Iterative methods for sparse matrices

Alexander Weiße

Ernst Moritz Arndt Universität Greifswald

September 25, 2006

Outline

Introduction

Construction of basis & matrix
- Fixed particle number
- Translation symmetry
- Phonons

Eigenstates of sparse matrices
- Lanczos algorithm
- Jacobi-Davidson algorithm

Correlation functions & time evolution
- Kernel polynomial method
- Time evolution

Applications to the polaron problem
- Low energy spectrum
- Static & dynamic correlations
- Time evolution

Conclusions

Introduction

Typical lattice models in solid state physics

- Hubbard Holstein model

$$H = -t \sum_{\langle ij \rangle,\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - g\omega_0 \sum_{i,\sigma} (b_i^{\dagger} + b_i) n_{i\sigma} + \omega_0 \sum_i b_i^{\dagger} b_i \,,$$

- Heisenberg type spin models

$$H = \sum_{ij} J_{ij} \; \vec{S}_i \cdot \vec{S}_j$$

Typical questions

- Ground-state properties, phase transitions, ...
- Correlations, linear response, ...

Introduction

Problem: Analytical techniques fail in many interesting cases

- Perturbation theory $\hat{=}$ expansion in small parameters
- But: Many effects result from competition of comparable parameters

Way out: Numerical simulations

- Microscopic model $\Rightarrow$ large matrix H
- Dimension $D(H) \propto \exp(\text{system size } L)$

Difficulty:

- Properties of a model depend on spectrum & eigenfunctions of H
- Full diagonalisation is prohibitive — resource consumption $O(D^3)$!

Efficient numerical techniques

- Quantum Monte Carlo (QMC):

  Advantages: Large systems, finite temperatures, stat. & dynamic correlations

  Drawbacks: Minus sign problem, limited resolution

see talks by Assaad, Mishchenko, Evertz, Hohenadler

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- Iterative methods for sparse matrices (ED, KPM, ...)

  Advantages: Stat. & dyn. correlations, finite temperatures, high resolution, simple algorithms

  Drawbacks: small systems (for interacting quantum models)

From a model to a matrix

- To use sparse matrix algorithms, we need a matrix!
- Consider the Hubbard model on a ring of L sites:

$$H = -t \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+1,\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- The Hilbert space of a single site consists of four states:

$$|0\rangle, \quad c^\dagger_{i\downarrow}|0\rangle, \quad c^\dagger_{i\uparrow}|0\rangle, \quad c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}|0\rangle\,,$$

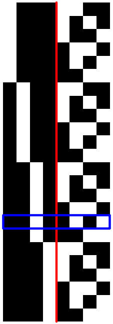
  thus for L sites we have 4^L states $\rightarrow$ Huge! Reduce with symmetries
- Typical symmetries: Particle number conservation, $SU(2)$ spin symmetry, translational invariance, other point groups
- How can we build a symmetric basis?

Fixed particle number

- The conservation of $N_e = N_\uparrow + N_\downarrow$ and $2S^z = N_\uparrow - N_\downarrow$ is equivalent to conservation of $N_\uparrow$ and $N_\downarrow$
- Choose normal order and translate into bit patterns:

$$c^\dagger_{3\uparrow} c^\dagger_{2\uparrow} c^\dagger_{0\uparrow} c^\dagger_{3\downarrow} c^\dagger_{1\downarrow} |0\rangle \to (\uparrow, \uparrow, 0, \uparrow) \times (\downarrow, 0, \downarrow, 0) \to 1101 \times 1010\,.$$

- Find all L-bit integers with a given number of set bits and assign index to each state
- Hilbert space dimension $\binom{L}{N_\uparrow}\binom{L}{N_\downarrow} \sim 4^L/L$

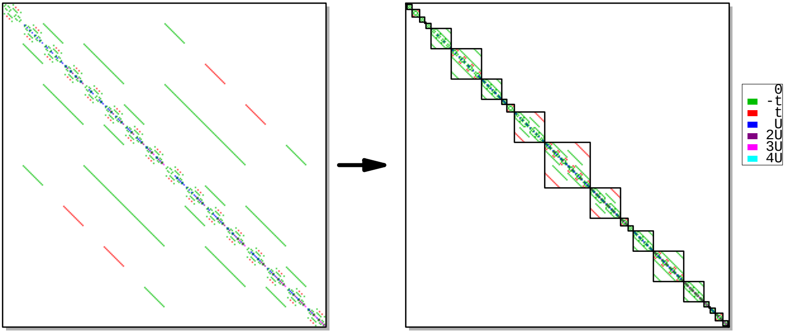


- Apply the Hamiltonian to all states, take care of minus signs,

$$\begin{aligned} \uparrow\text{-hopping}: &\quad 1101 \times 1010 \to -t\ (1011 + 1110) \times 1010 \\ \downarrow\text{-hopping}: &\quad 1101 \times 1010 \to -t\ 1101 \times (0110 + 1100 + 1001 - 0011) \\ U\text{-term}: &\quad 1101 \times 1010 \to U\ 1101 \times 1010 \end{aligned}$$

- Find the indices of the resulting states on the right

Block structure of the Hamiltonian



- Symmetrisation makes the Hamiltonian matrix block-diagonal
- We can treat each block separately

Translation symmetry
General concept

- For further $1/L$ reduction of block size use symmetry $T: \; c^{(\dagger)}_{i,\sigma} \to c^{(\dagger)}_{i+1,\sigma}$
- Eigenstates of T with eigenvalue $e^{-2\pi i k/L}$ are created by the projector

$$P_k = \frac{1}{L}\sum_{j=0}^{L-1} \exp\left(\frac{2\pi i}{L} jk\right) T^j \quad \text{where} \quad k = 0, 1, \ldots, (L-1)\,,$$

$$TP_k|n\rangle = \frac{1}{L}\sum_{j=0}^{L-1} \exp\left(\frac{2\pi i}{L} jk\right) T^{j+1}|n\rangle = e^{-2\pi i k/L} P_k|n\rangle\,.$$

- The old basis consists of R cycles formed by T, $|c_n\rangle = T^n|c_0\rangle$,

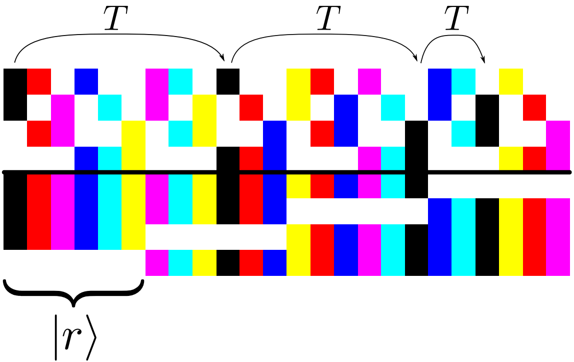
$$\longrightarrow 1101\times1010 \rightarrow 1110\times0101 \rightarrow 0111\times1010 \rightarrow 1011\times0101 \hookleftarrow$$

- Each cycle is represented by $|r\rangle \equiv |c_0\rangle$ and $P_k|c_n\rangle = e^{i\phi} P_k|r\rangle$
- The states $P_k|r\rangle$ with $k = 0, \ldots, (L-1)$ and $r = 0, \ldots, R$ form the new symmetrised basis. H does not mix states with different k, $[H, P_k] = 0$.
- The normalisation of $P_k|r\rangle$ requires some care!

Translation symmetry

Example

- For a system with $L = 4$ and $N_\uparrow = 3$, $N_\downarrow = 2$ we find



- There are $R = 6$ cycles represented by the 6 states $|r\rangle$
- From $P_k|r\rangle$ with $k = 0, \ldots, 3$ we obtain a total of $24 = \binom{4}{3}\binom{4}{2}$ states.
- Similar construction works for other lattice symmetries

Basis for phonon systems
Standard approach

- Problem: No particle number conservation – phonon space of a single site has infinite dimension → cut-off required
- Simple approach: Energy based cut-off

$$|m_0, \dots, m_{L-1}\rangle = \prod_{i=0}^{L-1} \frac{(b_i^\dagger)^{m_i}}{\sqrt{m_i!}} |0\rangle \quad \text{with} \quad \sum_{i=0}^{L-1} m_i \le M \,.$$

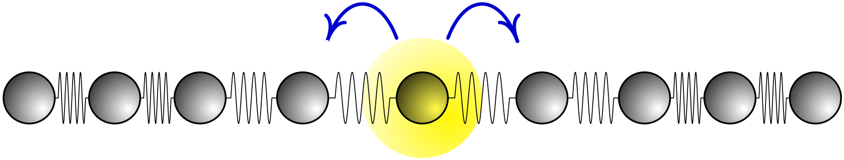
- Hilbert space dimension $\binom{L+M}{M}$ can be reduced using translation symmetry,

$$T|m_0, \dots, m_{L-1}\rangle = |m_{L-1}, m_0, \dots, m_{L-2}\rangle \,.$$

- Improvements:
  - Eliminate the phonon mode with momentum $q = 0$
  - Density matrix based optimisation of the basis (see talk of H. Fehske)

Basis for phonon systems

The polaron problem



- Basic model: Holstein model with a single electron:

$$H = -t \sum_i (c_i^\dagger c_{i+1} + \text{H.c.}) - g\omega_0 \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i \,.$$

- Bonča, Trugman et al. suggested a clever variational basis:
  - Work in reference frame of the electron
  - Starting from $|0\rangle$ add all states created by $\leq M$ applications of H
  - Equivalent to a mapping onto multi-band model
- Phonon occupation $m_i = 0$ for sites more than M steps away from e^-
- Allows solution of the problem on infinite lattice (momentum space)

Lanczos algorithm

General facts

- Developed by Cornelius Lanczos in the 1950s
- Fast convergence of extremal (smallest or largest) eigenstates
- Simple iterative algorithm (only sparse MVM), low memory requirements
- Belongs to the class of Krylov space methods

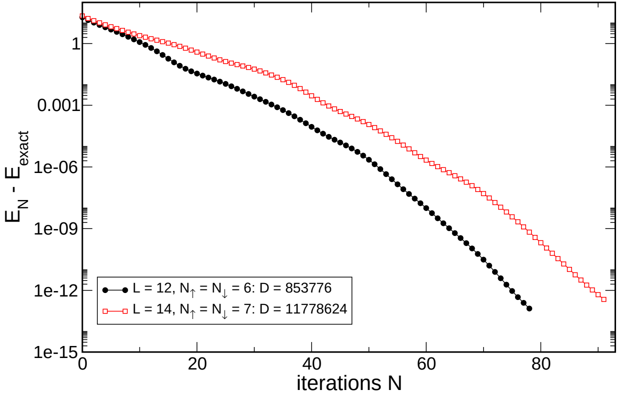
Algorithm

- Starting from random $|\phi_0\rangle$ build a tridiagonal matrix with:

$$
\begin{aligned}
|\phi'\rangle &= H|\phi_n\rangle - \beta_n|\phi_{n-1}\rangle\,, \\
\alpha_n &= \langle\phi_n|\phi'\rangle\,, \\
|\phi''\rangle &= |\phi'\rangle - \alpha_n|\phi_n\rangle\,, \\
\beta_{n+1} &= ||\phi''|| = \sqrt{\langle\phi''|\phi''\rangle}\,, \\
|\phi_{n+1}\rangle &= |\phi''\rangle/\beta_{n+1}\,,
\end{aligned}
\qquad
\tilde{H}_N = \begin{bmatrix}
\alpha_0 & \beta_1 & 0 & \ldots\ldots\ldots\ldots & & 0 \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \ldots\ldots & 0 \\
0 & \beta_2 & \alpha_2 & \beta_3 & 0 & 0 \\
 & & \ddots & \ddots & \ddots & \\
0 & \ldots & 0 & \beta_{N-2} & \alpha_{N-2} & \beta_{N-1} \\
0 & \ldots\ldots & & 0 & \beta_{N-1} & \alpha_{N-1}
\end{bmatrix}.
$$

Lanczos algorithm

- For increasing N the eigenstates of $\tilde{H}_N$ converge to the eigenstates of H:

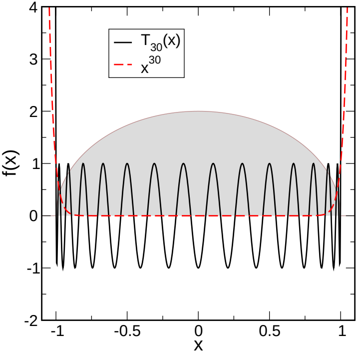


- Example: Ground state of the 1D Hubbard model with $L = 12$ and 14, compared with exact Bethe ansatz result. Note: $N \ll D$.

Jacobi-Davidson algorithm

- Generalisation of Lanczos suggested by Sleijpen and van der Vorst
- Combines Davidson's method and a procedure by Jacobi
- More reliable and faster for excited states,
  but higher memory consumption compared to Lanczos
- Algorithm:
  1. Initialise the set V with a random normalised start vector, $V_1 = \{|v_0\rangle\}$.
  2. Compute all unknown matrix elements $\langle v_i|H|v_j\rangle$ of $\tilde{H}_N$ with $|v_i\rangle \in V_N$.
  3. Compute an eigenstate $|s\rangle$ of $\tilde{H}_N$ with eigenvalue θ, and express $|s\rangle$ in the original basis, $|u\rangle = \sum_i |v_i\rangle\langle v_i|s\rangle$.
  4. Compute the associated residual vector $|r\rangle = (H - \theta)|u\rangle$ and stop the iteration, if its norm is sufficiently small.
  5. Otherwise, approximately solve the equation (e.g. with QMR)
  $$(1 - |u\rangle\langle u|)(H - \theta)(1 - |u\rangle\langle u|)|t\rangle = -|r\rangle\,.$$
  6. Orthogonalise $|t\rangle$ against V_N with the modified Gram-Schmidt method and append the resulting vector $|v_N\rangle$ to V_N, obtaining the set V_{N+1}.
  7. Return to step 2.

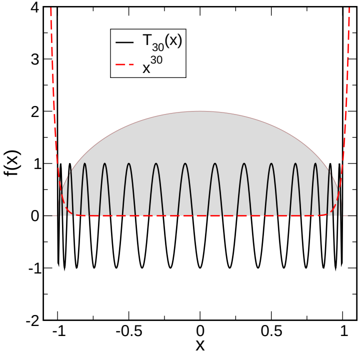
Polynomial expansions
Mathematical background



- Elementary task: Spectral density of a Hermitian matrix H:

$$\rho(E) = \sum_{k=0}^{D-1} \delta(E - E_k)$$

Polynomial expansions
Mathematical background



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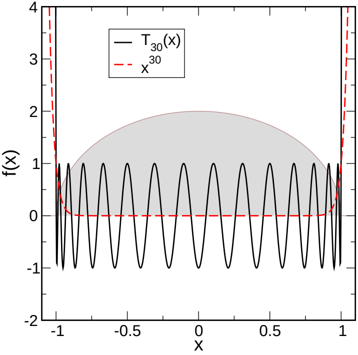
- Ill-conditioned: Reconstruction of $\rho(E)$ from standard *power moments*,

$$\mu_n = \int \rho(E)\, E^n\, dE = \mathrm{Tr}[H^n]$$

$\rightarrow$ most weight at boundaries, redundancy



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- Better: *Modified moments* from orthogonal polynomials $p_n(E)$,

$$\mu_n = \int \rho(E)\, p_n(E)\, dE = \mathrm{Tr}[p_n(H)]$$

$\rightarrow$ homogeneous weighting, stable reconstruction

Polynomial expansions
Chebyshev polynomials

- Prefered choice: Chebyshev polynomials of 1st kind

$$T_n(x) = \cos(n \arccos(x)) \quad \text{or} \quad T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

- With Re-scaling $H \to \tilde{H} = (H - b)/a$, $[E_{\min}, E_{\max}] \to [-1, 1]$ follows

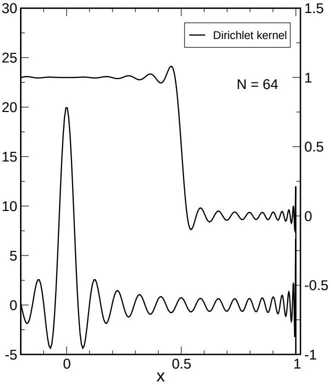
$$\mu_n = \int_{-1}^{1} \rho(\tilde{E})\, T_n(\tilde{E})\, d\tilde{E} = \mathrm{Tr}[T_n(\tilde{H})] \approx \sum_{r=0}^{R-1} \langle r | T_n(\tilde{H}) | r \rangle \Big/ R\,,$$

  where $|r\rangle$ denote normalised random vectors and $R \ll D$

- Stable recursion relations yield

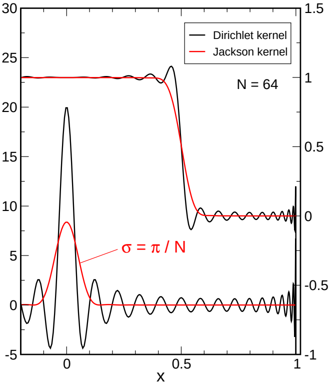
$$T_n(\tilde{H})|r\rangle = |r_n\rangle = 2\tilde{H}|r_{n-1}\rangle - |r_{n-2}\rangle$$

