An analysis of a quantum kinetic two-band model with inflow boundary conditions

Chiara Manzini, Omar Morandi

Dip. Matematica Applicata, Università Firenze,

chiara.manzini@unifi.it

Outlook

1- Multi-band model (MEF)

2- Quantum kinetic formulation

3- Well-posedness problem

4- Analytical difficulties

5- Final considerations

MEF model: derivation

[Morandi,Modugno05]: Ψ pure state of electron in a crystal lattice, subject to V external potential

$$\Psi(x,t) = \sum_n \int_{k\in\mathcal{B}} \varphi_n(k,t)\psi_n(k,x) \quad \text{with } \psi_n$$

$$(-\hbar^2/2\Delta + V_L)\psi_n(k,x) = E_n(k)\psi_n(k,x)$$

$$i\hbar\,\partial_t\varphi_n(k) = E_n(k)\varphi_n(k) + \int_{k'} \widehat{V}(k-k')\varphi_n(k')$$

$$+\frac{\hbar}{m}\sum_{n'\neq n}\int_{k'} \frac{P_{n,n'}(k,k')}{\Delta E_{n,n'}(k,k')}(k-k')\widehat{V}(k-k')\varphi_{n'}(k')$$

with $P_{n,n'}(k,k\prime)$ momentum matrix elements.

MEF model: derivation

[Morandi,Modugno05]: ($\mathcal{O}$(1)-in-k version)

$$i\hbar\,\partial_t\varphi_n(k) = E_n(k)\varphi_n(k) + \int_{k'} \widehat{V}(k-k')\varphi_n(k')$$

$$- i\frac{\hbar}{m}\sum_{n'\neq n}\frac{P_{n,n'}(0,0)}{E_n(0)-E_{n'}(0)}\int_{k'}\widehat{\nabla V}(k-k')\varphi_{n'}(k')$$

$$\chi_n(R_i) = \int_k \varphi_n(k)\exp\{ik\cdot R_i\},$$ R_i lattice sites,

$$\Psi(x) = \sum_n\sum_{R_i}\chi_n(R_i)\phi_n^W(x-R_i)$$

MEF model: derivation

[Morandi,Modugno05]: $\chi_n(x)$ can be considered cell-averaged wavefunction of the electron in the n-th band

$$\Rightarrow \quad n(x) \approx \sum_n |\chi_n(x)|^2$$

$$i\hbar\,\partial_t \chi_n(x) = E_n(-i\hbar\nabla)\chi_n(x) + V(x)\chi_n(x) - i\frac{\hbar}{m}\sum_{n'\neq n}\frac{P_{n,n'}(0,0)}{E_n(0)-E_{n'}(0)}\nabla V(x)\chi_{n'}(x)$$

Effective mass approx. : $E_n(k) = E_n + \dfrac{\hbar^2 k^2}{2m_n^*} + \mathcal{O}(k^3).$

