{P}^{a}(-hD_{\xi},\xi) = \begin{pmatrix} \xi^{2} - \mu & e^{i\phi/2}(E - \alpha hD_{\xi} - \alpha x_{E}) \\ e^{-i\phi/2}(E - \alpha hD_{\xi} - \alpha x_{E}) & -\xi^{2} + \mu \end{pmatrix}$$
(4)

By PT symmetry $\mathcal{P}^{a'} = \mathcal{I}\mathcal{P}^{a}\mathcal{I}$ near $a' = a'_{E} = (-x_{E}, \xi_{E})$. Solving the system $\mathcal{P}^{a}(-hD_{\xi}, \xi)\widehat{U} = 0$, $\widehat{U} = \begin{pmatrix}\widehat{\varphi}_{1}\\\widehat{\varphi}_{2}\end{pmatrix}$ gives second order ODE for $u(\xi) = \exp[-i\int^{\xi}g(s)ds/h]\widehat{\varphi}_{2}(\xi)$,

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

$$P^{a}(-hD_{\xi},\xi,h) = (hD_{\xi})^{2} + \alpha^{-2}(\xi^{2} - \mu)^{2} + h^{2}(\xi^{2} - \mu - E)^{-2}(2\xi^{2} + \mu + E)$$
(5)

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

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

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 $\Lambda_E^>$ where the linear approximation of $\Delta(x)$ breaks down. The linear approximation only holds for small ξ' . Consider the map

$$\iota^{a}: \sum_{\omega=\pm 1} \operatorname{Ker}_{h}(P_{\omega}^{a} - \left(\frac{E_{1}\omega}{\beta}\right)^{2}) \to \operatorname{Ker}_{h}(\mathcal{P}^{a} - E)$$
(6)

where Ker_h denotes the microlocal kernel. The index ω 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 Lorenzian structure and "diagonalize" ι^a in some orthogonal subspaces.

b) The normal form of Helffer-Sjöstrand

When $E_1 < \frac{1}{4}$, we take P^a_{ω} 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 $\phi_\beta(\xi',\theta) = \xi'\theta + g_\beta(\xi',\theta), g_\beta(\xi',\theta) = \mathcal{O}(|\xi',\theta|^3)$, parametrizing the canonical transformation $\kappa_\beta : (\partial_\theta \phi_\beta, \theta) \mapsto (\xi', \partial_{\xi'} \phi_\beta)$, 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)

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

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

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

The function F_0 , taking the period T(E) of Hamilton vector flow for P^a_{ω} at energy $(E_1/\beta)^2$ to 2π , involves an elliptic integral, which requires sometimes the use of formal calculus.

c) Weber equation and parabolic cylinder functions

Weber equation $P_0 v = \nu h v$, through change of variables $\eta = (h/2)^{1/2} \zeta$, $\tilde{v}(\zeta) = v(\eta)$ scales to

$$-\widetilde{v}'' + \frac{1}{4}\zeta^2 \widetilde{v} = \left(\nu + \frac{1}{2}\right)\widetilde{v}$$

Fundamental solutions express as parabolic cylinder functions D_{ν} , entire in **C**. The systems $(D_{\nu}(\pm\zeta), D_{-\nu-1}(\pm i\zeta))$ 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 ν , ${E'}_1^2 = 2\beta^2 F(\beta^{-2}E_1^2, \beta, h) = 2\beta^2(\nu+1)h$.

$$D_{\nu}(\varepsilon(h/2)^{-1/2}\eta) = \frac{\Gamma(\nu+1)}{-2i\pi\sqrt{h}}h^{E^2/4h} \int_{\infty}^{(0^+)} \exp\left[i\Phi_{\varepsilon}^{\nu}(s;\eta)/h\right] ds$$
$$D_{-\nu-1}(i\varepsilon(h/2)^{-1/2}\eta) = \frac{\Gamma(-\nu)}{2i\pi}h^{-E^2/4h} \int_{\infty}^{(0^+)} \exp\left[i\Phi_{\varepsilon}^{-\nu-1}(s;\eta)/h\right] \frac{ds}{s}$$

