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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 $\phi(x) = \mathrm{sgn}(x)\phi$. 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 (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 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

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

The energy surface: $\Sigma_E = \{\det(\mathcal{P} - E) = -(\xi^2 - \mu(x))^2 - \Delta(x)^2 + E^2 = 0\} = \Lambda_E^< \cup \Lambda_E^>$ 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 $(\pm x_E, \xi_E) \in \Lambda_E^>$, 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 $L^2(I) \otimes \mathbf{C}^2$, $I = [-(L+\ell), L+\ell]$, 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 ${}^\vee\mathcal{I}\mathcal{P}(x, hD_x) = \mathcal{P}(x, hD_x)\mathcal{I}^\vee$ 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

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

and outside supp V,

$$-h^2 u''(x) = k^2 u(x) \tag{3}$$

defines the state space $\mathcal{Z} \approx \mathbf{C}^2$ 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 $e^{-ikx/h} + B_2 e^{ikx/h}$ to the right of supp$V$, and $A_2 e^{-ikx/h}$ 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 $E = k^2 \in \mathbf{C}$, where k is a pole of S, and *physical resonances* those with 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 Im$E < 0$ to the second sheet Im$E > 0$.

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 $|x| \geq L + \ell$, so $\Delta(x) = \Delta_0$, $\mu(x) = \mu_0 > E$. Solutions are of the form

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

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

Let $\phi(x) = \mathrm{sgn}(x)\phi$, $\mathcal{Z}$ 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 $F_2^{\pm}(x) = \binom{e^{i\phi(x)/2}}{i} e^{\pm i\overline{k}x/h}$ (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 $\mathbf{C}^2$. Declare that $E \in \mathbf{C}$ 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.

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

Similarly we say that E is a $\overline{\mathcal{Z}}$-*resonance* iff the $\overline{\mathcal{Z}}$-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 $M^{\mathcal{Z}}(k)$ acting on $\mathcal{Z}$ according to the formula

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

and similarly for $M^{\overline{\mathcal{Z}}}(k)$. It is plausible to expect that $M^{\mathcal{Z}}(k), M^{\overline{\mathcal{Z}}}(k) \in \mathrm{U}(1,1)$, and that the corresponding scattering matrices $S^{\mathcal{Z}}(k)$, $S^{\overline{\mathcal{Z}}}(k)$ have a meromorphic extension to the complex plane, their poles defining the resonances $E^{\mathcal{Z}}$ and $E^{\overline{\mathcal{Z}}}$. 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:

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

Here $\oint_{\gamma_E}$ 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 :

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

By PT symmetry $\mathcal{P}^{a'} = \mathcal{I}\mathcal{P}^a\mathcal{I}$ near $a' = a'_E = (-x_E, \xi_E)$. Solving the system $\mathcal{P}^a(-hD_\xi, \xi)\widehat{U} = 0$, $\widehat{U} = \binom{\widehat{\varphi}_1}{\widehat{\varphi}_2}$ gives second order ODE for $u(\xi) = \exp[-i\int^\xi g(s)ds/h]\widehat{\varphi}_2(\xi)$,

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

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

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

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

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

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

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

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

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 $P_0v = \nu hv$, through change of variables $\eta = (h/2)^{1/2}\zeta$, $\widetilde{v}(\zeta) = v(\eta)$ scales to

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

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

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

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 $K_h^a(E) = \mathrm{Ker}_h(\mathcal{P}^a(-hD_\xi, \xi) - E)$ of ι^a is a 2-D vector space spanned by the spinors $\widehat{U}^j_{\varepsilon,\omega} = \binom{\widehat{\varphi}_1}{\widehat{\varphi}_2}^j_{\varepsilon,\omega}$, $(j, \varepsilon, \omega) \in \{\nu, -\nu-1\} \times \{-1, 1\}^2$, of the form:

