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FAST TRACK COMMUNICATION

Explicit Green functions for spin–orbit Hamiltonians

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Abstract
We derive explicit expressions for Green functions and some related characteristics of the Rashba and Dresselhaus Hamiltonians with a uniform magnetic field.

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1. Introduction

The Green function of a quantum Hamiltonian (integral kernel of the resolvent) is one of the characteristics whose knowledge usually permits us to perform the complete spectral analysis and to study various perturbations. The aim of the present communication is to obtain explicit expressions for the Green function for a class of spin–orbit Hamiltonians, namely, for the Rashba and Dresselhaus Hamiltonians with uniform magnetic fields, whose study plays a central role in the spintronics [1]. We use an abstract version of the construction [2], which permits us to reduce the problem to the well-known Green functions of the Landau Hamiltonian and the Laplacian.

2. Spin–orbit Hamiltonians

Below we use the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and denote the identity 2×2-matrix by σ_0.

We consider Hamiltonians of a charged two-dimensional particle in a uniform magnetic field B orthogonal to the plane and take into account the spin–orbit interaction. Let $\mathbf{A}$ be the

[3] Deceased (2 April 2007).

magnetic vector potential, i.e. $B = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}$. In what follows we use the symmetric gauge, $A(x, y) = \left(\frac{By}{2}, -\frac{Bx}{2}\right)$. Denote as usual $p_j := -\mathrm{i}\hbar\nabla_j$ and $\Pi_j := p_j - \frac{e}{c}A_j$, $j = x, y$. The Hamiltonian without spin–orbit interaction acts in the spinor space $L^2(\mathbb{R}^2, \mathbb{C}^2)$ and takes the form $\hat{H}_0 = \frac{1}{2m_*}\mathbf{\Pi}^2\sigma_0$. We are interested in the following two types of spin–orbit Hamiltonians. The first one, the Rashba Hamiltonian $\hat{H}_{\mathrm{R}}$, is of the form

$$\hat{H}_{\mathrm{R}} = \hat{H}_0 + \frac{\alpha_{\mathrm{R}}}{\hbar}\hat{U}_{\mathrm{R}} + \frac{g_*}{2}\mu_B B\sigma_z, \qquad \hat{U}_{\mathrm{R}} = \sigma_x\Pi_y - \sigma_y\Pi_x,$$

where $\mu_B \equiv \frac{|e|\hbar}{2m_e c}$ is the Bohr magneton (m_e is the electron mass), g_* is the effective g-factor, and α_{R} is the real-valued Rashba constant (whose dimension is ML^3T^{-2}) expressing the strength of the spin–orbit interaction. The second one, the Dresselhaus Hamiltonian, is given by

$$\hat{H}_{\mathrm{D}} = \hat{H}_0 + \frac{\alpha_{\mathrm{D}}}{\hbar}\hat{U}_{\mathrm{D}} + \frac{g_*}{2}\mu_B B\sigma_z, \qquad \hat{U}_{\mathrm{D}} = \sigma_y\Pi_y - \sigma_x\Pi_x,$$

and α_{D} is the real-valued Dresselhaus constant (whose dimension is ML^3T^{-2}) expressing the strength of the spin–orbit interaction.

In what follows we use mostly dimensionless coordinates introduced as follows. Denote $\varkappa_{\mathrm{J}} := \frac{m_*\alpha_{\mathrm{J}}}{\hbar^2}$, $\mathrm{J} = \mathrm{R}, \mathrm{D}$. Furthermore, denote by Φ_0 the magnetic flux quantum, $\Phi_0 := \frac{2\pi\hbar c}{e}$, and let $b := \frac{2\pi}{\Phi_0}B$ and $\mathbf{a} := \frac{2\pi}{\Phi_0}\mathbf{A} = \left(\frac{by}{2}, -\frac{bx}{2}\right)$. Now by setting $\mathbf{k} := \frac{1}{\hbar}\mathbf{p}$, $\mathbf{K} := \mathbf{k} - \mathbf{a}$ and introducing the coefficient $\gamma := -\frac{g_*}{2}\frac{m_*}{m_e}$ we rewrite the above Hamiltonians as $\hat{H}_{\mathrm{J}} = \frac{\hbar^2}{2m_*}H_{\mathrm{J}}$, $\mathrm{J} = 0, \mathrm{R}, \mathrm{D}$, where