Two-band model

ψ_c, ψ_v wavefunctions for electron in the c,v-bands

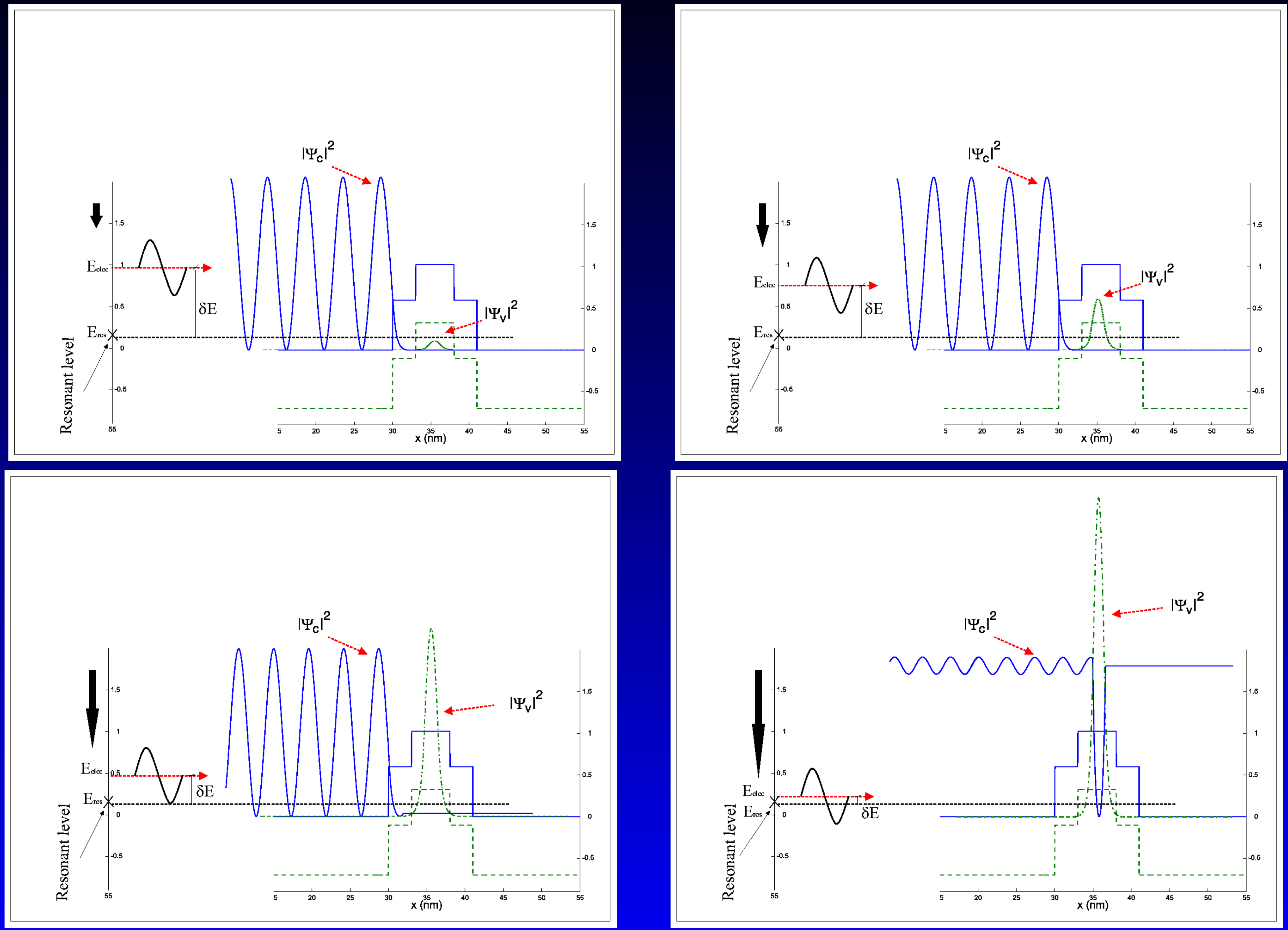
$$\Rightarrow \quad n(x) = |\psi_c|^2(x) + |\psi_v|^2(x)$$

$$i\hbar \frac{\partial \psi_c}{\partial t} = -\frac{\hbar^2}{2m_c^*}\Delta\psi_c + (E_c + V)\psi_c - i\nabla V \frac{\hbar P}{mE_g}\psi_v$$

$$i\hbar \frac{\partial \psi_v}{\partial t} = \frac{\hbar^2}{2|m_v^*|}\Delta\psi_v + (E_v + V)\psi_v - i\nabla V \frac{\hbar P}{mE_g}\psi_c$$

with $E_g = E_c - E_v$, E_c.

NEW: couplig reduces as E_g increases, no coupling when $V = 0$.


$|\Psi_c|^2$
$|\Psi_v|^2$
E_{elec}
E_{res}
δE
Resonant level
x (nm)

Quantum kinetic formulation

Density matices description:

$$\rho_{ij}(x,y) = \psi_i(x)\psi_j(y), \quad i,j \in \{c,v\}$$

Wigner matrices description:

$$w_{ij}(x,v) = \left(\mathcal{W}\,\rho_{ij}\right)(x,v), \quad i,j \in \{c,v\}.$$

The Wigner transform:

$$(\mathcal{W}\rho)(x,v) := \mathcal{F}_{\eta\to v}\rho\left(x+\frac{\eta}{2}, x-\frac{\eta}{2}\right)$$

$$\mathcal{W}\rho_{ij} \in L^2(\mathbb{R}^{2d};\mathbb{C}) \iff \rho_{ij} \in L^2(\mathbb{R}^{2d};\mathbb{C})$$

$$\rho_{ij}(x,y) = \overline{\rho_{ji}(y,x)} \implies w_{ij}(x,v) = \overline{w_{ji}(x,v)}.$$

Wigner-MEF system

$$\begin{aligned}
\left(\partial_t + v\cdot\nabla_x + i\Theta[V_{cc}]\right) w_{cc} &= \quad i\Theta[F_-]w_{cv} - i\Theta[F_+]w_{vc} \\
\Big(\partial_t - i\Delta_x + iv^2 + i\Theta[V_{cv}]\Big) w_{cv} &= \quad i\Theta[F_-]w_{cc} - i\Theta[F_+]w_{vv} \\
\Big(\partial_t + i\Delta_x - iv^2 + i\Theta[V_{vc}]\Big) w_{vc} &= -i\Theta[F_+]w_{cc} + i\Theta[F_-]w_{vv} \\
\left(\partial_t - v\cdot\nabla_x + i\Theta[V_{vv}]\right) w_{vv} &= -i\Theta[F_+]w_{cv} + i\Theta[F_-]w_{vc}
\end{aligned}$$