- We only need sparse MVM $\to$ linear in dimension D



- Partial sum needs regularisation

$$\rho(\tilde{E}) = \frac{1}{\pi\sqrt{1-\tilde{E}^2}}\left[\quad \mu_0 + 2\sum_{n=1}^{N-1} \quad \mu_n T_n(\tilde{E})\right]$$

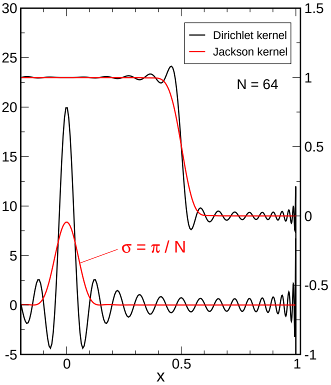


- Partial sum needs regularisation

$$\rho(\tilde{E}) = \frac{1}{\pi\sqrt{1-\tilde{E}^2}}\left[g_0\mu_0 + 2\sum_{n=1}^{N-1} g_n\mu_n T_n(\tilde{E})\right]$$

- Approximation theory $\rightarrow$ Jackson kernel:

$$g_n = \frac{1}{N+1}\left[(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}\right]$$



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- With $\tilde{E}_i = \cos[\pi(i+1/2)/\tilde{N}]$ we can use fast discrete Fourier transform:

$$\rho(\tilde{E}_i) = \frac{1}{\pi\sqrt{1-\tilde{E}_i^2}}\left\{g_0\mu_0 + 2\sum_{n=1}^{N-1} g_n\mu_n \cos[\pi n(i+1/2)/\tilde{N}]\right\}$$

- Dynamical correlations at $T = 0$: similar structure like $\rho(E)$

$$\chi(\omega) = \sum_k |\langle k|A|0\rangle|^2 \; \delta(\omega - E_k)$$

- Standard methods (Lanczos, Jacobi-Davidson) yield ground state $|0\rangle$
- Chebyshev moments follow from:

$$\begin{aligned} \mu_n &= \int_{-1}^{1} \chi(\tilde{\omega})\, T_n(\tilde{\omega})\, d\tilde{\omega} \\ &= \langle 0|A T_n(\tilde{H}) A|0\rangle \end{aligned}$$

- Advantage: Comparable effort for calculation of $\chi(\omega)$ and $|0\rangle$

Polynomial expansions

Dynamical correlations at $T > 0$ ($n > 0$)

- Double summation & thermal weights spoil simple expansion

$$\mathrm{Re}[\sigma(\omega)] = \frac{1}{\omega Z} \sum_{k,q} |\langle k|J|q\rangle|^2 \; [\mathrm{e}^{-\beta E_k} - \mathrm{e}^{-\beta E_q}] \, \delta(\omega - (E_q - E_k))$$
$$= \frac{1}{\omega Z} \int j(x, x+\omega) \, [\mathrm{e}^{-\beta x} - \mathrm{e}^{-\beta(x+\omega)}] \, dx$$

- Solution: 2D expansion of a matrix element density

$$j(x,y) = \sum_{k,q} |\langle k|J|q\rangle|^2 \, \delta(x - E_k) \, \delta(y - E_q)$$

$$\mu_{nm} = \int_{-1}^{1} \int_{-1}^{1} \tilde{j}(x,y) \, T_n(x) \, T_m(y) \, dx \, dy = \sum_{k,q} |\langle k|J|q\rangle|^2 \; T_n(\tilde{E}_k) \; T_m(\tilde{E}_q)$$
$$= \mathrm{Tr}\left(T_n(\tilde{H}) J T_m(\tilde{H}) J\right) \approx \frac{1}{R} \sum_{r=0}^{R-1} \langle r| \, T_n(\tilde{H}) J T_m(\tilde{H}) J |r\rangle$$

- Advantage: A single expansion yields $\mathrm{Re}[\sigma(\omega)]$ at all temperatures

- Chebyshev expansion can also be used to study quantum time evolution,

$$\mathrm{i}\,\partial_t|\psi\rangle = H|\psi\rangle\,,$$

- Simply expand the time evolution operator $U(t)$ in $T_k(\tilde{H})$:

$$|\psi_t\rangle = \exp(-\mathrm{i}\,Ht)|\psi_0\rangle =: U(t)|\psi_0\rangle\,,$$

$$U(t) = \exp(-\mathrm{i}(a\tilde{H}+b)t) = \mathrm{e}^{-\mathrm{i}\,bt}\left[c_0 + 2\sum_{k=0}^{N} c_k T_k(\tilde{H})\right]\,,$$

$$c_k = \int_{-1}^{1} \frac{T_k(x)\,\mathrm{e}^{-\mathrm{i}\,axt}}{\pi\sqrt{1-x^2}}\,dx = (-\mathrm{i})^k J_k(at)\,.$$

- For $k \to \infty$ the Bessel function $J_k(z)$ decays superexponentially,

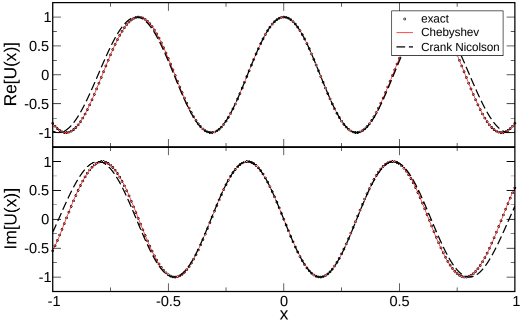
$$J_k(z) \sim \frac{1}{k!}\left(\frac{z}{2}\right)^k \sim \frac{1}{\sqrt{2\pi k}}\left(\frac{\mathrm{e}\,z}{2k}\right)^k\,,$$

hence we can truncate the series at $N \gtrsim 1.5at$.

- Chebyshev expansion method converges much faster than other methods, e.g., Crank-Nicolson

$$(1 + \tfrac{1}{2}\,\mathrm{i}\,H\Delta t)|\psi_{n+1}\rangle = (1 - \tfrac{1}{2}\,\mathrm{i}\,H\Delta t)|\psi_n\rangle \quad \text{with} \quad \Delta t = t/N\,,$$

$$U(t) = \left(\frac{1 - \mathrm{i}\,Ht/(2N)}{1 + \mathrm{i}\,Ht/(2N)}\right)^N .$$



- For illustration, substitute $H \to x$ and compare the approximation of $\exp(\mathrm{i}\,xt)$, where $t = 10$ and $N = 15$.

- We illustrate all techniques for the Holstein model with a single electron:

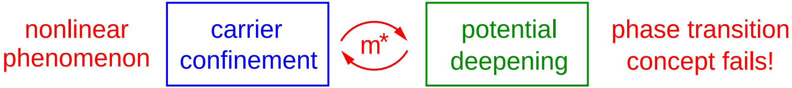
$$H = -t\sum_i (c_i^\dagger c_{i+1} + \text{H.c.}) - g\omega_0 \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i \,.$$

- Physics is governed by two dimension-less parameters:
  - phonon frequency *vs* electron transfer amplitude: $\boxed{\alpha = \omega_0/t}$
    $\rightsquigarrow$ retardation effects
    $\rightsquigarrow$ adiabatic regime ($\alpha \ll 1$) $\Leftrightarrow$ anti-adiabatic regime ($\alpha \gg 1$)
  - interaction strength: $\boxed{\lambda = \varepsilon_p/(2Dt)}$ or $\boxed{g^2 = \varepsilon_p/\omega_0}$
    $\rightsquigarrow$ weak- ($\lambda \ll 1$) $\Leftrightarrow$ strong-coupling ($\lambda \gg 1$) regime
    $\rightsquigarrow$ few- ($g^2 < 1$) $\Leftrightarrow$ multi-phonon ($g^2 \gg 1$) regime

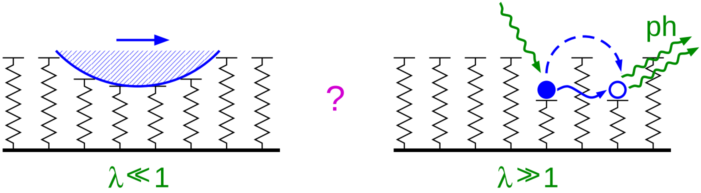
Application to the polaron problem
General aspects II

Questions:

- Polaron formation: Nature of “self-trapping” transition?

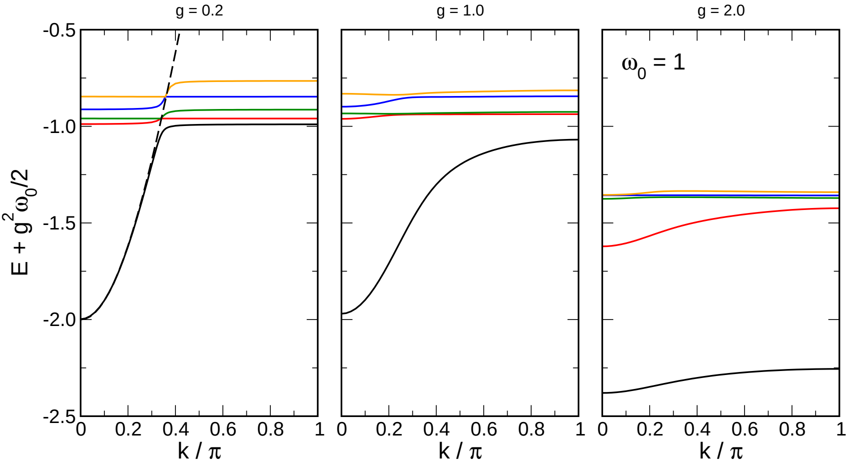


- Crossover regime: Polaron transport?



- Influence of dimensionality? . . .

- The Lanczos algorithm yields the low energy spectrum:



- We use the variational basis for the infinite system with cut-off $M = 16$

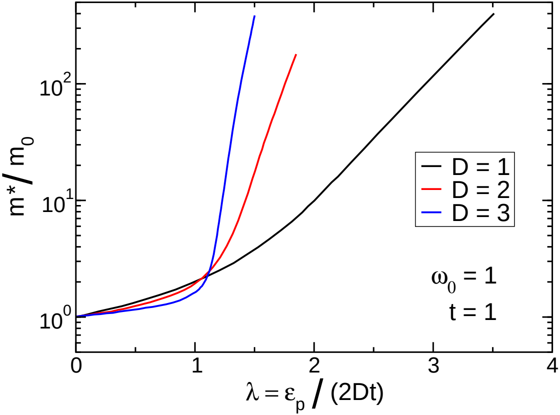
Application to the polaron problem

Effective mass

- From the dispersion we obtain the mass renormalisation:

$$\boxed{1/m^* = \partial^2 E(k)/\partial k^2\Big|_{k\to 0}}$$

- polaron crossover at about $\lambda \sim 1$ ($g^2 \sim 1$) is much sharper in higher D !

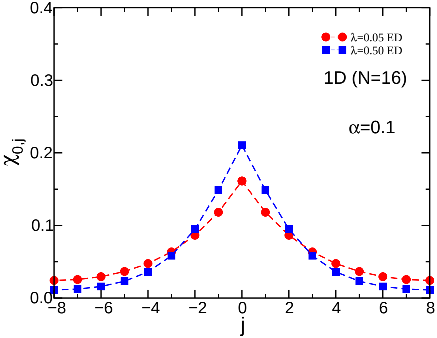


Application to the polaron problem
Static electron-lattice correlations

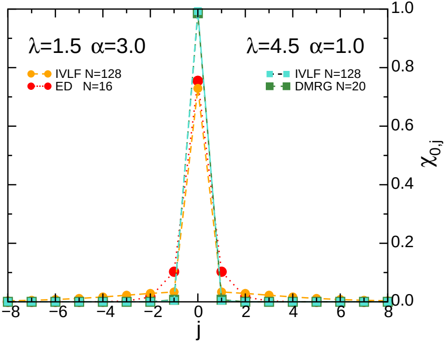
- Knowing the ground state, we can calculate static correlations, e.g.,

  the spatial extend of the polaron:
  $$\chi_{0,j} = \frac{\langle n_0 (b_j^\dagger + b_j) \rangle}{2g \langle n_0 \rangle}$$

weak coupling - adiabatic



strong coupling - non-adiabatic

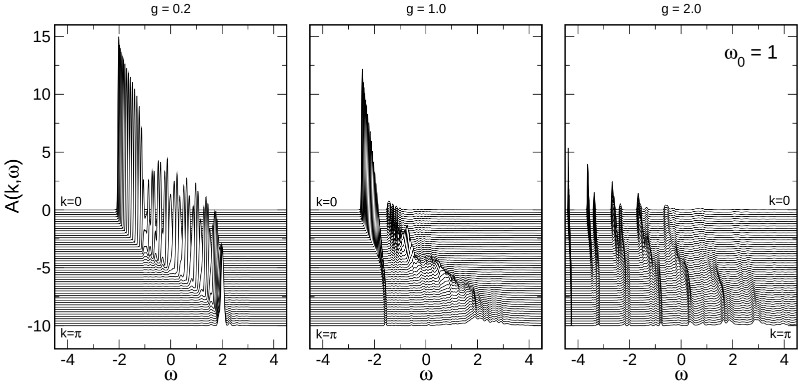


- Crossover from large to small size polarons (1D)

Application to the polaron problem
Dynamic correlations at $T = 0$

- Inverse photoemission spectra (ARPES) described by spectral function

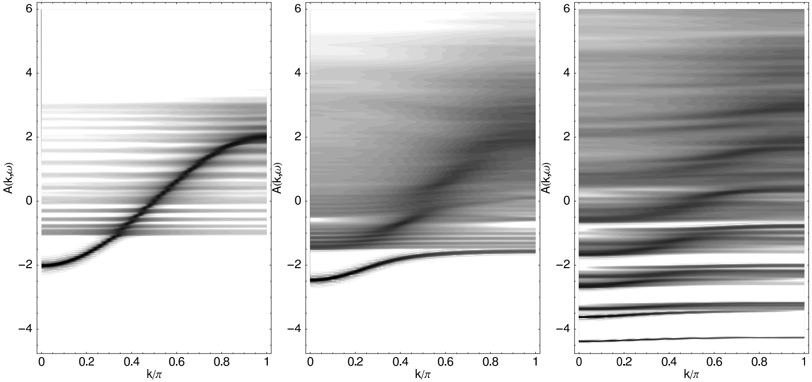
$$A(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\langle 0|c_k \frac{1}{\omega - H} c_k^\dagger|0\rangle$$



- The expansion order of KPM is $N = 1024$

- Inverse photoemission spectra (ARPES) described by spectral function

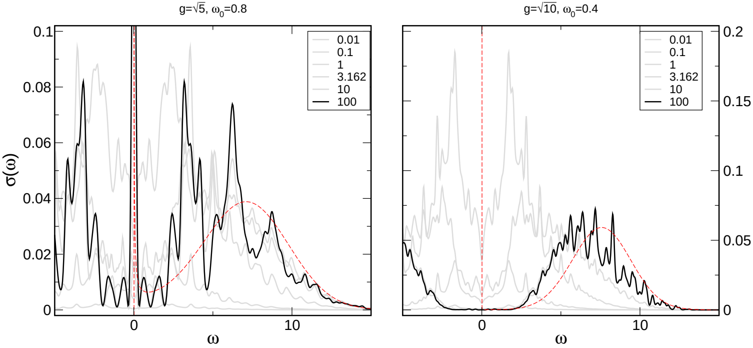
$$A(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\langle 0|c_k \frac{1}{\omega - H} c_k^\dagger|0\rangle$$



- The expansion order of KPM is $N = 1024$

- Temperature dependence of the optical conductivity

$$\mathrm{Re}[\sigma(\omega)] = \frac{1}{\omega Z}\sum_{k,q} |\langle k|J|q\rangle|^2\ [\mathrm{e}^{-\beta E_k} - \mathrm{e}^{-\beta E_q}]\,\delta(\omega - (E_q - E_k))$$