$$\begin{aligned} H_0 &= \mathbf{K}^2\sigma_0, & H_{\mathrm{R}} &= H_0 + 2\varkappa_{\mathrm{R}}U_{\mathrm{R}} + \gamma b\sigma_z,\\ U_{\mathrm{R}} &= \sigma_x K_y - \sigma_y K_x, & H_{\mathrm{D}} &= H_0 + 2\varkappa_{\mathrm{D}}U_{\mathrm{D}} + \gamma b\sigma_z,\\ U_{\mathrm{D}} &= \sigma_y K_y - \sigma_x K_x. \end{aligned}$$

In what follows we work with these new normalized Hamiltonians H_{J}.

3. Reduction to scalar case

We start with a simple resolvent identity which is an abstract version of the construction from [2] and which is of crucial importance in all our considerations.

For simplicity, for any self-adjoint operator A and a complex number E we use the notation $R(A, E) := (A - E)^{-1}$. Now let A be a self-adjoint operator acting in a certain Hilbert space, $\alpha \in \mathbb{R}$. Denote $B := A^2 + 2\alpha A$.

Let $E \in \mathbb{C}\backslash\operatorname{spec} B$, then $(B - E)^{-1} = [(A + \alpha)^2 - (E + \alpha^2)]^{-1} = [(A + \alpha - \eta)(A + \alpha + \eta)]^{-1}$, where $\eta = \sqrt{E + \alpha^2}$ (here and below in this section $\sqrt{z}$ is a fixed continuous branch of the square root on the complex plane $\mathbb{C}$ with an appropriate cut).

If both the numbers $\eta - \alpha$ and $-\eta - \alpha$ are outside of spec A (in particular, if $\Im\eta \neq 0$) and $\eta \neq 0$, then

$$((A + \alpha - \eta)(A + \alpha + \eta))^{-1} = \frac{1}{2\eta}((A - \eta + \alpha)^{-1} - (A + \eta + \alpha)^{-1}).$$

If, in addition, $-\eta + \alpha \notin \operatorname{spec} A$ and $\eta + \alpha \notin \operatorname{spec} A$, then $(A - \eta + \alpha)^{-1} - (A + \eta + \alpha)^{-1} = (A + \eta - \alpha)(A^2 - (\eta - \alpha)^2)^{-1} - (A - \eta - \alpha)(A^2 - (\eta + \alpha)^2)^{-1}$. As a result, we arrive at the identity

$$R(B;E) = \frac{1}{2\eta}((A+\eta-\alpha)R(A^2;(\eta-\alpha)^2) - (A-\eta-\alpha)R(A^2;(\eta+\alpha)^2))$$
$$= \frac{A-\alpha}{2\eta}(R(A^2;(\eta-\alpha)^2) - R(A^2;(\eta+\alpha)^2))$$
$$+ \frac{1}{2}(R(A^2;(\eta-\alpha)^2) + R(A^2;(\eta+\alpha)^2)). \tag{1}$$

Our aim now is to calculate the Green functions for H_R and H_D using equation (1).

Consider an operator $V_J = U_J + \beta_J\sigma_z$, where β_J is a real constant which will be chosen later, $J = R, D$. Using the commutation relation $K_xK_y - K_yK_x = ib$ and the elementary properties of the Pauli matrices one easily obtains

$$V_R^2 = (H_0 + \beta_R^2)\sigma_0 - b\sigma_z, \qquad V_D^2 = (H_0 + \beta_D^2)\sigma_0 + b\sigma_z. \tag{2}$$

Therefore,

$$H_J = V_J^2 + 2\varkappa_J V_J - \beta_J^2\sigma_0, \qquad J = R, D, \quad \text{for} \quad \beta_R := \frac{\gamma+1}{2\varkappa_R}b, \qquad \beta_D := \frac{\gamma-1}{2\varkappa_D}b. \tag{3}$$

3.1. The free case

We consider here the case without a magnetic field, $b = 0$. Then equation (3) reads simply as $H_J = U_J^2 + 2\varkappa_J U_J$ with $U_J^2 = H_0 \equiv -\Delta\sigma_0$. Clearly, $\operatorname{spec} H_J = f(\operatorname{spec} U_J)$ for $f(x) = x^2 + 2\varkappa_J x$. We see that $\operatorname{spec} U_J = \mathbb{R}$ (see the appendix), hence $\operatorname{spec} H_J = [-\varkappa_J^2, +\infty)$ and the spectrum contains no eigenvalues.

