Excitonic influence on transport coefficients in low dimensional quantum systems

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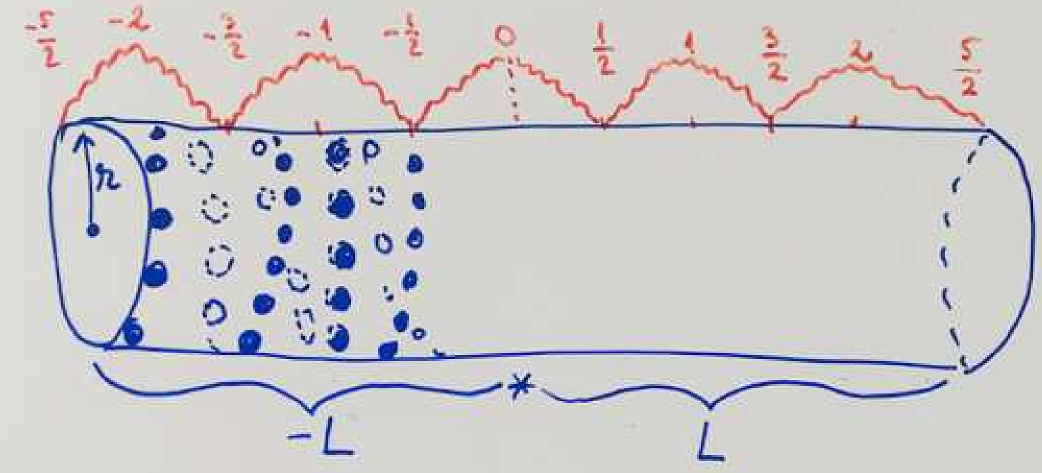


$2L \in \mathbb{N}$

$$\mathcal{H}_1 := L^2(\mathcal{C}) \otimes \mathbb{C}^2 \qquad ; \quad \Psi \in \mathcal{H}_1 \quad , \quad \Psi(x,\varphi,\alpha) \begin{cases} -L \le x \le L \\ \varphi \in [0,2\pi] \\ \alpha \in \{-1,1\} \end{cases}$$
$$= L^2([-L,L]) \otimes L^2([0,2\pi]) \otimes \mathbb{C}^2$$

Basis in $\mathcal{H}_1$: $\{e_p\}_{p=(n_p, j_p, \xi_p)}$ where

$$e_p = \psi_{n_p}(x)\, \phi_{j_p}(\varphi)\, \xi_p(\alpha) \quad \begin{cases} \{\psi_{n_p}\}_{n_p \geq 1} \text{ is a basis in } L^2([-L,L]) \\ \{\phi_{j_p}\}_{j_p \in \mathbb{Z}} \text{ is a basis in } L^2([0,2\pi]) \\ \xi_p \in \left\{ \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix} \right\} \end{cases}$$

The 1- particle Hamiltonian

$V_p(x) = V_p(x+1) \quad , V_p \in C^\infty(\mathbb{R})$

$h_x := -\frac{1}{2}\frac{d^2}{dx^2} + V_p(x)$, periodic boundary conditions in $L^2([-L,L])$

$h_\varphi := -\frac{1}{2}\frac{\partial^2}{\partial\varphi^2} \qquad ; \qquad \Phi_j(\varphi) = \frac{1}{\sqrt{2\pi r}}\, e^{ij\varphi/r}$

$h_x \psi_n = \varepsilon_n^{(x)} \psi_n \qquad , \qquad h_\varphi \phi_j = \frac{j^2}{2r^2}\phi_j$

$$h_1 := (h_x + h_\varphi) \otimes \mathbb{1}_{\mathbb{C}^2}$$

$$h_1 e_p = \varepsilon_p e_p \, , \qquad \varepsilon_p = \varepsilon^{(x)}_{n_p} + \frac{j_p^2}{2r^2}$$

