Condensed-matter effects in μCF

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Outline

Motivation of theoretical studies

Experimental data Some properties of hydrogenic molecular targets

Scattering in condensed targets

Method of response function Examples for solid tritium

Resonant formation in condensed targets

Resonance response function Examples for $dd\mu$ and $dt\mu$

Condensed-matter effects in μ CF experiments



Example of target-density effects in $dt\mu$ cycle

Condensed-matter effects in µCF experiments



Example of target-density effects in $dd\mu$ formation rate.

Interaction potential of hydrogenic molecules



• In liquid and solid deuterium, the interaction between neighboring D₂ molecules is important.

Mean kinetic energy of hydrogenic molecules



- Mean kinetic energy *ℰ*_T of H₂ molecule in liquid and solid para-H₂ at a fixed temperature of 19.3 K (Zoppi et al., 2001).
- Open circles O inelastic neutron scattering data, full circles • — path-integral quantum Monte Carlo.

Mean kinetic energy of hydrogenic molecules

<i>T</i> [K]	ϕ [LHD]	ℰ _Т [eV]
4.2	1.42	5.9 ± 1.0
20	1.21	5.2 ± 0.8
30	1.01	5.6 ± 0.8

- Mean kinetic energy *ε_T* of D₂ molecule in solid (4.2 K) and liquid (20 and 30 K) normal deuterium nD₂ versus temperature *T* and density φ (Mompeán et al., 1996).
- Energy \mathscr{E}_T is much greater than the classical limit $\frac{3}{2}k_{\rm B}T$.
- Energy $\mathscr{E}_{\mathcal{T}}$ in the solid is greater than in the liquid.
- Magnitude of *C_T* is mainly determined by the zero-point vibrations of the molecules in a target.

Method of response function

• Cross sections for scattering in condensed targets are calculated using the response function *S*, which depends only on target properties (Van Hove, 1954).

Partial differential cross section:

$$\left(\frac{\partial^2 \sigma}{\partial \Omega \partial \varepsilon'}\right) = N_{\text{mol}} \frac{k'}{k} \sigma_{\text{mol}} S(\vec{\kappa}, \omega)$$

Notation:

 $\sigma_{\rm mol} = \overline{|f_{\rm mol}|^2},$

 $f_{\rm mol}$ — scattering amplitude for a single molecule,

horizontal bar — averaging over the spins, rotational states, and isotopic concentration of the molecules,

 $\vec{\kappa} = \vec{k} - \vec{k}'$ — momentum transfer, $\omega = \varepsilon - \varepsilon'$ — energy transfer.

Impulse approximation of the response function

For large momentum κ and energy ω transfers:

$$\mathcal{S}(\vec{\kappa},\omega) = \int n(\vec{p}) \,\delta\left[\omega + p^2/2M - (\vec{p} + \vec{\kappa})^2/2M\right] \mathrm{d}^3 p \,,$$

 $n(\vec{p})$ — target-particle momentum distribution,

 \vec{p} and M — target-particle momentum and mass,

 δ function expresses the kinetic-energy conservation.

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- The target particle means a hydrogenic molecule or nucleus, depending on the magnitude of κ and ω .
- Application measurement of the momentum distribution (e.g., for proton in H₂, or for H₂ in solid/liquid hydrogen) using deep inelastic neutron scattering (ISIS, RAL).
- Effects of the target-particle movement are important even at high energies.

Averaging of nuclear amplitudes in molecules



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Scattering amplitude $t\mu(\uparrow\downarrow)+t$ and the same amplitude averaged over the triton motion in T_2 – –

Scattering of $t\mu$ in solid tritium at 3 and 20 K



Scattering of $t\mu$ in solid tritium at 3 and 20 K





 $t\mu(\uparrow\uparrow)+\mathsf{nT}_2$

10 -1

tµ energy (eV)

10⁻⁵ 10⁻⁴ 10⁻³ 10⁻²

Deceleration of muonic atoms in solid hydrogens



Mean energy of $t\mu$ atoms in a solid tritium nT₂ versus time, for T = 3 and 20 K.

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Mean energy of $d\mu$ atoms in a solid nD₂ and $t\mu$ atoms in a solid nT₂ at large times, as functions of target temperature.

Emission of cold $p\mu$ atoms from solid



Application of the calculated cross sections for $p\mu$ scattering from solid and gaseous nH₂ for description of the TRIUMF experiment using a solid multilayered target (Woźniak et al., 2003).

Energy balance in $dt\mu$ formation in a solid deuterium



The Vesman-type subthreshold resonance can contribute to the $dt\mu$ formation rate via the energy transfer ω to collective degrees of freedom of a condensed deuterium.

Resonance response function

- Van Hove's response function cannot be used for description of resonant formation of the muonic molecules.
- In particular, the function S does not take into account a significant change of the target-molecule mass in the formation process (e.g., [(dtm)dee] in the place of D₂).