$$\widehat{U}^\nu_{\varepsilon,\omega} = C^\nu_{h'} \textstyle\sum_{\theta_\omega = \pm\widehat{\theta}_\omega(\xi_1)} \binom{e^{i\phi/2}(\xi^2-\mu-E)^{-1/2}X^\nu_{\varepsilon,\omega}}{(\xi^2-\mu-E)^{1/2}} |\widetilde{a}^\nu_{\varepsilon,\omega}| \exp[i(\Phi^\nu_{\varepsilon,\omega} + h'R^\nu_\omega)/h'] + \mathcal{O}(h')$$
$$\widehat{U}^{-\nu-1}_{\varepsilon,\omega} = C^{-\nu-1}_{h'} \textstyle\sum_{\theta_\omega = \pm\widehat{\theta}_\omega(\xi_1)} \varepsilon\,\mathrm{sgn}(\theta_\omega) \binom{e^{i\phi/2}(\xi^2-\mu-E)^{-1/2}X^{-\nu-1}_{\varepsilon,\omega}}{(\xi^2-\mu-E)^{1/2}}$$
$$|\widetilde{a}^{-\nu-1}_{\varepsilon,\omega}| \exp[i(\Phi^{-\nu-1}_{\varepsilon,\omega} + h'R^{-\nu-1}_\omega)/h'] + \mathcal{O}(h')$$

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

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 $\mathcal{W}^a_\rho(U^a, V^a) = \big(\frac{i}{h}[\mathcal{P}, \chi^a]_\rho U^a | V^a\big) = \big(\frac{i}{h}[\mathcal{P}, \chi^a]_\rho \widehat{U}^a | \widehat{V}^a\big)$ the *microlocal Wronskian* of $(U^a, \overline{V^a})$ in ω^a_ρ. Here $\frac{i}{h}[\mathcal{P}, \chi^a]_\rho$ denotes the part of the commutator supported microlocally on ω^a_ρ (a small neighborhood of $\mathrm{supp}[\mathcal{P}, \chi^a] \cap \Lambda_E$ near ρ).

A crucial property of the microlocal Wronskian is to be invariant by Fourier transformation: $\mathcal{W}^a_\rho(U^a, V^a) = \mathcal{W}^a_\rho(\widehat{U}^a, \widehat{V}^a)$. 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 $\mathcal{W}_\rho$ on the space of microlocal solutions near a. In the basis $\widehat{U}^j_{\varepsilon,\omega}, j \in \{\nu, -\nu-1\}$ we have, up to a constant factor:

$$\rho\mathcal{W}_\rho = \begin{pmatrix} |C^\nu_{h'}|^2\mathcal{O}(h') & C^\nu_{h'}\overline{C^{-\nu-1}_{h'}}\exp[-i\pi {E'_1}^2/4h'](1+\mathcal{O}(h')) \\ \overline{C^\nu_{h'}}C^{-\nu-1}_{h'}\exp[i\pi {E'_1}^2/4h'](1+\mathcal{O}(h')) & |C^{-\nu-1}_{h'}|^2\mathcal{O}(h') \end{pmatrix}$$

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 $\mathcal{W}^a_\rho$ 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 $U^{a,j}_{\varepsilon,\omega}, U^{a',j}_{\varepsilon,\omega}$ 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