Fermions and their Fock space

$$\mathcal{H}_1 = L^2(\mathcal{C}) \otimes \mathbb{C}^2 \quad ; \quad \langle e_p , e_q \rangle_{\mathcal{H}_1} = \sum_{\alpha = \pm 1} \int_{\mathcal{C}} dx\, d\varphi \; e_p(x,\varphi,\alpha) \overline{e_q(x,\varphi,\alpha)}$$

$$\mathcal{H}_2 := \mathcal{H}_1 \otimes_a \mathcal{H}_1 \quad ; \quad e^{(2)}_{pq} = \frac{1}{\sqrt{2}} \left\{ e_p \otimes e_q - e_q \otimes e_p \right\}$$

$$\mathcal{H}_N := \mathcal{H}_1^{\otimes_a N} \quad ; \quad e^{(N)}_{p_1 \cdots p_N} = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \Sigma_N} (-1)^{m(\sigma)} e_{p_{\sigma(1)}} \otimes \cdots \otimes e_{p_{\sigma(N)}}$$

Occupation number basis:

$\mathcal{N} : \{p\} \to \mathbb{N}$ bijection

$$| n_1 , n_2 , n_3 , \ldots , n_j , \ldots \rangle \quad , \quad \sum_{j \geq 1} n_j = N \quad , \quad n_j \in \{0,1\}$$

$\downarrow$

how many times $e_{\mathcal{N}^{-1}(1)}$ appears in the tensor product

Instead of $e^{(3)}_{\mathcal{N}^{-1}(1)\, \mathcal{N}^{-1}(3)\, \mathcal{N}^{-1}(4)}$ we write

$$| 1, 0, 1, 1, 0, 0, \ldots \rangle$$

The Fock space:

$$\mathcal{F}_a := \bigoplus_{N \geq 0} \mathcal{H}_N \quad , \quad \mathcal{H}_0 := \mathbb{C}$$

The creation and annihilation operators:

$$a_s |\dots, n_s, \dots\rangle = \begin{cases} (-1)^{n_1+\dots+n_{s-1}} |\dots, 0, \dots\rangle & \text{if } n_s = 1 \\ 0 \quad , & n_s = 0 \end{cases}$$

$$a_s : \mathcal{H}_N \to \mathcal{H}_{N-1} \quad ; \quad a_s : \mathcal{F}_a \to \mathcal{F}_a$$

$$a_s^* |\dots, n_s, \dots\rangle = \begin{cases} (-1)^{n_1+\dots+n_{s-1}} |\dots, 1, \dots\rangle & \text{if } n_s = 0 \\ 0 \quad , \quad n_s = 1 \end{cases}$$

$$a_s^* : \mathcal{H}_N \to \mathcal{H}_{N+1}$$

$$\{a_s^\#, a_r^\#\} := a_s^\# a_r^\# + a_r^\# a_s^\# = 0$$

$$\{a_r, a_s^*\} = \delta_{rs} \quad , \quad a_s^* a_s |\dots, n_s, \dots\rangle = n_s |\dots, n_s, \dots\rangle$$

<u>The vacuum</u> $\Omega := |0, 0, 0, \dots\rangle \in \mathcal{H}_0$

$$|1, 0; 0, \dots\rangle = a_1^* \Omega$$

$$|1, 0, 1, 0, \dots\rangle = a_1^* a_3^* \Omega$$

$$|1, 0, 0, 1, 1, \dots\rangle = a_1^* a_4^* a_5^* \Omega$$

$$\vdots$$

N independent particles

$$h_N = h_1 \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + \dots + \mathbb{1} \otimes \dots \otimes h_1 \quad \text{in } \mathcal{H}_N$$

$$h_N \, |n_1, n_2, n_3, \dots\rangle = \left(\varepsilon_{\nu^{-1}(1)} n_1 + \varepsilon_{\nu^{-1}(2)} n_2 + \dots \right) |n_1, n_2, n_3, \dots\rangle$$

Assume $\varepsilon_{\nu^{-1}(j)} \le \varepsilon_{\nu^{-1}(k)}$ if $j \le k$

The groundstate energy is $E_0 = \sum_{j=1}^{N} \varepsilon_{\nu^{-1}(j)}$

The corresponding eigenvector : $\Psi_0 = |\underbrace{1, 1, 1, \dots, 1}_{N}, 0, 0, \dots\rangle$