Note that the Green function $G_0(x, y; z)$ of H_0 is known explicitly,

$$G_0(\mathbf{r}, \mathbf{r}'; z) = \frac{1}{2\pi}K_0(\sqrt{-z}|\mathbf{r}-\mathbf{r}'|),$$

where K_0 is the McDonald function and $\sqrt{x} > 0$ for $x > 0$. Hence, by (1), the Green function G_J, which is the integral kernel of the resolvent $(H_J - z)^{-1}$, has the form

$$G_J(\mathbf{r}, \mathbf{r}'; z) = \frac{1}{4\pi}\left[\frac{1}{i\sqrt{-(z+\varkappa_J^2)}}(U_J - \varkappa_J)\left(K_0(\zeta_J^+|\mathbf{r}-\mathbf{r}'|) - K_0(\zeta_J^-|\mathbf{r}-\mathbf{r}'|)\right)\right.$$
$$\left. + K_0(\zeta_J^+|\mathbf{r}-\mathbf{r}'|) + K_0(\zeta_J^-|\mathbf{r}-\mathbf{r}'|)\right]\sigma_0, \tag{4}$$

$$\zeta_J^\pm = \sqrt{-(z+\varkappa_J^2)} \pm i\varkappa_J,$$

where U_J acts as a differential expression with respect to $\mathbf{r}$. Applying the identity $K_0'(t) = -K_1(t)$ one concludes that

$$G_J(\mathbf{r}, \mathbf{r}'; z) = \begin{pmatrix} G_J^{11}(\mathbf{r}, \mathbf{r}'; z) & G_J^{12}(\mathbf{r}, \mathbf{r}'; z) \\ G_J^{21}(\mathbf{r}, \mathbf{r}'; z) & G_J^{22}(\mathbf{r}, \mathbf{r}'; z) \end{pmatrix},$$

with

$$G_J^{11}(\mathbf{r}, \mathbf{r}'; z) = G_J^{22}(\mathbf{r}, \mathbf{r}'; z) = \frac{1}{4\pi}\left[-\frac{\varkappa_J}{i\sqrt{-(z+\varkappa_J^2)}}\right.$$
$$\left.\times\left(K_0(\zeta_J^+|\mathbf{r}-\mathbf{r}'|) - K_0(\zeta_J^-|\mathbf{r}-\mathbf{r}'|)\right) + K_0(\zeta_J^+|\mathbf{r}-\mathbf{r}'|) + K_0(\zeta_J^-|\mathbf{r}-\mathbf{r}'|)\right]$$

for both J = R, D, and

$$G_{\mathrm{R}}^{12}(\mathbf{r},\mathbf{r}';z)=\frac{\mathrm{i}(y-y')-(x-x')}{4\pi\mathrm{i}\sqrt{-\big(z+\varkappa_{\mathrm{R}}^2\big)}|\mathbf{r}-\mathbf{r}'|}\times\big[\zeta_{\mathrm{R}}^{+}K_1\big(\zeta_{\mathrm{R}}^{+}|\mathbf{r}-\mathbf{r}'|\big)-\zeta_{\mathrm{R}}^{-}K_1\big(\zeta_{\mathrm{R}}^{-}|\mathbf{r}-\mathbf{r}'|\big)\big],$$

$$G_{\mathrm{D}}^{12}(\mathbf{r},\mathbf{r}';z)=\frac{(y-y')-\mathrm{i}(x-x')}{4\pi\mathrm{i}\sqrt{-\big(z+\varkappa_{\mathrm{D}}^2\big)}|\mathbf{r}-\mathbf{r}'|}\times\big[\zeta_{\mathrm{D}}^{+}K_1\big(\zeta_{\mathrm{D}}^{+}|\mathbf{r}-\mathbf{r}'|\big)-\zeta_{\mathrm{D}}^{-}K_1\big(\zeta_{\mathrm{D}}^{-}|\mathbf{r}-\mathbf{r}'|\big)\big],$$

and $G_{\mathrm{J}}^{21}(\mathbf{r},\mathbf{r}';z)=\overline{G_{\mathrm{J}}^{12}(\mathbf{r}',\mathbf{r};\bar{z})}$. We note that such a representation of the Green function was essentially obtained in [2] for special values of z.

