Towards spectral gaps in graphene in a magnetic field

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Joint work with H. Cornean, I. Herbst.

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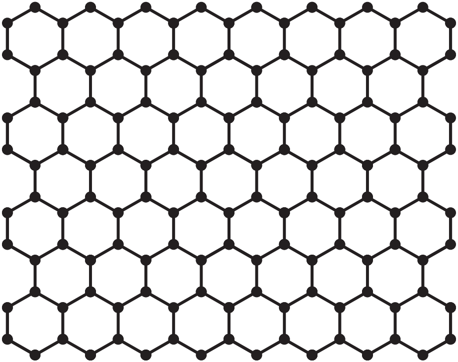
Aalborg University

Honeycomb lattice



Graphene

- Wallace 1947, Theoretical investigation of monolayer graphite.

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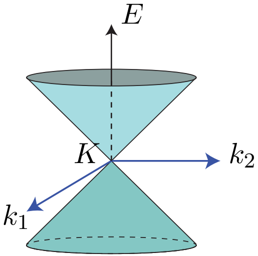

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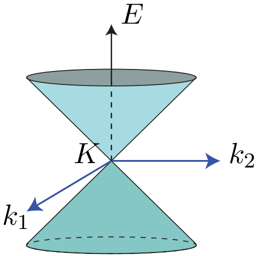

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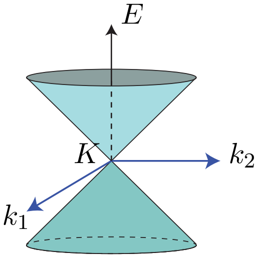

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- Nobel prize 2010. Huge interest.

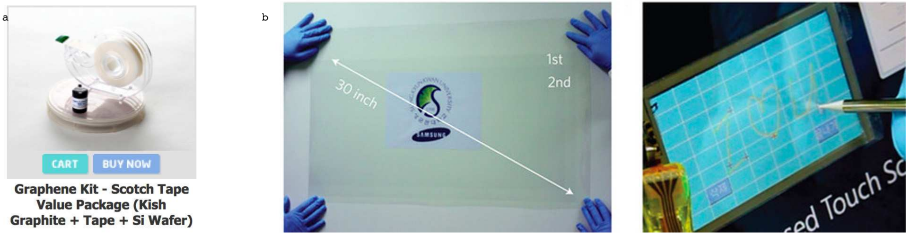

Figure: a) you can now order a graphene kit online at http://www.graphenesq.com. b) S. Bae and others : "Roll-to-roll production of 30-inch graphene films for transparent electrodes", Nature Nanotechnology, 2010.

The Setting

Two-dimensional crystal, two sites per unit cell. Notation and (solid state physics) nomenclature:

$$\Gamma = \text{Bravais lattice} = \{\gamma = (\gamma_1, \gamma_2) \in \mathbb{R}^2 \ : \ \gamma = m\mathfrak{a} + n\tilde{\mathfrak{a}},\ m, n \in \mathbb{Z}\},$$

$$\Omega = \text{unit cell} = \{(x_1, x_2) \ : \ x = \theta_1\mathfrak{a} + \theta_2\tilde{\mathfrak{a}}, -\frac{1}{2} < \theta_1, \theta_2 \leq \frac{1}{2}\}.$$

Choose numbering of $\mathfrak{a}$ and $\tilde{\mathfrak{a}}$ s.t. $|\Omega| = \mathfrak{a} \wedge \tilde{\mathfrak{a}} = \mathfrak{a}_1\tilde{\mathfrak{a}}_2 - \mathfrak{a}_2\tilde{\mathfrak{a}}_1$.