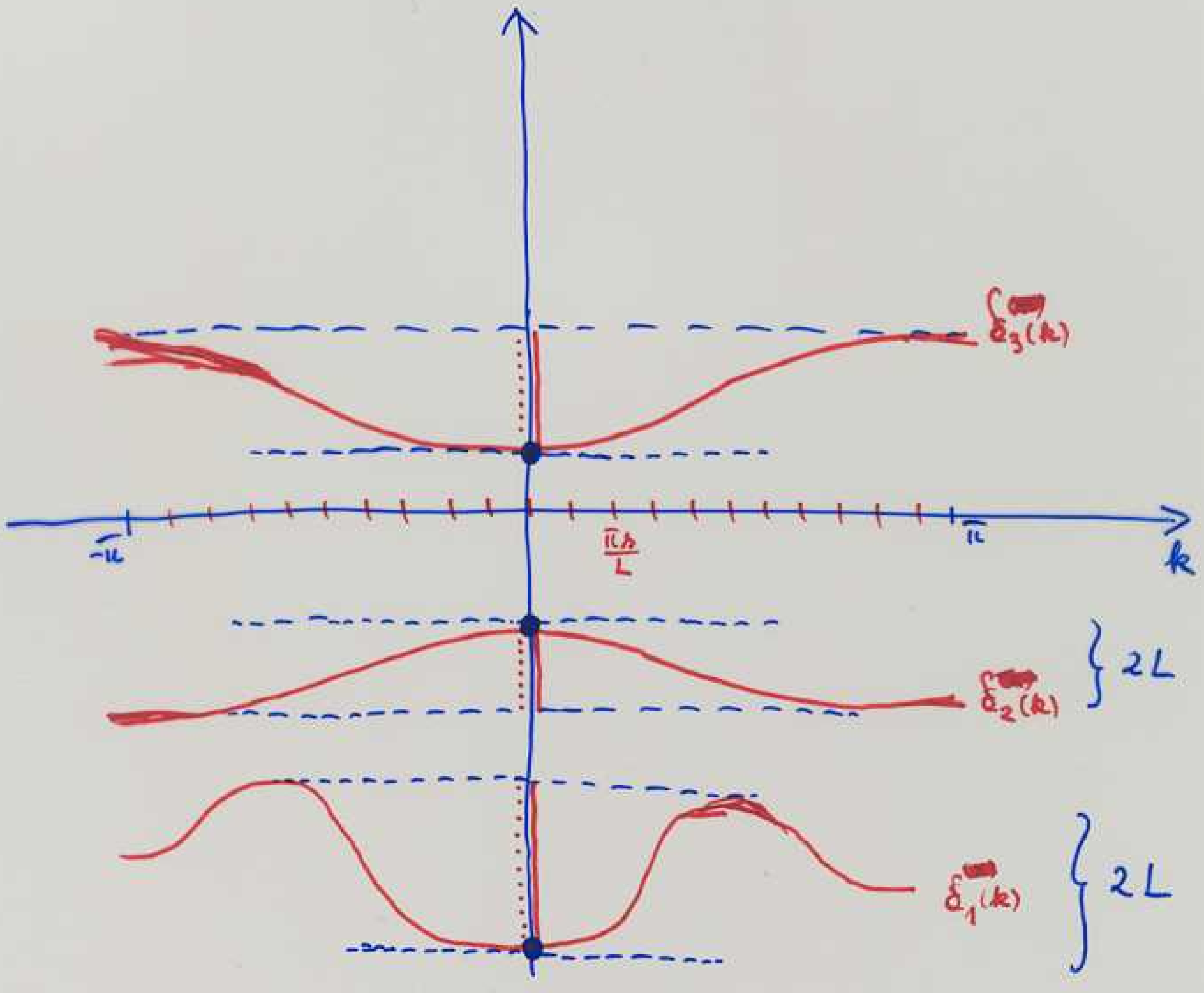
First excited state : $E_1 = \left(\sum_{j=1}^{N-1} \varepsilon_{\nu^{-1}(j)} \right) + \varepsilon_{\nu^{-1}(N+1)}$

An eigenvector: $\Psi_1 = |\underbrace{1, 1, \dots, 1}_{N-1}, 0, 1, 0, \dots\rangle$

$$d\Gamma(h_N) = \sum_{s \ge 1} \varepsilon_{\nu^{-1}(s)} \, a_s^* a_s \quad \text{in } \mathcal{F}_a$$