3.2. The magnetic case

Using (3) one can easily calculate the spectrum of H_{J}. Namely, spec $H_{\mathrm{J}}=g(\operatorname{spec}V_{\mathrm{J}})$ with $g(x)=x^2+2\varkappa_{\mathrm{J}}-\beta_{\mathrm{J}}^2$. The spectrum of V_{J} can be calculated using the results of the appendix. Note that the spectrum of H_0 consists of the Landau levels, spec $H_0=\{|b|(2n+1):n\in\mathbb{N}\}$.

Consider first the Rashba case. By (2) we have spec $V_{\mathrm{R}}^2=\big\{|b|(2n+1-s\operatorname{sign}b)+\beta_{\mathrm{R}}^2:n\in\mathbb{N},s=\pm1\big\}$ and, respectively, spec $V_{\mathrm{R}}=\big\{\pm\sqrt{|b|(2n+1-s\operatorname{sign}b)+\beta_{\mathrm{R}}^2}:n\in\mathbb{N},s=\pm1\big\}$. Hence, the spectrum of H_{R} consists of the Rashba levels, spec $H_{\mathrm{R}}=\{\varepsilon^{\pm}(n,s):n\in\mathbb{N},s=\pm1\}$, $\varepsilon^{\pm}(n,s)=|b|(2n+1-s\operatorname{sign}b)\pm2\varkappa_{\mathrm{R}}\sqrt{\beta_{\mathrm{R}}^2+|b|(2n+1-s\operatorname{sign}b)}$.

For the Dresselhaus case one has, exactly in the same way, spec $V_{\mathrm{D}}^2=\big\{|b|(2n+1+s\operatorname{sign}b)+\beta_{\mathrm{D}}^2:n\in\mathbb{N},s=\pm1\big\}$, spec $V_{\mathrm{D}}=\big\{\pm\sqrt{|b|(2n+1+s\operatorname{sign}b)+\beta_{\mathrm{D}}^2}:n\in\mathbb{N},s=\pm1\big\}$, and the spectrum of H_{D} consists of the Dresselhaus levels, spec $H_{\mathrm{D}}=\{\varepsilon^{\pm}(n,s):n\in\mathbb{N},s=\pm1\}$, $\varepsilon^{\pm}(n,s)=|b|(2n+1+s\operatorname{sign}b)\pm2\varkappa_{\mathrm{D}}\sqrt{\beta_{\mathrm{D}}^2+|b|(2n+1+s\operatorname{sign}b)}$. We note that the formulas for the eigenvalues were obtained e.g. in [3] by a different method.

Now let us pass to the calculation of the Green functions. Note that H_0 has the following Green function:

$$G_0(\mathbf{r},\mathbf{r}';z)=\frac{1}{4\pi}\Gamma\left(\frac{1}{2}-\frac{z}{2|b|}\right)\times\exp\left(\frac{\mathrm{i}b}{2}(\mathbf{r}\wedge\mathbf{r}')-\frac{|b|}{4}(\mathbf{r}-\mathbf{r}')^2\right)\Psi\left(\frac{1}{2}-\frac{z}{2|b|},1;\frac{|b|}{2}(\mathbf{r}-\mathbf{r}')^2\right),$$

where Ψ is the confluent hypergeometric function [4]. Clearly,

$$\big(V_{\mathrm{R/D}}^2-z\big)^{-1}=\begin{pmatrix}\big(H_0-\big(z-\beta_{\mathrm{R/D}}^2\pm b\big)\big)^{-1} & 0\\ 0 & \big(H_0-\big(z-\beta_{\mathrm{R/D}}^2\mp b\big)\big)^{-1}\end{pmatrix},\tag{5}$$