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 $K_h^a(E) = \operatorname{Ker}_h(\mathcal{P}^a(-hD_{\xi},\xi)-E)$ of ι^a is a 2-D vector space spanned by the spinors $\widehat{U}_{\varepsilon,\omega}^j = \left(\widehat{\varphi}_2^{j}\right)_{\varepsilon,\omega}^j$, $(j,\varepsilon,\omega) \in \{\nu, -\nu - 1\} \times \{-1,1\}^2$, of the form:

$$\begin{split} \widehat{U}_{\varepsilon,\omega}^{\nu} &= C_{h'}^{\nu} \sum_{\theta_{\omega} = \pm \widehat{\theta}_{\omega}(\xi_{1})} \binom{e^{i\phi/2} (\xi^{2} - \mu - E)^{-1/2} X_{\varepsilon,\omega}^{\nu}}{(\xi^{2} - \mu - E)^{1/2}} |\widetilde{a}_{\varepsilon,\omega}^{\nu}| \exp[i(\Phi_{\varepsilon,\omega}^{\nu} + h' R_{\omega}^{\nu})/h'] + \mathcal{O}(h') \\ \widehat{U}_{\varepsilon,\omega}^{-\nu-1} &= C_{h'}^{-\nu-1} \sum_{\substack{\theta_{\omega} = \pm \widehat{\theta}_{\omega}(\xi_{1})} \varepsilon \operatorname{sgn}(\theta_{\omega}) \binom{e^{i\phi/2} (\xi^{2} - \mu - E)^{-1/2} X_{\varepsilon,\omega}^{-\nu-1}}{(\xi^{2} - \mu - E)^{1/2}} \\ &|\widetilde{a}_{\varepsilon,\omega}^{-\nu-1}| \exp[i(\Phi_{\varepsilon,\omega}^{-\nu-1} + h' R_{\omega}^{-\nu-1})/h'] + \mathcal{O}(h') \end{split}$$

Here $\hat{\theta}_{\omega}(\xi_1)$ is a critical point (from stationary phase), $\Phi^j_{\varepsilon,\omega} + h'R^j_{\omega}$) the h'-dependent phase functions, and $X^j_{\varepsilon,\omega}$, $|\tilde{a}^j_{\varepsilon,\omega}|$ some positive amplitudes. Spinors $U^j_{\varepsilon,\omega}$ verify the symmetry $^{\dagger}\hat{U}^j_{-\varepsilon,-\omega} = \hat{U}^j_{\varepsilon,\omega}$ for the "local time" reversal operator $^{\dagger}u(\xi_1) = u(-\xi_1)$, and the constants $C^j_{h'}$ (from Whittaker normalization of $D_{\nu}, D_{-\nu-1}$) are related by $C^{\nu}_{h'}C^{-\nu-1}_{h'} = \left((2\sqrt{h'})^3\pi^2\sin\pi\nu\right)^{-1}$.

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 $U^a, V^a \in K_h(E)$ be supported on $\Lambda_E^>$. We call the sesquilinear form $\mathcal{W}^a_\rho(U^a, V^a) = \left(\frac{i}{\hbar}[\mathcal{P}, \chi^a]_\rho U^a | V^a\right) = \left(\frac{i}{\hbar}[\mathcal{P}, \chi^a]_\rho \widehat{U}^a | \widehat{V}^a\right)$ the microlocal Wronskian of $(U^a, \overline{V^a})$ in ω^a_ρ . Here $\frac{i}{\hbar}[\mathcal{P}, \chi^a]_\rho$ denotes the part of the commutator supported microlocally on ω^a_ρ (a small neighborhood of supp $[\mathcal{P}, \chi^a] \cap \Lambda_E$ near ρ).

A crucial property of the microlocal Wronskian is to be invariant by Fourier transformation: $\mathcal{W}^a_{\rho}(U^a, V^a) = \mathcal{W}^a_{\rho}(\hat{U}^a, \hat{V}^a)$. The relation $\mathcal{W}^a_+(U^a, V^a) + \mathcal{W}^a_-(U^a, V^a) = 0$ 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 ε, ω such that $\varepsilon \omega = 1$ we define a Lorenzian metric \mathcal{W}_{ρ} on the space of microlocal solutions near a. In the basis $\widehat{U}_{\varepsilon,\omega}^{j}, j \in \{\nu, -\nu - 1\}$ we have, up to a constant factor:

$$\rho \mathcal{W}_{\rho} = \begin{pmatrix} |C_{h'}^{\nu}|^2 \mathcal{O}(h') & C_{h'}^{\nu} \overline{C_{h'}^{-\nu-1}} \exp[-i\pi E_1'^2/4h'] (1 + \mathcal{O}(h')) \\ \overline{C_{h'}^{\nu}} \overline{C_{h'}^{-\nu-1}} \exp[i\pi E_1'^2/4h'] (1 + \mathcal{O}(h')) & |C_{h'}^{-\nu-1}|^2 \mathcal{O}(h') \end{pmatrix}$$