A simple semiconductor model

$$\mathcal{E}_p = \mathcal{E}^{(x)}_{n_p} + \frac{\dot{J}_p^2}{2r^2} \quad ; \qquad \boxed{\dot{J}_p = 0}$$



$$a(k) := \frac{1}{2}\left(-i\frac{d}{dx} + k\right)^2 + V_p \quad \text{in } L^2\left(\left(-\tfrac{1}{2}, \tfrac{1}{2}\right)\right), \quad k \in [-\pi, \pi] \; ; \text{PBC}$$

$$a(k)\, u_m(x,k) = \epsilon_m(k)\, u_m(x,k), \quad m \geq 1$$

$$h_x \psi_{\tilde{m}}(x) = \mathcal{E}^{(x)}_{\tilde{m}} \psi_{\tilde{m}}(x), \qquad \tilde{n} = (m, s) \; ; \quad k_s = \frac{\pi s}{L}$$

$$s \in \left\{-L + \tfrac{1}{2}, \dots, 0, \dots, L - \tfrac{1}{2}\right\}$$

$$\boxed{\psi_{\tilde{m}}(x) = \frac{1}{\sqrt{2L}}\, u_m(x, k_s)\, e^{i k_s x}} \qquad \boxed{\mathcal{E}^{(x)}_{\tilde{m}} = \epsilon_m(k_s)}$$

Assume that $N = 2(2L + 2L) = 8L$

The noninteracting ground state vector is

$$|1, 1, \dots, 1, 1, 0, 0, \dots\rangle$$

$$e_{\mathcal{N}^{-1}(N-1)} = \frac{1}{\sqrt{2L}} u_2(x,0) \frac{1}{\sqrt{2\pi r}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$e_{\mathcal{N}^{-1}(N)} = \frac{1}{\sqrt{2L}} u_2(x,0) \frac{1}{\sqrt{2\pi r}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

One noninteracting 1-excited state:

$$|1, 1, \dots, 1, 0, 1, 0, \dots\rangle$$

$$e_{\mathcal{N}^{-1}(N-1)}$$

$$e_{\mathcal{N}^{-1}(N+1)} = \frac{1}{\sqrt{2L}} u_3(x,0) \frac{1}{\sqrt{2\pi r}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Spectral gap: $\delta_3(0) - \delta_2(0)$

Interaction between particles

$$H_N = h_N + \frac{1}{2} \sum_{j \neq k} v(|\vec{x}_j - \vec{x}_k|) \otimes \mathbb{1}_{\mathbb{C}^4} \quad \text{in } \mathcal{H}_N$$

$$v(x, \varphi; x', \varphi') = + \frac{\lambda}{\sqrt{(x-x')^2 + 4r^2 \sin^2\left(\frac{\varphi-\varphi'}{2r}\right)}}$$

$$\widetilde{\mathcal{H}}_N := \left\{ L^2([-L,L]) \otimes \mathbb{C}^2 \right\}^{\otimes_a N}$$

$$\Pi_0 : \mathcal{H}_N \to \widetilde{\mathcal{H}}_N$$

$$(\Pi_0 \psi)(x_1, \alpha_1; \dots, x_N, \alpha_N) = \frac{1}{(2\pi r)^{N/2}} \int_0^{2\pi r} d\varphi_1 \dots \int_0^{2\pi r} d\varphi_N \; \psi(x_1, \varphi_1, \alpha_1; \dots, x_N, \varphi_N, \alpha_N)$$

$$(\Pi_0^* \psi)(x_1, \varphi_1, \alpha_1; \dots; x_N, \varphi_N, \alpha_N) = \frac{1}{(2\pi r)^{N/2}} \psi(x_1, \alpha_1; \dots; x_N, \alpha_N)$$

$$\widetilde{H}_N := \Pi_0 H_N \Pi_0^*$$

$$\widetilde{H}_N = h_{x,N} + \frac{1}{2} \sum_{j \neq k} v_r(|x-x'|) \otimes \mathbb{1}_{\mathbb{C}^4}$$

$$v_r(|x-x'|) = \frac{\lambda}{2\pi r} \int_0^{2\pi r}\int_0^{2\pi r} d\varphi \, d\varphi' \frac{1}{\sqrt{|x-x'|^2 + 4r^2 \sin^2\left(\frac{\varphi-\varphi'}{2r}\right)}}$$

$$\widetilde{H}_{N,L} = h_{x,N} + \frac{1}{2} \sum_{j \neq k} v_{r,L}(|x-x'|) \otimes \mathbb{1}_{\mathbb{C}^4}$$

$$v_{r,L}(t) := \frac{1}{\sqrt{2\pi}} \frac{\pi}{L} \sum_{m \in \mathbb{Z}^*} e^{i\frac{m\pi t}{L}} \hat{v}_r\left(\frac{m\pi}{L}\right), \quad \hat{v}_r(p) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} v_r(t) e^{-ipt} dt$$