$$\begin{aligned} U^\nu_{\varepsilon,\omega}(x,h) &= 2\omega\beta\xi_E e^{ix\xi_E/h}\textstyle\sum_{\rho=\pm}\left(\begin{smallmatrix} e^{i\phi/2}(\xi^2-\mu-E)^{-1/2}X^\nu_{\varepsilon,\omega} \\ (\xi^2-\mu-E)^{1/2}\end{smallmatrix}\right)|a^\nu_{\varepsilon,\omega}|\big|_{\theta_1=\theta_\omega(\xi_1),\xi_1=\xi^\rho_\omega(x)} \\ &\quad\times\left(\tfrac{L^\rho_\omega(x)}{i}\right)^{-1/2}\exp[i\big(\Psi^{\nu,\rho}_{\varepsilon,\omega}(x)+h'R^{\nu,\rho}_{\varepsilon,\omega}(x)\big)/h'](1+\mathcal{O}(h')) \\ U^{-\nu-1}_{\varepsilon,\omega}(x,h) &= 2\omega\beta\xi_E e^{ix\xi_E/h}\textstyle\sum_{\rho=\pm}\varepsilon\,\mathrm{sgn}(\theta_1)\left(\begin{smallmatrix} e^{i\phi/2}(\xi^2-\mu-E)^{-1/2}X^{-\nu-1}_{\varepsilon,\omega} \\ (\xi^2-\mu-E)^{1/2}\end{smallmatrix}\right)|\widetilde{a}^{-\nu-1}_{\varepsilon,\omega}|\big|_{\theta_1=\theta_\omega(\xi_1),\xi_1=\xi^\rho_\omega(x)} \\ &\quad\times\left(\tfrac{L^\rho_\omega(x)}{i}\right)^{-1/2}\exp[i\big(\Psi^{\nu,\rho}_{\varepsilon,\omega}(x)+h'R^{\nu,\rho}_{\varepsilon,\omega}(x)\big)/h'](1+\mathcal{O}(h')) \end{aligned}$$

Here $\big(L^\rho_\omega(x)\big)^{-1/2}$ is a real density (singular at $x = x_E$), and ρ labels the branch of the Lagrangian manifold. The phases $\Psi^{j,\rho}_{\varepsilon,\omega}(x) + h'R^{j,\rho}_{\varepsilon,\omega}(x)$, $j \in \{\nu, -\nu-1\}$ differ only by a constant.

b) WKB spinors away from the branching points

The Lagrangian manifold $\Lambda^>_E$ consists of 2 branches $\Lambda^{>,\rho}_E$ (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^ρ_E with fiber

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

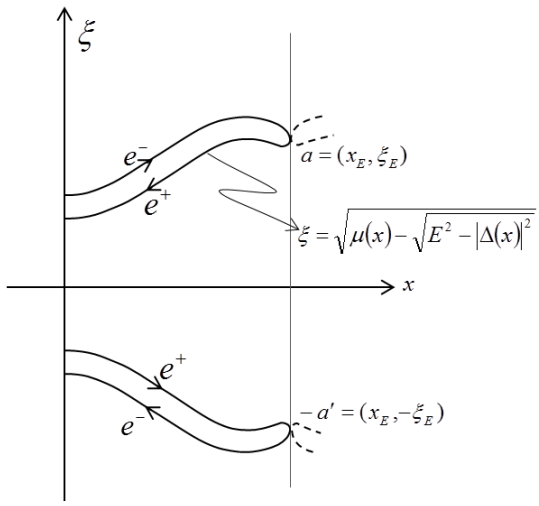

Figure 1. Phase-space picture

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 $\mathrm{Ker}_h(\mathcal{P} - E)$ on $\Lambda_E^{>,\rho}$ is one-dimensional space spanned by

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

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 $U_{\varepsilon,\omega}^{a',j,\rho}$ are related to the extension $U_{-\varepsilon,-\omega,\mathrm{ext}}^{a,k,\rho}$ of the normalized microlocal solutions $U_{\varepsilon,\omega}^{a,k,\rho}$ 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