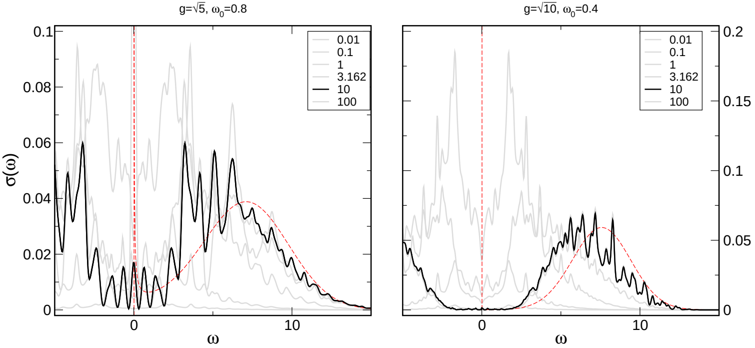
- Low T → deviations from analytic $\mathrm{Re}\,\sigma(\omega) = \frac{\sigma_0\,\mathrm{e}^{-(\omega-2\varepsilon_p)^2/(4\varepsilon_p\omega_0)}}{\omega\sqrt{\varepsilon_p\omega_0}}$
- High T → weight transfer to $\omega \sim 2t$

Application to the polaron problem

Dynamic correlations at $T > 0$

- Temperature dependence of the optical conductivity

$$\mathrm{Re}[\sigma(\omega)] = \frac{1}{\omega Z} \sum_{k,q} |\langle k|J|q\rangle|^2 \, [\mathrm{e}^{-\beta E_k} - \mathrm{e}^{-\beta E_q}] \, \delta(\omega - (E_q - E_k))$$



- Low $T \to$ deviations from analytic $\mathrm{Re}\,\sigma(\omega) = \frac{\sigma_0\, \mathrm{e}^{-(\omega-2\varepsilon_p)^2/(4\varepsilon_p\omega_0)}}{\omega\sqrt{\varepsilon_p\omega_0}}$
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Application to the polaron problem
Dynamic correlations at $T > 0$

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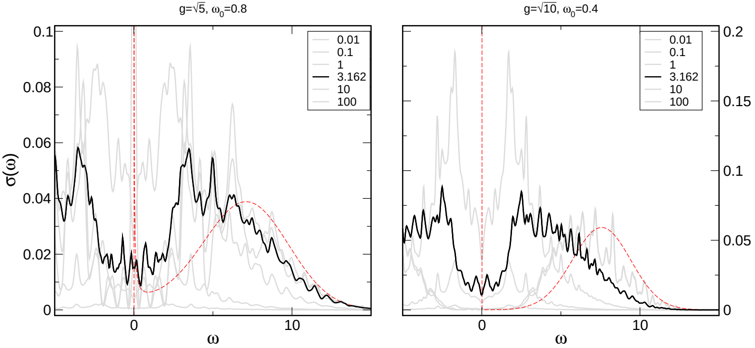

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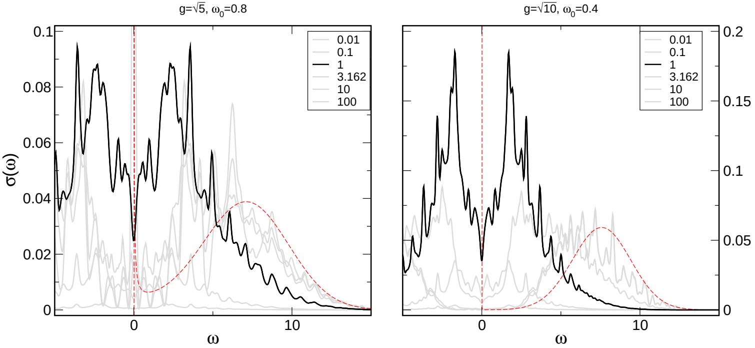

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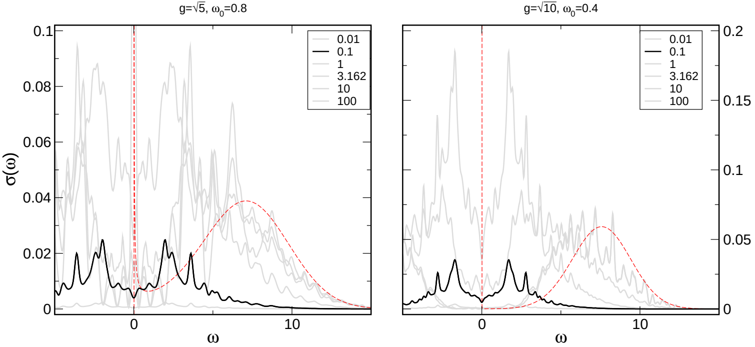

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Dynamic correlations at $T > 0$

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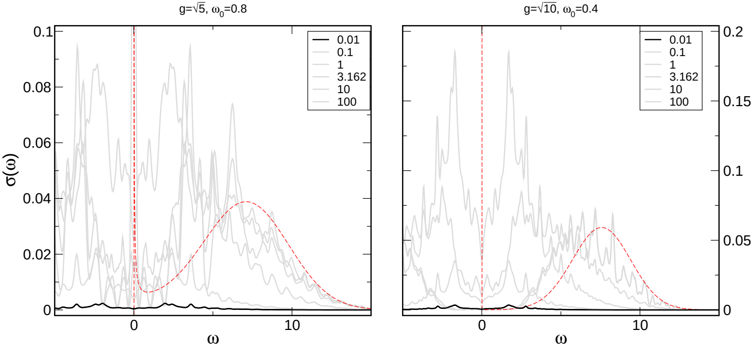

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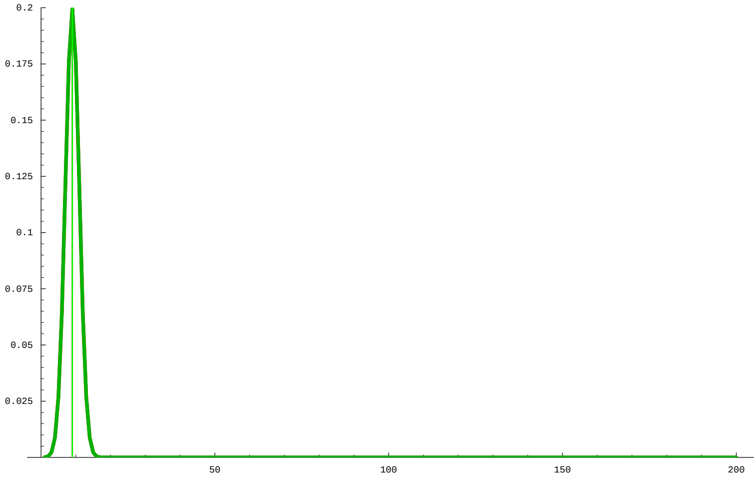
- Formation of a polaron, given a single-electron wave packet:



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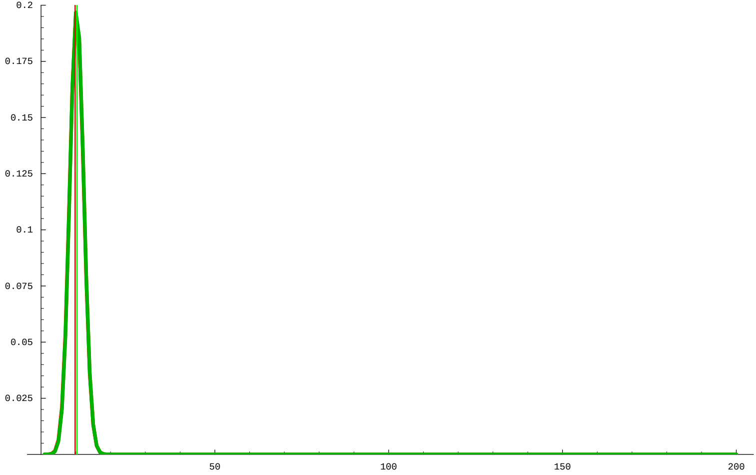

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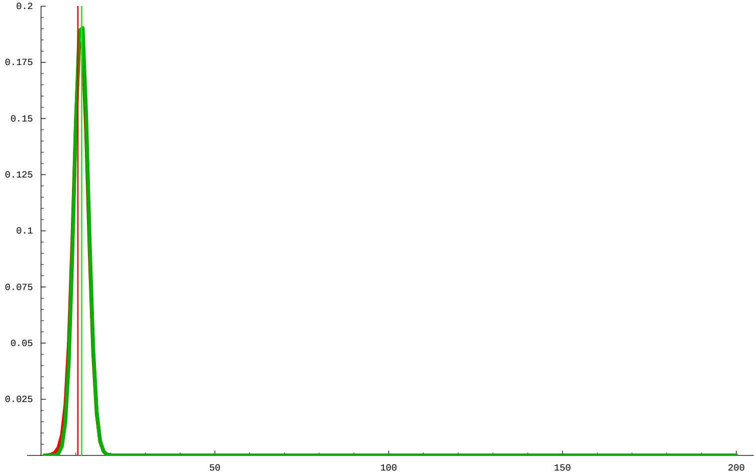

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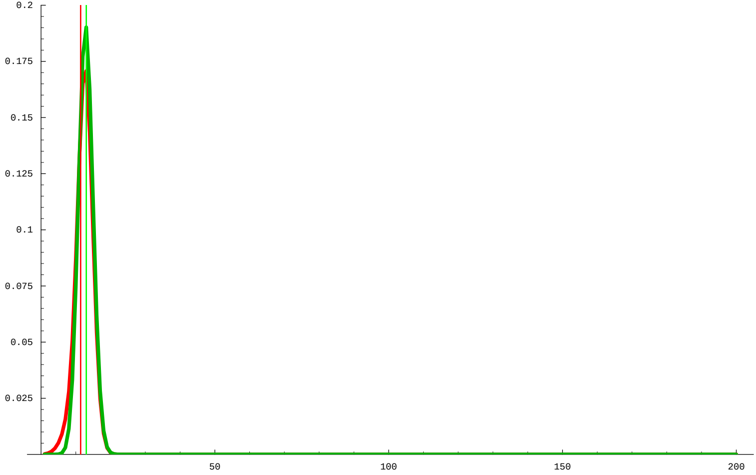

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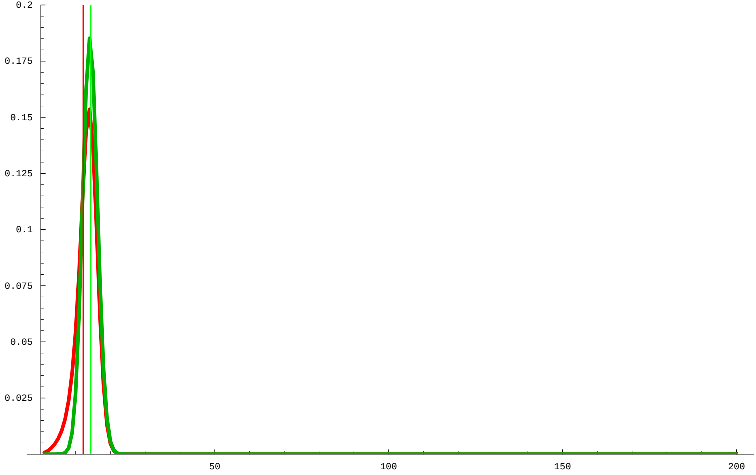

Application to the polaron problem
Time evolution

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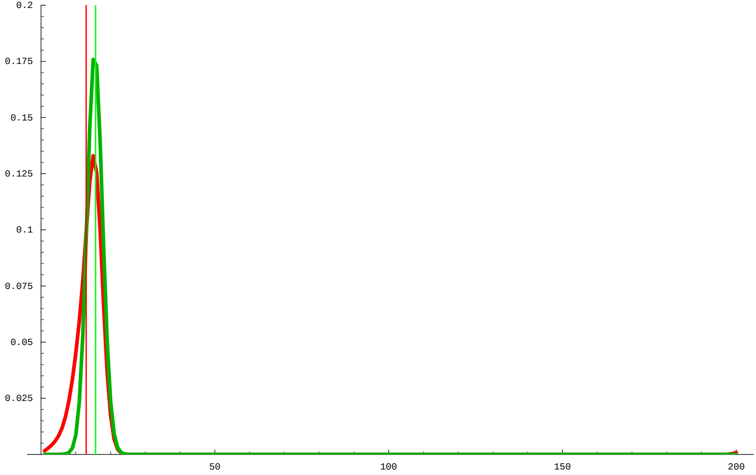

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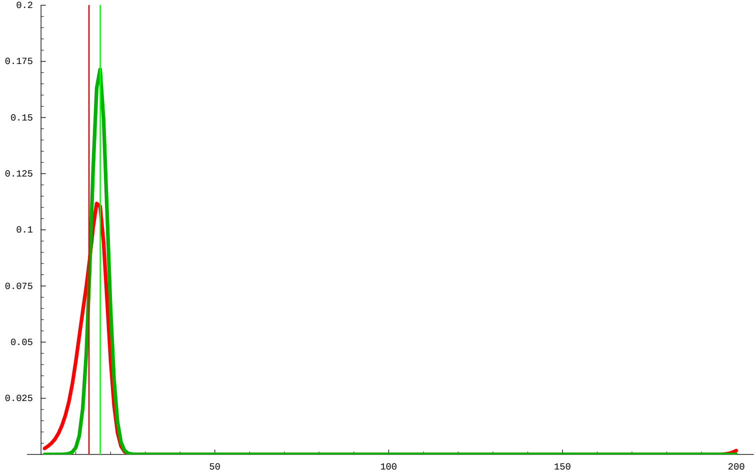

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Time evolution

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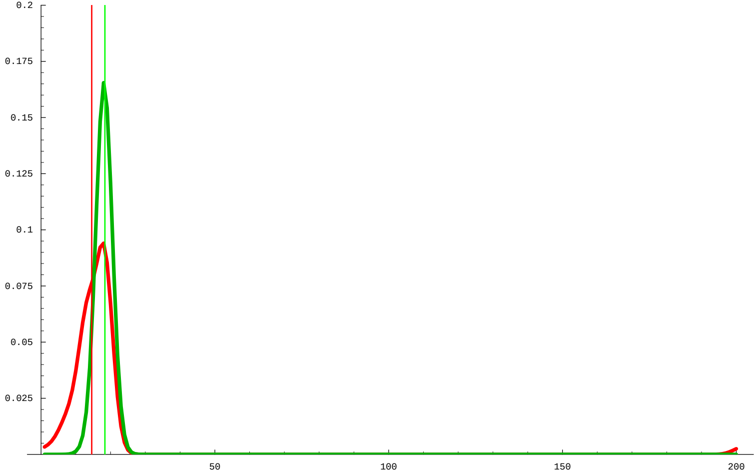

Application to the polaron problem
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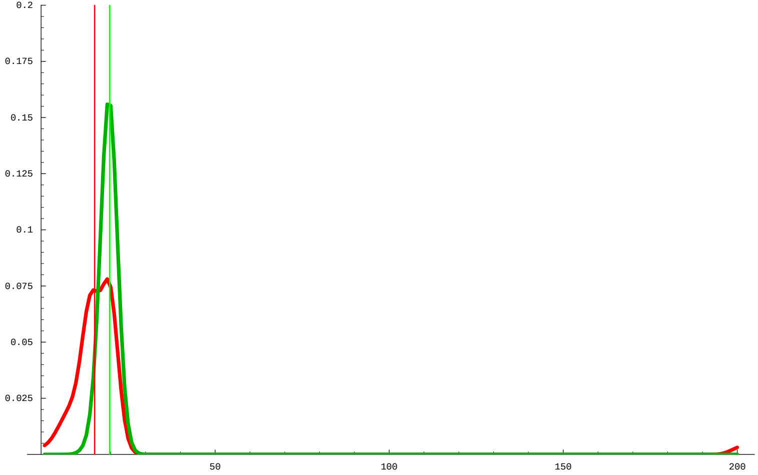

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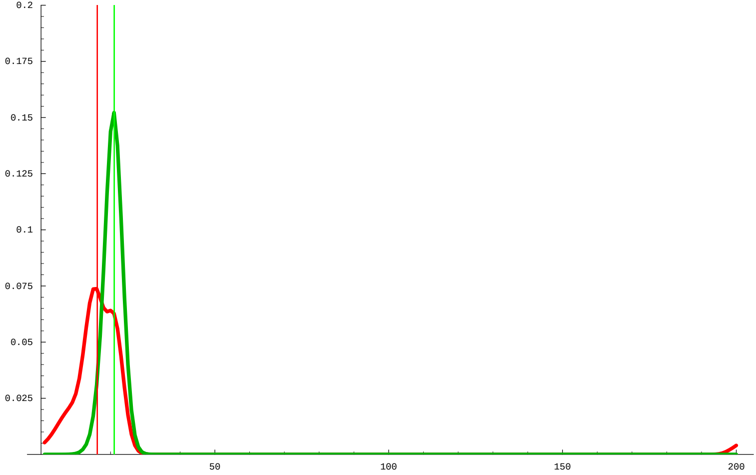