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Dual lattice:

$$\mathfrak{a} \cdot \mathfrak{a}^* = \tilde{\mathfrak{a}} \cdot \tilde{\mathfrak{a}}^* = 2\pi, \quad \mathfrak{a} \cdot \tilde{\mathfrak{a}}^* = \tilde{\mathfrak{a}} \cdot \mathfrak{a}^* = 0,$$

$$\Gamma^* = \text{reciprocal lattice} = \{(\gamma_1^*, \gamma_2^*) \ : \ \gamma^* = m\mathfrak{a}^* + n\tilde{\mathfrak{a}}^*,\ m, n \in \mathbb{Z}\},$$

$$\Omega^* = \text{1st Brillouin zone} = \{(k_1, k_2) \ : \ \|k\| \leq \|k - \gamma^*\|,\ \gamma^* \in \Gamma\}.$$

The Setting

A unit vector in $\ell^2(\Lambda)$ is the state vector of an electron. Γ-periodic zero-field Hamilton operator:

$$H_0 : \ell^2(\Lambda) \to \ell^2(\Lambda), \qquad H_0(x+\gamma, x') = H_0(x, x'-\gamma), \quad (x, x' \in \Lambda; \gamma \in \Gamma).$$

$\ell^2(\Lambda) \cong \int_{\Omega^*}^{\oplus} \mathbb{C}^2 \, dk$, Bloch-Floquet-Gelfand (BFG) decomposition
$\psi \in \ell^2_c(\Lambda)$, $\gamma \in \Gamma$, $\underline{x} \in \mathfrak{B}$, $k \in \Omega^*$

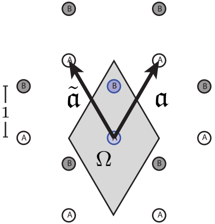
$$(U\psi)(k, \underline{x}) = \frac{1}{\sqrt{|\Omega^*|}} \sum_{\gamma \in \Gamma} e^{-ik\cdot(\gamma+\underline{x})} \psi(\gamma + \underline{x}),$$

$$UH_0U^* = \int_{\Omega^*}^{\oplus} h_0(k) \, dk,$$

$$h_0(k) = \begin{bmatrix} h_0(k; \underline{\boldsymbol{\xi}}, \underline{\boldsymbol{\xi}}) & h_0(k; \underline{\boldsymbol{\xi}}, \underline{\tilde{\boldsymbol{\xi}}}) \\ h_0(k; \underline{\tilde{\boldsymbol{\xi}}}, \underline{\boldsymbol{\xi}}) & h_0(k; \underline{\tilde{\boldsymbol{\xi}}}, \underline{\tilde{\boldsymbol{\xi}}}) \end{bmatrix}. \qquad (\mathfrak{B} = \{\underline{\boldsymbol{\xi}}, \underline{\tilde{\boldsymbol{\xi}}}\})$$

$$H_0(x, x') = \frac{1}{|\Omega^*|} \int_{\Omega^*} e^{ik\cdot(\gamma+\underline{x}-\gamma'-\underline{x}')} h_0(k; \underline{x}, \underline{x}') \, dk$$

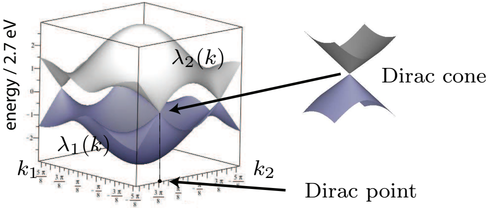
Graphene bandstructure calculation

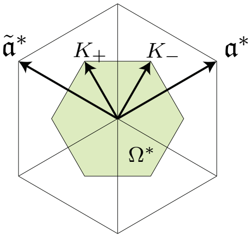


$$h_0^G(k;\underline{x},\underline{x}') = \frac{1}{|\Omega^*|}\sum_{\gamma\in\Gamma} e^{ik\cdot\gamma} H_0(\underline{x},\underline{x}'+\gamma).$$

$$h_0^G(k) = \begin{bmatrix} 0 & 2e^{-i\frac{3}{2}k_2}\cos(\frac{\sqrt{3}}{2}k_1)+1 \\ c.c. & 0 \end{bmatrix}$$

$$\lambda_{\substack{2\\1}}(k_1,k_2) = \pm\sqrt{3+2\cos(\sqrt{3}k_1)+4\cos(\frac{\sqrt{3}}{2}k_1)\cos(\frac{3}{2}k_2)},$$





Graphene bandstructure calculation

Dirac points:

$$K_\pm = \left(\pm\frac{2\pi}{3\sqrt{3}}, \frac{2\pi}{3}\right), \quad \lambda_1(K_\pm) = \lambda_2(K_\pm) = 0.$$