[Frosali, Morandi 05], where

$$\begin{aligned}
V_{ij}(x,\xi) &= (E_i+V)(x+\xi/2) - (E_j+V)(x-\xi/2) \\
F_\pm(x,\xi) &= (\nabla V\cdot P)\,(x\pm\xi/2) \\
(\Theta[\phi]f)\,(x,p) &= (2\pi)^{-d}\iint \mathrm{e}^{-i(v-v')\cdot\xi}\,\phi(x,\xi)\,f(x,v')\,d\xi\,dv'
\end{aligned}$$

Abstract formulation

$$\partial_t W + (A+B)W = FW \qquad \text{with}$$

$$\begin{aligned}
W &= (w_{cc}, w_{cv}, w_{vc}, w_{vv}) \\
A &= \operatorname{diag}\left(v\cdot\nabla_x, -i\Delta_x + iv^2, i\Delta_x - iv^2, -v\cdot\nabla_x\right) \\
B &= i\operatorname{diag}\left(\Theta[V_{cc}], \Theta[V_{cv}], \Theta[V_{vc}], \Theta[V_{vv}]\right) \\
F &= i\begin{pmatrix} & \Theta[F_-] & -\Theta[F_+] & \\ \Theta[F_-] & & & -\Theta[F_+] \\ -\Theta[F_+] & & & \Theta[F_-] \\ & -\Theta[F_+] & \Theta[F_-] & \end{pmatrix}
\end{aligned}$$

Difficulties and advantages

- $w_{cc}, w_{vv} \in L^2(\mathbb{R}^{2d}; \mathbb{R})$

$$\not\Longrightarrow \quad n(x) := \int (w_{cc} + w_{vv})(x, v)\, dv$$

is well-defined and non-negative ($\Rightarrow$ weighted space).

- conservation of the "L^2-norm":

Difficulties and advantages

- conservation of the "L^2-norm": set

$$\partial_t W + (A+B)W = FW$$

in $\left(L^2(\mathbb{R}^{2d}, dx\, dv; \mathbb{C})\right)^4$, with

$$<W, Z>_{(L^2)^4} := \sum_{i,j\in\{c,v\}} <W_{ij}, Z_{ij}>_{L^2} \; .$$

$$\partial_t \|W\|^2_{(L^2)^4} =$$

$$- <(A+B-F)W, W>_{(L^2)^4} - <W, (A+B-F)W>_{(L^2)^4}$$

where iA is self-adjoint and

$$\begin{aligned} <BW, W>_{(L^2)^4} &= - <W, BW>_{(L^2)^4} \\ <FW, W>_{(L^2)^4} &= - <W, FW>_{(L^2)^4} \end{aligned}$$

Existing results

- (single-band) Wigner-Poisson system, L^2-setting, $d = 1$ [Markowich, Ringhofer 91],...
- (single-band) WP system with inflow, time-dependent b.c. :

  $d = 1$, global-in-time well-p. [CM, Barletti 04]

  $d = 3$, local-in-time well-p. [CM 05]
- two-band Wigner-Kane system, $d = 1$ [Borgioli, Frosali, Zweifel 03]: global-in-time well-p.
- two-band Wigner-MEF system, $d = 1$ [Frosali, Morandi 05]: global-in-time well-p.

Wigner-MEF Poisson

$$
\begin{cases}
(\partial_t + A + B - F)W(x,v,t) = 0 \, (x,v,t) \in [0,1] \times \mathbb{R} \times \mathbb{R}^+ \\
-\partial_x^2 V(x,t) = n(x,t) = \int (w_{cc} + w_{vv})(x,v,t)\, dv
\end{cases}
$$

$$
\begin{cases}
w_{ii}(s,v,t) = \gamma_i(s,v,t), \; (s,v) \in \Phi_{\text{in}}, t \geq 0, \; i \in \{c,v\} \\
w_{ij} \equiv 0, \; (x,v) \in \{0,1\} \times \mathbb{R}, t \geq 0, \; i,j \in \{c,v\}, i \neq j \\
V(x,t) = 0, \; x \in \{0,1\}, t \geq 0, \\
W(x,v,0) = W_0(x,v)
\end{cases}
$$

$$\Phi_{\text{in}} := \{0\} \times \mathbb{R}^+ \bigcup \{1\} \times \mathbb{R}^-$$

Easy: non homogeneous Dirichlet/Neumann b.c.