The reduced operator in the second quantization

$\tilde{H}_N$ in $\tilde{\mathcal{H}}_N$; $\tilde{\mathcal{F}}_a = \bigoplus_{N\geq 0} \tilde{\mathcal{H}}_N$

$$\tilde{\mathbb{H}} = \sum_{s\geq 1} \tilde{\varepsilon}_{\nu^{-1}(s)} a_s^* a_s + \frac{1}{2} \sum_{\substack{p,q\\ r,s}} \langle \tilde{e}_{\nu^{-1}(p)} \otimes \tilde{e}_{\nu^{-1}(q)}, v_{2,L} \otimes 1_{\mathbb{C}^4}\, \tilde{e}_{\nu^{-1}(r)} \otimes \tilde{e}_{\nu^{-1}(s)} \rangle a_p^* a_q^* a_s a_r$$

$$\tilde{e}^{(x,\alpha)}_{(m,k_s,\xi_p)} = \frac{1}{\sqrt{2L}} u_m(x)\, e^{ik_s x} \xi_p(\alpha) \; , \quad \xi_p \in \Big\{ \underbrace{\begin{pmatrix}1\\0\end{pmatrix}}_{\uparrow}, \underbrace{\begin{pmatrix}0\\1\end{pmatrix}}_{\downarrow} \Big\}$$

Extracting a quadratic part of $\mathbb{H}$:

$$\mathcal{G}_{H\text{-}F} := \mathrm{Span}\Big\{ \Psi_0 \; , \; a^*_{(c,k_s,\uparrow/\downarrow)} a_{(v,k_s,\uparrow\downarrow)} \Psi_0 \; , \; a^*_{(c,k_s,\uparrow/\downarrow)} a_{(v,k_s,\downarrow/\uparrow)} \Psi_0 \Big\}$$

$k_s \in \{-\pi, \dots, \pi\}$

$k_s = \frac{\pi s}{L}$, $c = 3$, $v = 2$.

$H_{H\text{-}F} := \mathbb{P}_{\mathcal{G}} \tilde{\mathbb{H}} \mathbb{P}_{\mathcal{G}}$ is a matrix indexed by

$k_s = \frac{s\pi}{L}$ and $\sigma \in \{ (\uparrow\uparrow), (\uparrow\downarrow), (\downarrow\uparrow), (\downarrow\downarrow) \}$

$$
H_{H-F} = \begin{array}{cc}
 & \sigma=(\uparrow\uparrow), \quad \sigma=(\uparrow\downarrow), \quad \sigma=(\downarrow\uparrow), \quad \sigma=(\downarrow\downarrow) \\
\sigma=(\uparrow\uparrow) & \left[\begin{array}{c|c|c|c|c}
\langle \Psi_0, \tilde{H} \Psi_0 \rangle & & & & \\
\hline
G(\lambda) & (k_s, k_s') & & & \\
\hline
G(\lambda) & G(\lambda) & (k_s, k_s') & & \\
\hline
 & & & & \\
\hline
 & & & &
\end{array}\right]
\end{array}
$$

Up to errors of order λ^2 we can look at the diagonals!