When expanding the fibers around

$$\tilde{k} = k - K_+,$$

one gets

$$h_0^G(\tilde{k}_1, \tilde{k}_2) = \frac{3}{2}\begin{bmatrix} 0 & \tilde{k}_1 - i\tilde{k}_2 + \sum_{|\alpha|\geq 2} C_\alpha \tilde{k}^\alpha \\ \tilde{k}_1 + i\tilde{k}_2 + \dots & 0 \end{bmatrix}.$$

$\approx$ Weyl Hamiltonian (Dirac Hamiltonian for massless fermions) for $\|\tilde{k}\| << \min\{\|\mathfrak{a}^*\|, \|\tilde{\mathfrak{a}}^*\|\}$

- C. L. Fefferman and M. I. Weinstein, 2012;

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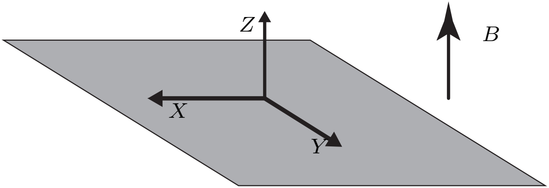
External magnetic field.

- Graphene sheet in orthogonal constant magnetic field.



- Energy gaps?

R. Rammal, 1985 (Hofstadter, 1976).

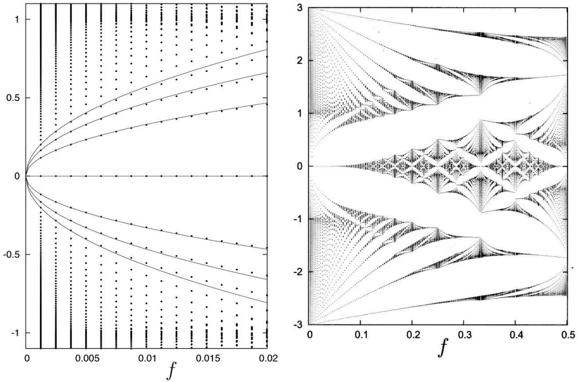


Figure: From Petra Dietl, Frederic Piechon and Gilles Montambaux, "A new magnetic field dependence of Landau levels on a graphene like structure", PRL 2008. $f = \phi/\phi_0$, $\phi = (d_{nn})^2 3b\sqrt{3}/2$, $\phi_0 = hc/e$. See also Guillement, Helffer, Treton: "Walk inside Hofstadter's butterfly", Journal de Physique 1989, and "C^*-Algebras in solid state physics: 2D Electrons in a uniform magnetic field", Jean Bellisard.

Single Dirac-cone fiber

$H_0 : \ell^2(\Lambda) \to \ell^2(\Lambda)$ generated by fibers $h_0(k)$. For $k \in \Omega^*$, $\{h_0(k; \underline{x}, \underline{x}')\}_{\underline{x},\underline{x}' \in \mathfrak{B}}$ is a self-adjoint matrix (2×2). Suppose:

(a) each $h_0(\,\cdot\,; \underline{x}, \underline{x}') : \Omega^* \to \mathbb{C}$, for fixed $\underline{x}, \underline{x}' \in \mathfrak{B}$, has an extension which is $C^\infty(\mathbb{R}^2)$ and Γ^*-periodic.

(b) 0 is an eigenvalue of $h_0(0)$ with degeneracy 2.

(c) Eigenvalues of $h_0(k)$, $k \neq 0$ satisfies $\lambda_1(k) < 0 < \lambda_2(k)$.

(d) $h_0(k) = h_0^{[1]}(k) + h_0^{Rem}(k)$,where

$$h_0^{[1]}(k_1, k_2) = \begin{bmatrix} 0 & k_1 - ik_2 \\ k_1 + ik_2 & 0 \end{bmatrix}, \tag{1}$$

$$\exists C_1 > 0, \qquad \|h_0^{Rem}(k)\| \leq C_1 \|k\|^2. \tag{2}$$

Theorem

Peierls subst. $H_b(\gamma + \underline{x}, \gamma' + \underline{x}') := e^{i \int_{\triangle(\gamma,\gamma')} B \, d^2 r} H_0(\gamma + \underline{x}, \gamma' + \underline{x}')$.