where +/− corresponds to R/D. Set now $\eta_{\mathrm{J}}:=\sqrt{z+\varkappa_{\mathrm{J}}^2+\beta_{\mathrm{J}}^2}$ and

$$\zeta_{\mathrm{R}}^{\pm}(b):=(\eta_{\mathrm{R}}\pm\varkappa_{\mathrm{R}})^2+b-\beta_{\mathrm{R}}^2,\qquad\zeta_{\mathrm{D}}^{\pm}(b):=(\eta_{\mathrm{D}}\pm\varkappa_{\mathrm{D}})^2-b-\beta_{\mathrm{D}}^2.$$

By (1), we have

$$(H_{\mathrm{J}}-z)^{-1}=\frac{V_{\mathrm{J}}-\varkappa_{\mathrm{J}}}{2\eta_{\mathrm{J}}}\big(\big(V_{\mathrm{J}}^2-(\eta_{\mathrm{J}}-\varkappa_{\mathrm{J}})^2\big)^{-1}-\big(V_{\mathrm{J}}^2-(\eta_{\mathrm{J}}+\varkappa_{\mathrm{J}})^2\big)^{-1}\big)+\frac{1}{2}\big(\big(V_{\mathrm{J}}^2-(\eta_{\mathrm{J}}-\varkappa_{\mathrm{J}})^2\big)^{-1}+\big(V_{\mathrm{J}}^2-(\eta_{\mathrm{J}}+\varkappa_{\mathrm{J}})^2\big)^{-1}\big).$$

Passing to the Green function, we obtain

$$G_{\mathrm{J}}(\mathbf{r},\mathbf{r}';z) = \frac{U_{\mathrm{J}} + \beta_{\mathrm{J}}\sigma_z - \varkappa_{\mathrm{J}}}{2\eta_{\mathrm{J}}}$$
$$\times\begin{pmatrix} G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(b)\big) - G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(b)\big) & 0 \\ 0 & G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) - G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\end{pmatrix}$$
$$+\frac{1}{2}\begin{pmatrix} G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(b)\big) + G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(b)\big) & 0 \\ 0 & G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) + G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\end{pmatrix}. \tag{6}$$

Here U_{J} is considered as a differentiation operator with respect to $\mathbf{r}$. Using the identity $\mathrm{d}\Psi(a,c,x)/\mathrm{d}x = -a\Psi(a+1,c+1,x)$ one can write more explicit expressions for the Green function. Namely,

$$G_{\mathrm{J}}(\mathbf{r},\mathbf{r}';z) = \begin{pmatrix} G_{\mathrm{J}}^{11}(\mathbf{r},\mathbf{r}';z) & G_{\mathrm{J}}^{12}(\mathbf{r},\mathbf{r}';z) \\ G_{\mathrm{J}}^{21}(\mathbf{r},\mathbf{r}';z) & G_{\mathrm{J}}^{22}(\mathbf{r},\mathbf{r}';z)\end{pmatrix},$$

with

$$G_{\mathrm{J}}^{11}(x,y;z) = \frac{\beta_{\mathrm{J}} - \varkappa_{\mathrm{J}}}{2\eta_{\mathrm{J}}}\big(G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(b)\big) - G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(b)\big)\big)$$
$$+\frac{1}{2}\big(G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(b)\big) + G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(b)\big)\big),$$
$$G_{\mathrm{J}}^{22}(\mathbf{r},\mathbf{r}';z) = -\frac{\beta_{\mathrm{J}} + \varkappa_{\mathrm{J}}}{2\eta_{\mathrm{J}}}\big(G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) - G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\big)$$
$$+\frac{1}{2}\big(G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) + G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\big)$$