Poisson coupling

- $(X_1)^4 := (L^2([0,1] \times \mathbb{R}; (1+v)\, dxdv; \mathbb{C}))^4$

cf. [Markowich,Ringhofer89]
(for $d \neq 1$[Barletti, CM 04])

$$\|n\|_{L^2} \leq C\|w_{cc} + w_{vv}\|_{X_1}$$

Poisson coupling

- $(X_1)^4 := (L^2([0,1]\times\mathbb{R};(1+v)\,dxdv;\mathbb{C}))^4$
cf. [Markowich,Ringhofer89]
(for $d \neq 1$[Barletti, CM 04])

$$\|n\|_{L^2} \leq C\|w_{cc}+w_{vv}\|_{X_1}$$

- V solution of Poisson pb. with $n[w] \in L^2([0,1])$:

$$V \in W_0^{1,2}([0,1]) \cap W^{2,2}([0,1]),\ \|V\|_{W^{2,2}} \leq C\|n[w]\|_{L^2}$$

- $\|\Theta[V]w_{ij}\|_{X_1} \leq C\|V\|_{W^{2,2}}\|w_{ij}\|_{X_1}$

Poisson coupling

- $(X_1)^4 := (L^2([0,1] \times \mathbb{R}; (1+v)\, dxdv; \mathbb{C}))^4$

cf. [Markowich,Ringhofer89]
(for $d \neq 1$[Barletti, CM 04])

$$\|n\|_{L^2} \leq C \|w_{cc} + w_{vv}\|_{X_1}$$

- V solution of Poisson pb. with $n[w] \in L^2([0,1])$

- $\|\Theta[V] w_{ij}\|_{X_1} \leq C \|w_{cc} + w_{vv}\|_{X_1} \|w_{ij}\|_{X_1}$
- $\|\Theta[F_\pm] w_{ij}\|_{X_1} \leq C \|w_{cc} + w_{vv}\|_{X_1} \|w_{ij}\|_{X_1}$

Inflow b.c. in $(X_1)^4$

$$\begin{cases} (\partial_t + A_{\gamma(t)} + B - F)W(x,v,t) = 0 \\ W(x,v,0) = W_0(x,v) \in (X_1)^4 \end{cases}$$

$$W(t) \in \mathcal{D}(A_{\gamma(t)}) := \{U \in \mathcal{D}(A) \mid w_{ii}|_{\Phi_{\text{in}}} = \gamma_i(t), i = c, v\}$$

$$\forall U_1, U_2 \in \mathcal{D}(A_{\gamma(t)}) \Rightarrow U_1 - U_2 \in \mathcal{D}(A_0)$$

Let $p_i : [0, +\infty) \to X_1, i = c, v$ such that

$$P(t) = (p_c, 0, 0, p_v) \in \mathcal{D}(A_{\gamma(t)}), \forall t \geq 0$$

$$\Rightarrow \mathcal{D}(A_{\gamma(t)}) = P(t) + \mathcal{D}(A_0)$$

(cf.[Barletti 00])

Inflow b.c. in $(X_1)^4$

$$\begin{cases} (\partial_t + A_{\gamma(t)} + B - F)W(x,v,t) = 0 \\ W(x,v,0) = W_0(x,v) \in (X_1)^4 \end{cases}$$

$$W(t) = P(t) + U(t), \text{ with } U : [0,+\infty) \longrightarrow \mathcal{D}(A_0)$$

$$\begin{cases} \{\partial_t - A_0 - L_P(t) - (B+F)[U](t)\}\, U(t) = Q_P(t) \\ U(x,v,0) = W_0(x,v) - P(x,v,0) \in \mathcal{D}(A_0) \end{cases}$$

with $L_P(t)$ bounded operator on $(X_1)^4$, $Q_P(t)$ source term: choose P such that $Q_P(t)$ is regular.

Local well-posedness

Theorem

$\forall\, \gamma_i, i = c, v$, s.t. $\exists$ suitable P, $\forall\, W_0 \in \mathcal{D}(A_{\gamma(0)})$, $\exists t_{\max} \leq \infty$ such that $\exists!$ classical solution $W(t), \forall\, t \in [0, t_{\max})$. If $t_{\max} < \infty$, then

$$\lim_{t \nearrow t_{\max}} \|W(t)\|_{(X_1)^4} = \infty.$$

$\Rightarrow$ A priori estimates *needed* for global-in-t result:

- $\|W(t)\|_{(L^2)^4} \leq \infty\ \forall\, t$
- $\|vW(t)\|_{(L^2)^4}$ necessitates different strategy.

TYPICAL problem with WP pb. in bounded domains ($d = 3$ [CM 05])