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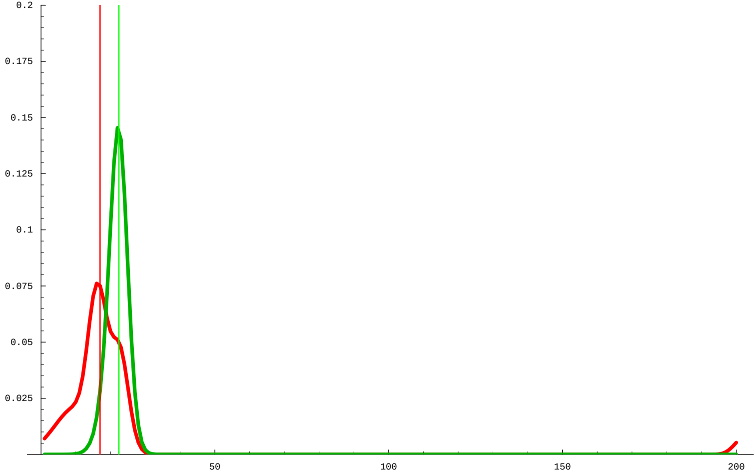

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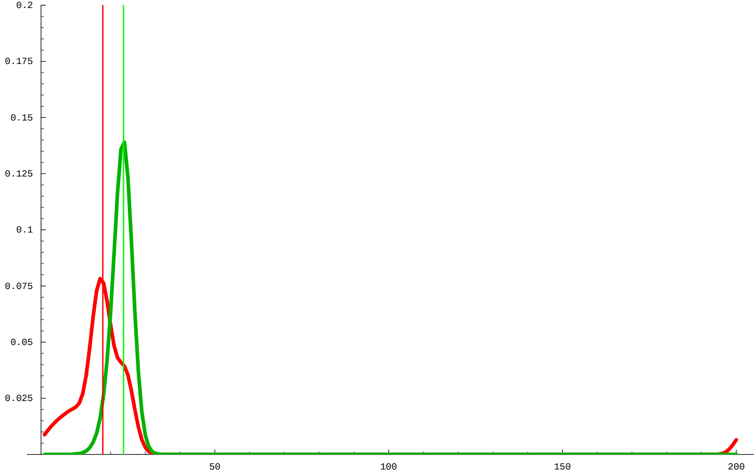

Application to the polaron problem
Time evolution

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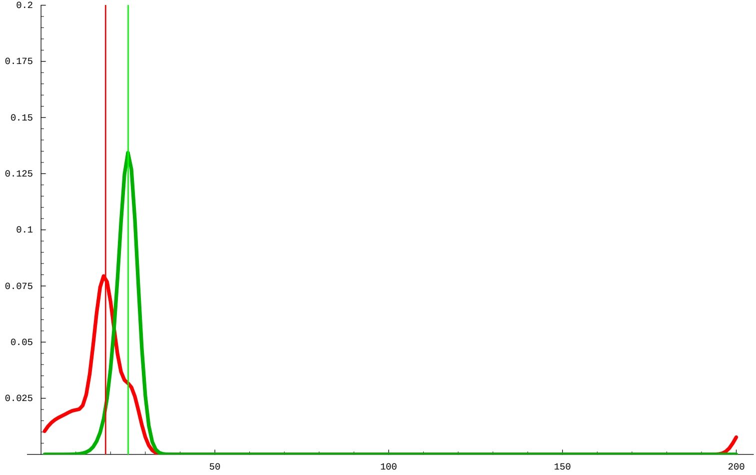

Application to the polaron problem
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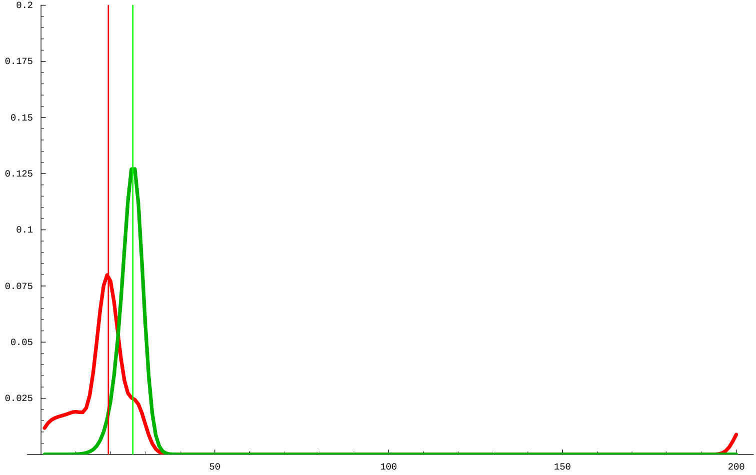

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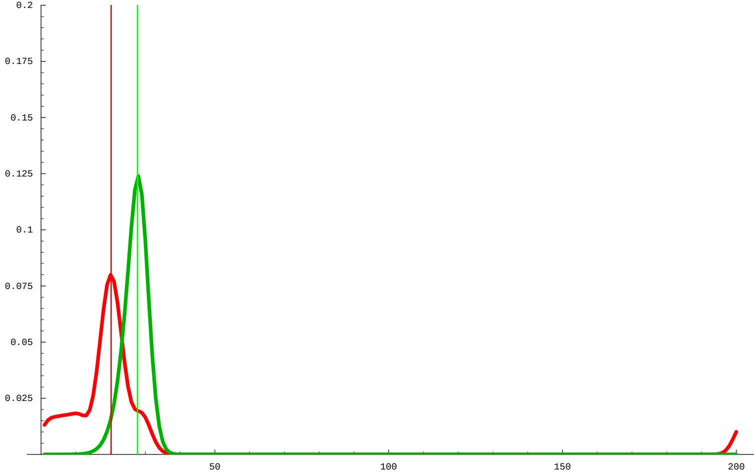

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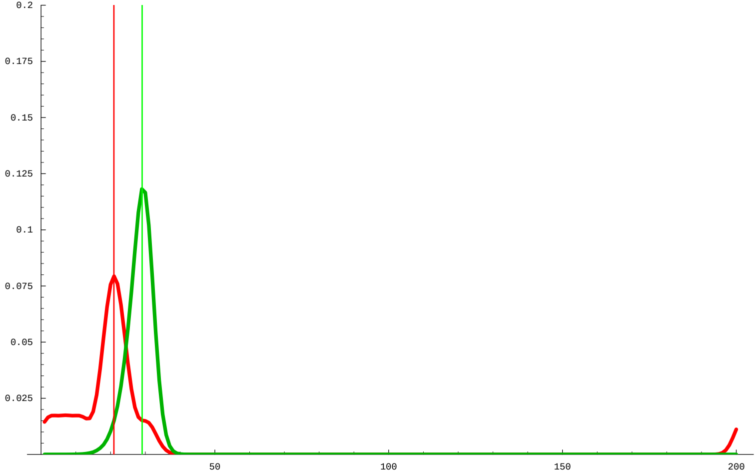

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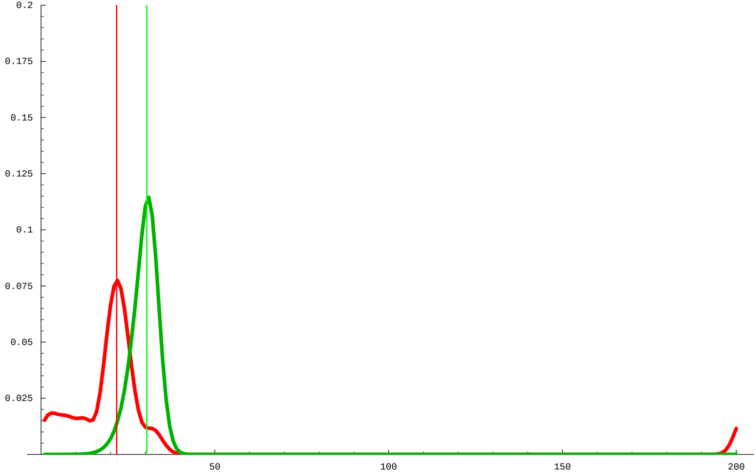

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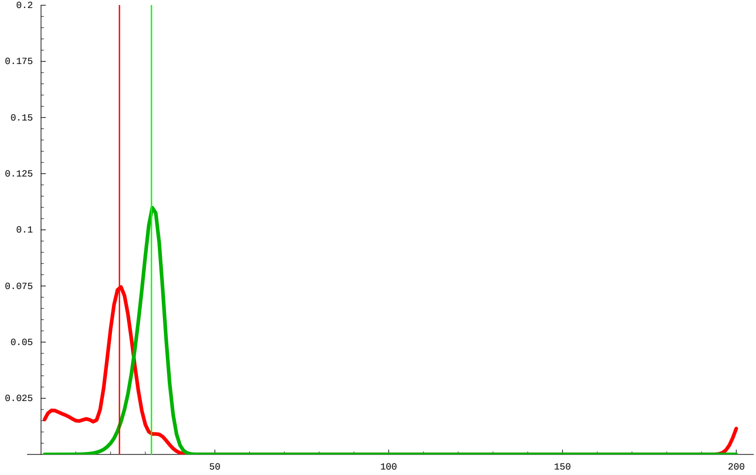

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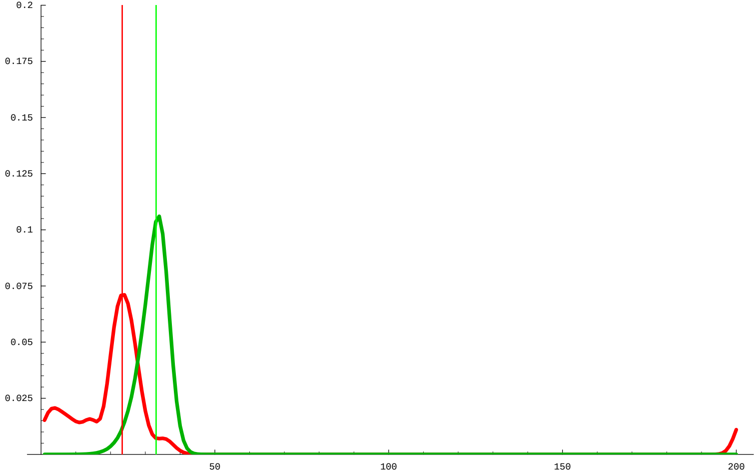

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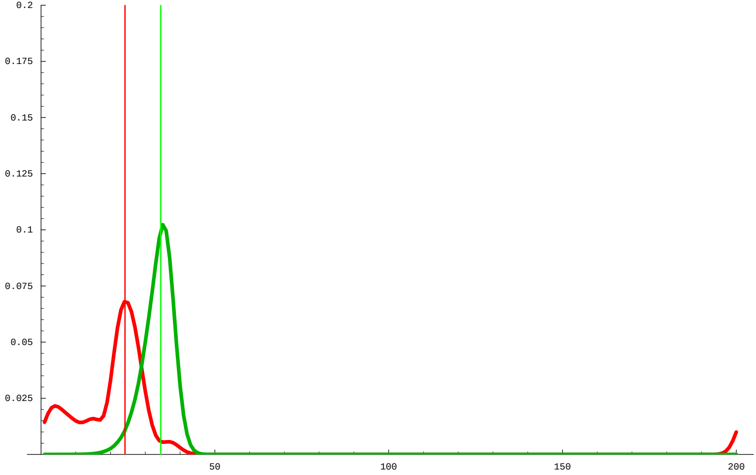

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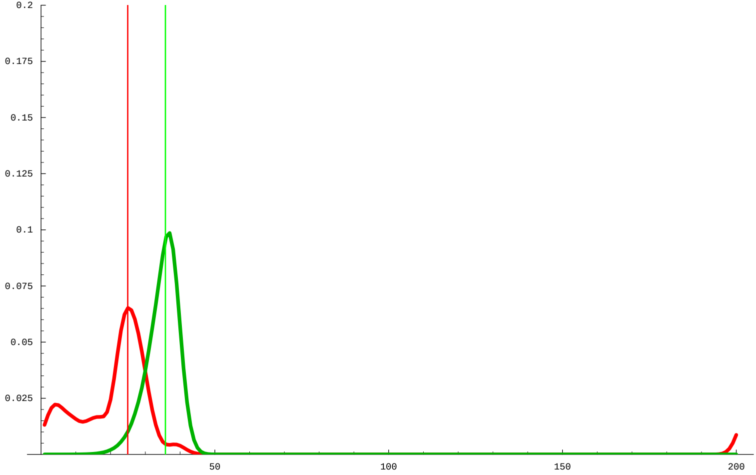

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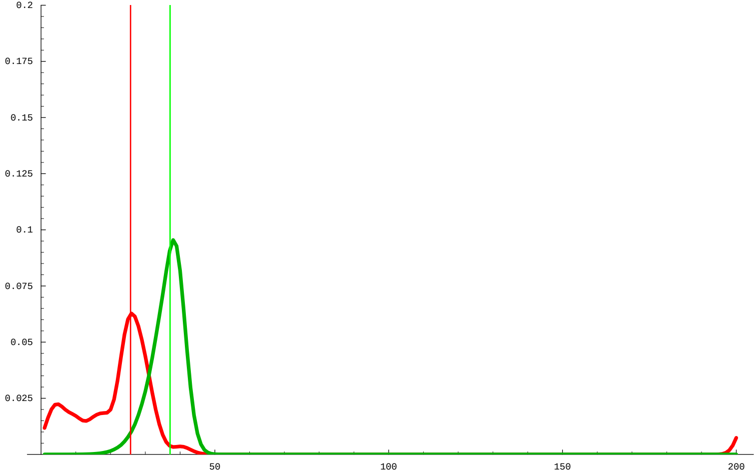

Application to the polaron problem
Time evolution

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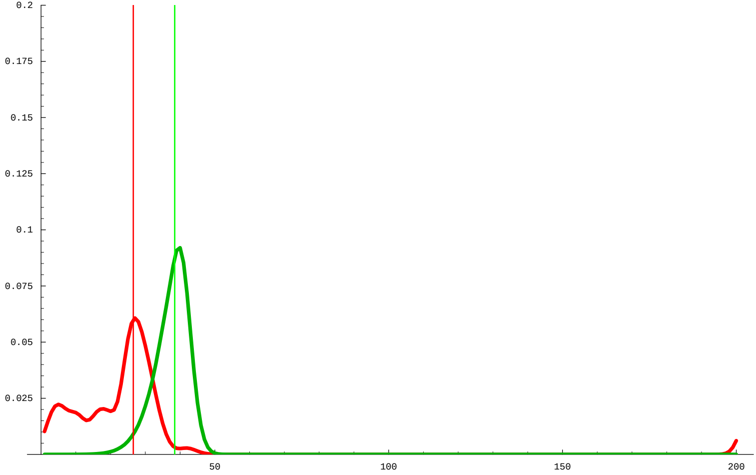

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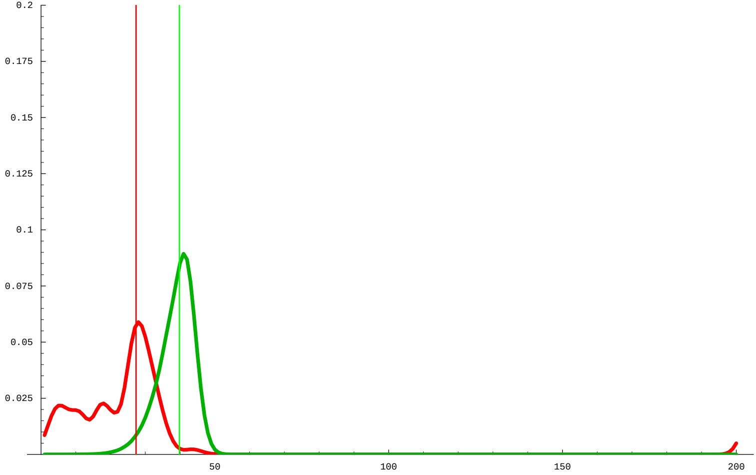

