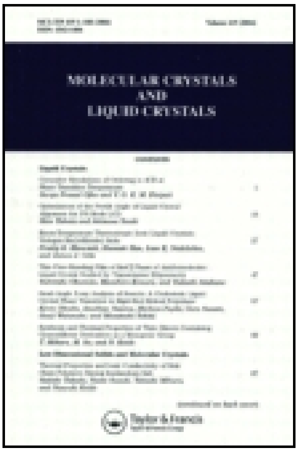

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Self-Trapping in Closed Systems

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SELF-TRAPPING IN CLOSED SYSTEMS

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Abstract We investigate the self-trapping (ST) in a closed one-dimensional (1d) system and show that there exists a critical size for the onset of the ST, $l_{cr}(g)$, depending on the coupling constant, g.

The problem of self-trapping is usually discussed as applied to infinite systems. There are the dimensionality of the system and the type of the electron-phonon coupling which control the ST patterns. Electronic properties of the systems like fullerenes (C_{60}, C_{70}, etc.) which are large but spatially restricted add a new dimension, the system size, to the ST problem. There is a believe that any restriction imposed on a spatial size of a "free" state facilitates the self-trapping. E.g., in 3d the ST barrier for particles confined in shallow centers is lower than for free particles. We consider a particle moving in a closed 1d system, a ring, and show that for such a system the spatial confinement has an opposite effect. As distinct from an infinite 1d system where ST sets in for arbitrary value of g, the confinement results in emerging of a critical value, $g_{cr}(l)$, for the coupling constant, depending on the ring size.

The ST at a ring is described by a non-linear Schroedinger equation:

$$-\tfrac{1}{2}d^2\psi/dx^2 - g\psi^3 = \lambda\psi \ , \tag{1}$$

where $-l \le x \le l$, and $\psi(-l) = \psi(l)$. The solution of this equation is:

$$2\sqrt{g}x = 2F(\mu(u), k)/\sqrt{u_M} \ , \tag{2}$$

where

$$\mu(u) = \arcsin\sqrt{(u_M - u)/(u_M - u_m)} \ , \qquad k = \sqrt{1 - u_m/u_M} \ . \tag{3}$$

Here $u = \psi^2$, u_M and u_m are the maximum and minimum values of u, and $F(\mu, k)$ is an elliptic integral of the first kind. The quantization condition has the form:[1]

$$\mathbf{K}(k)\mathbf{E}(k) = gl/2 \ , \tag{4}$$

where $\mathbf{K}$ and $\mathbf{E}$ are complete elliptic integrals of the first and the second kind, respectively. Eq. 4 has as solution only if

$$gl > (gl)_{\rm cr} = \pi^2/2 \quad . \tag{5}$$

This inequality establishes a lower bound for g for a given l, and for l for a given g. Near the threshold k is small:

$$k^2 \approx (u_M - u_m)/u_M \approx (8/\pi)\sqrt{gl - (gl)_{\rm cr}} \, . \tag{6}$$

Therefore, the density distribution shows a square-root singularity at $(gl)_{\rm cr}$. The total energy, $J(g)$, shows only is very soft singularity at the same point:

$$J(g) \approx -(\pi^2/8l^2)\{1 + (12/\pi^4)(gl - (gl)_{\rm cr})^2\Theta(gl - (gl)_{\rm cr})\} \, . \tag{7}$$

Here $\Theta(x) = 1$ or 0 for $x > 0$ and $x < 0$, respectively.

The above patterns differ drastically from the ST patterns in infinite systems. It is well known that the ST in 1d sets in at any value of g. In 2d a critical value of g exists, and the ground state energy shows an abrupt change at $g = g_{\rm cr}$.[2] The existence of the critical value of the parameter gl in closed 1d systems established above implies that some peculiar scenarios for the ST can emerge for closed 2D manifolds. E.g., a spontaneous symmetry breaking by a Jahn-Teller mechanism my result in squeezing a degenerate 2d state into a non-degenerate nearly-1d state, a string (there is no ST barrier and no critical value of g for this process). The latter state should be stable for $gl < gl_{\rm cr}$. String polarons[3] and excitons[4] circling C_{60} clusters have been found recently by numerical experiments. However, it is not clear now whether the mechanism described above is actually effective in fullerenes.

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