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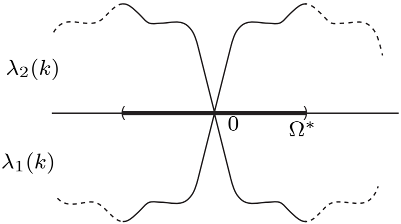
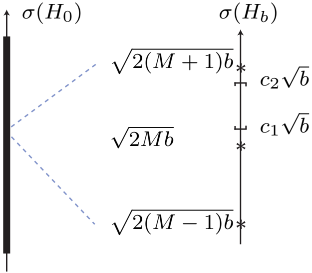
For fixed $M = 0, 1, 2, 3, \ldots$, choose c_1, c_2 such that

$$\sqrt{2M} < c_1 < c_2 < \sqrt{2(M+1)},$$

then there exists $b_0 > 0$, such that for all $0 < b < b_0$ we have

$$[c_1\sqrt{b}, c_2\sqrt{b}] \subset \rho(H_b).$$





The proof strategy: for $z \in \mathcal{K} \subset B_{\delta(b)}(0) \setminus \{\pm\sqrt{2mb}\}_{m\in\mathbb{Z}}$, $\mathcal{K}$ compact.

$$(H_b - z)S_b(z) - I = Err(b;z), \qquad \sup_{z\in\mathcal{K}} \|Err(b;z)\| \to 0, b \to 0.$$

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Symmetric gauge,

$$a(x) = \frac{1}{2}(-x_2, x_1), \qquad B = b(\partial_{x_1} a_2 - \partial_{x_2} a_1)$$

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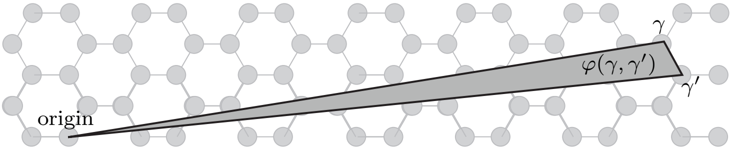
Auxilliary function (area of triangle):

$$\varphi(x, x') := \frac{1}{2} x' \wedge x, \qquad \int_{\triangle(\gamma,\gamma')} B \, d^2 r = b\varphi(\gamma, \gamma').$$



Dirac (Weyl) operator:

$$D_b := \begin{bmatrix} 0 & (-i\partial_{x_1} - ba_1(x)) - i\,(-i\partial_{x_2} - ba_2(x)) \\ (-i\partial_{x_1} - ba_1(x)) + i\,(-i\partial_{x_2} - ba_2(x)) & 0 \end{bmatrix},$$

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$$D_b^2 = \begin{bmatrix} (-i\nabla_x - ba(x))^2 - b & 0 \\ 0 & (-i\nabla_x - ba(x))^2 + b \end{bmatrix},$$

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Landau levels: $\sigma_L = (2n+1)b$, $n \in \mathbb{N}_0$. For $z^2 \pm b \notin \sigma_L$,

$$(D_b - z)^{-1} = (D_b + z)(D_b^2 - z^2)^{-1}.$$

Lemma 1.

$$\rho(D_b) \subseteq \mathbb{C} \setminus \{\pm\sqrt{2nb} \;:\; n \in \mathbb{N}_0\}.$$

We expand $(D_b - z)^{-1}$ acting in $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$ in Pauli matrices:

$$\sigma_0 := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

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Choose

$$g \in C_c^\infty(\mathbb{R}^2), \qquad g(k) = \begin{cases} 1, & \|k\| \leq 1 \\ 0, & \|k\| \geq 2 \end{cases}, \qquad g_\epsilon(k) := g\left(\frac{k}{\epsilon}\right),$$

for $\epsilon > 0$. (we will choose $\epsilon(b) \to 0$, as $b \to 0$)
$\tilde{G}_\epsilon : \ell^2(\Lambda) \to \ell^2(\Lambda)$, inverse BFG transform of $g_\epsilon(k) = g(\frac{k}{\epsilon})$:

$$\tilde{G}_\epsilon(x, x') = \frac{|\Omega|}{2\pi} \epsilon^2 \check{g}(\epsilon(x - x')).$$

Resolvent approximation, near part:

$$S_{b,near}(\gamma'' + \underline{x}'', \gamma' + \underline{x}'; z) = \sum_{j=0}^{3} \int_{\mathbb{R}^2} dy\, e^{ib\varphi(\gamma'',y)} \tilde{G}_\epsilon(\gamma'' + \underline{x}'', y) r_j(y, \gamma'; z) \sigma_j(\underline{x}'', \underline{x}')$$