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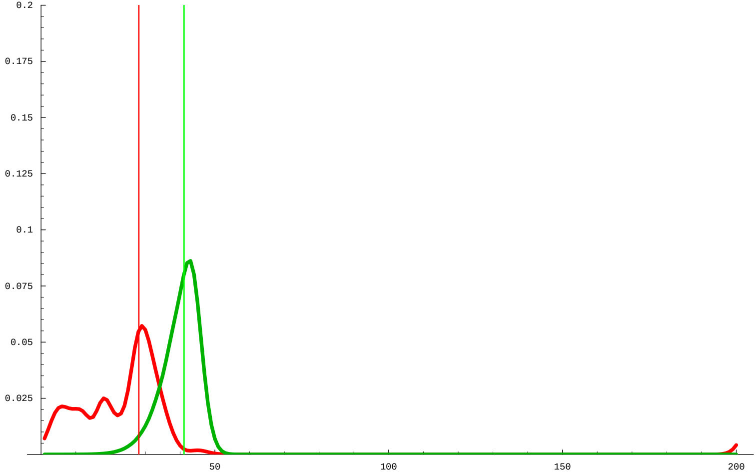

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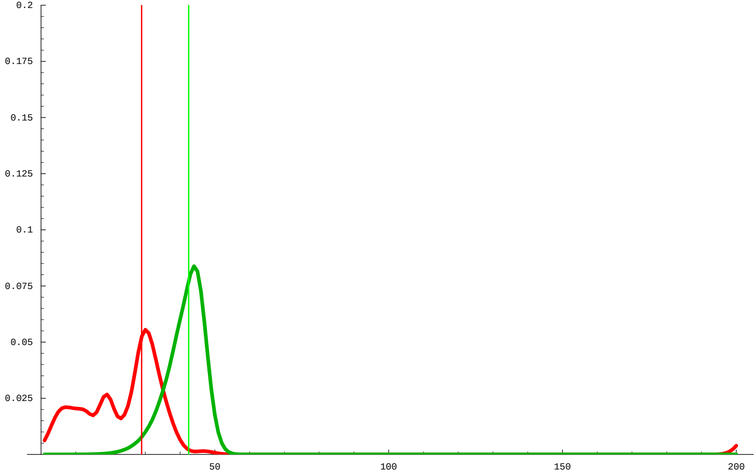

Application to the polaron problem
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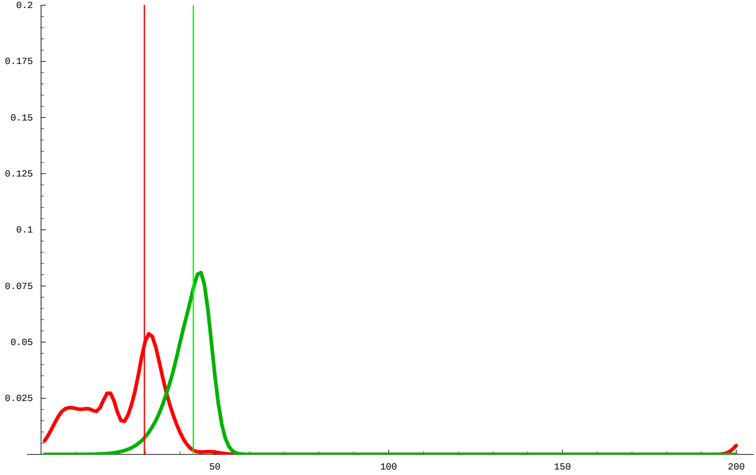

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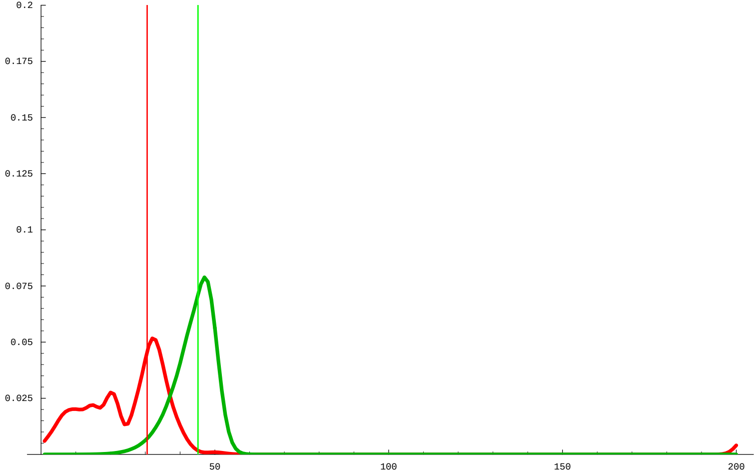

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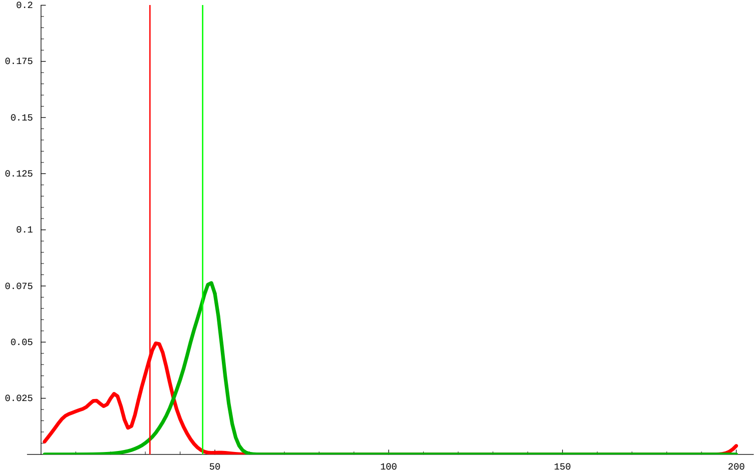

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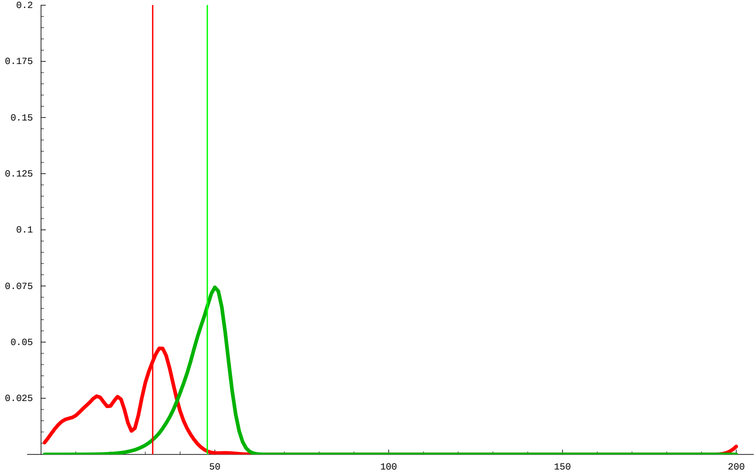

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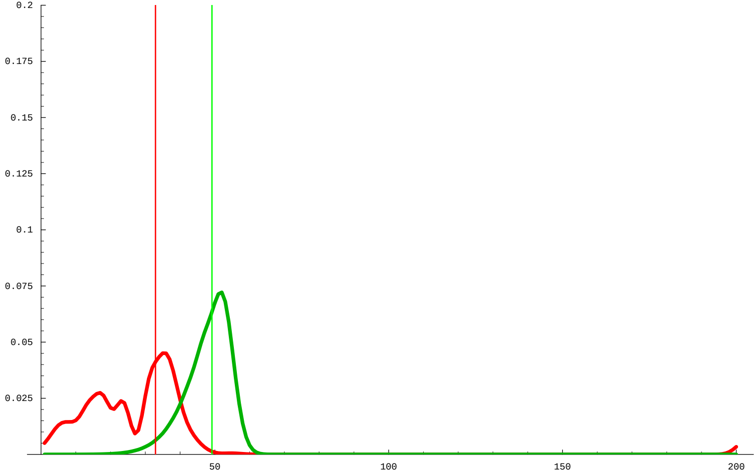

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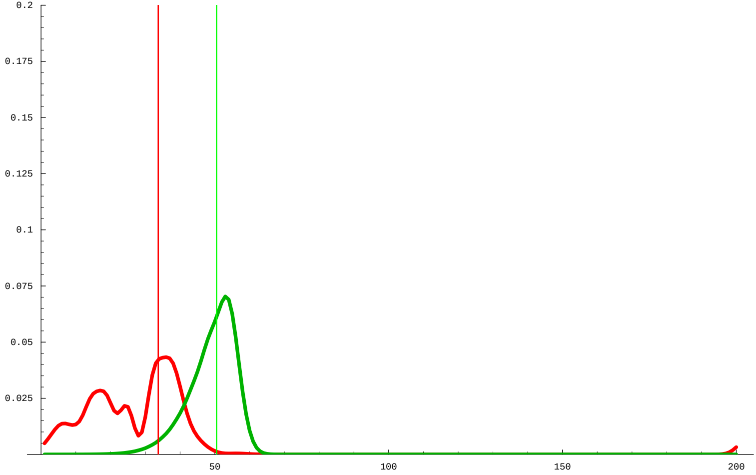

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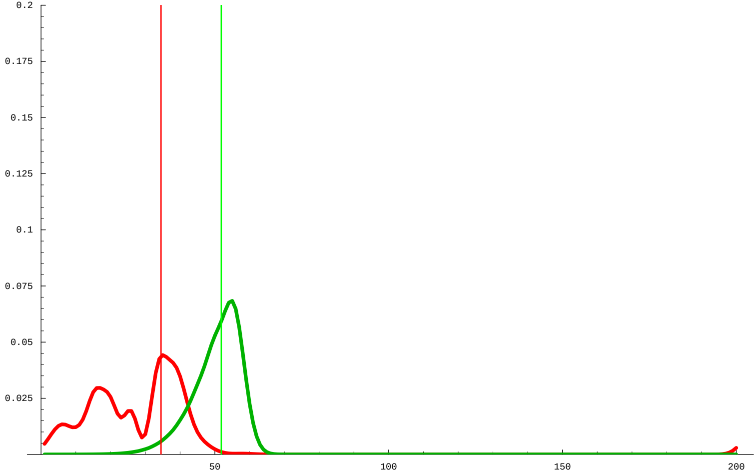

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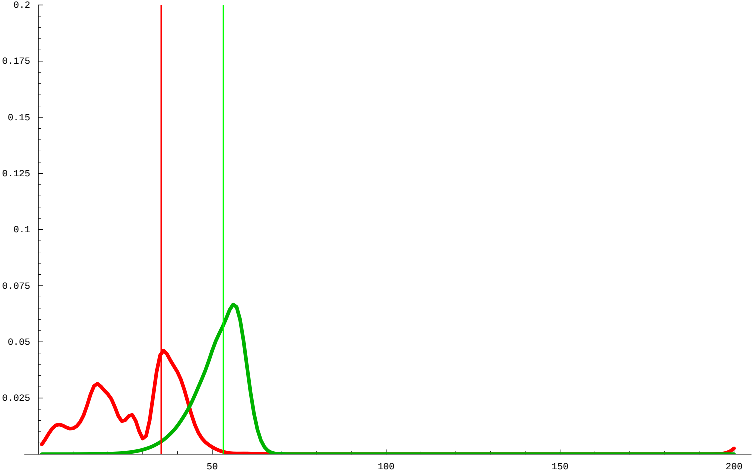

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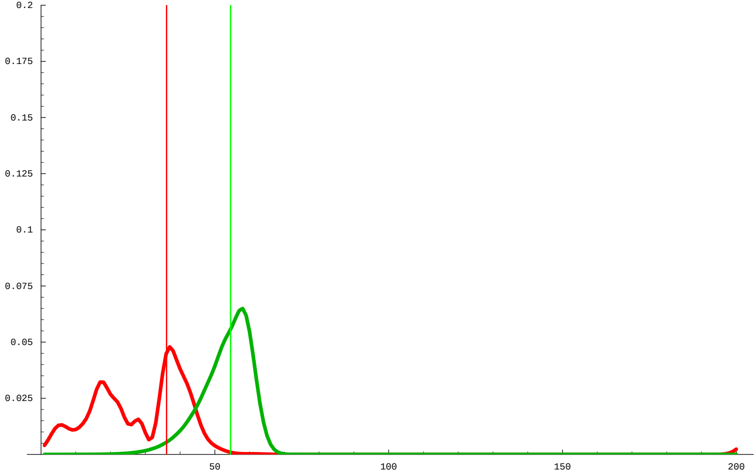

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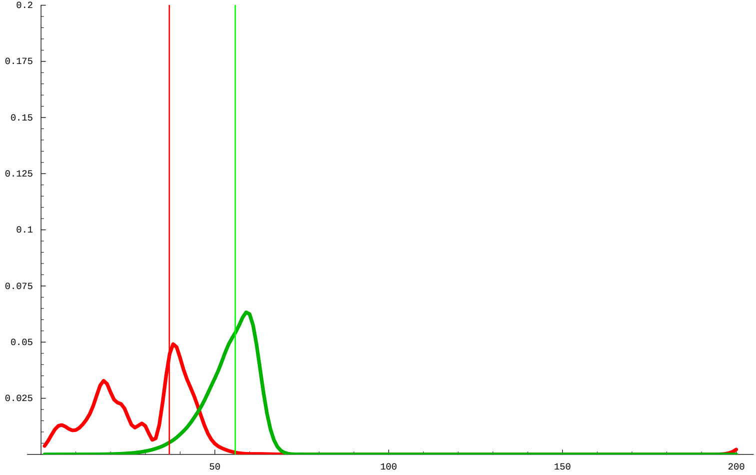

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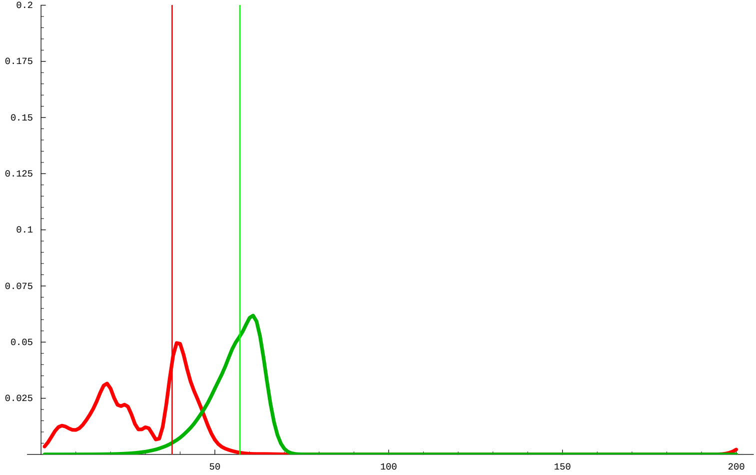

Application to the polaron problem
Time evolution

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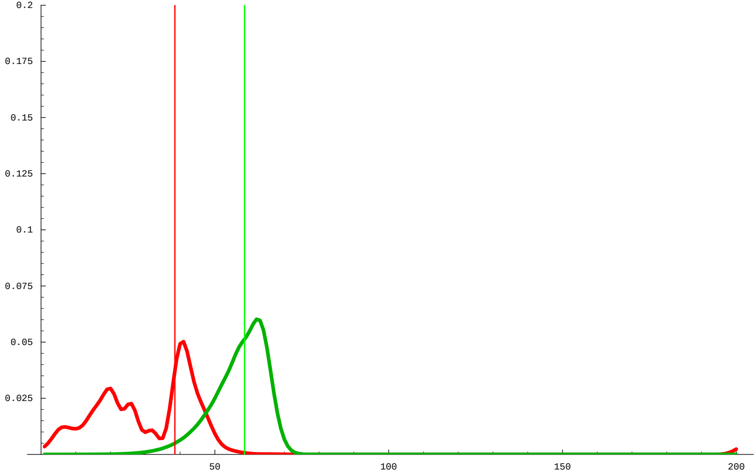

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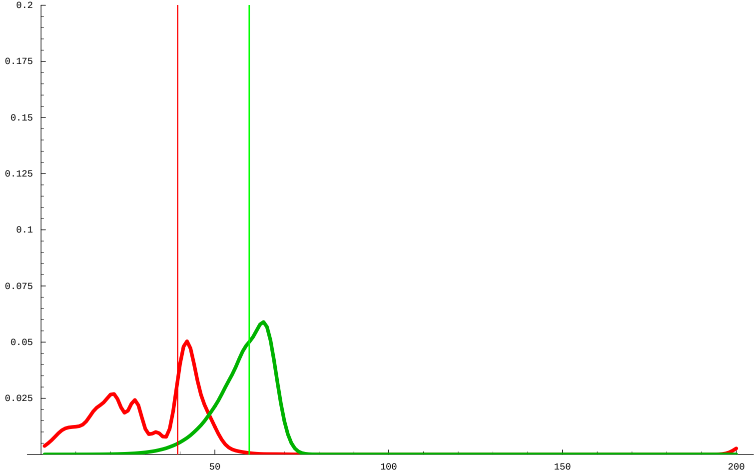