for both $\mathrm{J} = \mathrm{R}, \mathrm{D}$,

$$G_{\mathrm{R}}^{12}(\mathbf{r},\mathbf{r}';z) = |b|((x-x') - \mathrm{i}(y-y'))\bigg(\frac{\operatorname{sign} b - 1}{2}\big[G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) - G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\big]$$
$$+\big[F_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) - F_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\big]\bigg),$$
$$G_{\mathrm{D}}^{12}(\mathbf{r},\mathbf{r}';z) = |b|((y-y') - \mathrm{i}(x-x'))\bigg(\frac{\operatorname{sign} b + 1}{2}\big[G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) - G_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\big]$$
$$-\big[F_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^-(-b)\big) - F_0\big(\mathbf{r},\mathbf{r}';\zeta_{\mathrm{J}}^+(-b)\big)\big]\bigg).$$

and $G_{\mathrm{J}}^{21}(\mathbf{r},\mathbf{r}';z) = \overline{G_{\mathrm{J}}^{12}(\mathbf{r}',\mathbf{r};\bar{z})}$, where

$$F_0(\mathbf{r},\mathbf{r}';z) = \frac{1}{4\pi}\left(\frac{z}{2|b|} - \frac{1}{2}\right)\Gamma\left(\frac{1}{2} - \frac{z}{2|b|}\right)$$
$$\times\exp\left(\frac{\mathrm{i}b}{2}(\mathbf{r}\wedge\mathbf{r}') - \frac{|b|}{4}(\mathbf{r}-\mathbf{r}')^2\right)\Psi\left(\frac{3}{2} - \frac{z}{2|b|}, 2; \frac{|b|}{2}(\mathbf{r}-\mathbf{r}')^2\right).$$

4. Renormalized Green functions

In some applications it is necessary to know the renormalized Green function, namely the values $G_{\mathrm{J}}^{\mathrm{ren}}(\mathbf{r},\mathbf{r};z)$ given by $G_{\mathrm{J}}^{\mathrm{ren}}(\mathbf{r},\mathbf{r};z) = \lim_{\mathbf{r}'\to\mathbf{r}}[G_{\mathrm{J}}(\mathbf{r},\mathbf{r}';z) - S(\mathbf{r},\mathbf{r}')]$, where $S(\mathbf{r},\mathbf{r}';z) := -\frac{1}{2\pi}\log|\mathbf{r}-\mathbf{r}'|\sigma_0$ is the on-diagonal singularity. Terms of this kind appear e.g. when calculating the so-called Wigner R-matrix.

Consider first the case $b = 0$. We will use representation (4) for the Green function. Using the expansion

$$K_0(z) = \sum_{m=0}^{\infty} \frac{1}{(m!)^2}\left(\frac{z^2}{2}\right)^m (\psi(m+1) + \log 2 - \log z)$$

one easily sees that $G_{\mathrm{J}}^{12}(\mathbf{r}, \mathbf{r}'; z)$ are continuous functions vanishing at $\mathbf{r} = \mathbf{r}'$, which means that $G_{\mathrm{J}}^{\mathrm{ren}}$ is diagonal. To calculate the diagonal terms we use the equality

$$Q(z) := \lim_{r\to 0+} \frac{1}{2\pi}(K_0(\sqrt{-z}r) + \log r) = \frac{1}{2\pi}\left(\psi(1) - \frac{1}{2}\log(-z) + \log 2\right).$$

Hence,

$$\begin{aligned} G_{\mathrm{J}}^{\mathrm{ren}}(\mathbf{r}, \mathbf{r}; z) &= \left[-\frac{\varkappa_{\mathrm{J}}}{2\mathrm{i}\sqrt{-\left(z+\varkappa_{\mathrm{J}}^2\right)}}(Q(\zeta^+) - Q(\zeta^-)) + \frac{1}{2}(Q(\zeta^+) + Q(\zeta^-))\right]\sigma_0 \\ &= \frac{1}{2\pi}\left[\psi(1) - \frac{1}{2}\log\left(-\frac{z}{4}\right) + \frac{\varkappa_{\mathrm{J}}}{2\mathrm{i}\sqrt{-\left(z+\varkappa_{\mathrm{J}}^2\right)}}\log\frac{\sqrt{-\left(z+\varkappa_{\mathrm{J}}^2\right)} + \mathrm{i}\varkappa_{\mathrm{J}}}{\sqrt{-\left(z+\varkappa_{\mathrm{J}}^2\right)} - \mathrm{i}\varkappa_{\mathrm{J}}}\right]\sigma_0, \end{aligned}$$

which is independent of $\mathbf{r}$ due to the translational symmetry of the Hamiltonian.