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"Far" part of resolvent approximation:

$$h_\epsilon(k):=\begin{bmatrix}\epsilon g_{(\epsilon/4)}(k_1,k_2) & k_1-ik_2\\ k_1+ik_2 & -\epsilon g_{(\epsilon/4)}(k_1,k_2)\end{bmatrix}+h_0^{Rem}(k_1,k_2)$$

$$UH_\epsilon U^*:=\int_{\Omega^*}^{\oplus}h_\epsilon(k)\,dk,\qquad H_\epsilon:\ell^2(\Lambda)\to\ell^2(\Lambda).$$

Lemma 2. *H_ϵ has a spectral gap:*

$$\left(-\frac{\epsilon}{4},\frac{\epsilon}{4}\right)\subset\rho(H_\epsilon).$$

$$H_{\epsilon,b}(\gamma + \underline{x}, \gamma' + \underline{x}') := e^{ib\varphi(\gamma,\gamma')} H_\epsilon(\gamma + \underline{x}, \gamma' + \underline{x}')$$

Lemma 3. *If there exists $\epsilon_0, C' > 0$, s.t. $\|H_\epsilon\|' < C' < \infty$, for $\epsilon < \epsilon_0$, then there exists a constant $C > 0$ s.t.*

$$d_H(\sigma(H_\epsilon), \sigma(H_{\epsilon,b})) \leq C\sqrt{b}.$$

(H. Cornean, R. Purice: "On the regularity of the Hausdorff distance between spectra of perturbed magnetic Hamiltonians", Spectral Analysis of Quantum Hamiltonians 2011)

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Lemma 4. *Put $\epsilon = b^{1/4}$. We can find $b_0 > 0$ such that for $0 < b < b_0$, there exist $\delta(b) > 0$ s.t.*

$$B_{\delta(b)}(0) \in \rho(H_{\epsilon,b}).$$

Suppose $A : \ell^2(\Lambda) \to \ell^2(\Lambda)$.

$$\|A\|_{SH} := \max\left\{ \sup_{x\in\Lambda} \sum_{x'} |A(x,x')|, \sup_{x'\in\Lambda} \sum_{x} |A(x,x')| \right\}.$$

Lemma 5. *If $\|A\|_{SH} < \infty$, then A is bounded with $\|A\| \leq \|A\|_{SH}$.*

$$\|A\|' := \max\left\{ \sup_{x\in\Lambda} \sum_{x'\in\Lambda} (1 + |x_1 - x_1'| + |x_2 - x_2'|)\big|A(x,x')\big|, \right.$$
$$\left. \sup_{x'\in\Lambda} \sum_{x\in\Lambda} (1 + |x_1 - x_1'| + |x_2 - x_2'|)\big|A(x,x')\big| \right\}$$

Lemma 6. *If $\|A\|' < \infty$, then A is bounded with*

$$\|A\| \leq \|A\|_{SH} \leq \|A\|'.$$

Resolvent approximation

$$(D_b - z)^{-1} = \sum_{j=0}^{3} r_j(z) \otimes \sigma_j, \qquad h_\epsilon(k) = \epsilon g_{\epsilon/4}(k)\sigma_3 + h_0(k)$$

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$$\tilde{G}_\epsilon(x,x') = \frac{|\Omega|}{2\pi}\epsilon^2 \check{g}(\epsilon(x-x')), \qquad G_\epsilon(x,x') = \frac{|\Omega|}{2\pi}\epsilon^2 \check{g}(\epsilon(x-x'))\delta_{\underline{x},\underline{x}'},$$

