Quantum two–particle scattering on finite cavities

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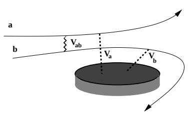
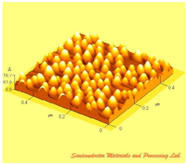
Motivation

Principle of two-particle scattering on finite structures:





- Up to now mostly one-particle properties, e.g. conductance and current, are investigated
- Exploratory example to study two-particle properties

Applications could be:

- Investigation of nano-structures, e.g. quantum-dots
- Analysis of correlated defects in SiO_2-structures

Coupled-channel scattering theory

Total T-matrix (Gell-Mann-Goldberger [Phys. Rev. 91 (1953) 398]):

$$\mathcal{T} = \mathcal{T}_1 + (1+\mathcal{V}_1\mathcal{G}_1)\mathcal{T}_{ab}(1+\mathcal{G}_1\mathcal{V}_1)$$

One-particle T-matrix: $\mathcal{T}_1 = \mathcal{V}_1 + \mathcal{V}_1\mathcal{G}_1\mathcal{V}_1$ mit $V_1 = V_a + V_b$

Correlated two-particle T-matrix: $\mathcal{T}_{ab} = \mathcal{V}_{ab} + \mathcal{V}_{ab}\mathcal{G}_1\mathcal{T}_{ab}$ mit $\mathcal{G}_1 = \frac{1}{\omega - \mathcal{H}_1}$

Assume one-particle wavefunction is known:

$$\mathcal{H}_1 \left|n_1\right\rangle = E_{n_1}\left|n_1\right\rangle$$

Introduce complete set $|n_1 n_2\rangle$:

$$\langle p_1 P|\,\mathcal{T}_{ab}\,|p_2 P'\rangle = V_{p_1p_2}\delta_{PP'} + \sum_{n_1n_2pp'\bar{P}} V_{p_1p}\frac{\langle pP|n_1n_2\rangle\langle n_1n_2|p'\bar{P}\rangle}{\omega + i\eta - E_{n_1n_2}}\langle p'\bar{P}|\,\mathcal{T}_{ab}\,|p_2P'\rangle$$

relative momentum $p = \frac{p_a - p_b}{2}$, center of mass motion $P = p_a + p_b$

Approximate solution

- concentrate on scattering states of cavity
- restrict to elastic scattering
- separable potential: $V_{p_1p_2} = \lambda g_{p_1}g_{p_2}$
- center of mass momenta $P \approx 0$; neglect medium effects $f \approx 0$

Consequently the T-matrix reads

$$\langle p_1 P|\,\mathcal{T}_{ab}\,|p_2 P'\rangle = \delta_{PP'}\frac{\lambda g_{p_1}g_{p_2}}{1 - \lambda J(P,\omega)}$$

with

$$J(P',\omega) = \sum_{n_1n_2}\frac{\sum\limits_{P} G_{n_1n_2}(P)G^*_{n_1n_2}(P')}{\omega - E_{n_1n_2} + i\eta}$$

and projected potential formfactors $G_{n_1n_2}(P) = \sum\limits_{p} g_p\langle pP|n_1n_2\rangle$

Model for cavity: Opaque wall

- Background Hamiltonian

$$\mathcal{H}_1 = -\frac{1}{2m}(\nabla^2 - \frac{\Omega}{R}\delta(r-R)),$$

$$\Omega = Opacity$$

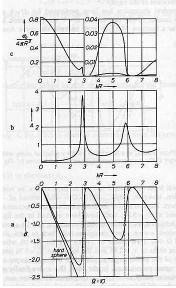
- Solution of the radial problem

$$\Psi(r) = \chi(r)/r$$

$$\chi(r) = c\begin{cases} A_k \sin kr & ; r < R \\ \sin(kr+\delta) & ; r > R \end{cases}$$

Three cases:

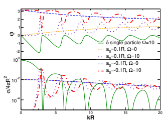
- $\Omega \to \infty$: Bound states in the interior
- $0 < \Omega < \infty$: Amplitude A_k maximal $\Longrightarrow$ resonance at virtual levels
- $\Omega = 0$ leads to case without cavity



Flügge: Rechenmethoden der Quantenmechanik

Results for contact interaction

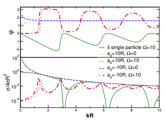
$\Omega = 10$, $a_0 = \pm 0.1R$:



$\delta =$ one-particle phase shift
$\varphi^\infty =$ free two-particle phase shift for contact potentials without cavity
$a_0 =$ two-particle scattering length
$\varphi =$ free two-particle phase shift for contact potentials with cavity

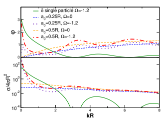
- $\delta < 0$ leads to repulsive potential
- cavity causes oscillations of φ around free particle case

$\Omega = 10$, $a_0 = \pm 10R$:



- second maximum in the cross section $\Rightarrow$ interference between one-particle and two-particle properties
- no bound state for case with cavity in contrary to the free problem without cavity

$\Omega = -1.2$, $a_0 > 0$:



- no bound states for φ^∞
- negative opacity enables bound state for φ

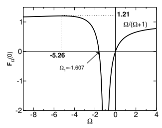
Occurrence of bound states

Two-particle phase shift φ from T-matrix: $\tan\varphi = \frac{\mathrm{Im}T}{\mathrm{Re}T}\Big|_{\omega=\frac{p^2}{m}}$,
Cross section (s-wave) $\sigma = \frac{4\pi}{p^2}\sin^2\varphi$

- positive/negative phase shift $\to$ attractive/repulsive potential
- Levinson theorem: $n\pi = \varphi(0)$ n...number of bound states
- negative/positive scattering length $a_0 \to$ odd/even $\#$ of bound states

Condition for bound states:

$$-\frac{R}{a_0} \geq F_\Omega(0)$$



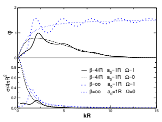
Results for finite potential range

Finite range effect of two-particle potential

- Chose exponential function as form factor $g_q = \beta^{-2}e^{-q^2/4\beta^2}$
- Limit $\beta \to \infty$ leads to contact interaction
- Opaque wall as background Hamiltonian

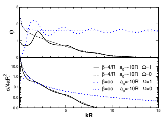
Consider case of contact potential (blue) and finite range (black):

$\beta = 4/R$, $a_0 = 1R$, $\Omega = 1$:



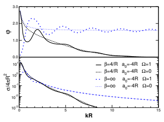
- no bound states for contact interaction and finite potential range
- $\varphi \to 0$ for $kR \to \infty$

$\beta = 4/R$, $a_0 = -10R$, $\Omega = 1$:



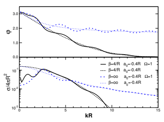
- finite potential range: bound state for cases with and without cavity
- contact interaction: no bound state for case with cavity

$\beta = 4/R$, $a_0 = -4R$, $\Omega = 1$:



- finite potential range: bound state for case with and without cavity
- contact interaction: no bound state for case with cavity

$\beta = 4/R$, $a_0 = -0.4R$, $\Omega = 1$:



- bound states for all cases

Summary

- T-matrix for two interacting particles and finite cavity considered:
  - Opaque wall as model for cavity: one-particle wave function known
  - Solution with separable potential for two-particle interaction
- Results
  - T-matrix equation analytically solved for cavities with virtual states
  - Exact solution for discrete states and approximate solution for additional scattering states
  - Two-particle phase shift φ shows additional oscillations besides standard ones at virtual levels
  - Interference effects cause splitting of maxima in cross section σ
  - Occurrence of bound states is dependent on scattering length and cavity strength
- Extension to realistic systems
  - Using realistic single-particle wave functions from ab-initio simulations as input to calculate two-particle T-matrix
  - Description of correlated defects in SiO_2 or other materials (degradation problem in FET structures) possible

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