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}^a_{ρ} endow $K^a_h(E)$ (mod h') with a Lorenzian form $\mathcal{W}^a = \frac{1}{2}(\mathcal{W}^a_+ - \mathcal{W}^a_-)$. The same holds at a', and the corresponding structures on $K^a_h \times K^{a*}_h$ and $K^{a'}_h \times K^{a'*}_h$ are anti-isomorphic. The group of automorphisms preserving \mathcal{W}^a and $\mathcal{W}^{a'}$ mod $\mathcal{O}(h')$ is therefore U(1,1).

6. Spinors in the spatial representation

We compute $U_{\varepsilon,\omega}^{a,j}, U_{\varepsilon,\omega}^{a',j}$ 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

$$\begin{aligned} U_{\varepsilon,\omega}^{\nu}(x,h) &= 2\omega\beta\xi_E e^{ix\xi_E/h} \sum_{\rho=\pm} {\binom{e^{i\phi/2}(\xi^2-\mu-E)^{-1/2}X_{\varepsilon,\omega}^{\nu}}{(\xi^2-\mu-E)^{1/2}}} |a_{\varepsilon,\omega}^{\nu}| \Big|_{\theta_1=\theta_\omega(\xi_1),\xi_1=\xi_\omega^{\rho}(x)} \\ &\times \left(\frac{L_{\omega}^{\rho}(x)}{i}\right)^{-1/2} \exp\left[i\left(\Psi_{\varepsilon,\omega}^{\nu,\rho}(x)+h'R_{\varepsilon,\omega}^{\nu,\rho}(x)\right)/h'\right](1+\mathcal{O}(h')) \\ U_{\varepsilon,\omega}^{-\nu-1}(x,h) &= 2\omega\beta\xi_E e^{ix\xi_E/h} \sum_{\rho=\pm} \varepsilon \operatorname{sgn}(\theta_1) {\binom{e^{i\phi/2}(\xi^2-\mu-E)^{-1/2}X_{\varepsilon,\omega}^{-\nu-1}}{(\xi^2-\mu-E)^{1/2}}} |\tilde{a}_{\varepsilon,\omega}^{-\nu-1}| \Big|_{\theta_1=\theta_\omega(\xi_1),\xi_1=\xi_\omega^{\rho}(x)} \\ &\times \left(\frac{L_{\omega}^{\rho}(x)}{i}\right)^{-1/2} \exp\left[i\left(\Psi_{\varepsilon,\omega}^{\nu,\rho}(x)+h'R_{\varepsilon,\omega}^{\nu,\rho}(x)\right)/h'\right](1+\mathcal{O}(h')) \end{aligned}$$

Here $(L_{\omega}^{\rho}(x))^{-1/2}$ is a real density (singular at $x = x_E$), and ρ labels the branch of the Lagrangian manifold. The phases $\Psi_{\varepsilon,\omega}^{j,\rho}(x) + h' R_{\varepsilon,\omega}^{j,\rho}(x)$, $j \in \{\nu, -\nu - 1\}$ 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 ρ) $\rho = \pm 1$ 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 \mathbf{C}^2 generated by $\binom{1}{0}$ the space of (pure) electronic states, or electronic spinors, and this by $\binom{0}{1}$ the space of (pure) hole states, or hole spinors.