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$$S_{b,far}(\gamma'' + \underline{x}'', x'; z) = \sum_{\underline{x}''' \in \mathfrak{B}} \sum_{\gamma''' \in \Lambda} e^{ib\varphi(\gamma'', \gamma''')} \left(I - G_\epsilon\right)(x'', x''') \left[\left(H_{\epsilon,b} - z\right)^{-1}\right](x''', x'; z),$$

$$S_b(x'', x'; z) := S_{b,near}(x'', x'; z) + S_{b,far}(x'', x'; z)$$

$$(D_b - z)^{-1} = \sum_{j=0}^{3} r_j(z) \otimes \sigma_j, \qquad h_\epsilon(k) = \epsilon g_{\epsilon/4}(k)\sigma_3 + h_0(k)$$

$$\tilde{G}_\epsilon(x, x') = \frac{|\Omega|}{2\pi}\epsilon^2 \check{g}(\epsilon(x - x')), \qquad G_\epsilon(x, x') = \frac{|\Omega|}{2\pi}\epsilon^2 \check{g}(\epsilon(x - x'))\delta_{\underline{x},\underline{x}'},$$

$$S_{b,near}(\gamma'' + \underline{x}'', \gamma' + \underline{x}'; z) = \sum_{j=0}^{3} \int_{\mathbb{R}^2} dy\; e^{ib\varphi(\gamma'',y)} \tilde{G}_\epsilon(\gamma'' + \underline{x}'', y) r_j(y, \gamma'; z)\sigma(\underline{x}'', \underline{x}')$$

$$S_{b,far}(\gamma'' + \underline{x}'', x'; z) = \sum_{\underline{x}''' \in \mathfrak{B}} \sum_{\gamma''' \in \Lambda} e^{ib\varphi(\gamma'',\gamma''')} \left(I - G_\epsilon\right)(x'', x''') \left[\left(H_{\epsilon,b} - z\right)^{-1}\right](x''', x'; z),$$

$$S_b(x'', x'; z) := S_{b,near}(x'', x'; z) + S_{b,far}(x'', x'; z)$$

Lemma 7. *There exists b_0 s.t. $\mathcal{K} \subset B_{\delta(b)}(0) \setminus \{\pm\sqrt{2mb}\}_{m \in \mathbb{N}_0}$ when $b < b_0$, $\mathcal{K} = [c_1\sqrt{b}, c_2\sqrt{b}]$. Furthermore, for $z \in \mathcal{K}$, we have*

$$(H_b - z)S_b(z) - I = Err(b; z), \qquad \sup_{z \in \mathcal{K}} \|Err(b; z)\|_{SH} \to 0, b \to 0.$$

Resolvent approximation

$$\left[H_b S_{b,near}(z)\right](x,x') = \sum_{\underline{x}''}\sum_{\gamma''} e^{ib\varphi(\gamma,\gamma'')} H_0(x,x'') \sum_{j=0}^{3}\int_{\mathbb{R}^2} dy\; e^{ib\varphi(\gamma'',y)}\tilde{G}_\epsilon(x'',y) r_j(y,\gamma';z)\sigma(\underline{x}'',\underline{x}')$$

collect the phases:

$$e^{ib\varphi(\gamma,\gamma'')}e^{ib\varphi(\gamma'',y)} = e^{ib[\varphi(\gamma,y)+\frac{1}{2}(\gamma''-y)\wedge(\gamma-\gamma')]}$$

consider

$$\begin{aligned}&\sum_{j=0}^{3}\int_{\mathbb{R}^2} dy\; e^{ib\varphi(\gamma,y)}\sum_{\underline{x}''}\sum_{\gamma''} H_0(x,x'')\tilde{G}_\epsilon(x'',y) r_j(y,\gamma';z)\sigma_j(\underline{x}'',\underline{x}')\\ &= \sum_{j=0}^{3}\int_{\mathbb{R}^2} dy\; e^{ib\varphi(\gamma,y)}\sum_{\underline{x}''}\sum_{\gamma''}\left(\frac{1}{|\Omega^*|}\int_{\Omega^*} dk\; e^{ik(x-x'')} h_0(k;\underline{x},\underline{x}'')\right)\tilde{G}_\epsilon(x'',y) r_j(y,\gamma';z)\sigma_j(\underline{x}'',\underline{x}').\end{aligned}$$

multiply with $e^{ik(y-y)}$, express $\tilde{G}_\epsilon(x'',y)$ in $\left\{e_{\gamma''}\right\}_{\gamma''\in\Gamma}$, $e_{\gamma''} = \frac{1}{\sqrt{|\Omega^*|}}e^{-ik(\gamma''+\underline{x}''-y)}$.