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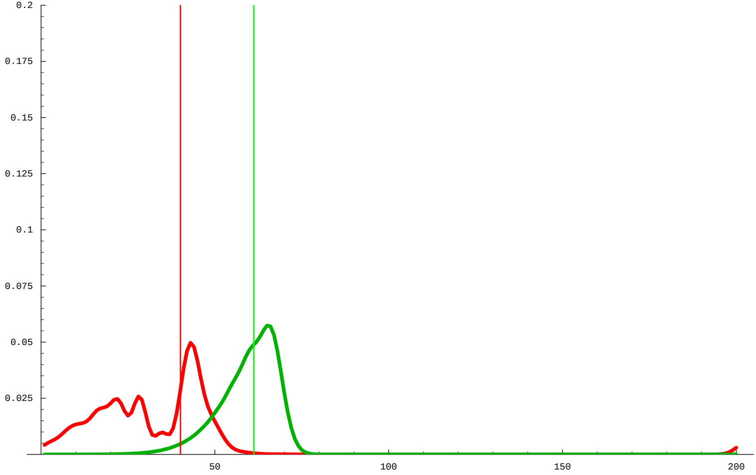

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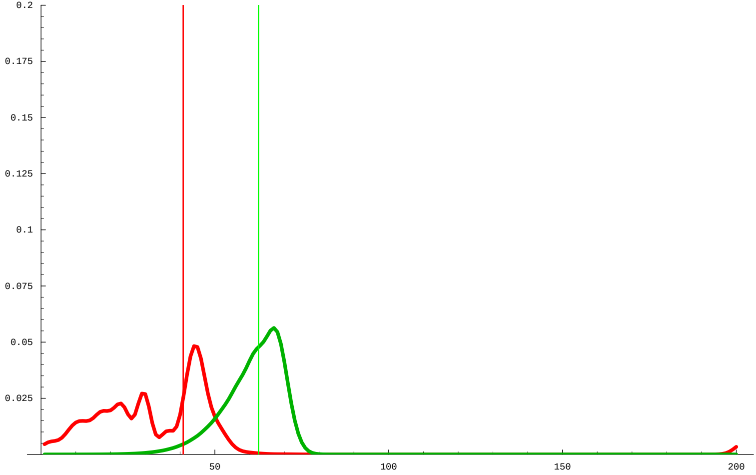

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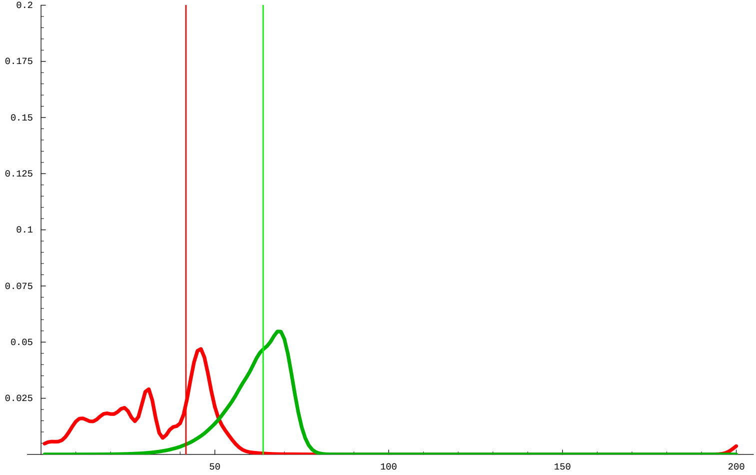

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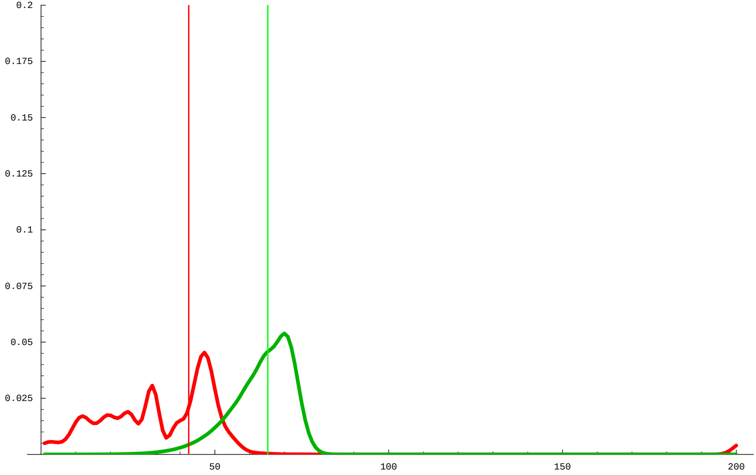

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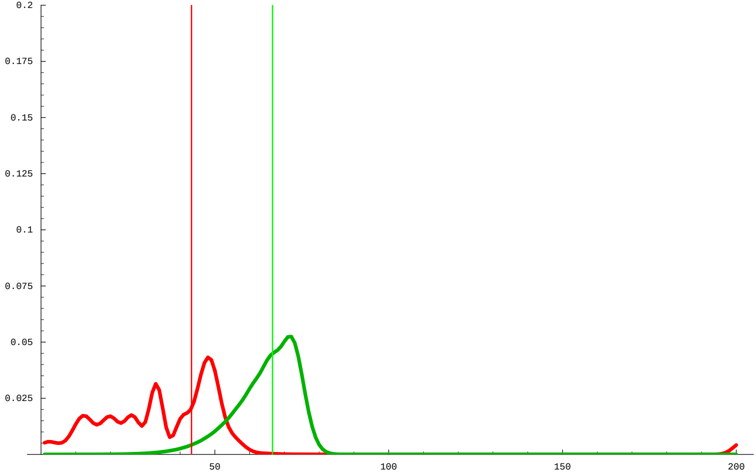

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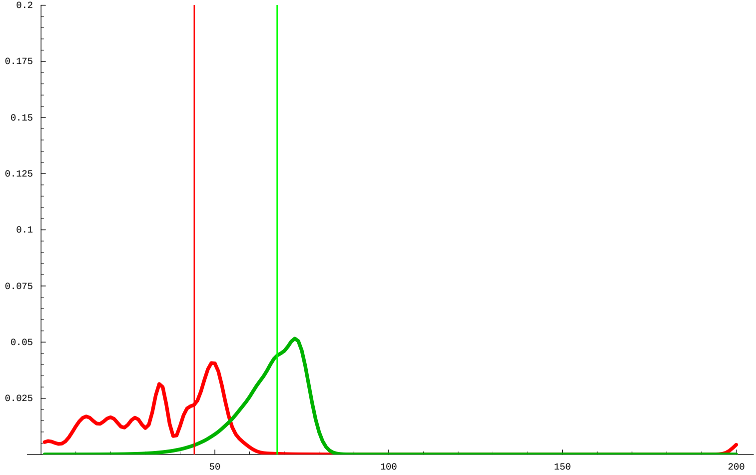

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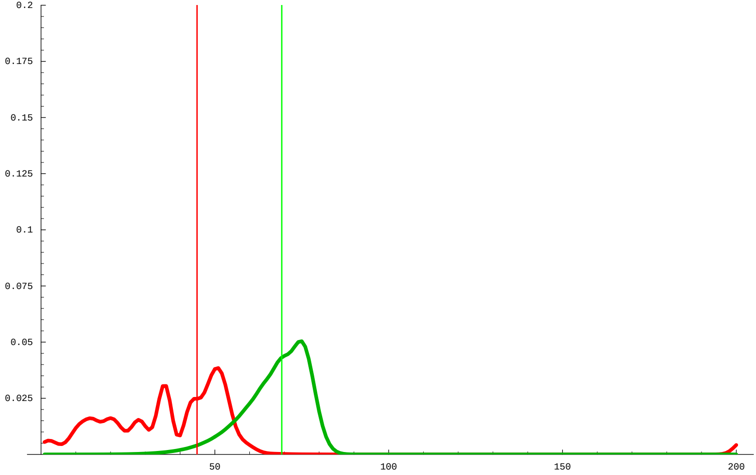

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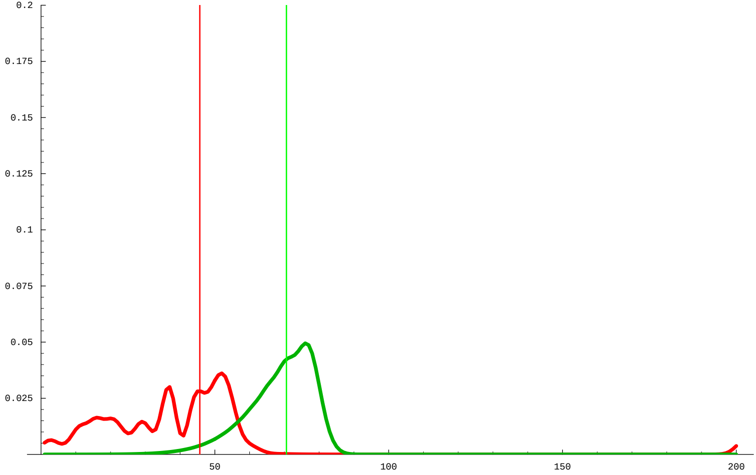

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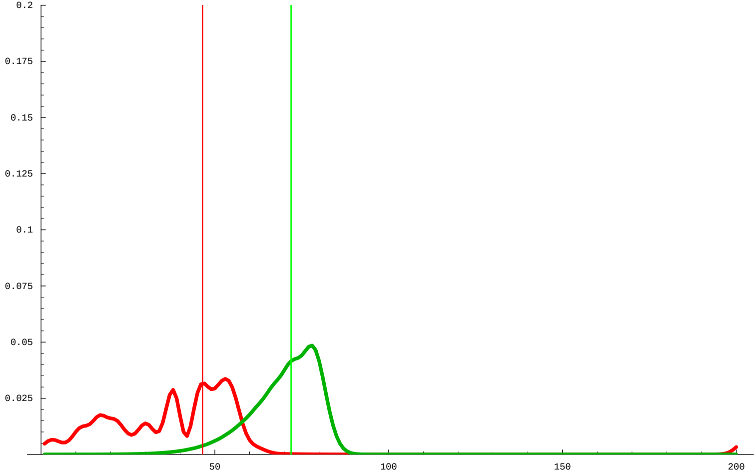

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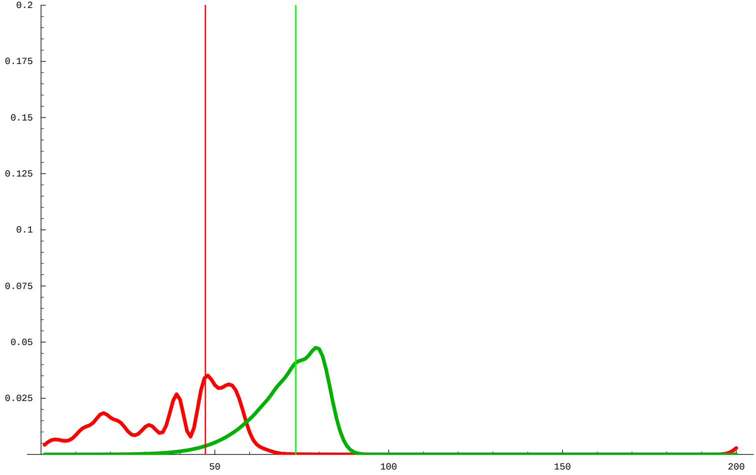

Application to the polaron problem
Time evolution

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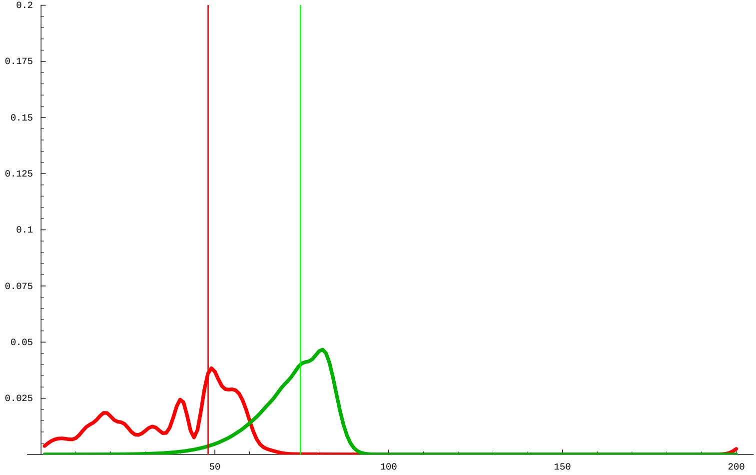

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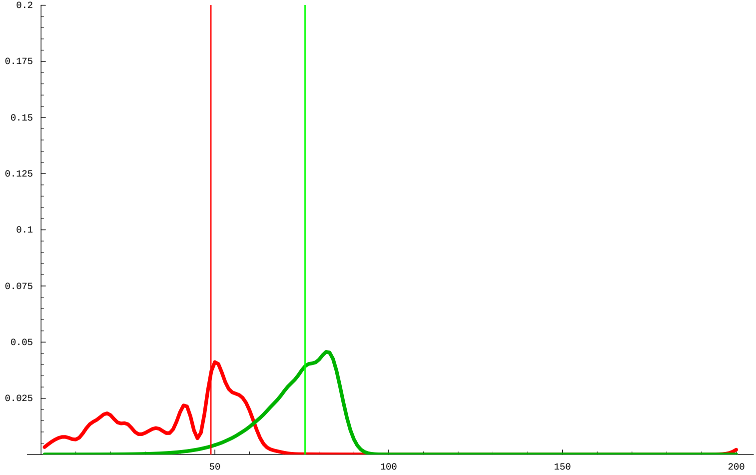

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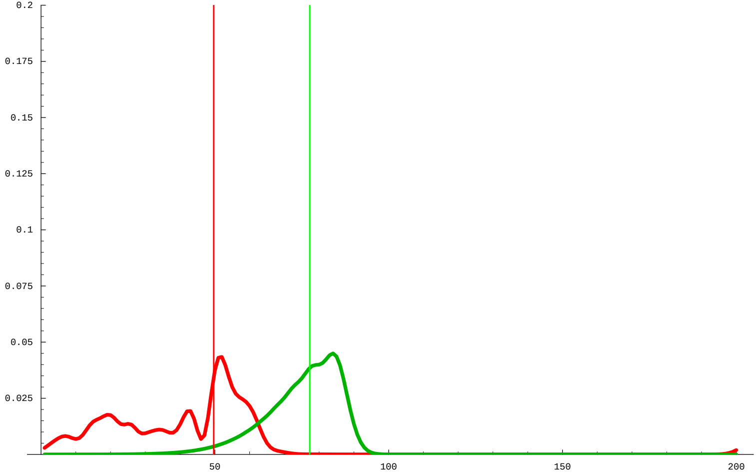

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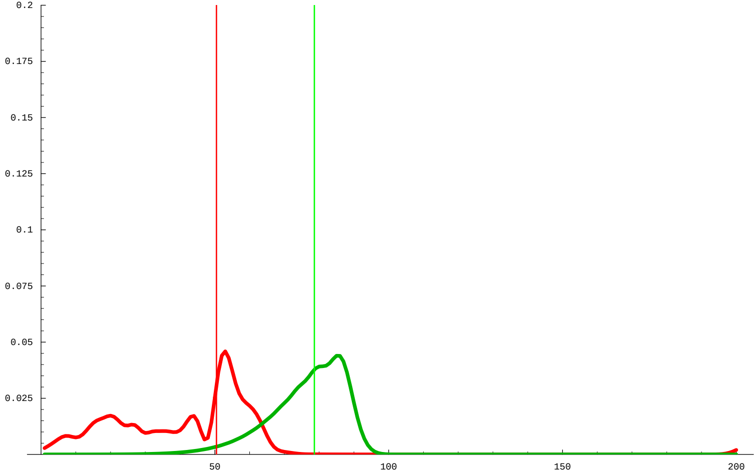

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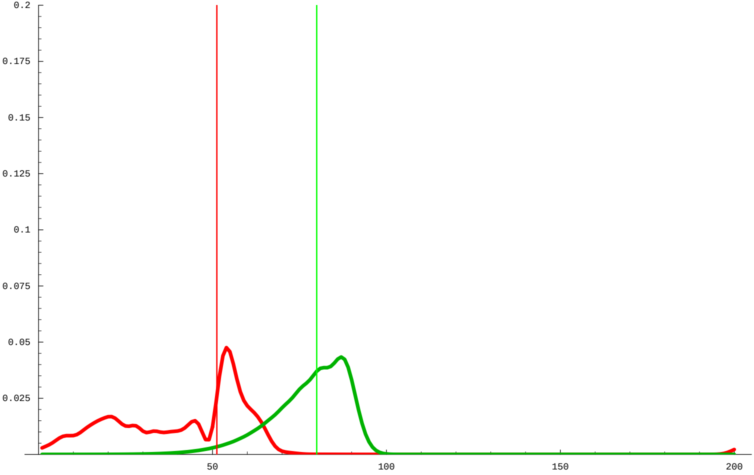