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

where $\mathcal{I}$ denotes complex conjugation. We compute the coefficients $d_{ij} = d_{ij}^\rho$. Considering behavior of $U_{\mathrm{e},\omega}^{a',j,\rho}$ 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 $U_1^{a',\rho} = U_{\varepsilon,\omega,\mathrm{ext}}^{\nu,a,\rho} = d_{21}^\rho U_{\varepsilon,\omega}^{-\nu-1,a',\rho}$. Similarly, take U_2 starting at a' and with $-\nu-1$ instead of ν, we get $U_1^{a,\rho} = U_{\varepsilon,\omega,\mathrm{ext}}^{-\nu-1,a',\rho} = e_{12}^\rho U_{\varepsilon,\omega}^{\nu,a,\rho}$, where $e_{12}^\rho = \rho\big(d_{21}^\rho\big)^{-1}$ 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

$$\begin{aligned}\big(\tfrac{i}{h}\,[\mathcal{P}^{a'},\chi^{a'}]_\rho U_1|U_{\varepsilon,\omega}^\nu\big) &= d_{21}^\rho\,\big(\tfrac{i}{h}\,[\mathcal{P}^{a'},\chi^{a'}]_\rho U_{\varepsilon,\omega}^{-\nu-1}|U_{\varepsilon,\omega}^\nu\big) = \\ &= d_{21}^\rho\,\mathcal{W}_\rho^{a'}\big(U_{\varepsilon,\omega}^{-\nu-1},U_{\varepsilon,\omega}^\nu\big) = d_{21}^\rho\,\mathcal{W}_\rho^{a'}\big(\widehat{U}_{\varepsilon,\omega}^{-\nu-1},\widehat{U}_{\varepsilon,\omega}^\nu\big) = \\ &= -d_{21}^\rho\,\overline{\mathcal{W}_\rho^{a}\big(\widehat{U}_{-\varepsilon,-\omega}^{-\nu-1},\widehat{U}_{-\varepsilon,-\omega}^\nu\big)} = -d_{21}^\rho\,\mathcal{W}_\rho^{a}\big(\widehat{U}_{-\varepsilon,-\omega}^{\nu},\widehat{U}_{-\varepsilon,-\omega}^{-\nu-1}\big) = -d_{21}^\rho\end{aligned}$$

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

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

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

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

$$\begin{aligned}\widetilde{S}_\rho(x,h) = S_\rho(x;h) - \big(x\xi_E + \widetilde{\Psi}_{\varepsilon,\omega}^{\nu,a',\rho)}(x) - h\,R_{-\omega}^\nu\big(\theta_{-\omega}(\xi_{-\omega}^\rho(-x))\big) = \\ \tfrac{(2\,\xi_E)^3}{\alpha}\,\Psi_{-\varepsilon,-\omega}^{\nu,a,\rho}(x_0) - \textstyle\int_{-x_0}^{x_0}\eta^\rho(y;h)\,dy + h\,R_{-\omega}^\nu\big(\theta_{-\omega}(0)\big)\end{aligned}$$

Moreover, $\beta(x,h)$ is also independent of x, so that, comparing the former expression (1) and (8) for a suitable choice of $\widetilde{C}^\rho$, 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 $\tau^\rho(h) = h\,\frac{\phi}{2} + h\,\frac{\pi}{4} - \int_{-x_0}^{x_0}\eta^\rho(y;h)\,dy + \mathrm{Const.}$, 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 $\mathcal{G}^\rho$ of vectors $\widehat{U}_1^\rho$ and $\widehat{U}_2^\rho$ in this basis, namely $\mathcal{G} = \begin{pmatrix} (\widehat{U}_1|\widehat{G}_{\varepsilon,\omega}^{-\nu-1,a}) & (\widehat{U}_2|\widehat{G}_{\varepsilon,\omega}^{-\nu-1,a}) \\ (\widehat{U}_1|\widehat{G}_{\varepsilon,\omega}^{\nu,a'}) & (\hat{U}_2|\widehat{G}_{\varepsilon,\omega}^{\nu,a'}) \end{pmatrix}$. 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 $\mathrm{Ker}_h(\mathcal{P} - E)$. Recall $e_{12}^\rho = \rho\big(\overline{d_{21}^\rho}\big)^{-1}$; for $\rho = +1$ (electronic state) we get $\mathrm{Im} d_{21}^+ = 0$, that is $\sin\big(\frac{\tau^{(+)}(h)}{h}\big) = 0$. 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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