The principal symbol $\mathcal{P}(x,\xi)$ 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 Λ_E^{ρ} with fiber

$$Y_{\rho}(x,\xi) = (\Delta^2 + (-\xi^2 + \mu + \rho\sqrt{\Delta^2 + (\xi^2 - \mu)^2})^2)^{-1/2} \begin{pmatrix} \Delta e^{i\phi/2} \\ -\xi^2 + \mu + \rho\sqrt{\Delta^2 + (\xi^2 - \mu)^2} \end{pmatrix}$$



Figure 1. Phase-space picture

Looking at the electronic state, we choose $\rho = +1$ so that $\lambda_{\rho}(x_{\rho}, \xi_{\rho}) - E = 0$, while $\lambda_{-\rho}(x_{\rho}, \xi_{\rho}) - E$ is elliptic. and similarly when looking at the hole state.

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

$$W^{\rho}(x,h) = e^{iS_{\rho}(x,h)/h} \left(w_0^{\rho}(x,h)Y_{\rho}(x,\partial_x S_{\rho}) + \mathcal{O}(h) \right) = e^{iS_{\rho}(x,h)/h} \widetilde{W}^{\rho}(x,h)$$

where $w_0^{\rho}(x)|dx|^{1/2}$ 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 $\Psi_{\varepsilon,\omega}^{j,\rho}(x) + h' R_{\varepsilon,\omega}^{j,\rho}(x)$ 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 $U^{a,k,\rho}_{-\varepsilon,-\omega,\text{ext}}$ of the normalized microlocal solutions $U^{a,k,\rho}_{\varepsilon,\omega}$ along the bicharacteristics by a monodromy matrix

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

(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 $\mathcal{M}^{a,a',\rho}$ and $\mathcal{M}^{a',a,\rho}$ is order 4; $\mathcal{M}^{a',a,\rho} \in U(1,1)$ is obtained by extending from the left to the right, and applying symmetry

$$\rho \mathcal{M}^{a',a,\rho} = \mathcal{I}(\mathcal{M}^{a,a',\rho})^{-1} \mathcal{I} =, \quad \rho = \pm 1$$
(7)

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

$$\mathcal{M}^{a,a',\rho} = \begin{pmatrix} 0 & d_{12}^{\rho} \\ d_{21}^{\rho} & 0 \end{pmatrix}, \quad \overline{d_{12}^{\rho}} \, d_{21}^{\rho} = 1$$

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 $\mathcal{M}^{a,a',\rho} = \begin{pmatrix} d_{11}^{\rho} & 0\\ 0 & d_{22}^{\rho} \end{pmatrix}$, with $\overline{d_{11}}^{\rho} d_{22}^{\rho} = 1$. 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 equal to $U_1^a = U_{\varepsilon,\omega}^{\nu,a}$ near *a*, extend it along to *a'* along the bicharacteristics $\rho = \pm 1$ by WKB. Evaluating on ρ near *a'* we find $U_1^{a',\rho} = U_{\varepsilon,\omega,\text{ext}}^{\nu,a,\rho} = d_{21}^{\rho} U_{\varepsilon,\omega}^{-\nu-1,a',\rho}$. Similarly, take U_2 starting at *a'* and with $-\nu - 1$ instead of ν , we get $U_1^{a,\rho} = U_{\varepsilon,\omega,\text{ext}}^{-\nu-1,a',\rho} = e_{12}^{\rho} U_{\varepsilon,\omega}^{\nu,a,\rho}$, where $e_{12}^{\rho} = \rho (d_{21}^{\rho})^{-1}$ is the matrix element of $\mathcal{M}^{a',a,\rho}$ given in (7). We compute d_{21}^{ρ} in two different ways and compare the result.

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

$$\begin{pmatrix} \frac{i}{\hbar} [\mathcal{P}^{a'}, \chi^{a'}]_{\rho} U_1 | U_{\varepsilon,\omega}^{\nu} \rangle = d_{21}^{\rho} \left(\frac{i}{\hbar} [\mathcal{P}^{a'}, \chi^{a'}]_{\rho} U_{\varepsilon,\omega}^{-\nu-1} | U_{\varepsilon,\omega}^{\nu} \right) = \\ = d_{21}^{\rho} \mathcal{W}_{\rho}^{a'} \left(U_{\varepsilon,\omega}^{-\nu-1}, U_{\varepsilon,\omega}^{\nu} \right) = d_{21}^{\rho} \mathcal{W}_{\rho}^{a'} \left(\widehat{U}_{\varepsilon,\omega}^{-\nu-1}, \widehat{U}_{\varepsilon,\omega}^{\nu} \right) = \\ = -d_{21}^{\rho} \overline{\mathcal{W}_{\rho}^{a}} \left(\widehat{U}_{-\varepsilon,-\omega}^{-\nu-1}, \widehat{U}_{-\varepsilon,-\omega}^{\nu} \right) = -d_{21}^{\rho} \mathcal{W}_{\rho}^{a} \left(\widehat{U}_{-\varepsilon,-\omega}^{\nu}, \widehat{U}_{-\varepsilon,-\omega}^{-\nu-1} \right) = -d_{21}^{\rho} \end{aligned}$$