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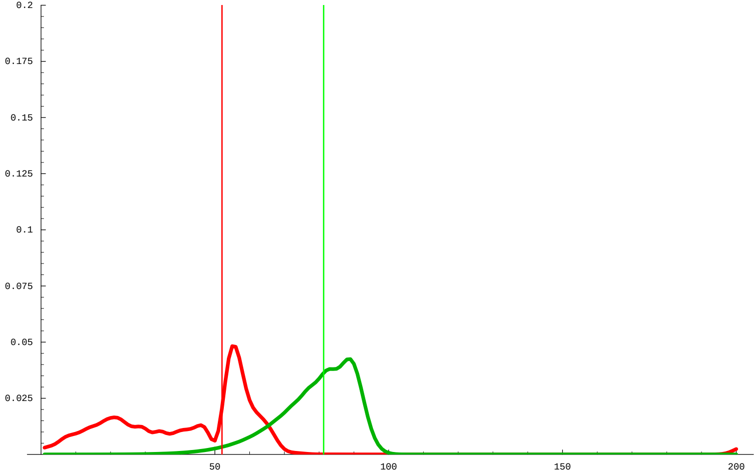

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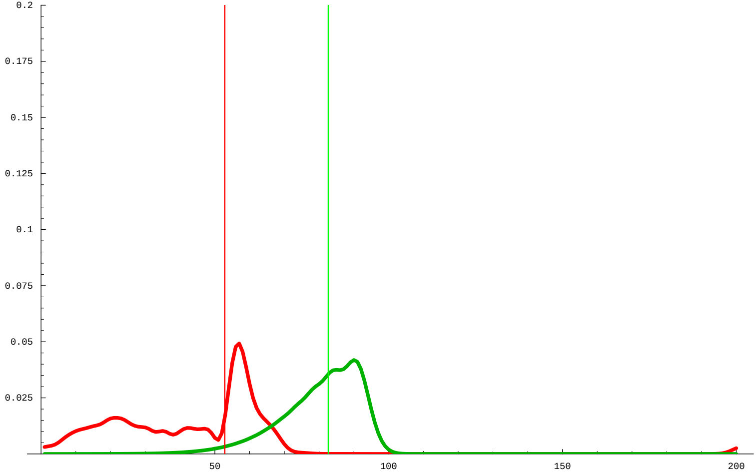

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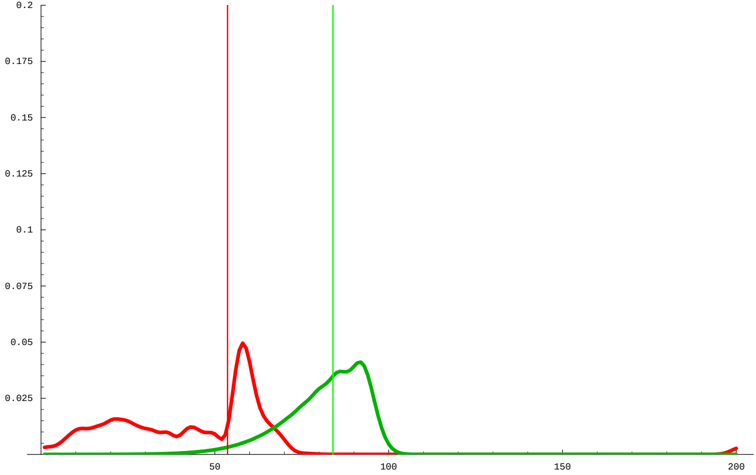

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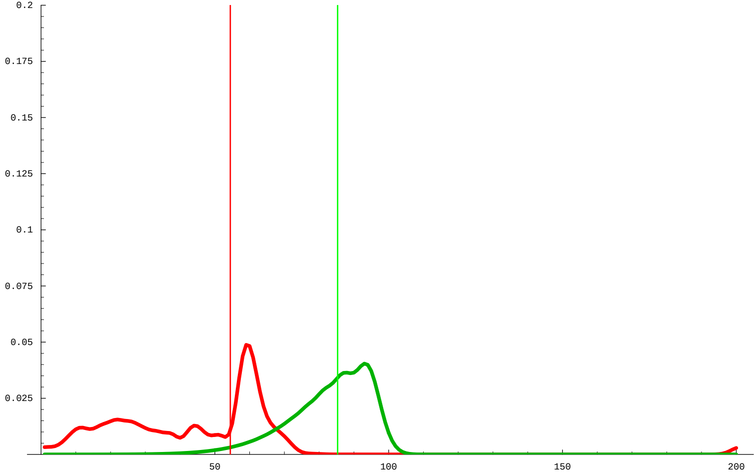

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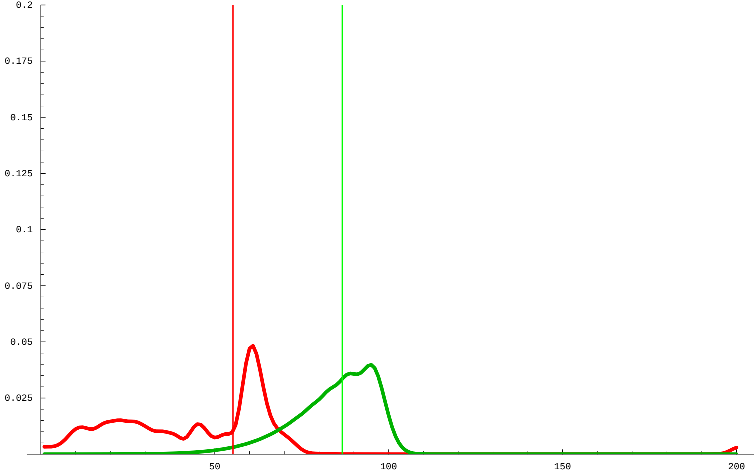

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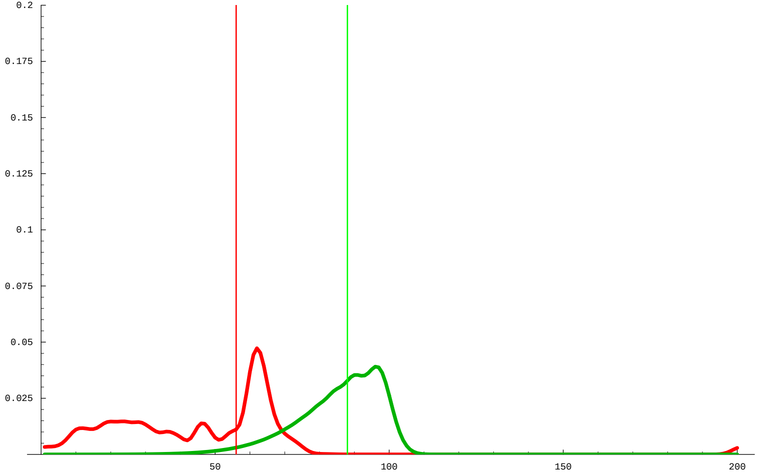

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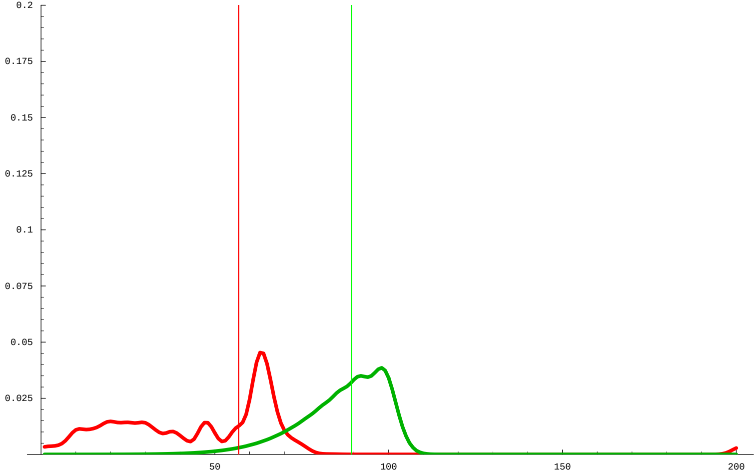

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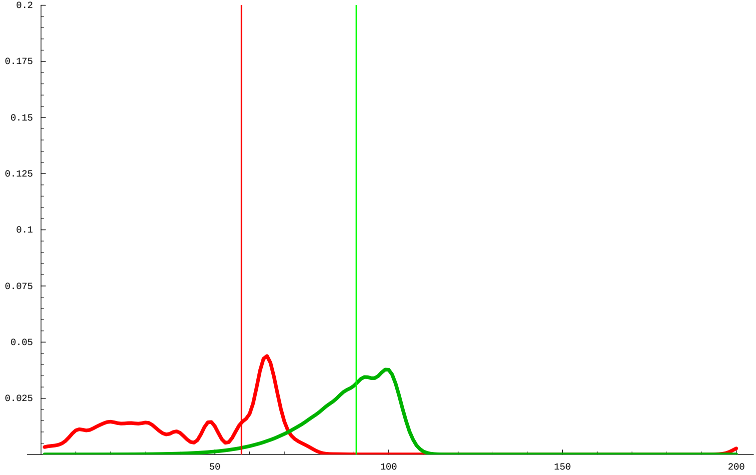

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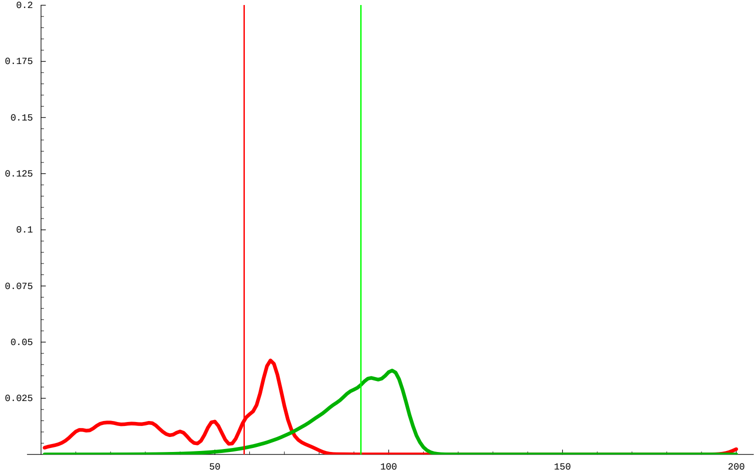

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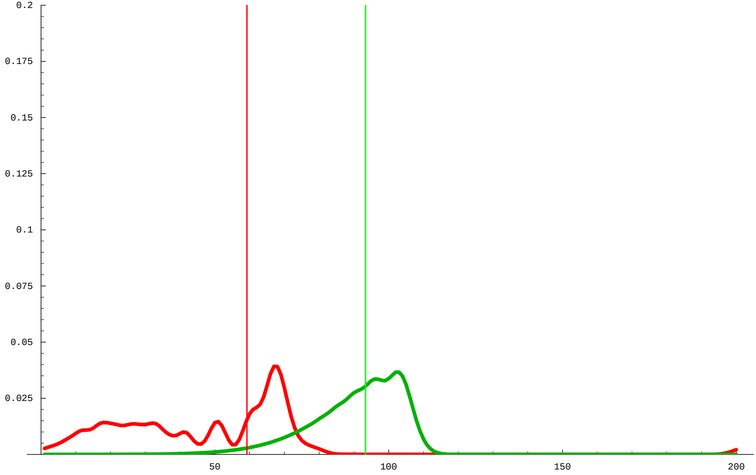

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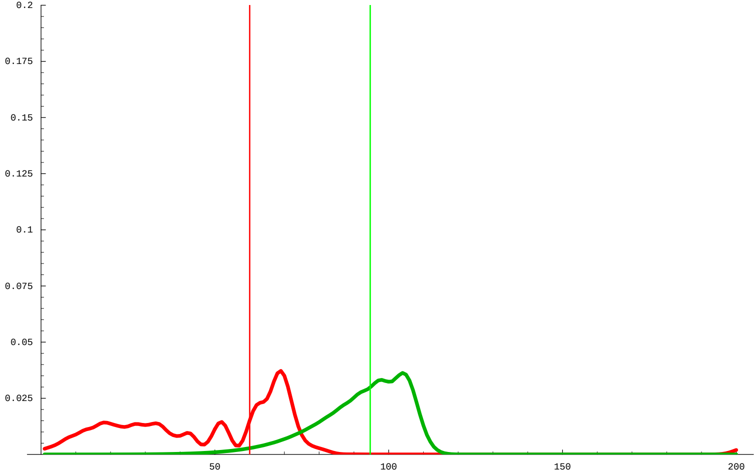

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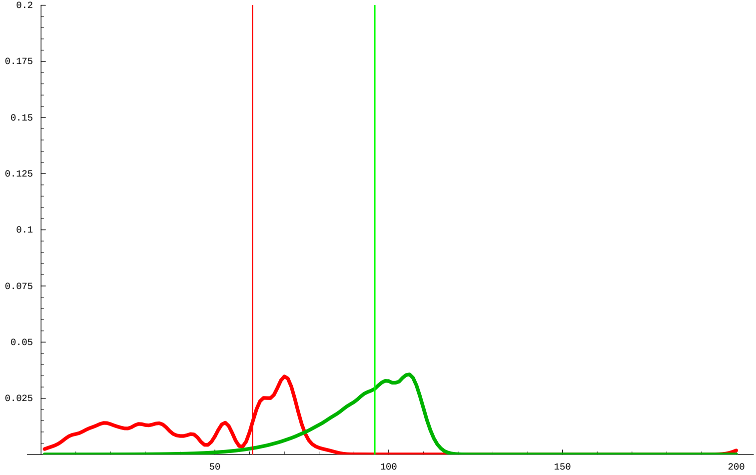

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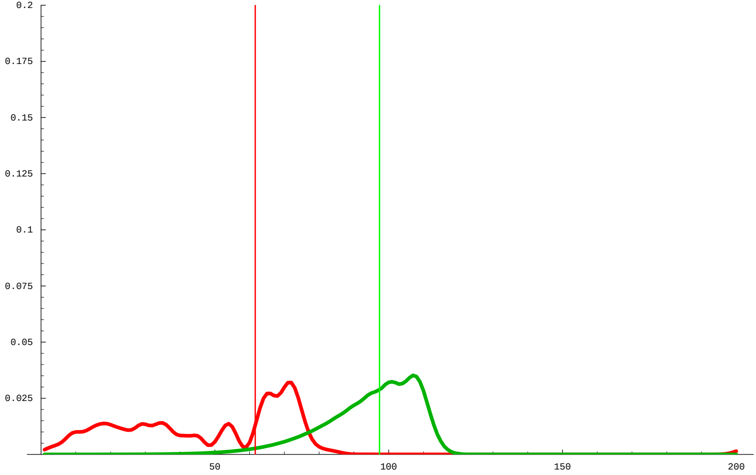

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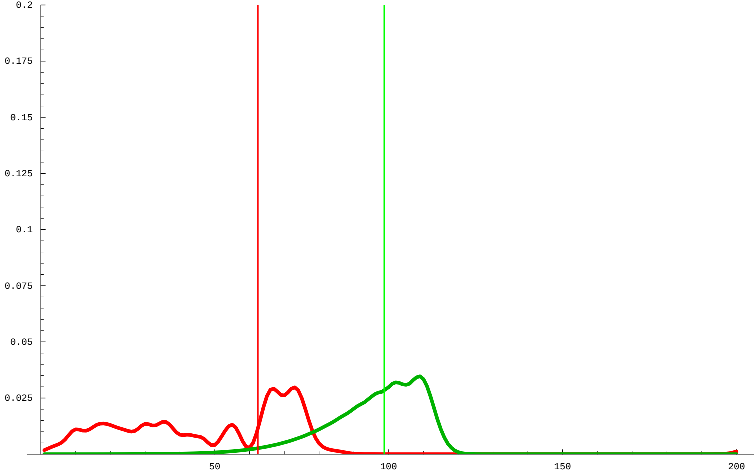