For the magnetic case ($b \neq 0$) we use the expansions [4]

$$\begin{aligned} \Psi(a, n+1, x) = &-\frac{(-1)^n}{\Gamma(a-n)}\left[\Phi(a, n+1, x)\log x + \sum_{r=0}^{\infty}\frac{(a)_r}{(n+1)_r r!}(\psi(a+r)\right. \\ &\left. - \psi(1+r) - \psi(1+n+r))x^r\right] + \frac{(n-1)!}{\Gamma(a)}\sum_{r=0}^{n-1}\frac{(a-n)_r}{(1-n)_r}\frac{x^{r-n}}{r!}, \end{aligned}$$

$$\Phi(a, c, x) = \sum_{r=0}^{\infty}\frac{(a)_r}{(c)_r r!}x^r, \qquad (a)_r := \frac{\Gamma(a+r)}{\Gamma(a)}.$$

The above expansions clearly show that the off-diagonal terms of $G_{\mathrm{J}}^{\mathrm{ren}}$ vanish. To express the diagonal terms we use the function

$$Q(z) := \lim_{\mathbf{r}\to\mathbf{r}'}\left(G_0(\mathbf{r}, \mathbf{r}'; z) + \frac{1}{2\pi}\log|\mathbf{r} - \mathbf{r}'|\right) = -\frac{1}{4\pi}\left(\psi\left(\frac{1}{2} - \frac{z}{2|b|}\right) - 2\psi(1) + \log\frac{|b|}{2}\right),$$

then

$$\begin{aligned} G_{\mathrm{J}}^{\mathrm{ren}}(\mathbf{r}, \mathbf{r}, z) = &\frac{\beta_{\mathrm{J}}\sigma_z - \varkappa_{\mathrm{J}}}{2\eta_{\mathrm{J}}}\begin{pmatrix} Q\left(\zeta_{\mathrm{J}}^-(b)\right) - Q\left(\zeta_{\mathrm{J}}^+(b)\right) & 0 \\ 0 & Q\left(\zeta_{\mathrm{J}}^-(-b)\right) - Q\left(\zeta_{\mathrm{J}}^+(-b)\right)\end{pmatrix} \\ &+ \frac{1}{2}\begin{pmatrix} Q\left(\zeta_{\mathrm{J}}^-(b)\right) + Q\left(\zeta_{\mathrm{J}}^+(b)\right) & 0 \\ 0 & Q\left(\zeta_{\mathrm{J}}^-(-b)\right) + Q\left(\zeta_{\mathrm{J}}^+(-b)\right)\end{pmatrix}. \end{aligned}$$

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Appendix. Supersymmetric spectral analysis

For the sake of completeness, here we are going to prove the following.

Proposition. *Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces, A be a closed densely defined linear operator from $\mathcal{H}_1$ to $\mathcal{H}_2$, and $m \geqslant 0$. On $\mathcal{H}_1 \oplus \mathcal{H}_2$ consider the operator $L := \left(\begin{smallmatrix} m & A^* \\ A & -m \end{smallmatrix}\right)$. Then*

$$\operatorname{spec} L = -\sqrt{\operatorname{spec}(AA^* + m^2)} \cup \sqrt{\operatorname{spec}(A^*A + m^2)}, \tag{A.1}$$

and the same correspondence holds for the eigenvalues.

Proof. First, it is well known [5] that $\operatorname{spec} AA^*\backslash\{0\} = \operatorname{spec} A^*A\backslash\{0\}$. Clearly,

$$L^2 = \begin{pmatrix} A^*A + m^2 & 0 \\ 0 & AA^* + m^2 \end{pmatrix}. \tag{A.2}$$

Therefore, $\operatorname{spec} L^2\backslash\{m^2\} = \operatorname{spec}(AA^* + m^2)\backslash\{m^2\}$, and for any $\lambda \in \operatorname{spec} AA^*\backslash\{0\} \equiv \operatorname{spec} AA^*\backslash\{0\}$ at least one of the numbers $-\sqrt{\lambda + m^2}, \sqrt{\lambda + m^2}$ lies in $\operatorname{spec} L$. Let us show that actually they both are in the spectrum of L.