$$\sum_{j=0}^{3}\int_{\mathbb{R}^2} dy\; e^{ib\varphi(\gamma,y)}\sum_{\underline{x}''}\frac{1}{|\Omega^*|}\int_{\Omega^*} dk\; g_\epsilon(k) e^{ik(x-y)} h_0(k;\underline{x},\underline{x}'') r_j(y,\gamma';z)\sigma_j(\underline{x}'',\underline{x}').$$

Substitute for $h_0(k)$ the leading order terms $k_1\sigma_1(\underline{x},\underline{x}'')+k_2\sigma_2(\underline{x},\underline{x}'')$:

$$\sum_{j=0}^{3}\int_{\mathbb{R}^2} dy\; e^{ib\varphi(\gamma,y)}\sum_{\underline{x}''}\frac{1}{|\Omega^*|}\int_{\Omega^*} dk\; e^{ik(x-y)}\left(k_1\sigma_1(\underline{x},\underline{x}'')+k_2\sigma_2(\underline{x},\underline{x}'')\right)g_\epsilon(k)r_j(y,\gamma';z)\sigma_j(\underline{x}'',\underline{x}')$$

commute the phase $e^{ib\varphi(\gamma,y)}$:

$$=-\int_{\mathbb{R}^2} dy\;\sum_{\underline{x}''}\left[\sum_{\nu=1}^{2}((-i\partial_{y_\nu}+ba_\nu(y))\sigma_\nu(\underline{x},\underline{x}'')+ba_\nu(x-y)\sigma_\nu(\underline{x},\underline{x}''))\left(e^{ib\varphi(x,y)}\tilde{G}_\epsilon(x,y)\right)\right]\dots$$

$$\dots\left(\sum_{j=0}^{3}r_j(y,\gamma';z)\sigma_j(\underline{x}'',\underline{x}')\right)$$

$$[(H_b-z)S_{b,near}(z)](x,x')\approx\int_{\mathbb{R}^2} dy\;\tilde{G}_\epsilon(x,y)e^{ib\varphi(\gamma,y)}\delta(\gamma'-y)\delta_{\underline{x},\underline{x}'}$$

$$=e^{ib\varphi(\gamma,\gamma')}\tilde{G}_\epsilon(x,\gamma')\delta_{\underline{x},\underline{x}'},$$

Resolvent approximation

$$\left(H_b S_{b,far}(z)\right)(x,x') = \sum_{x'',x'''\in\Lambda} e^{ib\varphi(\gamma,\gamma'')} H_0(x,x'') e^{ib\varphi(\gamma'',\gamma''')} (I - G_\epsilon)(x'',x''') \left(H_{\epsilon,b} - z\right)^{-1}(x''',x').$$

$$\begin{aligned}
&\approx \sum_{x'''} e^{ib\varphi(\gamma,\gamma''')} \left(\sum_{\underline{x}''} \frac{1}{|\Omega^*|} \int_{\Omega^*} dk\ e^{ik(x-x''')} h_0(k;\underline{x},\underline{x}'')(1-g_\epsilon(k)) \delta_{\underline{x}'',\underline{x}'''} \right) \left(H_{\epsilon,b} - z\right)^{-1}(x''',x') \\
&= \sum_{x'''} e^{ib\varphi(\gamma,\gamma''')} \left[(I - G_\epsilon) H_\epsilon\right](x,x''') \left(H_{\epsilon,b} - z\right)^{-1}(x''',x') \\
&= \sum_{x'',x'''} e^{ib(\varphi(\gamma,\gamma'') - \mathrm{fl}(\gamma,\gamma'',\gamma'''))} (I - G_\epsilon)(x,x'') H_{\epsilon,b}(x'',x''') \left(H_{\epsilon,b} - z\right)^{-1}(x''',x'),
\end{aligned}$$

$$\begin{aligned}
\left((H_b - z) S_{b,far}(z)\right)(x,x') &\approx \sum_{\gamma''} \sum_{\underline{x}''} e^{ib\varphi(\gamma,\gamma'')} (I - G_\epsilon)(\gamma + \underline{x}, \gamma'' + \underline{x}'') \delta_{\gamma'',\gamma'} \delta_{\underline{x}'',\underline{x}'} \\
&= e^{ib\varphi(\gamma,\gamma')} (I - G_\epsilon)(x,x').
\end{aligned}$$