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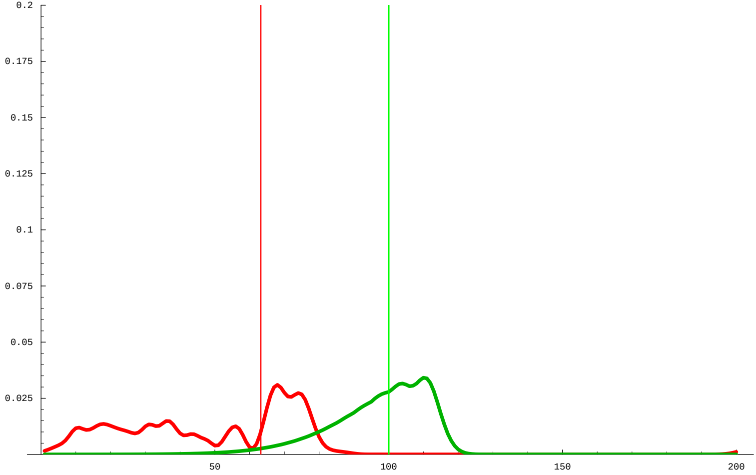

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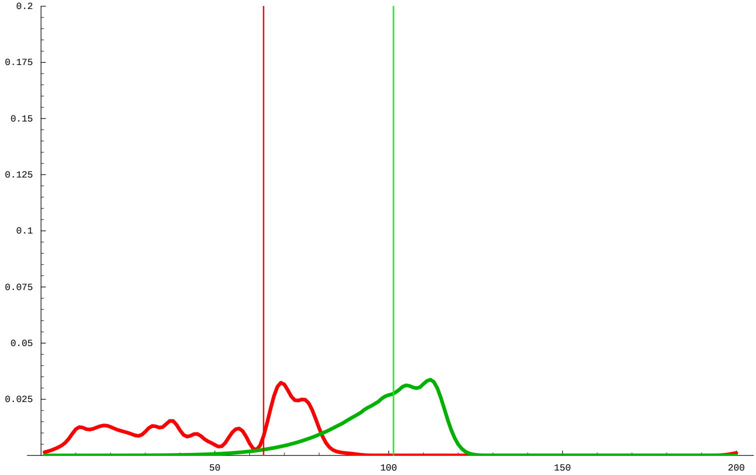

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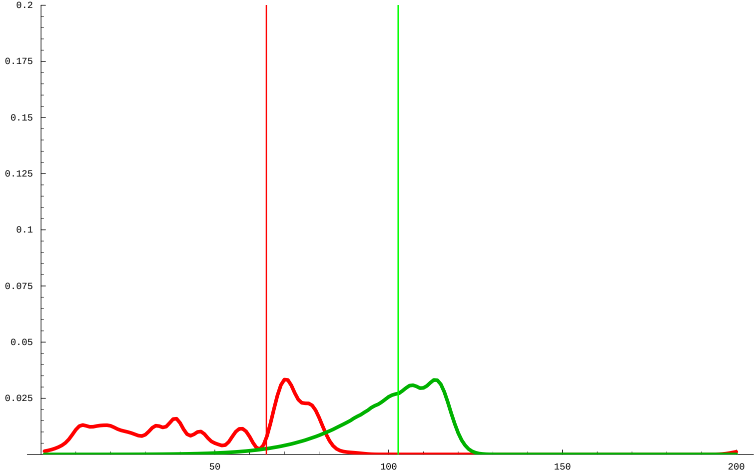

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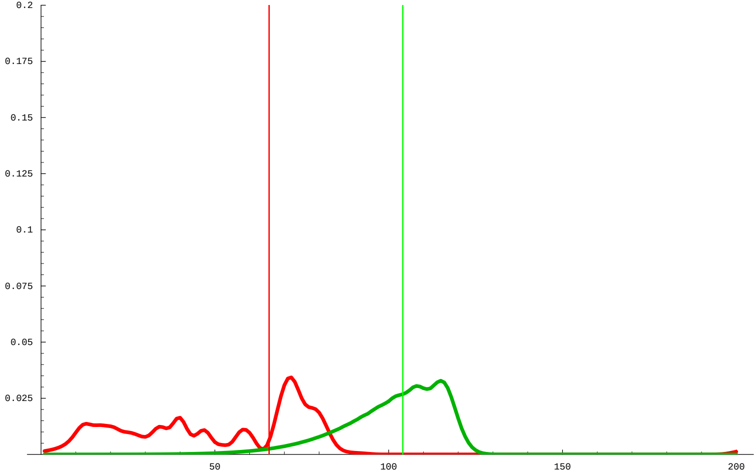

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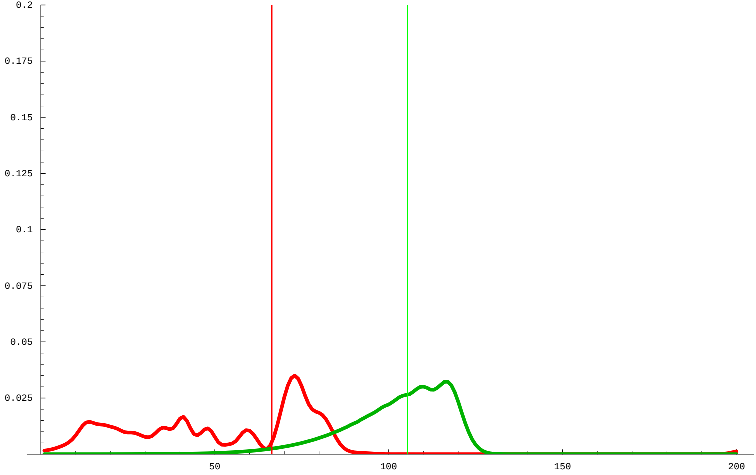

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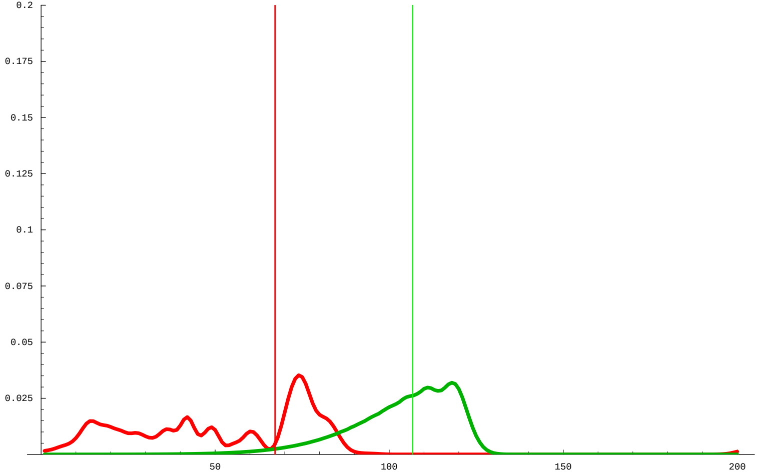

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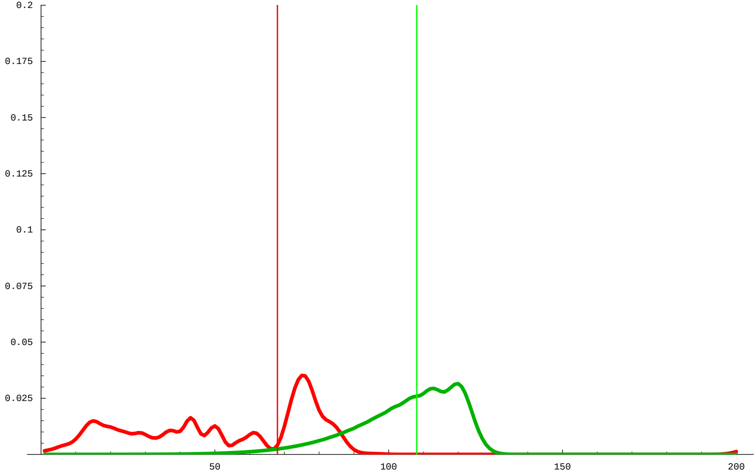

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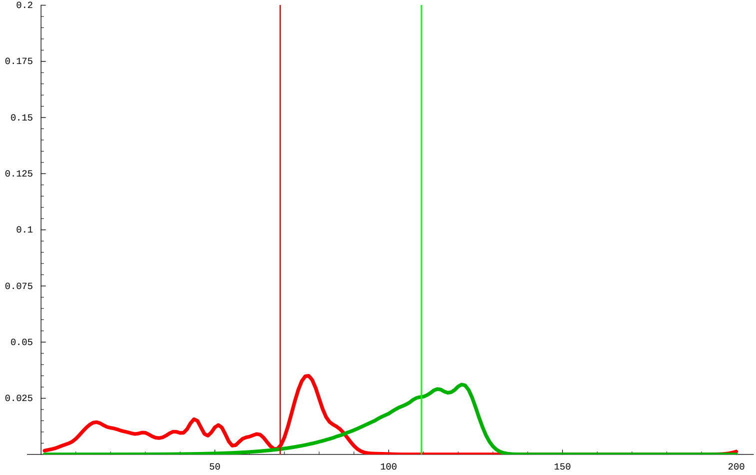

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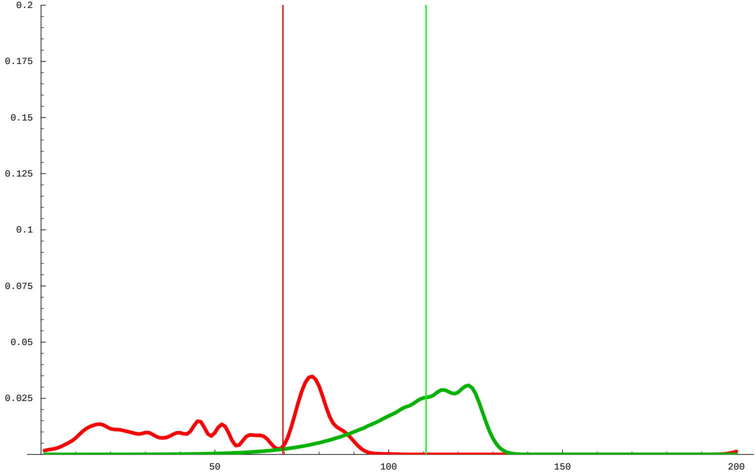

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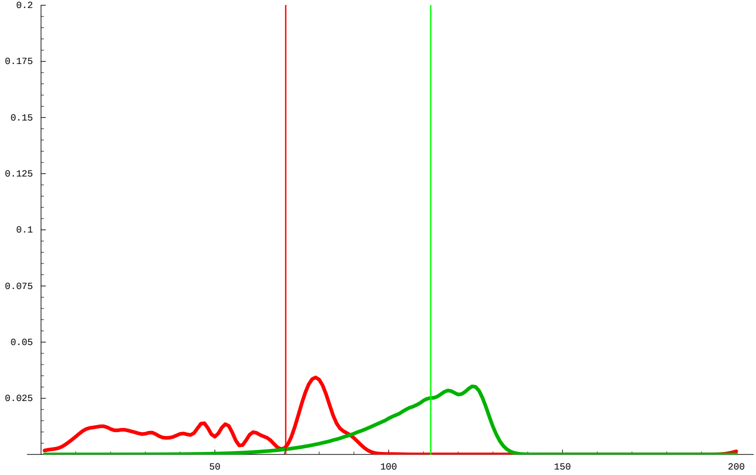

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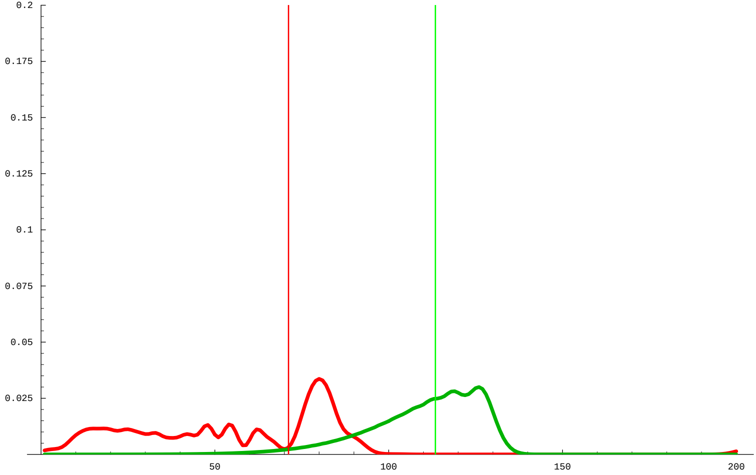

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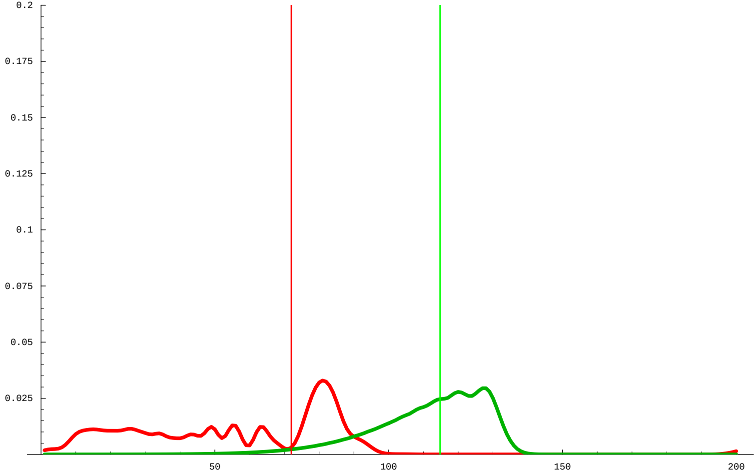

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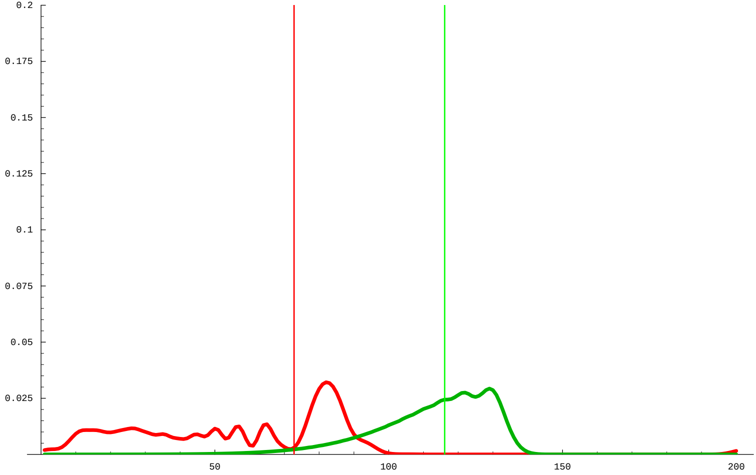

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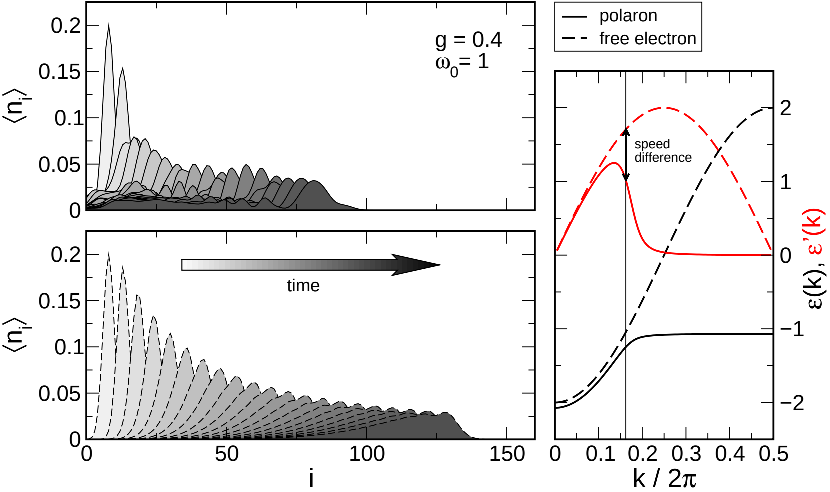

Summary

- Quantum many-particle problems $\rightarrow$ high-dimensional sparse matrix H
- Symmetries $\rightarrow$ substantial reduction of problem dimension D
- Some systems (phonons) require further tricks / cut-offs
- Usually iterative methods are *linear* in D (only sparse MVM)
- Dimensions can reach $D \sim 10^{10}$ or more
- We can calculate:
  - Extremal eigenstates & static correlations,
  - Approximations of spectral densities,
  - Dynamic correlations & linear response both at $T = 0$ and $T > 0$,
  - Quantum time evolution

Literature

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- Y. Saad, *Iterative Methods for Sparse Linear Systems*, *Numerical methods for large eigenvalue problems* see `http://www-users.cs.umn.edu/~saad/`
- A.Weiße, G. Wellein, A. Alvermann, H. Fehske, *The kernel polynomial method*, Reviews of Modern Physics **78**, 275 (2006)
- … "Computational Many-Particle Physics", Lecture Notes in Physics, Springer (2007)