$$(v/c, k_s) = \frac{1}{\sqrt{2L}}\, u_{v/c}(x)\, e^{ik_s x}$$

$$E_{c/v}(k_s) := \varepsilon_{c/v}(k_s) + \sum_k \Big\{ 2\big\langle (v,k)\otimes(c/v,k_s),\, v_{r,L}\, (v,k)\otimes(c/v,k_s)\big\rangle - \big\langle (v,k)\otimes(c/v,k_s),\, v_{r,L}\,(c/v,k_s)\otimes(v,k)\big\rangle \Big\}$$

$$\mathcal{H}_{symm}(k_s,k_s') = \delta_{k_s k_s'}\Big(\langle \psi_0, \tilde{H}\psi_0\rangle + E_c(k_s) - E_v(k_s)\Big) +$$

$$+ 2\big\langle (c,k_s)\otimes(v,k_s'),\, v_{r,L}\,(v,k_s)\otimes(c,k_s')\big\rangle -$$

$$- \big\langle (c,k_s)\otimes(v,k_s'),\, v_{r,L}\,(c,k_s')\otimes(v,k_s)\big\rangle$$

$$u_{v/c}(x,k_s) \simeq e^{i2n_{v/c}\pi x}, \quad |u_{v/c}(x,k_s)|^2 \sim 1$$

1) $E_{c/v}(k_s) \simeq \varepsilon_{c/v}(k_s) + C_1\,\hat{v}(0) + C_2\, v(0)$

2) The „direct term":

$$\big\langle (c,k_s)\otimes(v,k_s'),\, v_{r,L}\,(c,k_s')\otimes(v,k_s)\big\rangle \sim$$

$$\frac{1}{L^3}\sum_m \hat{v}_r\!\left(\frac{m\pi}{L}\right)\left(\int_{-L}^{L} |u_c(x)|^2\, e^{i(k_s'-k_s+\frac{m\pi}{L})x}\,dx\right)$$

$$\cdot\left(\int_{-L}^{L} |u_v(x')|^2\, e^{-i(k_s'-k_s+\frac{m\pi}{L})x'}\,dx'\right)$$

$$\sim \frac{1}{L}\,\hat{v}_r(k_s-k_s')$$

3) The „exchange term": $\displaystyle \frac{1}{L^3}\sum_m \hat{v}_r\!\left(\frac{\pi m}{L}\right)\left|\int_{-L}^{L} e^{i\frac{m\pi x}{L}}\, u_c(x)\,\overline{u_v(x)}\,dx\right|^2$

$$\sim \frac{1}{L}\,\hat{v}_r((n_v-n_c)\cdot 2\pi)$$

Eigenvalue problem for

$$\left(\tilde{E}_g + E_c(k_s) - E_v(k_s)\right) f(k_s) - \frac{\lambda}{L}\sum_{k_s'} \hat{v}_r(k_s - k_s') f(k_s') = \Lambda f(k_s)$$

in $k_s = \frac{s\pi}{L}$; $I_L = \left\{ k_s := \frac{s\pi}{L} \right\}_{s \in \{-L+\frac{1}{2}, \dots, 0, \dots, L+\frac{1}{2}\}}$; $2L \in \mathbb{N}^*$

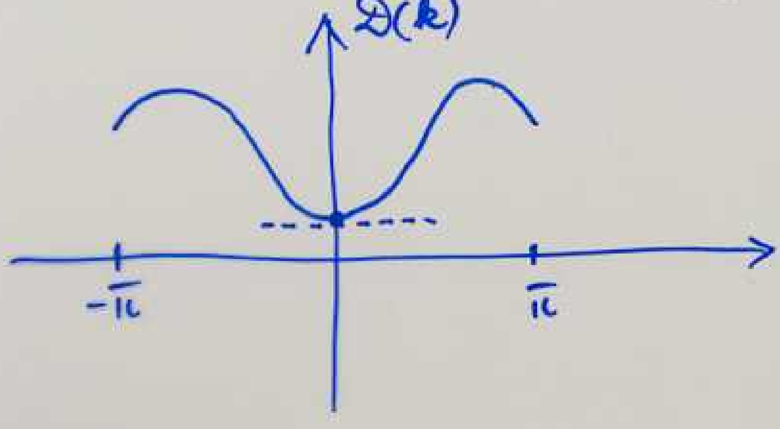
Assume $\hat{v} \in L^1([-3\pi, 3\pi]) \cap L^2([-3\pi, 3\pi])$

$$|\hat{v}(k)| \leq C_1 + |\ln|k||$$

$$|\hat{v}'(k)| \leq \frac{C_2}{|k|}$$

$$\begin{cases} H_\lambda : L^2([-\pi,\pi]) \to L^2([-\pi,\pi]) \\ (H_\lambda f)(k) = \mathcal{D}(k) f(k) - \lambda \displaystyle\int_{-\pi}^{\pi} \hat{v}(k-k') f(k')\, dk' \\ \mathcal{D}(k) = \mathcal{D}(k+2\pi) \quad , \quad \min \mathcal{D}(k) = \mathcal{D}(0) \quad , \quad \mathcal{D}''(0) > 0 . \end{cases}$$