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

Proposition 8: Let $\widetilde{\Psi}_{\varepsilon,\omega}^{\nu,a',\rho}(x) = x \xi_E + \frac{(2\xi_E)^3}{\alpha} \Psi_{\varepsilon,\omega}^{\nu,a',\rho}(x)$. We have

$$\left(\frac{i}{h} [\mathcal{P}^{a'}, \chi^{a'}]_{\rho} W^{\rho} | U^{\nu, a', \rho}_{\varepsilon, \omega}\right) = 2 \, \widetilde{C}^{\rho} \, e^{i\pi/4} \int \exp\left[i \left(\widetilde{S}_{\rho}(x; h)/h\right] \beta(x, h) \, (\chi_1^{a'})'(x) \, dx \right)$$
(8)

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

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

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

$$d_{21}^{\rho} = -e^{i\tau^{\rho}(h)/h} \int (\chi_1^{a'})'(x) \, dx = e^{i\tau^{\rho}(h)/h} \tag{9}$$

Here $\tau^{\rho}(h) = h \frac{\phi}{2} + h \frac{\pi}{4} - \int_{-x_0}^{x_0} \eta^{\rho}(y;h) dy + \text{Const.}$, 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 $F_{\varepsilon,\omega}^{j,a,\rho} = \frac{i}{h} [\mathcal{P}^a, \chi^a]_{\rho} U_{\varepsilon,\omega}^{j,a,\rho}$, and similarly with a'. The set $\{G_{\varepsilon,\omega}^{j,\flat} = F_{\varepsilon,\omega}^{j,\flat,+} - F_{\varepsilon,\omega}^{j,\flat,-} : j \in \{\nu, -\nu - 1\}, \flat \in \{a, a'\}\}$ (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 \mathcal{G}^{ρ} of vectors \widehat{U}_{1}^{ρ} and \widehat{U}_{2}^{ρ} in this basis, namely $\mathcal{G} = \begin{pmatrix} (\widehat{U}_{1} | \widehat{G}_{\varepsilon,\omega}^{-\nu-1,a}) & (\widehat{U}_{2} | \widehat{G}_{\varepsilon,\omega}^{-\nu-1,a}) \\ (\widehat{U}_{1} | \widehat{G}_{\varepsilon,\omega}^{\nu,a'}) & (\widehat{U}_{2} | \widehat{G}_{\varepsilon,\omega}^{\nu,a'}) \end{pmatrix}$. Using symmetries we get

$$\mathcal{G} = \mathcal{G}^{\rho} = 2 \begin{pmatrix} 1 & e_{12}^{\rho} \\ -d_{21}^{\rho} & -1 \end{pmatrix}$$

The condition $\det(\mathcal{G}^{(\rho)}) = 0$ means that U_1 is colinear to U_2 , i.e. there is a global section of $\operatorname{Ker}_h(\mathcal{P}-E)$. Recall $e_{12}^{\rho} = \rho(\overline{d_{21}^{\rho}})^{-1}$; for $\rho = +1$ (electronic state) we get $\operatorname{Im} d_{21}^+ = 0$, that is $\sin\left(\frac{\tau^{(+)}(h)}{h}\right) = 0$. We eventually obtain BS by "surgery": namely (ignoring tunneling) we cut and paste the half-bicharacteristic $\Lambda_E^{>,+}$ in the upper-half plane $\xi > 0$ with its symmetric part $\Lambda_E^{<,-}$ in $\xi < 0$ and add together the contributions. By symmetry, the constant term Const. in $\tau^+(h)$ drops out, while the other terms $h \frac{\phi}{2} + h \frac{\pi}{4} - \int_{-x_0}^{x_0} \eta^{\rho}(y;h) dy$ 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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