Let $\lambda > 0$, $\lambda \in \operatorname{spec} A^*A$, then there exists a sequence (ϕ_n) with $\phi_n \in \operatorname{dom} A^*A \subset \operatorname{dom} A$ such that $\|\phi_n\| \geqslant 1$ and $\lim(A^*A - \lambda)\phi_n = 0$. Denote $\psi_n := \left[\lambda + \left(\sqrt{\lambda + m^2} - m\right)\left(\begin{smallmatrix} 0 & A^* \\ A & 0 \end{smallmatrix}\right)\right]\left(\begin{smallmatrix} \phi_n \\ 0 \end{smallmatrix}\right)$. Clearly, $\left(\begin{smallmatrix} \phi_n \\ 0 \end{smallmatrix}\right) \perp \left(\begin{smallmatrix} 0 & A^* \\ A & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} \phi_n \\ 0 \end{smallmatrix}\right)$, which implies

$$\|\psi_n\| \geqslant \lambda\|\phi_n\| \geqslant \lambda. \tag{A.3}$$

By direct calculation, $(L - \sqrt{\lambda + m^2})\psi_n = \left(\sqrt{\lambda + m^2} - m\right)\left(\begin{smallmatrix} (A^*A-\lambda)\phi_n \\ 0 \end{smallmatrix}\right)$. Therefore, $\lim(L - \sqrt{\lambda + m^2})\psi_n = 0$. Together with (A.3) this implies $\sqrt{\lambda + m^2} \in \operatorname{spec} L$.

To show $-\sqrt{\lambda + m^2} \in \operatorname{spec} L$ one has to consider the functions

$$\psi_n := \left[\lambda - \left(\sqrt{\lambda + m^2} - m\right)\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}\right]\begin{pmatrix} 0 \\ \phi_n \end{pmatrix},$$

where $\phi_n \in \operatorname{dom} AA^* \subset \operatorname{dom} A^*$, $\|\phi_n\| \geqslant 1$, and $\lim(AA^* - \lambda)\phi_n = 0$ and to repeat the above steps. To finish the proof of equation (A.1) it is necessary to study the points $\pm m$. Not that it is sufficient to consider the situation when $\pm m$ is an isolated point in $\operatorname{spec} L$ (in particular, an eigenvalue of L), as for the continuous spectrum the result follows by taking the closure of $\operatorname{spec} L\backslash\{-m, m\}$.

For $m = 0$, equation (A.2) reads as $\operatorname{spec} L^2 = \operatorname{spec} AA^* \cup \operatorname{spec} A^*A$, and the conditions $0 \in \operatorname{spec} L$ and $0 \in \operatorname{spec} AA^* \cup \operatorname{spec} A^*A$ are equivalent.

Assume $m \neq 0$ and m is an eigenvalue of L, then there are $\phi \in \operatorname{dom} A$ and $\varphi \in \operatorname{dom} A^*$ with $\|\phi\| + \|\varphi\| > 1$ such that $(L - m)\left(\begin{smallmatrix} \phi \\ \varphi \end{smallmatrix}\right) \equiv \left(\begin{smallmatrix} A^*\varphi \\ A\phi - 2m\varphi \end{smallmatrix}\right) = 0$. Clearly, this implies $A\phi_n \in \operatorname{dom} A^*$ and $A^*A\phi = 0$. If $\phi = 0$, then also $\varphi = 0$, which contradicts to the choice. Therefore, ϕ is an eigenvector of A^*A.

Assume now that 0 is an eigenvalue of A^*A, then there is a nonzero vector $\phi \in \operatorname{dom} A^*A \subset \operatorname{dom} A$ with $\langle A^*A\phi_n, \phi_n\rangle \equiv \|A\phi\| = 0$. Then $(L - m)\left(\begin{smallmatrix} \phi \\ 0 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 \\ A\phi \end{smallmatrix}\right) = 0$, from which $m \in \operatorname{spec} L$.

The relationship between the conditions $-m \in L$ and $0 \in \operatorname{spec} AA^*$ can be proved in a completely similar way. $\square$

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