$$\begin{cases} H_\lambda^{(d)} : \ell^2(I_L) \to \ell^2(I_L) \\ (H_\lambda^{(d)} f)(k_s) = \mathcal{D}(k_s) f(k_s) - \dfrac{\lambda\pi}{L} \displaystyle\sum_{s' \neq s} \hat{v}(k_s - k_s') f(k_s') \end{cases}$$



<u>Proposition 1</u> :

a) $\sigma_{ess}(H_\lambda) = \operatorname{Ran} \mathcal{D} = [\mathcal{D}(0), \max \mathcal{D}]$

b) $\sigma(H_\lambda) \cap (-\infty, \mathcal{D}(0)) \subseteq \sigma_{disc}(H_\lambda)$

c). Assume $E \in \sigma_{disc}(H_\lambda)$, $E < \mathcal{D}(0)$

$\mathrm{mult}(E) = M < \infty$. Fix $\varepsilon_0 > 0$ s.t

$B_{2\varepsilon_0}(E) \setminus \{E\} \subset \rho(H_\lambda)$.

Then $\exists\, L_0 > 0$ s.t $\forall L > L_0$, the interval $[E - \varepsilon_0, E + \varepsilon_0]$ contains exactly M eigenvalues of $H_\lambda^{(d)}$ (with multiplicities), $\{E_j(L)\}_{j=1}^{M}$, and $\exists\, \alpha > 0$ s.t

$$|E_j(L) - E| \leq C L^{-\alpha}.$$

d). Assume $M = 1$, $H_\lambda \phi = E\phi$, $H_\lambda^{(d)} \phi^{(d)} = E_1(L) \phi^{(d)}$.

Then $\sup_s |\phi^{(d)}(k_s) - \phi(k_s)| \leq C L^{-\alpha}$.

$\sqrt{2L}$

The low-lying spectrum of H_N

$\boxed{\lambda=0}$

E_0

$E_1 = \delta_3(0) - \delta_2(0) + E_0$

$\delta_3(\frac{\pi}{L}) - \delta_2(0) + E_0$

$\boxed{\lambda \ll 1}$

$\tilde{E}_0$

$\underbrace{* \quad * \quad *}$ $\underbrace{\qquad\qquad}_{\text{Ran } \mathcal{D}}$

discrete eigenvalues of H_λ

E_1: excited state for H_N

An approximation for its eigenvector is

$$\Psi_1 \sim \sum_{k_s} \Phi(k_s)\, a^*_{(c,k_s,\uparrow)}\, a_{(v,k_s,\uparrow)}\, \Psi_0$$

$$\mathcal{U}_\lambda : L^2(-\pi,\pi) \to L^2\left(-\frac{\pi}{\lambda}, \frac{\pi}{\lambda}\right) \; ; \; (\mathcal{U}_\lambda f)(k) = \sqrt{\lambda}\, f(\lambda k)$$

$$\mathcal{U}_\lambda H_\lambda \mathcal{U}_\lambda^* = \lambda^2 \left\{ \frac{\mathcal{D}(\lambda k)}{\lambda^2} - \hat{v}(\lambda \cdot) * \right\}$$

$$\approx \lambda^2 \left\{ -\frac{1}{2} \frac{d^2}{dx^2} - \frac{1}{\lambda} v\left(\frac{x}{\lambda}\right) \right\} \text{ on } L^2(\mathbb{R})$$

$$v(x) = \frac{1}{2\pi r} \int_0^{2\pi r} dy \, \frac{1}{\sqrt{x^2 + 4r^2 \sin^2\left(\frac{y}{2r}\right)}}$$

$$\left\| \frac{1}{\lambda} v\left(\frac{\cdot}{\lambda}\right) - \left\{ -2 \ln\frac{\lambda}{2}\, \delta + \text{f.p.}\, \frac{1}{|x|} \right\} \right\|_{\mathcal{B}(H^1; H^{-1})} = \mathcal{O}(\sqrt{\lambda})$$