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- In particular, the function S does not take into account a significant change of the target-molecule mass in the formation process (e.g., [(dtm)dee] in the place of D₂).
- However, a generalized resonance response function $S_{res}(\kappa, \omega)$ can be applied for estimation of condensed-matter effects in the resonant formation (Adamczak&Faifman, 2005).
- For the Vesman-type resonances at the lowest resonance energies ε_{if} , function S_{res} tends to the incoherent part of Van Hove's function S ($dd\mu$ resonances below 10 meV).

Resonance response function for $dd\mu$ in 3-K solid D₂



- Function S_{res} and matrix elements $|V_{if}|^2$ versus $d\mu$ energy.
- Recoil-less $dd\mu$ formation is described by the δ function.
- The wide spectrum of S_{res} corresponds to the formation with simultaneous phonon annihilation or creation.

Resonant $dd\mu$ formation in solid deuterium



- The resonant $dd\mu$ -formation rate in solid deuterium at 3 K.
- The rate is proportional to the product of S_{res} and $|V_{if}|^2$.
- It is assumed that rotational-vibrational levels of the D₂ molecule are not changed in the condensed target!

Resonant $dd\mu$ formation in solid nD₂ at 3 K



- The calculated Monte Carlo time spectra of *dd*-fusion products agree well with the experimental results for normal nD₂ target at 3 K (Knowles et al., 1997).
- Broadening of molecular rotational levels in the solid $(\sim 0.5 \text{ meV})$ taken into account to obtain reasonable fits.

Ortho-para effects in $dd\mu$ formation in solid D₂



 The calculated ortho-para effect in ddµ formation is opposite to that found in experiments (Toyoda et al., 2003).

Ortho-para effects in $dd\mu$ formation in solid D₂



- The calculated ortho-para effect in *dd*µ formation is opposite to that found in experiments (Toyoda et al., 2003).
- The calculated time spectra are very sensitive to the locations and widths of the lowest $dd\mu$ resonances.
- Possible explanation of this discrepancy: widths (values?) of the rotational levels of D₂ and $[(dd\mu)dee]$ significantly ($\sim 1 \text{ meV}$) changed in a solid/liquid deuterium.

Resonance response function for $dt\mu$ in 3-K solid D₂



- Function S_{res} and matrix elements $|V_{if}|^2$ versus $t\mu$ energy.
- Recoil-less *dt*µ formation is described by the Breit-Wigner function.
- Broadening of molecular levels is not significant in the case of wide $dt\mu$ resonances!

Resonant $dt\mu$ formation in a 3-K solid deuterium



Resonant $dt\mu$ -formation rate in solid nD₂ for the $t\mu$ spin states F = 0 and F = 1.

Resonant $dt\mu$ formation in a 3-K solid deuterium





Resonant $dt\mu$ -formation rate in solid nD₂ for the $t\mu$ spin states F = 0 and F = 1. Ortho-para effects in low-energy resonant $dt\mu$ -formation for the state F = 0.

Resonant $dt\mu$ formation in solid D/T



Resonant $dt\mu$ -formation rate in $t\mu(F = 0)$ scattering on nD₂ molecule bound in a solid D/T ($C_t = 0.4, \phi = 1.45$).

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The same rate averaged over the steady-state $t\mu$ energies versus target temperature. Experimental point (Ackerbauer et al., 1999), dashed line — the rate scaled by the factor of 0.86.

Resonant $dt\mu$ formation in liquid D₂



- Resonant dtμ-formation rate in liquid deuterium at T = 23 K and φ = 1.16, calculated using a crude model of liquid.
- The rate at small κ and ω is described by the Lorentzian function (its width equals $D_{\rm s}\kappa^2$, $D_{\rm s}$ is the self-diffusion coefficient of D₂ in deuterium).

Resonant $dt\mu$ formation in liquid D₂



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- The rate at small κ and ω is described by the Lorentzian function (its width equals $D_{\rm s}\kappa^2$, $D_{\rm s}$ is the self-diffusion coefficient of D₂ in deuterium).
- Averaged $dt\mu$ -formation rates: $4.0 \times 10^8 \text{ s}^{-1}$ (T = 23 K, $\phi = 1.16$) and $3.6 \times 10^8 \text{ s}^{-1}$ (T = 33.3 K, $\phi = 0.928$).

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- Condensed-matter effects are very significant in solid, liquid, and cool dense gaseous hydrogenic targets.
- These effects can be described using a generalized response function.
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- Outlook
 - Estimation of intermolecular-interaction effects in rotational energies of D₂ and $[(dd\mu)dee]$ is necessary to solve the ortho-para problem in $dd\mu$ formation.
 - A more accurate model needed for mixed D/T crystals.